

DFT study of the role of substituents in tin(II) bis(amidoethyl)amine complexes used for ϵ -caprolactone polymerization

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Computational methods

Calculations were carried out by the density functional theory (DFT) using the non-empirically generalized gradient approximation and the PBE functionalⁱⁱ implemented in the PRIRODA program using TZ2P basis.^{iii,iv} Full geometry optimization was performed for all stable compounds, and a saddle point search was performed for transition states. The type of stationary points was confirmed by vibrational frequency calculations; saddle points were confirmed also by the intrinsic reaction coordinate (IRC) calculation. The charges were calculated using the Hirshfeld population analysis.

Calculated Cartesian coordinates and energies of transition states and minima

Pre-reaction complexes (RCa)

Compound RCa isomer 1

Atomic N.	X	Y	Z
50	0.38295301	-0.12473106	-0.95687242
7	1.08525984	-0.96798116	1.37777196
6	2.25359531	-1.85448249	1.22093190
1	2.58596400	-2.25766137	2.19474646
1	2.00313930	-2.69360457	0.55984475
1	3.07852241	-1.29047656	0.76827085
7	-0.92262212	-1.81679429	-0.32770756
6	-0.07926201	-1.70505674	1.92722814
1	0.22155964	-2.29076406	2.81658263
1	-0.82473553	-0.96445932	2.24193212
6	-0.72021556	-2.61108801	0.88116514
1	-1.67756559	-2.98121024	1.28507848
1	-0.08380237	-3.49745829	0.69420648
16	-1.75161098	-2.52941284	-1.56042171
7	0.15330969	1.66979568	0.62889466
6	1.42216849	0.21328132	2.20490791
1	1.52033204	-0.07360745	3.27017104
1	2.39143231	0.59827689	1.85990661
6	0.38086878	1.32526034	2.04142724
1	0.72097951	2.19449922	2.62831297
1	-0.58638420	1.02747349	2.47511085
16	1.10312758	2.92334613	0.08296818
8	0.80967252	3.01274038	-1.37280442
8	2.51527771	2.81145545	0.53664320
6	0.43930477	4.41644543	0.87367205
6	1.16427152	5.04009748	1.88900461
6	0.64592807	6.19060203	2.49051024
6	-0.58232158	6.73097551	2.08540375
6	-1.28744628	6.08694669	1.05264392
6	-0.78575712	4.93773854	0.44647228
1	2.12964374	4.63164139	2.18598606
1	-1.32837314	4.45852910	-0.36837849

ⁱⁱ J.P. Perdew, K. Burke, M. Ernzerhoff, *Phys. Rev. Lett.*, 1996, **77**, 3865.

ⁱⁱⁱ M. Ernzerhoff, G.E. Scuseria, *J. Chem. Phys.*, 1999, **110**, 5029.

^{iv} D.N. Laikov, *Chem. Phys. Lett.*, 1997, **281**, 151.

^v D.N. Laikov, Y.A. Ustynuk, *Russ. Chem. Bull. (Int. Ed.)*, 2005, **54**, 820.

1	-2.24131106	6.49779050	0.71609277
6	-1.12704958	7.98758826	2.71678920
1	1.21177938	6.67991542	3.28549219
8	-3.07217866	-3.03275101	-1.11886678
8	-1.65038386	-1.55898234	-2.68725744
6	-0.79230699	-3.99616448	-2.04269322
6	0.39529530	-3.83328801	-2.76288398
6	1.13687520	-4.95748855	-3.12068782
6	0.71158215	-6.25126540	-2.76870150
6	-0.48146907	-6.38583105	-2.04503859
6	-1.23743428	-5.26740133	-1.68093815
1	0.72111285	-2.83434866	-3.05644663
1	2.05982088	-4.83166823	-3.69044998
6	1.50957393	-7.46098511	-3.18718094
1	-0.83048723	-7.38182807	-1.76573707
1	-2.17566855	-5.37005484	-1.13631186
1	-0.60455067	8.22559194	3.65196090
1	-1.00919665	8.84808708	2.04021237
1	-2.20014400	7.89328268	2.93415579
1	1.19770350	-8.35749095	-2.63632556
1	1.37564058	-7.66588233	-4.26060589
1	2.58518178	-7.30893743	-3.02038754
8	-1.71846078	1.04517152	-1.19396861
1	-1.42084901	1.73391763	-0.54714369
6	-2.10199211	1.64495674	-2.45669851
1	-1.30013562	2.28843725	-2.84473562
1	-3.02370072	2.22605856	-2.31410922
1	-2.29446047	0.81325363	-3.14114449

Energy = -8139.845304 Hartree

Number of imaginary frequencies = 0.

Compound RCa isomer 2

Atomic N.	X	Y	Z
50	1.61987039	-1.76975843	0.67362775
7	1.22217363	-0.57423389	2.92008674
6	1.98776637	-1.27967750	3.96626014
1	1.87166805	-0.78615824	4.94800195
1	1.64150550	-2.31727989	4.05088496
1	3.05076454	-1.29039391	3.69486460
7	-0.46488570	-2.19357309	1.36875696
6	-0.23568967	-0.62718449	3.19510011
1	-0.42934559	-0.43708460	4.26742140
1	-0.71656384	0.17171143	2.61715285
6	-0.84137874	-1.95706530	2.76889155
1	-1.93725224	-1.88093198	2.88284132
1	-0.51312756	-2.77876735	3.42736894
16	-1.06009363	-3.59701907	0.72102705
7	1.64276324	0.58666698	0.28241320
6	1.69314450	0.82232004	2.76728715
1	1.33754467	1.44477529	3.61151057
1	2.79123324	0.81247315	2.78361422
6	1.23852340	1.41624908	1.43034289
1	1.63876172	2.44133037	1.35764459
1	0.14269224	1.51682616	1.39615264
16	3.13286855	0.99519246	-0.33873486
8	3.38474161	-0.00615766	-1.41004230
8	4.16202589	1.20616629	0.71367503

6	2.89783404	2.60935205	-1.13673591
6	3.43474683	3.75464483	-0.54826660
6	3.25427782	4.99211527	-1.17242214
6	2.55287726	5.09992369	-2.38148301
6	2.02983579	3.92810932	-2.95684086
6	2.19783473	2.68834672	-2.34413705
1	4.00069087	3.66515418	0.37839392
1	1.80870615	1.78285271	-2.80959341
1	1.48878055	3.98981534	-3.90306587
6	2.38957504	6.43174575	-3.06988501
1	3.67336354	5.88928965	-0.71296337
8	-0.18309706	-3.88833221	-0.44769966
8	-1.26452637	-4.64107619	1.75501451
6	-2.70636405	-3.18003800	0.08450167
6	-3.81799659	-3.88413821	0.54533014
6	-5.08176067	-3.56892260	0.03753946
6	-5.24625018	-2.56305372	-0.92472141
6	-4.10658134	-1.86598433	-1.36539772
6	-2.83957982	-2.16610433	-0.86950031
1	-3.68345104	-4.66775516	1.29007125
1	-5.95481581	-4.11745426	0.39638331
6	-6.60714092	-2.24653923	-1.49342373
1	-4.21699898	-1.07486446	-2.11009790
1	-1.95638194	-1.62263831	-1.20867774
1	2.54742785	7.26534894	-2.37369863
1	3.11898410	6.53997152	-3.88766476
1	1.38955713	6.53418716	-3.51304968
1	-6.73306774	-2.70712244	-2.48572810
1	-7.40976366	-2.62662322	-0.84839690
1	-6.74733519	-1.16408941	-1.61991549
8	0.48637820	-1.19002871	-1.44094366
1	0.81905311	-0.26313953	-1.36021195
6	0.95122550	-1.79400583	-2.67566462
1	2.03862731	-1.68247529	-2.77793430
1	0.43963892	-1.32328139	-3.52726507
1	0.67598607	-2.85161615	-2.61799887

Energy = -8139.847842 Hartree

Number of imaginary frequencies = 0.

Compound RCa isomer 3

Atomic N.	X	Y	Z
50	2.33700661	-1.01039197	0.18702235
7	2.21599260	-0.46021062	2.63406357
6	3.50458450	-0.78410455	3.28692024
1	3.51159691	-0.44898658	4.33851213
1	3.66575136	-1.86955397	3.26172490
1	4.31591177	-0.29074755	2.73760886
7	0.48964738	-1.90892328	1.06629202
6	1.08188106	-1.21304846	3.26462434
1	1.36398178	-1.51403779	4.28668191
1	0.22293043	-0.53442033	3.33683309
6	0.66184839	-2.42082363	2.42529439
1	-0.27654399	-2.82623707	2.83937587
1	1.41311587	-3.23005519	2.48246766
16	-0.26641200	-2.82460915	-0.06812945
7	1.39104931	0.97465450	0.27212463
6	1.96408728	1.00964293	2.65517802

1	1.63700704	1.32211683	3.66426064
1	2.91415825	1.51044760	2.42474696
6	0.93174148	1.40957084	1.59631171
1	0.81220829	2.50271148	1.62678019
1	-0.04856537	0.95409910	1.80950328
16	1.89556537	2.12906505	-0.79203938
8	3.04379265	1.51348834	-1.53620861
8	2.08903592	3.44140859	-0.12970898
6	0.56536202	2.33397208	-2.00123241
6	0.08031402	3.61606214	-2.25737719
6	-0.93500098	3.78152789	-3.20328250
6	-1.46838639	2.68477290	-3.89469707
6	-0.96376216	1.40380641	-3.60824397
6	0.04849110	1.21899958	-2.66871695
1	0.49722516	4.46569020	-1.71813501
1	0.41473378	0.21426839	-2.45421949
1	-1.37147254	0.53411633	-4.12675667
6	-2.54180399	2.87097583	-4.93773105
1	-1.31775309	4.78355472	-3.40604245
8	0.20408054	-2.20966364	-1.35217811
8	-0.11952692	-4.28420540	0.14491226
6	-2.03133213	-2.45044581	0.08767651
6	-2.92280804	-3.46438637	0.43446745
6	-4.28310884	-3.16299449	0.55296010
6	-4.76091685	-1.86527707	0.32544258
6	-3.83681369	-0.86268022	-0.02317150
6	-2.47852571	-1.14522604	-0.14346795
1	-2.54722135	-4.47377617	0.59891433
1	-4.98480330	-3.95407274	0.82397556
6	-6.23169386	-1.54741547	0.42978131
1	-4.19011963	0.15439181	-0.20462009
1	-1.76827501	-0.36502677	-0.41866907
1	-3.05811910	3.83189719	-4.81602580
1	-2.10843063	2.85296743	-5.94988709
1	-3.28827160	2.06621816	-4.89289326
1	-6.67115679	-1.39434777	-0.56794618
1	-6.78437988	-2.36112902	0.91619615
1	-6.40176944	-0.62396999	1.00111152
8	4.88255326	0.77272437	0.49091163
1	4.39175099	1.17554731	-0.26502721
6	6.04180399	0.12519321	-0.04771590
1	5.77140922	-0.69335055	-0.73695632
1	6.60300636	-0.29854704	0.79527343
1	6.69334858	0.83877350	-0.57686992

Energy = -8139.851739 Hartree

Number of imaginary frequencies = 0.

Compound RCa isomer 4

Atomic N.	X	Y	Z
50	1.25784087	-0.82047206	0.68667760
7	0.80347624	-0.30773892	3.05886713
6	1.79821610	-0.99034930	3.91839550
1	1.66633887	-0.70335926	4.97560354
1	1.67942852	-2.07761003	3.82942960
1	2.80684870	-0.71369650	3.58705347
7	-0.81396557	-1.45885434	1.13100320
6	-0.59122567	-0.74434082	3.39340630

1	-0.64499848	-1.01027435	4.46252909
1	-1.25796672	0.10859185	3.21754088
6	-1.05748573	-1.89552438	2.50740377
1	-2.13081350	-2.06445142	2.69908992
1	-0.53475364	-2.83755884	2.75270136
16	-1.38615205	-2.39099704	-0.10611835
7	0.95123768	1.40419414	0.74495336
6	0.93326547	1.17575107	3.17564532
1	0.46713510	1.51875173	4.11657922
1	2.00484411	1.41026515	3.21519263
6	0.29651334	1.88227968	1.98459303
1	0.45407899	2.96693036	2.09906049
1	-0.79412667	1.70985965	1.96123752
16	0.42003677	2.27686960	-0.60083710
8	0.67721218	3.71721985	-0.35499410
8	-0.95112695	1.87526005	-1.00827544
6	1.57047083	1.69132375	-1.86235738
6	1.25457497	0.55489075	-2.61175316
6	2.15444286	0.12006520	-3.58690854
6	3.35033427	0.81211187	-3.83354021
6	3.63148732	1.95905604	-3.07192387
6	2.74995433	2.40434488	-2.08682412
1	0.31939274	0.02036884	-2.44095735
1	2.95577285	3.30216949	-1.50421105
1	4.55436662	2.51243034	-3.25558737
6	4.29620754	0.35197696	-4.91420310
1	1.91832156	-0.77510135	-4.16446007
8	-0.55886507	-1.92957522	-1.26759065
8	-1.43179623	-3.83506822	0.22665979
6	-3.08858608	-1.85594106	-0.38678963
6	-4.12475420	-2.78036231	-0.25799409
6	-5.43840914	-2.36060665	-0.48584545
6	-5.72342862	-1.03473321	-0.84113753
6	-4.65515194	-0.12685218	-0.96003216
6	-3.33887668	-0.52434229	-0.73649199
1	-3.89520875	-3.81094044	0.01019068
1	-6.25453791	-3.07888745	-0.38766794
6	-7.13912189	-0.58865168	-1.10900501
1	-4.85617638	0.91057223	-1.23418787
1	-2.51962123	0.19060597	-0.83183537
1	4.31200399	-0.74331207	-4.99151836
1	3.98559206	0.74346505	-5.89541916
1	5.31958790	0.70335230	-4.72905332
1	-7.29697680	-0.41296236	-2.18422954
1	-7.86659059	-1.34280622	-0.78278210
1	-7.36429640	0.35570806	-0.59356885
8	3.71843274	1.10938930	1.64072082
1	2.96767698	1.48349432	1.11955047
6	4.87167119	1.01140735	0.79695426
1	4.69324224	0.35068920	-0.06834267
1	5.67930429	0.58188720	1.40281971
1	5.19570269	2.00008776	0.43258426

Energy = -8139.843496 Hartree

Number of imaginary frequencies = 0.

Compound RCa isomer 5

Atomic N. X Y Z

50	1.55571940	-1.57493433	-0.24287437
7	1.51922726	-1.84106873	2.28715776
6	2.39997986	-2.94839265	2.70663615
1	2.39514826	-3.07049123	3.80464792
1	2.06763323	-3.88694930	2.24653348
1	3.42550726	-2.74288076	2.37495871
7	-0.32322630	-2.57066981	0.31645706
6	0.10033139	-2.11067636	2.64101115
1	0.03072715	-2.48719179	3.67854813
1	-0.44497747	-1.16116225	2.58259165
6	-0.55224039	-3.08720625	1.66763346
1	-1.62960379	-3.12654683	1.90685925
1	-0.15974321	-4.11116018	1.78849667
16	-0.90039994	-3.46658939	-0.94982373
7	1.30303876	0.48987792	0.77881435
6	1.99268100	-0.55418380	2.85511047
1	1.86666867	-0.54023083	3.95403382
1	3.06638354	-0.47659683	2.63200015
6	1.27090960	0.65038663	2.23692854
1	1.81535202	1.55562914	2.55650698
1	0.23755447	0.73958841	2.60766707
16	0.11808581	1.17032986	-0.12915498
8	-1.15726382	1.37077162	0.59687062
8	0.14319185	0.27797389	-1.35205294
6	0.68160340	2.79492257	-0.68051001
6	1.63867097	2.88633988	-1.69569189
6	2.08816119	4.14417188	-2.08998703
6	1.59731531	5.31546542	-1.48546227
6	0.63466101	5.19126261	-0.47364729
6	0.16934036	3.93806189	-0.06734230
1	2.00836642	1.98243799	-2.17959738
1	-0.59315493	3.84181429	0.70468525
1	0.23667248	6.08914199	0.00232294
6	2.08172073	6.67002090	-1.93736588
1	2.83126627	4.22113168	-2.88593898
8	-0.12057891	-2.95272399	-2.11506896
8	-0.91251639	-4.91785272	-0.64542008
6	-2.62178710	-2.96204328	-1.17466366
6	-3.64230778	-3.88956293	-0.96873963
6	-4.96926441	-3.48819841	-1.14782465
6	-5.28353624	-2.17674405	-1.53021644
6	-4.23095667	-1.26474899	-1.72871599
6	-2.90267277	-1.64571611	-1.55546005
1	-3.39060972	-4.90973050	-0.68132718
1	-5.77312369	-4.20961733	-0.98926186
6	-6.71466286	-1.75189821	-1.74648362
1	-4.45663901	-0.23778544	-2.02236784
1	-2.09066084	-0.93467821	-1.71087148
1	3.17781051	6.69631401	-2.01355629
1	1.68331200	6.91581495	-2.93365730
1	1.76489832	7.46079336	-1.24589366
1	-6.93555894	-1.65318053	-2.82062331
1	-7.41812009	-2.48281976	-1.32756653
1	-6.91548597	-0.77448940	-1.28578206
8	4.20756801	0.87805267	0.79667544
1	3.26177750	0.91334158	0.52645701
6	5.01478281	0.94189832	-0.38040864
1	4.79648776	0.11611337	-1.08083057

1 6.06123942 0.85594593 -0.06108092
 1 4.89529721 1.90111842 -0.91433430
 Energy = -8139.849771 Hartree
 Number of imaginary frequencies = 0.

Compound RCa isomer 6

Atomic N.	X	Y	Z
50	1.06524365	-0.74457417	0.08097189
7	0.57356204	0.10320881	2.51342902
6	1.76744096	-0.07273094	3.36552477
1	1.59179007	0.31675269	4.38488484
1	2.02152331	-1.13780542	3.43820171
1	2.61081579	0.46121725	2.91018413
7	-0.26491367	-2.24047286	1.17688963
6	-0.58229483	-0.67308936	3.02972347
1	-0.64262710	-0.57241187	4.13028824
1	-1.49729115	-0.24832447	2.59699771
6	-0.51659038	-2.14516273	2.61108049
1	-1.46321443	-2.62971223	2.89900971
1	0.29100917	-2.67518395	3.14181193
16	-1.52078373	-2.37589422	0.14235748
7	0.13349799	1.30330505	-0.00089406
6	0.21984064	1.54303272	2.40136114
1	-0.32084740	1.87670327	3.30671918
1	1.15882974	2.10795587	2.33727349
6	-0.61629647	1.81944753	1.15253084
1	-0.75371116	2.91260720	1.08052868
1	-1.62193798	1.37202996	1.21946035
16	-0.44894405	1.68555332	-1.51606117
8	-1.92653944	1.68746546	-1.56473795
8	0.35558089	0.82551796	-2.42537670
6	0.07081672	3.39972339	-1.80397564
6	1.34800692	3.65661504	-2.31029571
6	1.74292101	4.97527417	-2.52778923
6	0.87937013	6.04852701	-2.24660548
6	-0.39960072	5.76175547	-1.74825518
6	-0.81326020	4.44459701	-1.53125867
1	2.00808008	2.82393764	-2.55355593
1	-1.81932197	4.22080798	-1.17757491
1	-1.08876970	6.58119605	-1.53562490
6	1.31205042	7.46964109	-2.50813113
1	2.73727370	5.17795382	-2.93094560
8	-2.81632846	-1.88771267	0.67093172
8	-0.91960638	-1.73157244	-1.09338557
6	-1.74546706	-4.12141543	-0.26490761
6	-0.70677299	-4.82354906	-0.88425787
6	-0.88633753	-6.17006934	-1.18724191
6	-2.09067056	-6.83057117	-0.88127632
6	-3.11321075	-6.10032337	-0.26096454
6	-2.95073810	-4.74685101	0.04902735
1	0.22523959	-4.31563752	-1.13161202
1	-0.07998357	-6.72114107	-1.67493548
6	-2.27355247	-8.28596538	-1.23156720
1	-4.05619508	-6.59419317	-0.01982905
1	-3.74808704	-4.17193213	0.51818314
1	2.33511870	7.64872809	-2.14890726
1	1.30537277	7.68898947	-3.58700324

1	0.64341323	8.18895454	-2.01842361
1	-2.30440463	-8.42611519	-2.32275838
1	-1.43992791	-8.89477887	-0.85298660
1	-3.20707667	-8.68452043	-0.81497520
8	2.96250143	1.94972837	0.74331458
1	2.11727087	1.95907533	0.23623833
6	4.05944221	1.99507311	-0.17450274
1	4.02916825	1.15962964	-0.89488740
1	4.97878911	1.90913973	0.41826475
1	4.09133418	2.94756642	-0.72968434

Energy = -8139.843223 Hartree
Number of imaginary frequencies = 0.

Compound RCa isomer 7

Atomic N.	X	Y	Z
50	0.24181176	0.52084086	0.38225342
7	-0.47171832	1.20852025	2.63850945
6	0.28006577	0.44828199	3.66368035
1	0.01732516	0.79338615	4.67817665
1	0.04386381	-0.62004903	3.58143515
1	1.35502501	0.59031395	3.49738181
7	-1.83979225	-0.15203284	0.65749333
6	-1.94477553	0.97148489	2.76206750
1	-2.21715963	0.91283075	3.83024015
1	-2.45560260	1.83530969	2.32031212
6	-2.39092152	-0.27301210	2.00324249
1	-3.49302952	-0.29127907	1.98538971
1	-2.05201292	-1.19493748	2.51467498
16	-2.46785954	-1.06112056	-0.56237306
7	0.13408814	2.74990673	0.32870923
6	-0.17533553	2.66808206	2.74495774
1	-0.71675449	3.09713921	3.60699239
1	0.90253969	2.77108369	2.92519563
6	-0.55387304	3.40166997	1.46331240
1	-0.22001956	4.44827447	1.55942529
1	-1.64757196	3.42280749	1.31658878
16	-0.04220470	3.66446509	-1.08807816
8	0.68683322	4.94424882	-0.90262889
8	-1.45915830	3.71521192	-1.51595697
6	0.87749671	2.65184030	-2.26548784
6	0.20922801	1.65260989	-2.97623820
6	0.92753461	0.88418307	-3.89546965
6	2.29263868	1.11162873	-4.12231077
6	2.93353974	2.13404431	-3.39998253
6	2.23561944	2.90739944	-2.47378107
1	-0.85389067	1.47574497	-2.81585430
1	2.72173392	3.71530464	-1.92727065
1	3.99430196	2.32825407	-3.57029102
6	3.05359563	0.29925821	-5.13980761
1	0.41157039	0.09088969	-4.43812858
8	-3.93710375	-0.91556307	-0.64590201
8	-1.59449664	-0.72142371	-1.72312203
6	-2.15524993	-2.80085745	-0.15035357
6	-0.87305854	-3.33181190	-0.32168988
6	-0.63440886	-4.66197096	0.01838368
6	-1.65967382	-5.47716833	0.53015914
6	-2.93574907	-4.91904246	0.69190487

6	-3.19185111	-3.58741269	0.35308465
1	-0.07812822	-2.71065238	-0.73601452
1	0.36483028	-5.07947789	-0.12086140
6	-1.39421677	-6.92326595	0.86673246
1	-3.74647975	-5.53697610	1.08245642
1	-4.18843039	-3.15919311	0.45631067
1	2.54666739	-0.65020013	-5.35359771
1	3.14209871	0.84917866	-6.08960903
1	4.07378756	0.08048849	-4.79592942
1	-1.33787044	-7.53359988	-0.04789195
1	-0.43722253	-7.04303189	1.39343537
1	-2.19020934	-7.34158628	1.49582678
8	2.73689369	2.26700732	1.56694539
1	2.08353034	2.67719259	0.94953599
6	4.01176018	2.19478823	0.91939718
1	3.97858971	1.56164717	0.01621997
1	4.71282734	1.74570726	1.63392111
1	4.38603237	3.19464023	0.64427852

Energy = -8139.838052 Hartree

Number of imaginary frequencies = 0.

Compound RCa isomer 8

Atomic N.	X	Y	Z
50	2.03442997	0.04537126	0.31340805
7	1.46924289	1.05873052	2.57889442
6	2.65958409	1.04287146	3.45417912
1	2.45233753	1.54369590	4.41648243
1	2.96301201	0.00772599	3.65558884
1	3.48354615	1.56075460	2.94752019
7	0.69196397	-1.39990632	1.42370919
6	0.34333350	0.28629373	3.17150608
1	0.29904937	0.46239197	4.26236689
1	-0.59092181	0.65042783	2.72764920
6	0.45266581	-1.20809071	2.85236966
1	-0.47203527	-1.70403672	3.18846261
1	1.28427033	-1.67070768	3.40994902
16	-0.55471038	-1.74495383	0.42520842
7	0.61660758	1.71413068	-0.02377777
6	1.06540839	2.45723135	2.27724184
1	0.60957829	2.92656494	3.16992233
1	1.98166311	3.00646729	2.02353948
6	0.09925808	2.51526257	1.09041585
1	-0.01034123	3.57301642	0.80390178
1	-0.90237184	2.15034439	1.37110045
16	0.95879837	2.48348925	-1.43191934
8	1.76526594	1.49952918	-2.20698758
8	1.54174870	3.84627236	-1.20474953
6	-0.61186902	2.73638268	-2.28102239
6	-0.98328450	4.01248883	-2.70085751
6	-2.19822398	4.17463503	-3.37302128
6	-3.03715831	3.08088604	-3.62697395
6	-2.63261895	1.80674122	-3.18757052
6	-1.42693110	1.62319492	-2.51581621
1	-0.32665937	4.85833459	-2.50147682
1	-1.11923710	0.63426963	-2.17185029
1	-3.27540042	0.94401637	-3.37279522
6	-4.34524633	3.25573011	-4.35733546

1	-2.49728900	5.17045708	-3.70531891
8	-1.86338564	-1.19855736	0.86739600
8	0.00405841	-1.33954771	-0.91281356
6	-0.73783054	-3.54501189	0.39119882
6	0.30841246	-4.33151258	-0.10160012
6	0.16512192	-5.71601108	-0.12231339
6	-1.01042607	-6.33301174	0.34445584
6	-2.04176811	-5.51952981	0.83242510
6	-1.91525187	-4.12721663	0.85751550
1	1.21828848	-3.85824193	-0.47031991
1	0.97813938	-6.33289316	-0.51012805
6	-1.15340233	-7.83391892	0.30379096
1	-2.96251530	-5.97958071	1.19593224
1	-2.71947161	-3.49038376	1.22401730
1	-4.54368743	4.31205253	-4.57829483
1	-4.34125438	2.70468823	-5.30976462
1	-5.18547331	2.86523483	-3.76482307
1	-1.19081126	-8.19782479	-0.73420341
1	-0.29820059	-8.32847113	0.78655899
1	-2.07011908	-8.16309254	0.80902004
8	3.76208361	2.93108395	0.38705656
1	3.10558991	3.39892549	-0.18044468
6	4.93669224	2.71976664	-0.40779529
1	4.70971193	2.15323515	-1.32572229
1	5.64087296	2.13617482	0.19921108
1	5.41716075	3.67363117	-0.68229830

Energy = -8139.855223 Hartree

Number of imaginary frequencies = 0.

Compound RCa isomer 9

Atomic N.	X	Y	Z
50	0.28835159	-0.22599250	-0.42661519
7	-0.67364868	-0.29038443	1.92118733
6	0.43572084	-0.10204048	2.89062889
1	0.08573336	-0.32127283	3.91462636
1	1.27467852	-0.76026239	2.64013690
1	0.77715467	0.93715134	2.85705421
7	0.43369975	-2.30038666	0.47222953
6	-1.24960172	-1.65016972	2.05362460
1	-1.63759727	-1.81219917	3.07592508
1	-2.09104512	-1.72113264	1.34801607
6	-0.20800430	-2.71890739	1.71127352
1	-0.73696748	-3.68281213	1.60118114
1	0.51571977	-2.84072267	2.53514513
16	1.53570938	-3.27515005	-0.23551045
7	-0.29993534	2.01116103	0.40712410
6	-1.69493155	0.78909873	2.08703400
1	-2.69509445	0.33636450	2.15853937
1	-1.49612534	1.32461436	3.02506323
6	-1.65746988	1.78301315	0.90344334
1	-2.17709420	2.70877506	1.19883036
1	-2.23327414	1.35510887	0.06188624
16	0.53180918	3.21294001	1.09932510
8	1.98065869	2.95392656	0.74085292
8	0.22903188	3.44204726	2.53996393
6	0.10533575	4.75285146	0.24374727
6	-0.20362650	5.89111448	0.98715934

6	-0.51878604	7.07626544	0.31646562
6	-0.52679474	7.13821288	-1.08403758
6	-0.21933821	5.97147162	-1.80681162
6	0.09427483	4.78185851	-1.15361890
1	-0.19736247	5.83792888	2.07516415
1	0.31951002	3.87634506	-1.71711278
1	-0.23031078	5.99715558	-2.89821523
6	-0.83938613	8.42623123	-1.80403435
1	-0.76382525	7.96899518	0.89500290
8	2.06032291	-2.43488295	-1.35851756
8	2.48613989	-3.88124210	0.72803175
6	0.61539184	-4.64761144	-0.98063253
6	0.76139313	-5.93587120	-0.46814993
6	0.03901891	-6.98499750	-1.04526351
6	-0.82180453	-6.76334789	-2.12861549
6	-0.94811897	-5.45291831	-2.62557156
6	-0.23864405	-4.39697835	-2.05920911
1	1.44429900	-6.10591824	0.36359081
1	0.15215295	-7.99510304	-0.64708737
6	-1.58137219	-7.90000454	-2.76602927
1	-1.61086758	-5.26116425	-3.47185527
1	-0.33165205	-3.38548360	-2.45585812
1	-1.33958732	9.14478675	-1.14221464
1	0.08287434	8.90095678	-2.17362779
1	-1.48430925	8.25165332	-2.67637947
1	-1.17002680	-8.13863217	-3.75884807
1	-1.52862558	-8.80993195	-2.15496272
1	-2.64025356	-7.64232862	-2.91027195
8	2.33094111	0.44160171	0.37967796
1	2.23605580	1.45649204	0.55521696
6	3.57776733	0.21295611	-0.33253601
1	3.63029609	0.84235345	-1.23224740
1	3.61312692	-0.84311105	-0.61514132
1	4.40831306	0.45752893	0.34182709

Energy = -8139.840809 Hartree

Number of imaginary frequencies = 0.

Pre-reaction complexes (RCb)

Compound RCb isomer 1

Atomic N.	X	Y	Z
50	-0.65973492	-0.70823841	0.00063325
7	0.29033060	-2.39181444	1.40870781
6	-0.32702084	-3.72533030	1.21829238
1	0.09671704	-4.45143959	1.93290251
1	-0.13368549	-4.07907156	0.19865277
1	-1.41343875	-3.65341208	1.35601592
7	1.22160990	-1.16652540	-0.95700499
6	1.74293830	-2.41321353	1.05421473
1	2.20807753	-3.32546565	1.46803239
1	2.20721239	-1.53912129	1.52670675
6	1.95498594	-2.31874488	-0.45212398
1	3.04318383	-2.20801427	-0.62315832
1	1.67290638	-3.27903713	-0.93045497
6	1.38418598	-0.83236965	-2.32960364
6	1.87547689	0.45880275	-2.66045227
6	2.03638236	0.82284343	-4.00164914

6	1.72911731	-0.05114432	-5.05072360
6	1.21881581	-1.30869768	-4.71695607
6	1.03092436	-1.71270901	-3.38784246
7	-0.28652584	0.30678419	1.86914651
6	0.08054397	-1.90467195	2.80053536
1	0.68710434	-2.50490573	3.50364979
1	-0.98252523	-2.05941115	3.03331910
6	0.41510206	-0.41744186	2.91627721
1	0.07915789	-0.07890296	3.91330996
1	1.51679369	-0.28429438	2.91499708
6	-0.54968725	1.68745515	2.08065011
6	0.49528738	2.62972142	2.27225245
6	0.18550179	3.98041469	2.47929013
6	-1.13086949	4.44957003	2.49399827
6	-2.15322528	3.51337396	2.30382954
6	-1.89281272	2.15272244	2.10368201
6	2.23392824	1.44306036	-1.57513164
1	2.42219486	1.81949950	-4.23196070
6	1.95044615	0.34789697	-6.48980587
1	0.93272628	-1.99690367	-5.51722159
6	0.38950256	-3.05367352	-3.12724482
6	1.94521206	2.21539628	2.21765981
1	1.00671801	4.68930637	2.61638443
6	-1.43993135	5.91599630	2.67735119
1	-3.19375483	3.84850168	2.32679448
6	-3.05535128	1.20471524	1.93767027
1	2.76924525	2.30476188	-1.99540817
1	2.86059482	0.97237144	-0.80544075
1	1.34211317	1.82869428	-1.05598291
1	1.12927840	-3.84205701	-2.91478843
1	-0.18898289	-3.37885720	-4.00188124
1	-0.29358709	-3.00385417	-2.26571897
1	1.31241960	-0.23400679	-7.16877433
1	2.99534583	0.17685021	-6.79456174
1	1.73762348	1.41431544	-6.64838345
1	2.58270981	3.07381320	1.96811425
1	2.10090911	1.43321323	1.46217769
1	2.29945658	1.81596476	3.18163710
1	-2.87805434	0.25992123	2.46999329
1	-3.21990938	0.94320951	0.87992187
1	-3.98128082	1.66112569	2.31250782
1	-1.58147735	6.41733677	1.70656439
1	-0.62457788	6.43536682	3.19865981
1	-2.36403953	6.06204803	3.25420694
1	-3.05252256	-2.10324004	-0.24422213
8	-3.50999816	-2.86643131	0.16831963
6	-4.80506384	-2.42091188	0.59012882
1	-5.29717828	-3.27952571	1.06337852
1	-5.42348212	-2.09009281	-0.26080398
1	-4.74406247	-1.60152194	1.32673378

Energy = -7200.151446 Hartree

Number of imaginary frequencies = 0.

Compound RCb isomer 2

Atomic N.	X	Y	Z
50	1.11076020	-1.11060133	0.09202687
7	1.06925070	-1.32214152	2.46040758

6	2.39920015	-1.54192622	3.07694666
1	2.30911321	-1.59661017	4.17511198
1	3.08823766	-0.73786606	2.79566120
1	2.81278115	-2.48667055	2.70315165
7	1.14554372	1.01833056	0.82137045
6	0.45120261	-0.04587587	2.92497988
1	0.51676917	0.01409945	4.02699030
1	-0.60711947	-0.07491276	2.64037292
6	1.10155628	1.17178187	2.28056190
1	0.49450021	2.04731921	2.56828717
1	2.09953295	1.32646735	2.73031649
6	1.02661683	2.19913103	0.03996722
6	0.19483117	2.21439283	-1.11948179
6	0.06713351	3.37778336	-1.88573699
6	0.72521238	4.56726635	-1.56399005
6	1.54554411	4.54580181	-0.43563595
6	1.72690093	3.40438890	0.35930066
7	-0.79997394	-2.06182145	0.54105176
6	0.16940847	-2.47953176	2.72906818
1	-0.04338260	-2.54393490	3.81186281
1	0.71884936	-3.38283565	2.42667116
6	-1.12342271	-2.37241802	1.92363198
1	-1.63621579	-3.34956374	1.99512590
1	-1.80531142	-1.64826590	2.41629571
6	-1.80344329	-2.31811954	-0.43089310
6	-3.06426180	-1.66255673	-0.40078527
6	-4.02032237	-1.94435494	-1.38562377
6	-3.78040325	-2.85296937	-2.41991736
6	-2.53269909	-3.48557037	-2.44745689
6	-1.54982116	-3.24365769	-1.48043473
6	-0.59752849	1.00844435	-1.55802049
1	-0.59073649	3.35142698	-2.75864398
6	0.58333749	5.80348248	-2.41831297
1	2.09511883	5.45100277	-0.16312658
6	2.73013944	3.52350971	1.48876533
6	-3.39209231	-0.62493834	0.64581068
1	-4.97824928	-1.41814575	-1.34916569
6	-4.83658614	-3.16161700	-3.45370654
1	-2.31740172	-4.20542591	-3.24171181
6	-0.24361166	-3.99527442	-1.56740272
1	-1.39450571	1.30032200	-2.25493107
1	-1.07196386	0.49347874	-0.71059336
1	0.02214615	0.26992732	-2.09737719
1	3.42563167	2.67315955	1.52399890
1	2.25786281	3.59686237	2.47982652
1	3.32793722	4.43376940	1.35051158
1	1.24441707	5.76148552	-3.29884326
1	0.84418834	6.71013839	-1.85578325
1	-0.44431913	5.91735641	-2.79200540
1	-4.17228900	0.05622309	0.28147576
1	-2.50595916	-0.02817839	0.90566694
1	-3.76463797	-1.07773985	1.57871285
1	0.10090342	-4.31349528	-0.57373463
1	0.56273878	-3.37628413	-1.99257177
1	-0.35089769	-4.87986150	-2.20930795
1	-4.39152199	-3.34491548	-4.44153628
1	-5.55550294	-2.33657818	-3.54920748
1	-5.40756816	-4.06389210	-3.18205060

1	3.09115353	0.70841479	0.68027932
8	4.00665689	0.37441322	0.86995024
6	4.76570849	0.43579520	-0.34102533
1	5.75975455	0.02518791	-0.12329327
1	4.88567919	1.47306153	-0.69763788
1	4.30542994	-0.16567362	-1.14421314

Energy = -7200.149596 Hartree
Number of imaginary frequencies = 0.

Compound RCb isomer 3

Atomic N.	X	Y	Z
50	0.98184642	-1.38027114	0.59000842
7	0.20578593	-1.58734245	2.93960497
6	1.06656907	-2.50669632	3.70933767
1	0.67031922	-2.66218276	4.72889910
1	2.07964093	-2.09202354	3.78319719
1	1.12549789	-3.47308357	3.19258697
7	1.33076470	0.59402682	1.50852588
6	0.23015992	-0.21897834	3.52927954
1	0.28361808	-0.29050381	4.63145965
1	-0.71155157	0.27604170	3.26038609
6	1.38071307	0.60569386	2.96332114
1	1.28698377	1.62878338	3.36741282
1	2.34873602	0.22284495	3.36100593
6	1.81577243	1.74612607	0.84975118
6	3.03250788	1.72682854	0.10794413
6	3.44001909	2.86823714	-0.60108226
6	2.70357166	4.05611517	-0.59128244
6	1.52435318	4.07957052	0.16396490
6	1.06954603	2.96359687	0.87403043
7	-1.17054344	-1.62278139	0.46552338
6	-1.18403758	-2.10883520	2.83969333
1	-1.71146080	-1.96497857	3.80231681
1	-1.11361700	-3.18667113	2.63613338
6	-1.93525224	-1.44042378	1.68687016
1	-2.92282521	-1.92884918	1.60609447
1	-2.14465664	-0.38126024	1.95034006
6	-1.87171494	-1.73054564	-0.75865919
6	-2.73470415	-0.70419545	-1.22982745
6	-3.41335948	-0.86395551	-2.44451475
6	-3.25912259	-2.00283025	-3.24119323
6	-2.38765505	-2.99725468	-2.78317970
6	-1.70183533	-2.88918871	-1.56663959
6	3.92738358	0.50960072	0.10386596
1	4.38051651	2.82956204	-1.15749649
6	3.14970848	5.26426099	-1.37905007
1	0.92404893	4.99334138	0.18638681
6	-0.23361950	3.05125003	1.62604757
6	-2.87426440	0.59213595	-0.47395376
1	-4.06469120	-0.05582359	-2.78942227
6	-4.02344941	-2.16546247	-4.53338952
1	-2.24843746	-3.90130268	-3.38258800
6	-0.81006750	-4.02541885	-1.12825295
1	4.95345637	0.78938990	-0.17090598
1	3.59431208	-0.26137971	-0.60928317
1	3.94257979	0.02497509	1.08918047
1	-0.08007697	3.25234940	2.69867704

1	-0.78183604	2.10187143	1.55247794
1	-0.86050674	3.86076989	1.23017342
1	4.21022399	5.19127710	-1.65478334
1	3.00761073	6.19207902	-0.80703745
1	2.57240544	5.36882638	-2.31143261
1	-3.28770826	1.37577299	-1.12238132
1	-1.89207209	0.92070617	-0.10621692
1	-3.53948231	0.50281245	0.39968050
1	-0.94417224	-4.24482931	-0.05964040
1	0.25825480	-3.79025532	-1.26018458
1	-1.02457970	-4.93157984	-1.71079071
1	-3.44737898	-2.73943454	-5.27264017
1	-4.27343030	-1.19102808	-4.97551137
1	-4.97196854	-2.70289857	-4.37254391
1	1.19685953	1.03239263	-1.20120922
8	0.64644604	0.26589583	-1.47210487
6	1.01222826	-0.12742488	-2.80811650
1	2.05531187	-0.47914111	-2.85964582
1	0.87023921	0.70879489	-3.50807707
1	0.34208675	-0.94709867	-3.09114025

Energy = -7200.154308 Hartree

Number of imaginary frequencies = 0.

Compound RCb isomer 4

Atomic N.	X	Y	Z
50	1.04957670	-1.43599286	0.58059154
7	0.29662590	-1.60128003	2.92390467
6	1.17763403	-2.49438474	3.70189132
1	0.79000541	-2.63984458	4.72601951
1	2.18402124	-2.06177622	3.76228117
1	1.24953869	-3.46763832	3.19979226
7	1.37553083	0.56242048	1.44551713
6	0.30438623	-0.22217235	3.48997278
1	0.36911072	-0.27332006	4.59238514
1	-0.64663784	0.25402401	3.22142078
6	1.43665497	0.61068262	2.89960353
1	1.31924253	1.64261142	3.27755591
1	2.41462516	0.26124734	3.30542935
6	1.92839322	1.67735462	0.76985048
6	3.20515483	1.62511180	0.14316846
6	3.67791102	2.73732758	-0.57369225
6	2.94657889	3.92259198	-0.68087071
6	1.70271368	3.97817628	-0.03746454
6	1.18707110	2.89385144	0.67876155
7	-1.13020573	-1.61274848	0.45578742
6	-1.08183302	-2.15045862	2.83294991
1	-1.60207253	-2.03419278	3.80327055
1	-0.99044499	-3.22350856	2.61164529
6	-1.86394262	-1.47606356	1.70581319
1	-2.84365811	-1.98124328	1.63624557
1	-2.08762798	-0.42911691	1.99817737
6	-1.88509447	-1.74160664	-0.73181177
6	-2.89264041	-0.80185509	-1.09221047
6	-3.63149124	-0.98090437	-2.26863137
6	-3.40801846	-2.05330851	-3.13677219
6	-2.39945340	-2.95872232	-2.78947776
6	-1.64642813	-2.83304588	-1.61572312

6	4.08304148	0.39890258	0.24410706
1	4.66079262	2.67372293	-1.04798368
6	3.46960048	5.10239803	-1.46452015
1	1.10668101	4.89252451	-0.10593856
6	-0.16692391	3.00974502	1.33059141
6	-3.12655183	0.44614723	-0.27673806
1	-4.39089202	-0.23666751	-2.52524472
6	-4.23552226	-2.24013962	-4.38578919
1	-2.19972049	-3.81031849	-3.44569983
6	-0.60914082	-3.88399760	-1.30880014
1	5.13777402	0.67115213	0.10243403
1	3.83397929	-0.35558681	-0.51874165
1	3.97248804	-0.09399533	1.21862766
1	-0.69721019	2.04893608	1.27455777
1	-0.77098773	3.79170688	0.85175842
1	-0.08701390	3.26727985	2.39947423
1	3.46005775	6.02155895	-0.86038629
1	2.85135592	5.29711243	-2.35452339
1	4.49917997	4.92988138	-1.80418546
1	-3.64539343	1.20503952	-0.87738312
1	-2.17045259	0.86603758	0.06790140
1	-3.73941308	0.26373828	0.61996699
1	-0.61465774	-4.14884143	-0.24172501
1	0.41260060	-3.53948179	-1.53577199
1	-0.79040009	-4.78960663	-1.90341641
1	-3.64594041	-2.69234783	-5.19549985
1	-4.63542551	-1.28265070	-4.74741434
1	-5.09594316	-2.90348275	-4.20126829
1	1.64276502	0.84270273	-1.33623849
8	1.19237380	0.06157651	-1.72408282
6	0.15090130	0.54326813	-2.59845130
1	-0.38516357	-0.33455210	-2.97398671
1	0.58652729	1.09334499	-3.44692433
1	-0.55859209	1.19267746	-2.06408590

Energy = -7200.153521 Hartree

Number of imaginary frequencies = 0.

Transition state 1a (TS1a)

Compound TS1a isomer 1

Atomic N.	X	Y	Z
50	0.62015045	-0.20800047	-1.00087714
7	1.11028552	-0.78617638	1.44328225
6	2.30082178	-1.66309059	1.42040443
1	2.51461792	-2.07258415	2.42362881
1	2.14504290	-2.49337387	0.72129118
1	3.16738439	-1.08022046	1.08480501
7	-0.26388830	-2.17199898	-0.44858137
6	-0.09886465	-1.53024459	1.88055789
1	0.04237089	-1.92699313	2.90420556
1	-0.93491054	-0.81899142	1.89639878
6	-0.44197354	-2.66753507	0.91257715
1	-1.48465371	-2.97270346	1.09684896
1	0.19964726	-3.54600072	1.10663140
16	-1.26064003	-2.67821813	-1.64644301
7	0.17960404	1.94267356	0.78286630
6	1.38440919	0.39181313	2.30669594

1	1.45187950	0.06797974	3.36372042
1	2.36052370	0.79555172	2.00613236
6	0.35239145	1.51762235	2.16851640
1	0.68480897	2.34095335	2.82365847
1	-0.63029760	1.20111382	2.55298424
16	1.13165843	3.17301559	0.23639110
8	0.91086179	3.20994473	-1.23133099
8	2.51107240	3.06088209	0.78128153
6	0.44249955	4.70303679	0.92694527
6	1.09543943	5.34659338	1.97828722
6	0.54331434	6.51473141	2.51271605
6	-0.64811134	7.05189848	2.00655699
6	-1.28155315	6.38597012	0.94172567
6	-0.74604833	5.21959209	0.40066713
1	2.03419733	4.94088268	2.35386467
1	-1.23137105	4.71820450	-0.43663636
1	-2.20587516	6.79371452	0.52744687
6	-1.22800291	8.32706547	2.56610155
1	1.05405009	7.02114916	3.33406043
8	-2.64232993	-2.94494295	-1.18598354
8	-1.00533497	-1.65866399	-2.71992922
6	-0.60910529	-4.25204611	-2.25926232
6	0.57020277	-4.26501608	-3.01016378
6	1.07481599	-5.48208666	-3.46227360
6	0.41943771	-6.69311142	-3.17535233
6	-0.76126665	-6.64944887	-2.42072201
6	-1.28305435	-5.43649292	-1.96262932
1	1.07354963	-3.32823896	-3.24973917
1	1.99211574	-5.49503565	-4.05418158
6	0.96293980	-8.00056648	-3.69478655
1	-1.28726649	-7.57821894	-2.19205976
1	-2.21122217	-5.39831257	-1.39352322
1	-0.75645548	8.59729385	3.51952767
1	-1.07692409	9.16578293	1.86907840
1	-2.31101155	8.23599052	2.73010659
1	0.51912540	-8.85635757	-3.17037058
1	0.74278682	-8.11682320	-4.76733017
1	2.05473018	-8.05356216	-3.58240414
8	-1.39902532	0.74441689	-0.65845495
1	-0.86690134	1.49424458	0.00944744
6	-2.10426641	1.35493755	-1.76043761
1	-1.49706376	2.14366770	-2.23131967
1	-3.03947210	1.78745759	-1.37798417
1	-2.33984518	0.57687533	-2.49663353

Energy = -8139.841571 Hartree

Number of imaginary frequencies = 0.

Compound TS1a isomer 2

Atomic N.	X	Y	Z
50	0.67878079	-0.73277181	-0.63350093
7	0.46561879	-0.31698677	1.88194048
6	1.29987335	-1.34973085	2.53350019
1	1.16977310	-1.33479011	3.63017106
1	1.03372598	-2.34409928	2.15562963
1	2.35416365	-1.15667987	2.30015206
7	-0.86944330	-2.04772925	0.26739377
6	-0.97762787	-0.53807515	2.15652180

50	1.16953075	-2.03031158	1.00581682
7	-1.11148345	-1.68546045	2.28282714
6	-1.11016083	-2.74490333	3.31179428
1	-2.05246854	-2.74562097	3.88914442
1	-0.98640192	-3.72951508	2.84320450
1	-0.27148062	-2.58032513	3.99938774
7	-0.52946901	-2.84648323	-0.15542617
6	-2.19285512	-1.90815210	1.29306626
1	-3.15729642	-2.07774997	1.80906677
1	-2.28349257	-0.99521440	0.68992174
6	-1.87690353	-3.07206106	0.35434338
1	-2.62582207	-3.06528091	-0.45691222
1	-1.97270393	-4.04414320	0.86770225
16	0.06951302	-3.81403160	-1.33403718
7	0.64702260	0.62060046	1.60084283
6	-1.22758329	-0.35163376	2.92049909
1	-2.27473021	-0.17144369	3.23336244
1	-0.59765983	-0.35263368	3.81921601
6	-0.74484152	0.79139292	2.01690125
1	-0.90587431	1.73768115	2.56169963
1	-1.35647881	0.85800636	1.10315597
16	1.81892073	1.21423757	2.61413693
8	3.10097003	0.72736788	2.05106568
8	1.47219288	0.94197541	4.03283024
6	1.78567350	3.01733947	2.42228866
6	1.21131575	3.81052446	3.41617942
6	1.18155026	5.19801331	3.24952292
6	1.72420096	5.80380487	2.10762382
6	2.30188441	4.98011112	1.12491262
6	2.33650041	3.59549737	1.27433360
1	0.81329799	3.33990550	4.31444740
1	2.80380011	2.96375179	0.51898485
1	2.73752356	5.43399334	0.23257682
6	1.72207201	7.30354738	1.94769895
1	0.73459852	5.82092333	4.02670574
8	1.53333712	-3.47325706	-1.30101240
8	-0.34571573	-5.23070002	-1.21570027
6	-0.60455817	-3.20401740	-2.89983821
6	-1.17097068	-4.10672712	-3.79841995
6	-1.66587842	-3.63138366	-5.01629257
6	-1.60377824	-2.26952910	-5.34200382
6	-1.03034472	-1.38321841	-4.41157389
6	-0.53053331	-1.83806801	-3.19343901
1	-1.21762788	-5.16385317	-3.53951812
1	-2.10738397	-4.33404970	-5.72537804
6	-2.14437175	-1.75633955	-6.65333128
1	-0.97427648	-0.31873065	-4.64893293
1	-0.08921172	-1.15006053	-2.46924019
1	0.97860020	7.77589417	2.60248756
1	2.70625401	7.72491646	2.20542598
1	1.50700092	7.59643698	0.91086227
1	-1.38483369	-1.17396402	-7.19479418
1	-2.47100616	-2.57892466	-7.30182171
1	-3.00535440	-1.09003985	-6.49237537
8	1.25101817	-0.38535473	-0.54776955
1	1.01319599	0.33798355	0.35411885
6	2.51295257	-0.12321894	-1.19465625
1	3.30581474	0.08374889	-0.45939106

1 2.39623713 0.74701309 -1.85766149
 1 2.78857279 -0.99826658 -1.79862916
 Energy = -8139.842267 Hartree
 Number of imaginary frequencies = 0.

Compound TS1a isomer 4

Atomic N.	X	Y	Z
50	1.47137129	-1.69124162	-1.22553194
7	1.37246764	-2.39008284	1.31536639
6	2.25267148	-3.57322478	1.39749718
1	2.25493002	-4.00250816	2.41581249
1	1.91788471	-4.34540749	0.69321305
1	3.27623749	-3.28184485	1.13165772
7	-0.40762272	-2.76692629	-0.76409578
6	-0.03545073	-2.75521970	1.60380554
1	-0.09664812	-3.33852983	2.54248929
1	-0.59806740	-1.82276726	1.74320817
6	-0.67201865	-3.52970672	0.45036858
1	-1.75431800	-3.61008000	0.65333164
1	-0.28221977	-4.56028557	0.39022747
16	-1.10374641	-3.21831894	-2.17709517
7	1.70854175	0.45569807	0.50070447
6	1.85411739	-1.32810533	2.23170137
1	1.57368600	-1.57246959	3.27499843
1	2.94952607	-1.30130589	2.16951513
6	1.33402824	0.06736450	1.86038911
1	1.71162331	0.77636683	2.61726618
1	0.23513713	0.10953488	1.92469847
16	3.18343282	1.18978071	0.30268469
8	3.37789130	1.28044426	-1.16408253
8	4.21103191	0.53984559	1.15621638
6	2.99444079	2.87852788	0.93637258
6	3.53584003	3.21911025	2.17647004
6	3.37130880	4.52073526	2.65847015
6	2.68034196	5.48813915	1.91531551
6	2.15068316	5.11844873	0.66611516
6	2.30294919	3.82437873	0.17311490
1	4.09444094	2.47315359	2.74072790
1	1.90776563	3.54919362	-0.80469936
1	1.61690724	5.86028385	0.06878702
6	2.53565121	6.90100002	2.42295957
1	3.79543018	4.79036808	3.62763095
8	-0.31171954	-2.42720151	-3.18032074
8	-1.22319841	-4.68503761	-2.34410310
6	-2.78955388	-2.55786848	-2.16091633
6	-3.85633922	-3.39616227	-2.48335338
6	-5.15209723	-2.87327290	-2.48891115
6	-5.39221811	-1.52739298	-2.17686558
6	-4.29610968	-0.71030533	-1.84644914
6	-2.99643350	-1.21330655	-1.83662820
1	-3.66387606	-4.44146824	-2.72216320
1	-5.99110222	-3.52516222	-2.73935509
6	-6.78909492	-0.95980906	-2.21385431
1	-4.46621656	0.33785295	-1.59185028
1	-2.14599943	-0.58080763	-1.57339907
1	2.68428731	6.95430040	3.50912189
1	3.28065157	7.56250143	1.95389485

1	1.54459476	7.31250525	2.18770981
1	-6.96592617	-0.42091867	-3.15779996
1	-7.54618835	-1.75091088	-2.13868594
1	-6.95290184	-0.24337929	-1.39726436
8	0.19277576	0.16918275	-1.40030384
1	0.83751965	0.57195318	-0.49664196
6	0.30746108	0.96011758	-2.60063076
1	1.35032260	1.26067615	-2.78557444
1	-0.31600958	1.86010242	-2.49182200
1	-0.06287327	0.36946180	-3.44944477

Energy = -8139.842294 Hartree

Number of imaginary frequencies = 0.

Compound TS1a isomer 5

Atomic N.	X	Y	Z
50	1.47826779	-2.00420022	0.58649844
7	1.11486006	-0.60211807	2.78932834
6	1.91308570	-1.31682765	3.80585885
1	1.80065501	-0.85433334	4.80320978
1	1.59644139	-2.36568332	3.86905670
1	2.97145557	-1.29095352	3.51872039
7	-0.49239704	-2.43899417	1.49556732
6	-0.33206865	-0.67087173	3.10607862
1	-0.51017755	-0.37150052	4.15669155
1	-0.84867758	0.04560317	2.45400786
6	-0.90917742	-2.06090760	2.84088922
1	-2.00808930	-1.99231935	2.92280483
1	-0.57825381	-2.78890753	3.60126734
16	-1.08883154	-3.80297780	0.81098932
7	1.68678713	0.72179323	0.18384977
6	1.57629418	0.80223340	2.66931033
1	1.19243574	1.40077639	3.51860380
1	2.67271590	0.80188578	2.71935272
6	1.17286420	1.45552623	1.34030592
1	1.52435219	2.50145364	1.36265385
1	0.07689453	1.50411487	1.24046791
16	3.21166182	1.11162317	-0.34205353
8	3.54491973	0.08639329	-1.35958111
8	4.11850882	1.34680665	0.81080419
6	3.05743480	2.70312691	-1.19792283
6	3.49492550	3.87206101	-0.57392186
6	3.35636687	5.09340906	-1.23912668
6	2.79425240	5.16189194	-2.52173328
6	2.36799526	3.96728015	-3.12896156
6	2.49576879	2.74224162	-2.47786140
1	3.95487547	3.81381798	0.41189709
1	2.18205190	1.81729507	-2.96166325
1	1.93571460	3.99923062	-4.13103199
6	2.67940950	6.47745275	-3.25038552
1	3.69939709	6.00910807	-0.75369626
8	-0.16656230	-3.99137378	-0.36088422
8	-1.28125012	-4.91810274	1.76642883
6	-2.72708797	-3.38524961	0.16270231
6	-3.80908442	-4.21697378	0.44916022
6	-5.06574488	-3.89873838	-0.07249413
6	-5.25192070	-2.76290059	-0.87336713
6	-4.14257002	-1.93896031	-1.13605142

6	-2.88129783	-2.24056053	-0.62595463
1	-3.65899801	-5.09623241	1.07455420
1	-5.91663599	-4.54556322	0.14929257
6	-6.60378027	-2.43850327	-1.45821536
1	-4.27176476	-1.04550314	-1.75043535
1	-2.02093148	-1.59751713	-0.82350284
1	2.71442246	7.32574129	-2.55475593
1	3.50784373	6.60130930	-3.96523952
1	1.74504054	6.53787041	-3.82492709
1	-6.65314770	-2.73917389	-2.51639414
1	-7.40778255	-2.96392941	-0.92712301
1	-6.80928993	-1.35986233	-1.41925001
8	0.32973704	-0.91348058	-1.03218496
1	0.91420478	0.04144164	-0.65852404
6	0.59677857	-1.26424444	-2.40520430
1	1.66808176	-1.17292452	-2.64210677
1	0.02136990	-0.59291190	-3.05998993
1	0.26765108	-2.29818702	-2.57580876

Energy = -8139.842275 Hartree

Number of imaginary frequencies = 0.

Compound TS1a isomer 6

Atomic N.	X	Y	Z
50	1.52296853	-0.86136293	0.76856023
7	0.81482422	-0.25448361	3.08374405
6	1.79470456	-0.84429830	4.02601671
1	1.59425056	-0.51567292	5.06028652
1	1.73000848	-1.93920624	3.98544073
1	2.80199838	-0.52991945	3.72566748
7	-0.66904324	-1.42613721	1.07525337
6	-0.57028085	-0.75842375	3.35933518
1	-0.64769042	-1.05214357	4.41932440
1	-1.27057362	0.06726197	3.18285012
6	-0.95283878	-1.90443540	2.43001413
1	-2.02398062	-2.12538314	2.57874036
1	-0.40177149	-2.82984591	2.68127775
16	-1.24185443	-2.33839083	-0.17109481
7	0.99629241	1.49829698	0.73348910
6	0.85551596	1.23470318	3.16923285
1	0.32611027	1.57153213	4.07840443
1	1.91009176	1.52739215	3.24549174
6	0.23440465	1.90094960	1.94389367
1	0.28162283	2.99316096	2.08208704
1	-0.82003635	1.61752629	1.81453395
16	0.52372730	2.43146276	-0.65220875
8	0.86613786	3.84512353	-0.38444293
8	-0.86841220	2.06760478	-0.98678851
6	1.64004219	1.78437448	-1.90152228
6	1.31145298	0.59975195	-2.56764007
6	2.18670893	0.11896581	-3.54140377
6	3.36969018	0.80575615	-3.86110544
6	3.66431093	1.99556220	-3.17521644
6	2.80707097	2.49300814	-2.19369149
1	0.39484644	0.05713977	-2.33178616
1	3.02588058	3.41964173	-1.66432142
1	4.58001184	2.54004574	-3.41159439
6	4.29042292	0.28621998	-4.93560934

1	1.94457316	-0.81302530	-4.05415678
8	-0.46367553	-1.86200714	-1.35470927
8	-1.26964104	-3.79026771	0.13858543
6	-2.96378207	-1.82556617	-0.40353894
6	-3.98612046	-2.76036191	-0.24512695
6	-5.31170273	-2.35684776	-0.43273205
6	-5.62427139	-1.03503108	-0.77837259
6	-4.57082081	-0.11443933	-0.92890912
6	-3.24427962	-0.49759549	-0.74434400
1	-3.73556828	-3.78851891	0.01383701
1	-6.11569548	-3.08531332	-0.31090853
6	-7.05296850	-0.60572594	-1.00257254
1	-4.79322338	0.92034495	-1.19708431
1	-2.43666196	0.22597231	-0.86366427
1	4.34719753	-0.81031007	-4.91602468
1	3.92394805	0.57481825	-5.93301105
1	5.30473995	0.69066745	-4.82612324
1	-7.24178362	-0.41354316	-2.06993818
1	-7.76038313	-1.37643039	-0.67090571
1	-7.27934885	0.32569775	-0.46429506
8	3.18920970	0.75238872	1.48561239
1	2.14775896	1.49918222	0.96058464
6	4.46057749	0.68211555	0.86327416
1	4.50286961	-0.10226099	0.07951837
1	5.24525452	0.44894466	1.60483897
1	4.72718430	1.64133561	0.38494787

Energy = -8139.824288 Hartree

Number of imaginary frequencies = 0.

Compound TS1a isomer 7

Atomic N.	X	Y	Z
50	1.88877535	-1.97418261	-0.32551152
7	1.46451354	-1.50467777	2.15146565
6	2.58975720	-2.10394001	2.90321565
1	2.52905512	-1.85531342	3.97758412
1	2.56338024	-3.19585967	2.79389143
1	3.53136778	-1.72443092	2.48681450
7	-0.22704148	-2.61205888	0.28294000
6	0.15598822	-2.09524775	2.57626128
1	0.23758516	-2.46530581	3.61234879
1	-0.59798205	-1.29832864	2.55995417
6	-0.30324382	-3.19349670	1.62360513
1	-1.33366096	-3.47953081	1.89753580
1	0.31481111	-4.10450029	1.73203504
16	-0.89571273	-3.47909021	-0.95159262
7	1.20665622	0.40626150	-0.05203419
6	1.45990634	-0.02837173	2.33579803
1	1.07397962	0.22801873	3.33963799
1	2.50158930	0.31006104	2.26336837
6	0.62683284	0.69338173	1.27462614
1	0.65224236	1.77350008	1.49985552
1	-0.42248094	0.36941174	1.27920580
16	0.53154057	1.21391165	-1.40404081
8	-0.93781102	1.15830219	-1.27779341
8	1.24785471	0.63817173	-2.55591249
6	1.04114544	2.93435717	-1.21270812
6	2.33866477	3.30501223	-1.57987773

6	2.72645497	4.63460970	-1.43278134
6	1.83729112	5.60075617	-0.92822492
6	0.54164100	5.19781494	-0.57273912
6	0.13392271	3.86901426	-0.71246868
1	3.02257633	2.56284356	-1.99129021
1	-0.87777531	3.55691791	-0.45572737
1	-0.16330560	5.93564558	-0.18590114
6	2.26513267	7.04067469	-0.80142415
1	3.73632550	4.93194532	-1.72086692
8	-0.25320247	-2.90276027	-2.16929722
8	-0.84706706	-4.94474697	-0.71402866
6	-2.64905381	-3.02300811	-0.98864508
6	-3.61555767	-3.98108840	-0.68372416
6	-4.96590948	-3.62020063	-0.71491206
6	-5.35926580	-2.31757402	-1.05121756
6	-4.36126614	-1.37340558	-1.35384166
6	-3.01071048	-1.71431303	-1.32573545
1	-3.30366397	-4.99591351	-0.43902048
1	-5.72606039	-4.36764002	-0.47909936
6	-6.81791162	-1.93715417	-1.11389852
1	-4.64731550	-0.35375416	-1.61995888
1	-2.24728608	-0.97359949	-1.56549644
1	3.27226806	7.12146139	-0.36969766
1	2.29781008	7.52494431	-1.78951120
1	1.57113743	7.61257648	-0.17288689
1	-7.15500736	-1.84828532	-2.15832543
1	-7.45018244	-2.68829393	-0.62317824
1	-6.99911261	-0.96510297	-0.63386834
8	3.53014970	-0.35369512	0.24692857
1	2.33082342	0.44035456	-0.03851196
6	4.72772503	-0.38754940	-0.50602573
1	4.80530024	-1.30842459	-1.12091970
1	5.61109400	-0.35827017	0.15721960
1	4.80228901	0.46916690	-1.20159638

Energy = -8139.822535 Hartree

Number of imaginary frequencies = 0.

Compound TS1a isomer 8

Atomic N.	X	Y	Z
50	1.45837128	-0.86791575	0.16736603
7	0.63000470	0.14793649	2.47328210
6	1.75859916	0.05188102	3.42288542
1	1.50795102	0.52446538	4.39014864
1	2.00206232	-1.00282276	3.60546184
1	2.63022423	0.54727137	2.97781920
7	-0.09766564	-2.27267337	1.19990289
6	-0.54395562	-0.62056100	2.95568848
1	-0.67014617	-0.46998215	4.04484749
1	-1.43981588	-0.23735093	2.45109725
6	-0.42940396	-2.10995817	2.61015582
1	-1.37819839	-2.60082269	2.88100004
1	0.36156261	-2.59505105	3.20560694
16	-1.32076478	-2.33693838	0.11859803
7	0.36355609	1.33366871	-0.15711862
6	0.26775411	1.57265031	2.26061535
1	-0.33876088	1.94500744	3.10721922
1	1.20487106	2.14321160	2.22889853

6	-0.49097598	1.79954159	0.95209861
1	-0.70386612	2.87925076	0.86949831
1	-1.45154893	1.26658762	0.92095447
16	-0.13959189	1.72325802	-1.75007784
8	-1.59579134	1.53135109	-1.84667301
8	0.82389182	1.00602722	-2.60775065
6	0.18875298	3.49555087	-1.89829898
6	1.48859608	3.93306160	-2.16892815
6	1.73100877	5.30002785	-2.28520799
6	0.69358474	6.23804283	-2.13828111
6	-0.60077870	5.76808023	-1.87151206
6	-0.86300468	4.40106678	-1.75245595
1	2.29009342	3.20683479	-2.30334568
1	-1.87149215	4.03147650	-1.56916928
1	-1.41947567	6.48141479	-1.76151299
6	0.96707785	7.71250343	-2.29545569
1	2.74324369	5.64761972	-2.49996424
8	-2.59864664	-1.76358640	0.61473030
8	-0.67988229	-1.75864720	-1.11816490
6	-1.64573181	-4.07837582	-0.25079784
6	-0.65097415	-4.84915495	-0.86059141
6	-0.90376353	-6.19031763	-1.13402259
6	-2.13925314	-6.77936077	-0.80677980
6	-3.11747980	-5.98189354	-0.19834302
6	-2.88060641	-4.63242817	0.08136527
1	0.30458009	-4.39607048	-1.12486255
1	-0.13130295	-6.79378986	-1.61479044
6	-2.39902449	-8.23222256	-1.11813164
1	-4.08451128	-6.41925573	0.05700295
1	-3.64394212	-4.00508118	0.54004270
1	1.90484035	8.00030899	-1.80065250
1	1.06769729	7.97844934	-3.35910344
1	0.15364830	8.31885147	-1.87736130
1	-2.37551665	-8.41367149	-2.20319939
1	-1.63154864	-8.87879562	-0.66800767
1	-3.37902927	-8.55329037	-0.74329388
8	2.71254301	1.15722263	0.57994300
1	1.47796798	1.56998718	0.01962798
6	3.95172668	1.25835919	-0.09388092
1	4.13118076	0.40427133	-0.78050268
1	4.79088974	1.28497028	0.62526989
1	4.01016998	2.17980886	-0.70288861

Energy = -8139.822379 Hartree

Number of imaginary frequencies = 0.

Compound TS1a isomer 9

Atomic N.	X	Y	Z
50	0.53550810	0.50836557	0.51955712
7	-0.41524050	1.38374138	2.68567491
6	0.33477566	0.74697798	3.79278064
1	0.01012412	1.14519167	4.76979542
1	0.16339876	-0.33703214	3.78182817
1	1.40405202	0.94592917	3.65015864
7	-1.52907443	-0.33664349	0.85792816
6	-1.86984062	1.05913925	2.76749969
1	-2.20143247	1.11783946	3.81993794
1	-2.41168880	1.81821823	2.19055963

6	-2.18931866	-0.30093691	2.15531397
1	-3.28395271	-0.38517952	2.05808544
1	-1.85072696	-1.12398815	2.81303024
16	-2.23656464	-1.13019097	-0.39155003
7	0.23333187	2.93079185	0.32380900
6	-0.22260006	2.86136341	2.72874522
1	-0.83413076	3.29517126	3.54071355
1	0.83631521	3.04296684	2.94934630
6	-0.58265585	3.53338170	1.40599430
1	-0.36512482	4.60995579	1.50251043
1	-1.64915240	3.43149400	1.16044950
16	0.05102051	3.81586337	-1.15724874
8	0.77622819	5.09733057	-1.01303542
8	-1.38420677	3.81283665	-1.50258064
6	0.95067024	2.76851201	-2.30774522
6	0.29316014	1.68841863	-2.90315914
6	0.99893075	0.89036250	-3.80331540
6	2.34006548	1.16130638	-4.11857462
6	2.96914077	2.25715423	-3.50397539
6	2.28352141	3.06690836	-2.59886670
1	-0.74715579	1.46706951	-2.66636848
1	2.76193595	3.92509460	-2.12833738
1	4.01174116	2.47955394	-3.73769236
6	3.08239222	0.30816364	-5.11552954
1	0.49567920	0.03430730	-4.25457048
8	-3.69806147	-0.89110547	-0.44306710
8	-1.37407482	-0.79345018	-1.56084406
6	-2.02520084	-2.90577221	-0.07731217
6	-0.75606418	-3.48007417	-0.19589035
6	-0.59552473	-4.83987427	0.06046598
6	-1.68758321	-5.64272833	0.43691730
6	-2.94855905	-5.04095078	0.54852939
6	-3.12604952	-3.67806458	0.29159123
1	0.09250168	-2.86627674	-0.50142717
1	0.39433536	-5.29071760	-0.03587630
6	-1.50394273	-7.11896133	0.68687838
1	-3.80956936	-5.64775324	0.83533913
1	-4.10838318	-3.21154022	0.35874104
1	2.71568012	-0.72650832	-5.10691547
1	2.94376850	0.69606340	-6.13680363
1	4.16120958	0.29927480	-4.91211987
1	-1.38249421	-7.66497183	-0.26147106
1	-0.60545701	-7.31480694	1.28873098
1	-2.36898732	-7.54791832	1.20850813
8	2.23649979	2.02674627	1.39178360
1	1.35829747	2.79488969	0.70870084
6	3.55079412	1.85031557	0.88982838
1	3.59565735	1.09272540	0.07992186
1	4.23093414	1.51675534	1.69288194
1	3.95114803	2.79526591	0.48173976

Energy = -8139.821412 Hartree

Number of imaginary frequencies = 0.

Compound TS1a isomer 10

Atomic N.	X	Y	Z
50	0.94696212	-0.45126349	1.59780705
7	-1.03967357	0.05282110	3.02402067

6	-0.67807341	-0.25239250	4.42826319
1	-1.48283088	0.05428015	5.11835337
1	-0.51161104	-1.33170462	4.53828669
1	0.24686468	0.28327394	4.67573023
7	-0.89367360	-1.50926423	0.75583106
6	-2.22259235	-0.75633323	2.58309174
1	-2.83150125	-1.02213752	3.46311092
1	-2.83375502	-0.12800600	1.92353117
6	-1.80327570	-1.99284804	1.79656553
1	-2.71147013	-2.45684600	1.37449980
1	-1.33754158	-2.75102186	2.45342517
16	-0.49304169	-2.57266974	-0.43669799
7	0.12632912	1.71285880	0.89929682
6	-1.31840706	1.51083398	2.87261939
1	-2.31867933	1.74437058	3.27913260
1	-0.56392044	2.04898214	3.45973563
6	-1.24337971	1.96529472	1.41695833
1	-1.47686970	3.04148459	1.37755108
1	-1.96921980	1.43409145	0.78458881
16	0.36661294	2.46146369	-0.64880610
8	0.24529378	3.92406869	-0.46692434
8	-0.50322562	1.77129173	-1.62320638
6	2.08541560	2.05034089	-0.96840209
6	2.40238094	0.80004734	-1.50723851
6	3.74238348	0.50320774	-1.75762033
6	4.75775671	1.43506241	-1.48779809
6	4.40127468	2.68367267	-0.95114893
6	3.06920838	3.00097108	-0.68741494
1	1.62409019	0.06695541	-1.72403777
1	2.78572774	3.97046280	-0.27937508
1	5.17899275	3.41790676	-0.73441386
6	6.19812155	1.11105967	-1.79203379
1	3.99855947	-0.47659862	-2.16306949
8	0.71876359	-1.96701062	-1.06776047
8	-0.43562135	-3.97900105	0.03593903
6	-1.84149742	-2.48615837	-1.64336979
6	-2.10721135	-1.27304339	-2.28835487
6	-3.14102578	-1.21644127	-3.22024679
6	-3.91640210	-2.35178351	-3.51986265
6	-3.62834430	-3.55144477	-2.85494328
6	-2.59342527	-3.62778664	-1.91760409
1	-1.51354480	-0.38547999	-2.06510425
1	-3.34914637	-0.27200857	-3.72709322
6	-5.02018118	-2.27513719	-4.54533625
1	-4.21909857	-4.44298840	-3.07419634
1	-2.35799837	-4.55966139	-1.40461671
1	6.39906216	0.03806401	-1.67638552
1	6.44418383	1.38011467	-2.83114409
1	6.88194990	1.66786754	-1.13829136
1	-5.68762732	-1.42346919	-4.35036516
1	-4.60790825	-2.13484740	-5.55625057
1	-5.62447071	-3.19118452	-4.55343437
8	1.59855342	1.53577065	2.83168769
1	0.92459071	1.99507558	1.71168590
6	2.98689461	1.74781966	3.02129769
1	3.60427356	0.98077780	2.50966883
1	3.24340987	1.71382904	4.09514809
1	3.29858851	2.73441124	2.63472080

Energy = -8139.824291 Hartree
 Number of imaginary frequencies = 0.

Compound TS1a isomer 11

Atomic N.	X	Y	Z
50	1.89184320	0.02028760	-0.07464397
7	1.19000804	1.10975826	2.14589071
6	2.04641819	0.53386766	3.20685339
1	1.84093332	1.00693357	4.18346024
1	1.85513556	-0.54343516	3.29358196
1	3.09639382	0.69220704	2.93197370
7	-0.14996555	-0.73833400	0.60873610
6	-0.24933390	0.83163232	2.41109085
1	-0.46764833	0.99139506	3.48315382
1	-0.83927286	1.54942405	1.82789886
6	-0.65655321	-0.56888914	1.96346819
1	-1.75642562	-0.63344210	2.00068021
1	-0.25770369	-1.33821249	2.65158153
16	-1.01491940	-1.61920822	-0.46877614
7	1.57017016	2.45398974	-0.36744052
6	1.41494703	2.57997608	2.06226993
1	0.91520894	3.08715153	2.90809727
1	2.49628472	2.74493313	2.14378190
6	0.92020202	3.17623782	0.74396020
1	1.18775451	4.24503994	0.72351480
1	-0.17351237	3.10325813	0.64662945
16	1.39836943	3.16020370	-1.93379939
8	2.16523385	2.25269723	-2.80930638
8	1.73114097	4.59827328	-1.84314907
6	-0.36185470	3.01765609	-2.27576995
6	-1.15186322	4.16850376	-2.24610353
6	-2.52027678	4.05126715	-2.49894214
6	-3.10369205	2.80391073	-2.76909351
6	-2.27891755	1.66537178	-2.79300523
6	-0.90979940	1.76260185	-2.55742621
1	-0.69265813	5.13402557	-2.03761482
1	-0.29272279	0.86432672	-2.58726454
1	-2.71053624	0.68179703	-2.98354554
6	-4.58126163	2.67828465	-3.03977251
1	-3.14552641	4.94568443	-2.48215580
8	-2.46916318	-1.32976329	-0.38604349
8	-0.29222885	-1.42431629	-1.75920939
6	-0.81970268	-3.36485934	-0.01509075
6	0.39578503	-4.00750017	-0.26967308
6	0.54936123	-5.34348583	0.09272134
6	-0.49533758	-6.05415154	0.71161914
6	-1.70296478	-5.38548040	0.95383424
6	-1.87412393	-4.04553938	0.59231281
1	1.20290673	-3.46692395	-0.76573968
1	1.49513674	-5.84906054	-0.11270311
6	-0.31827205	-7.50521660	1.08375776
1	-2.52806997	-5.92191076	1.42633545
1	-2.81965208	-3.53056645	0.75914216
1	-5.11173487	3.61414957	-2.82362700
1	-4.76396942	2.42143846	-4.09426785
1	-5.02547073	1.87642980	-2.43352747
1	-0.23012643	-8.13404369	0.18479398

1	0.59755599	-7.65720415	1.67297864
1	-1.16877186	-7.87519503	1.67016411
8	3.65171146	1.47776115	0.51928204
1	2.69708729	2.29041862	-0.11129405
6	4.89382982	1.23714411	-0.13040067
1	4.87261820	0.31044245	-0.73921895
1	5.70174837	1.13168991	0.61363977
1	5.15624809	2.06656933	-0.80859894

Energy = -8139.825627 Hartree
Number of imaginary frequencies = 0.

Compound TS1a isomer 12

Atomic N.	X	Y	Z
50	1.12986767	-0.00847207	0.32512996
7	-0.01819348	-0.12251750	2.72611022
6	0.56097198	-1.19372213	3.57111025
1	0.00435833	-1.27947831	4.52260923
1	0.53159451	-2.15984893	3.05687499
1	1.60776269	-0.94682467	3.77737737
7	-0.41349182	-1.74935651	0.52593243
6	-1.40668476	-0.45444605	2.33923221
1	-2.05030489	-0.55322897	3.23433137
1	-1.79652071	0.38355881	1.74095786
6	-1.48062849	-1.76032925	1.52123094
1	-2.47523737	-1.80520356	1.04565954
1	-1.39539182	-2.63180685	2.18888712
16	0.55315226	-3.04072928	0.34164575
7	1.21374786	2.28714252	1.68481314
6	0.05301713	1.15693355	3.48675680
1	-0.78734535	1.21784782	4.20280886
1	0.98255885	1.12222385	4.07024527
6	0.09330447	2.41121149	2.62098861
1	0.21588729	3.27647138	3.29434705
1	-0.86082673	2.55333185	2.07983947
16	1.74180770	3.68976974	0.95541888
8	2.93726158	3.28730845	0.17649567
8	1.81869733	4.80028009	1.93505943
6	0.44094050	4.13912821	-0.22363745
6	-0.52438390	5.07996607	0.13909759
6	-1.52996016	5.41216230	-0.77213067
6	-1.57951224	4.82374287	-2.04458499
6	-0.59134603	3.88398671	-2.38486981
6	0.41636690	3.53850269	-1.48545539
1	-0.46823522	5.55764484	1.11684036
1	1.19275963	2.82436562	-1.75883830
1	-0.60926050	3.41985130	-3.37294984
6	-2.64443135	5.21455383	-3.03891397
1	-2.28447104	6.14962292	-0.49164855
8	1.87762415	-2.38174868	-0.02166039
8	0.53864276	-4.00821877	1.46662426
6	0.04223459	-3.94765306	-1.13606501
6	-0.31043229	-5.29126692	-1.02446568
6	-0.71558100	-5.98313236	-2.16976023
6	-0.76940864	-5.35099936	-3.41919184
6	-0.40747601	-3.99340439	-3.49877882
6	-0.00363025	-3.28886652	-2.36833405
1	-0.25939894	-5.78183317	-0.05335228

1	-0.99134254	-7.03596592	-2.08780646
6	-1.19000196	-6.10328341	-4.65666580
1	-0.44189712	-3.48362041	-4.46348858
1	0.27696273	-2.23748589	-2.43956566
1	-3.52748203	5.63215780	-2.53806448
1	-2.26676846	5.98034000	-3.73432827
1	-2.96257091	4.35524225	-3.64471602
1	-0.34146217	-6.23022604	-5.34601498
1	-1.57352006	-7.10081625	-4.40847969
1	-1.97235715	-5.56070185	-5.20641136
8	2.72010875	0.34289438	1.90255499
1	2.18840528	1.43083215	1.94897091
6	4.10730505	0.37661552	1.51409566
1	4.29427576	1.16058362	0.76449960
1	4.39181280	-0.60451245	1.10835838
1	4.71812677	0.58142722	2.40527320

Energy = -8139.825469 Hartree

Number of imaginary frequencies = 0.

Compound TS1a isomer 13

Atomic N.	X	Y	Z
50	2.75698996	-1.11839557	0.22887301
7	2.24995208	-0.26104134	2.56043959
6	3.19637012	-0.92454940	3.48883247
1	3.09606862	-0.51693320	4.50981998
1	2.98579431	-2.00144625	3.51852131
1	4.21646070	-0.76515651	3.11893582
7	0.49047601	-1.43906760	0.74647564
6	0.83651644	-0.56971222	2.93752909
1	0.77320480	-0.72832137	4.02758837
1	0.21848191	0.30090383	2.68339825
6	0.29946119	-1.76471698	2.16437793
1	-0.76741421	-1.89027488	2.42173004
1	0.80772591	-2.70066142	2.46286201
16	-0.16897324	-2.51955175	-0.30728710
7	2.54962659	1.33298266	0.13293135
6	2.47966027	1.21254933	2.57003713
1	2.03790855	1.65446150	3.48123980
1	3.56479168	1.37217665	2.59488845
6	1.90282476	1.90507650	1.33449852
1	2.11157417	2.98398662	1.40800190
1	0.81346571	1.76703954	1.26264691
16	2.48405981	2.29391527	-1.31331921
8	3.39810705	1.58980405	-2.23131752
8	2.70695591	3.70460820	-0.93154055
6	0.79781562	2.14454532	-1.91529965
6	-0.08283391	3.21320009	-1.73348570
6	-1.37243783	3.11848617	-2.25976396
6	-1.78615379	1.97682738	-2.96372843
6	-0.87537825	0.91805106	-3.12441754
6	0.41595545	0.99285191	-2.60883737
1	0.25113049	4.10740805	-1.20885885
1	1.10667920	0.16203769	-2.74095559
1	-1.18046904	0.01175837	-3.64899445
6	-3.17110276	1.88541818	-3.55165768
1	-2.06607056	3.95064640	-2.12766027
8	0.34168538	-2.11280465	-1.64702153

8	0.00186290	-3.93426394	0.11747313
6	-1.96043301	-2.20339799	-0.26064256
6	-2.84094524	-3.28303671	-0.18213481
6	-4.21696663	-3.04296398	-0.17230298
6	-4.72702265	-1.73745131	-0.23531772
6	-3.81695914	-0.66846460	-0.30092558
6	-2.44017053	-0.89252424	-0.31676117
1	-2.43944335	-4.29402065	-0.12034082
1	-4.90705299	-3.88661122	-0.10852746
6	-6.21454954	-1.48679376	-0.25258645
1	-4.19424868	0.35594282	-0.33556119
1	-1.73801208	-0.06050340	-0.36315072
1	-3.82387948	2.68178058	-3.17226529
1	-3.13500810	1.97389865	-4.64821720
1	-3.63373899	0.91462326	-3.32452893
1	-6.58952045	-1.43329477	-1.28684413
1	-6.76327419	-2.29250503	0.25246960
1	-6.46767187	-0.53589505	0.23523867
8	4.60441923	0.13769081	0.84790874
1	3.64372063	1.13155746	0.34814319
6	5.80621624	-0.12538485	0.13344561
1	5.78196812	-1.11651874	-0.36265457
1	6.66904497	-0.11697293	0.82104135
1	5.98275614	0.62900752	-0.65244067

Energy = -8139.822147 Hartree

Number of imaginary frequencies = 0.

Transition state 1b (TS1b)

Compound TS1b isomer 1

Atomic N.	X	Y	Z
50	0.04802457	-0.09648205	-0.76433325
7	0.84069765	-0.82470113	2.53665209
6	1.98026061	-0.88091749	3.44666243
1	1.66635454	-0.96674651	4.51038933
1	2.59886909	0.02125806	3.34701204
1	2.60759497	-1.75055087	3.20701408
7	0.93828946	1.45727062	0.72920823
6	0.02457071	0.36431861	2.77707744
1	-0.15576555	0.53666687	3.86194706
1	-0.95752537	0.21160719	2.30775023
6	0.63768226	1.61835527	2.16369414
1	-0.06641280	2.45236754	2.33456135
1	1.56083524	1.90075779	2.70695186
6	1.09722972	2.74247169	0.08690799
6	-0.02808722	3.49908376	-0.32928836
6	0.16346087	4.73518610	-0.96007961
6	1.43728304	5.26292658	-1.19011390
6	2.53618240	4.52086020	-0.74752390
6	2.39322543	3.27991366	-0.11295773
7	-0.79743010	-1.81153810	0.23491330
6	0.08918380	-2.07955933	2.57797694
1	-0.28782991	-2.30235839	3.60423970
1	0.79287219	-2.88492155	2.31169081
6	-1.10931981	-2.12860370	1.63066781
1	-1.49879265	-3.16016221	1.68558669
1	-1.91901410	-1.49488389	2.04393148

6	-1.62967944	-2.48796892	-0.71721196
6	-3.02392840	-2.23955131	-0.81626683
6	-3.78571081	-2.93101907	-1.76771009
6	-3.21757102	-3.86432409	-2.63941574
6	-1.83894432	-4.08633804	-2.54695749
6	-1.03994513	-3.42262793	-1.60887480
6	-1.44469714	3.00651884	-0.13818280
1	-0.71493405	5.30191803	-1.27971888
6	1.62027347	6.57900000	-1.90623832
1	3.54332137	4.91994667	-0.89349371
6	3.63772535	2.55036306	0.33501208
6	-3.70233917	-1.20791149	0.05017129
1	-4.85568190	-2.71767688	-1.83822560
6	-4.06227255	-4.61868429	-3.63763762
1	-1.36784756	-4.80548668	-3.22216868
6	0.43885350	-3.72183394	-1.55524361
1	-2.15020227	3.84642601	-0.18812609
1	-1.59183383	2.49521542	0.82175934
1	-1.73163950	2.29666352	-0.93218184
1	3.51652622	2.09280014	1.32642353
1	4.48863316	3.24243903	0.38054821
1	3.89593172	1.74049234	-0.36391503
1	1.70767200	6.42687607	-2.99379277
1	2.53287482	7.09281778	-1.57472396
1	0.76664847	7.24971628	-1.73842776
1	-4.63437843	-0.86283010	-0.41602144
1	-3.05002332	-0.33594996	0.21141544
1	-3.95773292	-1.60477889	1.04496872
1	0.77949423	-3.87325573	-0.52243412
1	1.03906190	-2.89348936	-1.96505070
1	0.67064810	-4.61871958	-2.14475965
1	-3.53459692	-4.74924898	-4.59275627
1	-5.00790930	-4.09672642	-3.83615732
1	-4.31297779	-5.62480116	-3.26561356
1	2.03792405	0.47223526	0.37662029
8	2.34902024	-0.29075092	-0.35149249
6	3.10343885	-1.40300572	0.13859610
1	3.49634004	-1.95925260	-0.72370118
1	2.48437500	-2.07472324	0.75118339
1	3.95364380	-1.04409182	0.73926342

Energy = -7200.131906 Hartree

Number of imaginary frequencies = 0.

Compound TS1b isomer 2

Atomic N.	X	Y	Z
50	0.97366500	-0.99763733	-0.09869952
7	0.97950113	-1.16129589	2.37933826
6	2.29628897	-1.34417498	3.03410840
1	2.17366290	-1.38157511	4.13108063
1	2.98115039	-0.54204142	2.74670815
1	2.73586249	-2.28736162	2.68918085
7	1.25548136	1.25361180	0.83225209
6	0.32784161	0.10134709	2.82208157
1	0.28942642	0.13179775	3.92777228
1	-0.70305800	0.08239164	2.44529152
6	1.02240753	1.35231256	2.28757548
1	0.37565804	2.21248531	2.52218294

1	1.97111237	1.51353323	2.83031893
6	1.15151799	2.49646449	0.10887414
6	0.06973329	2.74078202	-0.77019817
6	0.02335673	3.93910384	-1.49489391
6	1.01433659	4.91786194	-1.37959945
6	2.06480098	4.67285013	-0.49047625
6	2.15369511	3.49043417	0.25564173
7	-0.84571207	-2.07366538	0.49340725
6	0.11292576	-2.32999063	2.69499111
1	-0.10160545	-2.35436821	3.77994633
1	0.69180959	-3.22809553	2.43542552
6	-1.17830873	-2.31652904	1.88406169
1	-1.66141903	-3.30273461	2.01470804
1	-1.88696623	-1.58239019	2.32153225
6	-1.78431821	-2.50297761	-0.48537737
6	-3.09357667	-1.95418382	-0.56113535
6	-3.97460413	-2.38337851	-1.56108975
6	-3.61599565	-3.34984541	-2.50555897
6	-2.32973003	-3.89058924	-2.41849875
6	-1.41536081	-3.49726939	-1.43264508
6	-1.05111969	1.74822927	-0.94468087
1	-0.82076842	4.10961914	-2.16790295
6	0.96482682	6.18190861	-2.20311284
1	2.84982896	5.42414331	-0.37119374
6	3.31426883	3.33179426	1.21166945
6	-3.55771565	-0.88900644	0.40140736
1	-4.97066593	-1.93429279	-1.60782456
6	-4.59253979	-3.81564260	-3.55864382
1	-2.02532125	-4.65789986	-3.13532925
6	-0.06443154	-4.17336369	-1.39509642
1	-1.92018843	2.22514224	-1.41647196
1	-1.36907959	1.32245958	0.01529197
1	-0.75733471	0.90233302	-1.58895874
1	3.70451951	2.30534816	1.23614061
1	3.02091432	3.59186244	2.24131179
1	4.13394403	4.00544500	0.93016964
1	1.48004007	6.04548788	-3.16716743
1	1.45591080	7.01751518	-1.68620372
1	-0.07023874	6.47482014	-2.42601848
1	-4.38159990	-0.30682144	-0.03208455
1	-2.73986125	-0.20091209	0.65427130
1	-3.92410994	-1.31979001	1.34694278
1	0.27631074	-4.33017874	-0.36271188
1	0.71150380	-3.57451749	-1.89696443
1	-0.10966980	-5.14461279	-1.90613770
1	-4.07368755	-4.14564514	-4.46894073
1	-5.29464912	-3.01677513	-3.83456135
1	-5.19249868	-4.66638184	-3.19766712
1	2.40763307	0.76250899	0.68069732
8	3.31501555	-0.10351362	0.55713719
6	4.12458134	0.06814086	-0.59227860
1	4.87398529	-0.73967081	-0.65342152
1	4.67056131	1.02971709	-0.56510681
1	3.53805661	0.04767685	-1.53486609

Energy = -7200.138317 Hartree

Number of imaginary frequencies = 0.

Compound TS1b isomer 3

Atomic N.	X	Y	Z
50	0.64832854	-1.10022664	0.01061992
7	0.28627428	-1.31829393	2.48527598
6	1.47343266	-1.74415171	3.24901915
1	1.23263144	-1.85490060	4.32224846
1	2.27865911	-1.00939429	3.14530921
1	1.82851887	-2.70757866	2.86249614
7	1.04998827	1.08888841	1.05650067
6	-0.17450999	0.02821056	2.91260839
1	-0.31824496	0.04646303	4.00973749
1	-1.15234935	0.20149764	2.44269466
6	0.78119719	1.14234746	2.49361706
1	0.31312764	2.09630036	2.80738854
1	1.72372890	1.07438016	3.07082820
6	2.05477381	2.03467631	0.64551097
6	3.40272760	1.65843201	0.41933730
6	4.32794571	2.61603117	-0.01943768
6	3.97372985	3.94849372	-0.24658126
6	2.64860320	4.31569767	0.00443588
6	1.69112301	3.39561844	0.44994643
7	-1.30789053	-1.99623871	0.29408234
6	-0.79453760	-2.32775164	2.63024259
1	-1.19289851	-2.31014991	3.66320205
1	-0.33648258	-3.31081343	2.44908905
6	-1.90509260	-2.10255361	1.61014676
1	-2.58471990	-2.97316027	1.66593397
1	-2.51903415	-1.22963905	1.91810536
6	-2.13961053	-2.21463919	-0.83520675
6	-3.30575180	-1.44172692	-1.09206367
6	-4.08005142	-1.71050322	-2.22823238
6	-3.74512601	-2.71285129	-3.14365172
6	-2.59009910	-3.45897436	-2.88963270
6	-1.79163134	-3.23767877	-1.76064527
6	3.89493680	0.24766734	0.63564163
1	5.36223888	2.30356526	-0.18652332
6	4.97913647	4.94866991	-0.76384920
1	2.34351397	5.35399342	-0.15122548
6	0.29449946	3.90265179	0.73178804
6	-3.70793295	-0.29409626	-0.19886813
1	-4.96639013	-1.09637201	-2.41115308
6	-4.61369467	-2.99738216	-4.34563112
1	-2.30560327	-4.25484753	-3.58334684
6	-0.58504844	-4.11982727	-1.54129565
1	4.97632599	0.24508964	0.82828844
1	3.71125817	-0.38690880	-0.24484324
1	3.39043140	-0.23910432	1.47936821
1	0.17436428	4.16791344	1.79452109
1	-0.48125720	3.16254497	0.49728855
1	0.09149723	4.81152534	0.15015967
1	5.99768591	4.69900227	-0.43653756
1	4.74665689	5.96595287	-0.42061391
1	4.98624897	4.96909285	-1.86524546
1	-4.40733957	0.37011567	-0.72392493
1	-2.82437634	0.29127070	0.09156201
1	-4.21104050	-0.63589233	0.71980757
1	-0.47743708	-4.38883305	-0.48156199
1	0.35327491	-3.62063146	-1.83219397

1	-0.66661406	-5.03744459	-2.13946533
1	-4.02270651	-3.39136434	-5.18389797
1	-5.13233232	-2.09109616	-4.68793726
1	-5.38740587	-3.74624443	-4.11140490
1	0.05072679	1.21392643	0.07644767
8	-0.55861938	0.79663277	-0.79515702
6	-0.24858066	1.37619388	-2.06743741
1	0.83779752	1.41245663	-2.25725079
1	-0.64818382	2.40134692	-2.12226748
1	-0.72279119	0.77462101	-2.85616565

Energy = -7200.144459 Hartree

Number of imaginary frequencies = 0.

Compound TS1b isomer 4

Atomic N.	X	Y	Z
50	0.87579191	-1.16831076	-0.00020340
7	0.45092297	-1.32706070	2.46097136
6	1.63400710	-1.63965654	3.28089714
1	1.35852766	-1.74587059	4.34629536
1	2.38448024	-0.84970731	3.18538499
1	2.07753158	-2.58167338	2.93377376
7	1.07678008	1.07743883	0.92623949
6	-0.12638348	-0.00515846	2.80827260
1	-0.30439389	0.06250975	3.89871478
1	-1.09775221	0.06844285	2.30222464
6	0.75794291	1.15580165	2.35565281
1	0.22005329	2.09109592	2.61191487
1	1.68463159	1.18119276	2.95849562
6	2.11052608	2.01912665	0.56219566
6	3.49359703	1.72776771	0.67974031
6	4.43906975	2.68238997	0.28045353
6	4.07388592	3.93687034	-0.21573202
6	2.70973444	4.22773933	-0.28951609
6	1.72917438	3.30046630	0.08641239
7	-1.16958225	-1.93291843	0.26731652
6	-0.53891778	-2.42377901	2.57344079
1	-0.92425996	-2.49230814	3.60963988
1	-0.00030198	-3.35588264	2.34488916
6	-1.68793309	-2.24235535	1.58989573
1	-2.26062775	-3.18881965	1.57842803
1	-2.38881660	-1.48399472	1.99699366
6	-2.07052684	-2.12233305	-0.81028718
6	-3.31781149	-1.44019723	-0.88042325
6	-4.18122149	-1.66702187	-1.95991635
6	-3.86243224	-2.54186535	-3.00185156
6	-2.63014174	-3.20049477	-2.93281746
6	-1.74129879	-3.01904511	-1.86647975
6	4.00849056	0.42620388	1.24437153
1	5.49975204	2.43099475	0.36396137
6	5.11424971	4.92996120	-0.67382765
1	2.39121485	5.20881033	-0.65199775
6	0.27934706	3.71308398	-0.03608900
6	-3.71393657	-0.40661606	0.14563955
1	-5.12629223	-1.11760318	-1.99616230
6	-4.81967974	-2.78786111	-4.14314461
1	-2.35368299	-3.89798045	-3.72830009
6	-0.45758027	-3.81342554	-1.85702419

1	5.05793333	0.27416649	0.96045309
1	3.43335128	-0.43998557	0.88852966
1	3.97031116	0.42414957	2.34600019
1	-0.35955393	3.24163795	0.72079718
1	-0.13041854	3.44230485	-1.02093315
1	0.18553385	4.80264950	0.06453261
1	6.03795481	4.84513474	-0.08494535
1	4.74674654	5.96185780	-0.59153551
1	5.38368130	4.76143074	-1.72859907
1	-4.44076300	0.29779837	-0.28082868
1	-2.83615613	0.16191170	0.48612827
1	-4.18021584	-0.85405475	1.03791702
1	-0.21012168	-4.15697908	-0.84297252
1	0.40471834	-3.22133541	-2.20508385
1	-0.54039294	-4.68481588	-2.52059269
1	-4.28566599	-2.92874026	-5.09332705
1	-5.51961231	-1.94993293	-4.26496458
1	-5.42140818	-3.69491744	-3.97194266
1	0.21603163	1.13134742	-0.18102327
8	0.02768326	0.62964249	-1.19567120
6	-1.06649160	0.97460085	-2.04053783
1	-1.33075976	0.11581450	-2.67220116
1	-0.78119588	1.81405830	-2.69674778
1	-1.95732760	1.26429951	-1.46089506

Energy = -7200.139811 Hartree

Number of imaginary frequencies = 0.

Intermediate 1a (I1a)

Compound I1a isomer 1

Atomic N.	X	Y	Z
8	-0.04856382	-1.40625859	-0.83033860
6	0.69223026	-1.10723315	-2.00763216
1	0.61948659	-0.04007494	-2.28466621
1	0.29450566	-1.70516628	-2.84444554
1	1.76233177	-1.35813140	-1.89140499
50	-0.09249236	-0.13310781	0.84517273
7	-2.61697225	-0.16353169	0.71453261
6	-3.17765828	-0.17221918	2.08384204
1	-4.28161461	-0.16204169	2.06445108
1	-2.83464044	-1.06027515	2.62666879
1	-2.82445627	0.71848884	2.61730347
7	-1.44369584	-2.85920618	0.94196978
6	-3.09039184	-1.32879531	-0.08022312
1	-4.17601446	-1.22539103	-0.26715935
1	-2.56774145	-1.29587911	-1.04592574
6	-2.86041505	-2.69412030	0.56890211
1	-3.19850960	-3.45973893	-0.15075055
1	-3.46512276	-2.81114248	1.47724045
16	-1.13386222	-4.29893442	1.82833061
7	-0.60309521	1.53787360	-0.52572142
6	-2.97356479	1.10700628	0.01548646
1	-3.99748319	1.03385066	-0.39537169
1	-2.95598817	1.91666646	0.75639974
6	-1.96100634	1.46093445	-1.07788341
1	-2.26923117	2.41407698	-1.53646843
1	-1.96057032	0.70519378	-1.87943679

16	-0.10076509	3.02612083	0.00282506
8	1.08893245	2.73953799	0.84782379
8	-1.22069590	3.83771561	0.54955137
6	0.47155854	3.89100687	-1.48253743
6	-0.24098527	4.98936494	-1.96151171
6	0.21369163	5.64927758	-3.10742322
6	1.37198456	5.22931406	-3.77500714
6	2.07292258	4.12055181	-3.26573931
6	1.63180392	3.45059654	-2.12768141
1	-1.13048843	5.32413612	-1.42907246
1	2.18475972	2.59976403	-1.73035085
1	2.98071949	3.78200414	-3.76908484
6	1.87319334	5.95452263	-4.99888103
1	-0.34071862	6.51082694	-3.48421593
8	-2.03118150	-4.24345381	3.00225942
8	-1.15265513	-5.48026590	0.93759524
6	0.56418132	-4.00254534	2.34154762
6	1.60515263	-4.56825035	1.60589755
6	2.92057990	-4.33095322	2.00977467
6	3.20324255	-3.54116152	3.13423018
6	2.12968101	-2.99499847	3.85975189
6	0.81108689	-3.21703681	3.47055351
1	1.38128363	-5.19170959	0.74111960
1	3.74204782	-4.77000357	1.44131911
6	4.62503478	-3.26492189	3.55219160
1	2.33193939	-2.38327537	4.74057358
1	-0.02165247	-2.80122291	4.03635087
1	1.14368797	6.69334530	-5.35382696
1	2.81251724	6.48619833	-4.78315995
1	2.08201199	5.25447868	-5.82049968
1	4.76022932	-3.41716862	4.63210036
1	5.33360341	-3.91197440	3.02030725
1	4.89572273	-2.21983266	3.33697204
1	-0.82789024	-2.81283137	0.10337535

Energy = -8139.848628 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 2

Atomic N.	X	Y	Z
8	-0.45936625	-2.07139314	1.89920771
6	-0.30006055	-3.49365707	1.94377616
1	0.74962509	-3.79069023	1.79201128
1	-0.92180863	-4.00348554	1.18635775
1	-0.62019477	-3.84480966	2.93722835
50	0.07663808	-0.96777742	0.20396131
7	-0.28482985	0.88987284	1.95254597
6	-0.41541367	2.17255209	1.23443130
1	-0.46302063	3.02436305	1.93734814
1	-1.32304238	2.16302361	0.61980629
1	0.44184323	2.31172809	0.56484126
6	-1.42629668	0.67331177	2.88411287
1	-1.47487496	1.51663076	3.59976372
1	-1.19544125	-0.24116964	3.44713756
6	-2.80277340	0.51454343	2.24484982
1	-3.52966846	0.39535628	3.06583186
1	-3.09660178	1.41547643	1.68429829
6	0.96474644	0.84294460	2.76489331

1	0.92297467	-0.09323790	3.33806870
1	0.98900196	1.69461883	3.47217953
6	2.23204537	0.82382442	1.90927978
1	2.43736905	1.81779728	1.47594841
1	3.07488602	0.57683770	2.57478716
1	-2.23403531	-1.43892357	1.69726396
7	-2.80612457	-0.64071314	1.33828494
16	-4.32180416	-1.20853547	0.81747350
8	-5.36140643	-0.95285989	1.84029759
8	-4.06149966	-2.57169910	0.31615746
6	-4.67381410	-0.12124403	-0.58063069
6	-3.86432335	-0.18485310	-1.71862917
6	-4.16295042	0.63242367	-2.80632112
6	-5.26268852	1.50916514	-2.77763071
6	-6.05479996	1.55106605	-1.62120248
6	-5.76892526	0.73965896	-0.51999716
1	-3.01417774	-0.86652529	-1.74781331
1	-6.38551176	0.76099720	0.37792457
1	-6.91143746	2.22620197	-1.58020724
6	-5.59456024	2.36194975	-3.97620913
1	-3.53330531	0.58886917	-3.69694222
1	-4.68597699	2.74648827	-4.45917804
1	-6.13925840	1.77476097	-4.73187032
1	-6.22889682	3.21390051	-3.69992640
7	2.07713785	-0.16923944	0.85182192
16	3.08601793	-1.44923112	0.76280214
8	3.70468774	-1.83036956	2.05357739
8	2.22960491	-2.44824019	0.01865359
6	4.44337810	-1.01965011	-0.35376701
6	4.16899857	-0.72964574	-1.69357032
6	5.21846027	-0.39019591	-2.54349407
6	6.54425465	-0.33499586	-2.07615308
6	6.78852732	-0.62900563	-0.72758791
6	5.74697357	-0.97393227	0.13835310
1	3.14498806	-0.77801473	-2.06429512
1	5.93451330	-1.21620770	1.18368182
1	7.81069531	-0.59299866	-0.34632035
6	7.67394883	0.00775579	-3.01467101
1	5.00850456	-0.16633533	-3.59117903
1	7.40460635	0.84087422	-3.67860742
1	7.92170301	-0.85080927	-3.65798498
1	8.58275946	0.28345284	-2.46477023

Energy = -8139.850005 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 3

Atomic N.	X	Y	Z
8	-1.39438642	-1.35206999	1.04799114
6	-0.96754275	-2.51057218	1.75428847
1	0.11965988	-2.49934176	1.95025550
1	-1.20967316	-3.43592143	1.20237342
1	-1.49159360	-2.54879399	2.72367653
50	-0.44530170	-0.55468688	-0.62034067
7	0.19594598	1.39677147	0.91175600
6	0.42749020	2.57321153	0.05108530
1	0.70429084	3.46009681	0.64973045
1	-0.47382490	2.79560784	-0.53217257

1	1.23737624	2.35670414	-0.65623099
6	-0.82937492	1.66554486	1.95431398
1	-0.46935520	2.46761811	2.62770202
1	-0.92432612	0.74102461	2.54078293
6	-2.21299015	2.06578949	1.44882488
1	-2.84399536	2.25702351	2.33261426
1	-2.17125296	3.00638109	0.87972255
6	1.45540435	0.97601665	1.59049542
1	1.16592787	0.31643193	2.41988243
1	1.97165989	1.85809510	2.01331774
6	2.38933373	0.19410814	0.67109257
1	2.79804323	0.82815044	-0.13549638
1	3.24849386	-0.13729987	1.28180032
1	-2.73899985	0.07046898	1.00521460
7	-2.77536826	1.01913506	0.58308944
16	-4.36596347	1.30384319	0.01365330
8	-5.12445576	2.11629156	0.99110893
8	-4.85125871	-0.01479640	-0.43013447
6	-4.06212112	2.34610614	-1.42794421
6	-3.45395760	1.79097228	-2.55774694
6	-3.25146233	2.59364860	-3.67782584
6	-3.65346372	3.94172483	-3.68939802
6	-4.26174742	4.46896445	-2.54080847
6	-4.47170418	3.67920241	-1.40745197
1	-3.14705011	0.74520577	-2.55661646
1	-4.95543269	4.07967432	-0.51706313
1	-4.58115379	5.51254415	-2.53221850
6	-3.45838690	4.78793015	-4.92194411
1	-2.77413622	2.16673381	-4.56165364
1	-2.48972234	4.58483463	-5.39855104
1	-4.23776661	4.57064766	-5.66872039
1	-3.51377089	5.85863534	-4.68772673
7	1.62378043	-0.94273982	0.15982678
16	2.36883315	-1.97345791	-0.88812664
8	1.21543433	-2.72684885	-1.47555237
8	3.34169184	-1.29473360	-1.77858383
6	3.31764202	-3.13613256	0.12243218
6	4.69478004	-2.95881751	0.26368611
6	5.41686332	-3.84834443	1.06332381
6	4.78370460	-4.91745655	1.71369977
6	3.39672292	-5.07567924	1.54571193
6	2.66010184	-4.19404440	0.75716272
1	5.18976607	-2.14503512	-0.26524080
1	1.58818909	-4.32800681	0.61589663
1	2.88787377	-5.90680366	2.03789773
6	5.57248336	-5.89649048	2.54681554
1	6.49431996	-3.71359368	1.17556570
1	6.53840054	-5.47541859	2.85400066
1	5.77778285	-6.81652063	1.97763580
1	5.01954304	-6.19153272	3.44912067

Energy = -8139.848390 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 4

Atomic N.	X	Y	Z
8	1.15099293	-0.04496453	-1.08115731
6	0.57898332	-0.97916645	-1.98827480

1	-0.50981716	-0.83383302	-2.10396119
1	0.75246091	-2.02067614	-1.66335676
1	1.05103517	-0.85009995	-2.97662208
50	0.35750026	0.43712770	0.78479194
7	-0.38359298	2.67920936	-0.22064796
6	-0.47468086	3.63867313	0.89780025
1	-0.78222151	4.63897205	0.54264954
1	0.49395986	3.71628380	1.40535094
1	-1.20976194	3.28110511	1.62925489
6	0.53492007	3.15938042	-1.28512884
1	0.14004555	4.09751125	-1.72181547
1	0.53099832	2.38966032	-2.06975688
6	1.97679895	3.41547408	-0.85293428
1	2.52289450	3.76122750	-1.74824190
1	2.04659739	4.21367962	-0.10310005
6	-1.72413835	2.43537099	-0.82570128
1	-1.55356918	1.98900278	-1.81490842
1	-2.25755631	3.39393556	-0.96613127
6	-2.57002883	1.46146401	-0.01003449
1	-2.86200050	1.88907567	0.96552731
1	-3.50416549	1.28622871	-0.57347137
1	2.48606589	1.38726132	-0.92542713
7	-1.78584268	0.23346739	0.12538292
16	-2.44980667	-1.01876165	0.96521501
8	-1.26766246	-1.89961599	1.22818355
8	-3.30617465	-0.57497618	2.09220394
6	-3.53312225	-1.89442955	-0.19036363
6	-4.91092470	-1.67774408	-0.13875842
6	-5.73877806	-2.33998093	-1.04883489
6	-5.21006471	-3.22332285	-2.00121525
6	-3.81926061	-3.42848661	-2.02338312
6	-2.97843885	-2.77095401	-1.12754449
1	-5.32283127	-1.01300124	0.61997457
1	-6.81696459	-2.17327156	-1.01117269
6	-6.11076678	-3.96367309	-2.95806547
1	-3.39032904	-4.11866036	-2.75258252
1	-1.90266718	-2.94262603	-1.13685815
1	-6.28988881	-4.99248655	-2.60876853
1	-7.08746782	-3.47185019	-3.05176874
1	-5.66101222	-4.03548804	-3.95782755
7	2.55957569	2.19156180	-0.27366303
16	4.19700541	2.37841429	0.22940460
8	5.10832443	2.27152587	-0.93084887
8	4.21173293	3.58580885	1.08168501
6	4.39829537	0.91021527	1.24634330
6	4.00839268	0.95040181	2.58710856
6	4.15996903	-0.19496667	3.36554761
6	4.68497427	-1.37948570	2.82092589
6	5.07440014	-1.38336319	1.47260827
6	4.93624047	-0.24464399	0.67767772
1	3.60513485	1.87034535	3.00833764
1	3.85956840	-0.17283145	4.41434732
6	4.79737981	-2.62497887	3.66219863
1	5.49295825	-2.29187082	1.03668274
1	5.24949542	-0.24239845	-0.36546502
1	5.08374216	-2.38706701	4.69536278
1	3.82893174	-3.14750635	3.70470209
1	5.53416230	-3.32520251	3.24852481

Energy = -8139.848548 Hartree
Number of imaginary frequencies = 0.

Compound 11a isomer 5

Atomic N.	X	Y	Z
50	1.87479980	-2.78501623	-0.49888366
7	1.81610401	-2.02157624	2.07320137
6	2.34673165	-3.24287683	2.71692032
1	2.23873237	-3.19632468	3.81622262
1	1.81902524	-4.13050567	2.34717482
1	3.41013813	-3.34807379	2.46898304
7	-0.07826443	-3.14804215	0.43278453
6	0.37630783	-1.84844211	2.39318551
1	0.23167037	-1.78265877	3.48953921
1	0.05004640	-0.90223679	1.94362641
6	-0.48592059	-2.97516452	1.81603123
1	-1.54198701	-2.66417719	1.89704294
1	-0.38040930	-3.90384170	2.40278456
16	-0.96626303	-3.95309416	-0.66974622
7	2.83166409	0.53010685	0.51685735
6	2.61433153	-0.86366945	2.55906135
1	2.45080562	-0.75451384	3.65068989
1	3.67357653	-1.10964229	2.40273012
6	2.34776191	0.48962645	1.89728078
1	2.92331381	1.22510758	2.47758749
1	1.28486223	0.77582370	1.97198482
16	3.56982225	1.94774856	-0.01758986
8	4.00903369	1.66144828	-1.39556679
8	4.51270571	2.36302023	1.04172321
6	2.28666633	3.22281998	-0.10930904
6	2.11907036	4.11303673	0.95301573
6	1.11443150	5.08063527	0.87852133
6	0.27882267	5.17504970	-0.24426705
6	0.47427730	4.26869210	-1.30074817
6	1.47119034	3.29620395	-1.24242722
1	2.78672556	4.05887443	1.81225985
1	1.63531689	2.61008068	-2.07302313
1	-0.15930616	4.33298040	-2.18753402
6	-0.77949691	6.24562458	-0.33558335
1	0.98452960	5.78169819	1.70512942
8	-0.00645770	-3.94092535	-1.84153702
8	-1.51731053	-5.24716742	-0.21349231
6	-2.37392760	-2.90246804	-1.10090808
6	-3.65719944	-3.44891527	-1.11957687
6	-4.73478274	-2.63126296	-1.46778551
6	-4.54357898	-1.28068044	-1.79532415
6	-3.23816400	-0.75907783	-1.75664253
6	-2.14886373	-1.55821280	-1.41307037
1	-3.79908543	-4.49780509	-0.86186650
1	-5.74213616	-3.05135248	-1.48338170
6	-5.70674929	-0.41148721	-2.20269620
1	-3.07362011	0.29263233	-1.99990786
1	-1.13290273	-1.15340346	-1.37636291
1	-1.05766979	6.62112747	0.65754530
1	-0.41631294	7.10308950	-0.92333808
1	-1.68544994	5.87319338	-0.83260206
1	-5.80106562	-0.37767954	-3.29943208

1	-6.65461709	-0.79477208	-1.80322418
1	-5.57576919	0.62257397	-1.85651666
8	1.19556010	-0.93174803	-1.22594078
1	2.17329207	0.13572832	-0.19954648
6	1.53279206	-0.62537369	-2.58920274
1	2.58473445	-0.31000497	-2.69464573
1	0.89212540	0.20480364	-2.92784559
1	1.34634266	-1.47953320	-3.26235827

Energy = -8139.851144 Hartree
Number of imaginary frequencies = 0.

Compound I1a isomer 6

Atomic N.	X	Y	Z
50	0.69110307	-0.18070855	-0.79153550
7	1.53642181	-0.86585595	1.54764833
6	2.73311560	-1.67892295	1.22266478
1	3.07922053	-2.24655105	2.10483706
1	2.50904094	-2.37921045	0.40953603
1	3.53797427	-1.00934622	0.89503720
7	0.03283389	-2.26700132	-0.29624777
6	0.42439681	-1.72103554	2.04676228
1	0.69630652	-2.16883227	3.02265589
1	-0.44852627	-1.06989493	2.18259553
6	0.05674534	-2.82844527	1.05266120
1	-0.93121421	-3.22273799	1.33944984
1	0.77856905	-3.66120645	1.11808992
16	-1.22769852	-2.56801457	-1.29067214
7	0.35434296	2.11210500	2.21452385
6	1.95694138	0.12978714	2.57827660
1	2.36417446	-0.43054336	3.44446086
1	2.78769539	0.70662768	2.14893277
6	0.90725342	1.10619499	3.12953051
1	1.39504268	1.63157668	3.96297953
1	0.04569100	0.57066780	3.55282255
16	1.47900061	3.20035595	1.57786996
8	1.97980710	2.72779501	0.25792199
8	2.44713908	3.50356261	2.65702134
6	0.45857468	4.65471224	1.27197355
6	0.09035496	5.46846482	2.34696814
6	-0.68104200	6.60157183	2.10243901
6	-1.08911600	6.93619365	0.79842427
6	-0.69978547	6.10217603	-0.25908038
6	0.07602956	4.96239601	-0.03235380
1	0.41426732	5.21532526	3.35593157
1	0.39324967	4.31997685	-0.85293114
1	-1.00464695	6.34765778	-1.27781837
6	-1.90808115	8.17759515	0.54868913
1	-0.97187012	7.24189283	2.93731263
8	-2.49827639	-2.85643634	-0.58668860
8	-1.14708407	-1.39824548	-2.24223894
6	-0.83224122	-4.03972553	-2.26649142
6	0.21913541	-3.99479728	-3.18721128
6	0.52816743	-5.13679499	-3.92153552
6	-0.19767943	-6.32989301	-3.75118434
6	-1.24600217	-6.34515388	-2.82096034
6	-1.57120266	-5.20677103	-2.07772010
1	0.77810720	-3.07026930	-3.33236051

1	1.34541253	-5.10367817	-4.64468669
6	0.13458357	-7.55160981	-4.57076233
1	-1.82333712	-7.26030239	-2.67710635
1	-2.39550592	-5.21081585	-1.36557241
1	-2.73468865	8.26161737	1.26806986
1	-1.29074524	9.08238305	0.65929025
1	-2.32996414	8.18283205	-0.46417914
1	-0.35588656	-8.44826057	-4.17122081
1	-0.19645291	-7.42577765	-5.61318317
1	1.21827648	-7.73300417	-4.59700951
8	-0.89785148	0.69478467	0.25964362
1	-0.19327368	1.66622784	1.42278991
6	-1.97045879	1.32032083	-0.45059275
1	-1.61189897	2.05985002	-1.19078135
1	-2.60888200	1.84888958	0.27451036
1	-2.58556265	0.57630164	-0.98019562

Energy = -8139.851748 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 7

Atomic N.	X	Y	Z
50	1.55202382	-1.31264729	-0.62709075
7	1.27477787	-0.46029273	1.79168754
6	1.70342949	-1.61697129	2.61298991
1	1.42282111	-1.47857494	3.67243348
1	1.24768758	-2.54021083	2.23741084
1	2.79412343	-1.71540036	2.54706117
7	-0.33283167	-2.09719056	0.27368670
6	-0.19854878	-0.26035359	1.87201725
1	-0.48940672	0.03450037	2.89890682
1	-0.45259008	0.55389955	1.18135544
6	-0.97082975	-1.51839858	1.45486083
1	-2.00985731	-1.22080625	1.24191785
1	-0.99621902	-2.24773067	2.28306378
16	-1.23546131	-2.57503631	-1.00315071
7	2.38395924	2.06434449	0.23954493
6	2.01589612	0.73353609	2.29610940
1	1.75096460	0.87189523	3.36338843
1	3.08687650	0.49390270	2.24322002
6	1.79727333	2.06611046	1.57968838
1	2.32787030	2.81738149	2.18248498
1	0.73018829	2.34673767	1.56743439
16	3.09018248	3.48936166	-0.31566184
8	3.61730513	3.16334303	-1.65317980
8	3.95321364	3.99295385	0.77375935
6	1.75935292	4.69852460	-0.53454036
6	1.48252717	5.61452834	0.48156532
6	0.43873299	6.52728134	0.30971101
6	-0.32905765	6.53972426	-0.86378090
6	-0.02280691	5.60985783	-1.87289887
6	1.01450486	4.69235645	-1.71797116
1	2.09648384	5.62317857	1.38158915
1	1.26347516	3.98712493	-2.51057850
1	-0.60349083	5.60956262	-2.79741975
6	-1.43862432	7.54280298	-1.05706986
1	0.22279760	7.24848559	1.10020723
8	-2.52375631	-1.85902771	-1.13557003

8	-0.21890668	-2.50872652	-2.12120414
6	-1.63272681	-4.32574735	-0.78763305
6	-0.61215029	-5.27907608	-0.85385331
6	-0.92585945	-6.62285192	-0.66683174
6	-2.24735948	-7.03316592	-0.41320253
6	-3.24936963	-6.05467522	-0.35294982
6	-2.95261294	-4.70200102	-0.54132815
1	0.41164292	-4.96919091	-1.06326760
1	-0.13254813	-7.37071031	-0.72318197
6	-2.57492835	-8.49469759	-0.23790297
1	-4.28155164	-6.35362459	-0.16160621
1	-3.73191255	-3.94144330	-0.51209525
1	-1.71101768	8.02713311	-0.11075494
1	-1.13394929	8.33262674	-1.76090902
1	-2.33779311	7.06847490	-1.47438856
1	-2.55560374	-9.01842908	-1.20614402
1	-1.84313540	-8.99360869	0.41264687
1	-3.57362855	-8.63311001	0.19521570
8	0.66970253	0.49691821	-1.19715639
1	1.75447177	1.62327175	-0.47975959
6	0.42254095	0.76793031	-2.58263955
1	1.35744062	0.97185427	-3.13484757
1	-0.21965653	1.65993561	-2.65027573
1	-0.10407531	-0.06583940	-3.07311214

Energy = -8139.851194 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 8

Atomic N.	X	Y	Z
50	0.73737012	-0.63528863	-0.42473766
7	0.84910075	-0.43871799	2.14556344
6	1.76516980	-1.54794478	2.50492328
1	1.73447909	-1.75278688	3.58996570
1	1.49348585	-2.45895284	1.95900113
1	2.78840854	-1.26637315	2.22712233
7	-0.63073694	-2.12832677	0.53992643
6	-0.55159823	-0.74641210	2.54604001
1	-0.63184311	-0.78963741	3.64990092
1	-1.18160470	0.07121999	2.17319995
6	-1.05033688	-2.06228359	1.93806233
1	-2.14832731	-2.07835082	2.02723386
1	-0.65799528	-2.92342710	2.50668829
16	-1.70108467	-2.54455336	-0.62166908
7	0.56491228	2.71977194	1.34014460
6	1.35439169	0.78228947	2.84122797
1	1.38610763	0.56444043	3.92825746
1	2.39199533	0.93384017	2.51313320
6	0.58224382	2.09900162	2.67033416
1	1.03996276	2.80855096	3.37433849
1	-0.46941450	1.98807317	2.97032637
16	2.07779278	3.17193885	0.73904482
8	2.65172554	2.09205829	-0.11015557
8	2.86114550	3.68990634	1.88436841
6	1.65052484	4.53983207	-0.35478277
6	1.34324255	5.78633449	0.19787230
6	1.03462732	6.84421856	-0.65313701
6	1.02993535	6.67665092	-2.04998870

6	1.34749764	5.41554222	-2.57342662
6	1.66174375	4.34322944	-1.73436901
1	1.35581231	5.91958419	1.27911002
1	1.92331125	3.36539640	-2.13697798
1	1.35219144	5.26776990	-3.65469510
6	0.70879084	7.83720309	-2.95778961
1	0.79404763	7.82061118	-0.22836162
8	-3.10983081	-2.23565270	-0.28549128
8	-1.07069430	-1.92777144	-1.84761787
6	-1.60694935	-4.33663183	-0.85496883
6	-0.44326325	-4.90359647	-1.38301660
6	-0.37280685	-6.28541063	-1.54211115
6	-1.44966253	-7.11524692	-1.18093056
6	-2.60325075	-6.51848233	-0.65337492
6	-2.69164613	-5.13327761	-0.49007163
1	0.39042264	-4.26520671	-1.67568177
1	0.53283457	-6.73109944	-1.95809582
6	-1.37008122	-8.60735316	-1.38551038
1	-3.45087539	-7.14525218	-0.37007641
1	-3.59284461	-4.66504780	-0.09603212
1	-0.20198958	8.35866351	-2.63113953
1	1.52382758	8.57710748	-2.95169108
1	0.56404338	7.50716703	-3.99413683
1	-1.53183160	-8.86559922	-2.44365689
1	-0.38220398	-8.99842014	-1.10549385
1	-2.13100473	-9.13441342	-0.79586035
8	-0.66798041	0.91452219	-0.27982831
1	0.06867237	2.11040462	0.62733138
6	-1.32519631	1.40197839	-1.45327839
1	-0.61028073	1.73045438	-2.23063080
1	-1.94277424	2.26921962	-1.17229459
1	-1.98170859	0.63453651	-1.89203617

Energy = -8139.851742 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 9

Atomic N.	X	Y	Z
50	1.41718015	-2.03628352	0.82377855
7	-0.85171977	-2.08872798	2.24531183
6	-0.56707823	-3.25799718	3.10695865
1	-1.46970608	-3.57785869	3.65933372
1	-0.20473746	-4.09943665	2.50355346
1	0.21445416	-2.98998030	3.82852590
7	-0.17331105	-3.16556379	-0.19395455
6	-1.91886014	-2.41189736	1.26388303
1	-2.84815639	-2.70467358	1.79148499
1	-2.12001611	-1.50205648	0.68456779
6	-1.49872005	-3.51364099	0.28699752
1	-2.23985345	-3.53743364	-0.53074497
1	-1.52194651	-4.50713652	0.76715717
16	0.46536820	-3.76276792	-1.56658299
7	-0.35895170	1.11824782	1.92750433
6	-1.26661322	-0.96637594	3.13065199
1	-2.19989162	-1.25875586	3.65539588
1	-0.49054613	-0.85281758	3.89991088
6	-1.51466720	0.40358794	2.48161957
1	-1.96164549	1.03349530	3.26330424

1	-2.25334164	0.33822249	1.66983607
16	0.82529558	1.57802177	3.04496433
8	1.97592086	0.63895201	2.99888581
8	0.12567595	1.82596967	4.32656651
6	1.39935223	3.15581734	2.38449652
6	0.53423694	4.25356715	2.38054548
6	0.99854544	5.47847015	1.90860922
6	2.31834762	5.62626924	1.44456662
6	3.16275673	4.50734733	1.46402391
6	2.71311707	3.27070725	1.93401159
1	-0.48661285	4.14562590	2.74557425
1	3.36707303	2.40001083	1.95853611
1	4.18969856	4.60204605	1.10687567
6	2.81562020	6.96601474	0.96333203
1	0.32688815	6.33887465	1.90050023
8	1.84873370	-3.15428795	-1.50967540
8	0.33607842	-5.22620276	-1.73895195
6	-0.41923478	-2.99628485	-2.94796047
6	-0.88362864	-3.79528157	-3.99176348
6	-1.54657299	-3.19100170	-5.06373099
6	-1.75086406	-1.80463739	-5.10080802
6	-1.27533563	-1.02744668	-4.02841529
6	-0.61098051	-1.61035834	-2.95136622
1	-0.72279561	-4.87212740	-3.95692455
1	-1.91065780	-3.81025688	-5.88555489
6	-2.46446755	-1.15313640	-6.25905089
1	-1.42783730	0.05390873	-4.04013388
1	-0.24589405	-1.00766011	-2.11424792
1	2.05189042	7.48739402	0.37020232
1	3.06495526	7.61786867	1.81507091
1	3.71979144	6.86197500	0.35019358
1	-1.82094239	-0.40893510	-6.75110048
1	-2.76598266	-1.89250011	-7.01154873
1	-3.36744898	-0.62311185	-5.92134387
8	0.83326592	-0.27935423	-0.17993573
1	0.09259821	0.63171589	1.10844858
6	1.88048107	0.51769268	-0.74372094
1	2.77657024	0.56226543	-0.09724662
1	1.51534537	1.54775633	-0.88354679
1	2.18977715	0.12416293	-1.72686963

Energy = -8139.851342 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 10

Atomic N.	X	Y	Z
50	0.69254071	-0.45409140	-0.66186905
7	1.45889170	-0.39352767	1.80109096
6	2.61196129	-1.32575436	1.79342552
1	2.90992355	-1.59752539	2.82180661
1	2.36155276	-2.23755917	1.23870651
1	3.45945274	-0.83679480	1.29730584
7	-0.09262443	-2.23618934	0.45118503
6	0.29141221	-0.98769920	2.50896909
1	0.52087027	-1.11139942	3.58546486
1	-0.54481213	-0.28540435	2.39969121
6	-0.12271767	-2.33610477	1.90880063
1	-1.13613022	-2.56873361	2.27299930

1	0.54922320	-3.13815913	2.26087466
16	-1.35214044	-2.77757578	-0.43694654
7	0.44014001	2.69582905	1.44188027
6	1.91896555	0.85778436	2.47408802
1	2.27838886	0.58508664	3.48726629
1	2.78885371	1.22470194	1.91205441
6	0.91837275	2.01000364	2.64854956
1	1.42141505	2.75006508	3.28719908
1	0.02022150	1.68158305	3.19051271
16	1.63816316	3.46455030	0.53147896
8	2.14248653	2.56545879	-0.54280764
8	2.59661467	4.05858562	1.49163649
6	0.70753065	4.78416489	-0.27001680
6	0.36775773	5.92304144	0.46451156
6	-0.33490493	6.94760160	-0.16538597
6	-0.70107372	6.85249114	-1.51975544
6	-0.34224216	5.69795548	-2.23062295
6	0.36461191	4.66201153	-1.61577211
1	0.65879094	6.00139726	1.51148034
1	0.65822965	3.77002202	-2.16788479
1	-0.61692936	5.60715342	-3.28295893
6	-1.43736291	7.98129165	-2.19629428
1	-0.60412391	7.84018319	0.40230248
8	-2.64867249	-2.76162847	0.27848806
8	-1.18863814	-1.98038489	-1.70905298
6	-1.02707709	-4.50228627	-0.87776758
6	0.04294013	-4.80832244	-1.72427324
6	0.29587874	-6.13943328	-2.04531728
6	-0.50496396	-7.17631946	-1.53264470
6	-1.57006667	-6.83938707	-0.68613232
6	-1.83947868	-5.50801530	-0.35611693
1	0.66038700	-4.00890866	-2.13412683
1	1.12764226	-6.38138976	-2.70981004
6	-0.23268211	-8.61124752	-1.90882601
1	-2.20494749	-7.62947828	-0.28092743
1	-2.67601446	-5.24165781	0.28877923
1	-2.16488497	8.44799814	-1.51853162
1	-0.73632459	8.76940036	-2.51271956
1	-1.96942379	7.63396236	-3.09118160
1	-0.54050222	-8.80891034	-2.94722754
1	0.83878088	-8.84630282	-1.84063565
1	-0.78071610	-9.30682443	-1.26073864
8	-0.86005428	0.78963125	0.00051290
1	-0.11870672	2.04724854	0.81544082
6	-1.88445163	1.20577493	-0.90704983
1	-1.47349935	1.66572685	-1.82516449
1	-2.51300889	1.95712873	-0.40398111
1	-2.52282458	0.35918198	-1.20396150

Energy = -8139.851747 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 11

Atomic N.	X	Y	Z
50	1.44430530	-1.58866711	-1.51275317
7	1.48112857	-2.65965487	0.94228340
6	2.36304853	-3.81976524	0.68392733
1	2.36698312	-4.51872493	1.54044282

1	2.03306878	-4.35982581	-0.21209416
1	3.38580817	-3.46187490	0.51308152
7	-0.25456303	-2.94457303	-1.17328705
6	0.08780541	-3.10931749	1.19224180
1	0.05566404	-3.78831168	2.06724244
1	-0.50974919	-2.21819582	1.42173341
6	-0.53162837	-3.79472659	-0.02884659
1	-1.61523528	-3.89479933	0.15645374
1	-0.13531660	-4.81631892	-0.16081658
16	-1.09185720	-3.02141296	-2.56683317
7	1.46635338	0.52708686	1.62326736
6	2.02483801	-1.93319325	2.12211464
1	1.99030152	-2.61157784	2.99989462
1	3.08482414	-1.72734235	1.91961546
6	1.34210622	-0.61926154	2.53043286
1	1.78064948	-0.33712630	3.49771870
1	0.26530528	-0.75995432	2.70265873
16	3.03247164	1.12756950	1.40283611
8	3.58512317	0.66750765	0.10288113
8	3.77137144	0.85753690	2.65770379
6	2.75911312	2.90573792	1.26538511
6	2.31973587	3.62083031	2.38348983
6	2.15090107	4.99872757	2.28122002
6	2.41946654	5.67724517	1.07802329
6	2.86326692	4.93327113	-0.02368849
6	3.03778449	3.54913885	0.06141615
1	2.11860441	3.10084542	3.31956019
1	3.39049314	2.96745791	-0.78927244
1	3.07797804	5.44212127	-0.96497284
6	2.24962812	7.17307339	0.99038328
1	1.80662024	5.56221293	3.15045796
8	-0.32176541	-2.02324823	-3.40211850
8	-1.30541462	-4.38439081	-3.10048185
6	-2.73192206	-2.32412958	-2.24733768
6	-3.86534545	-3.00922253	-2.68485274
6	-5.12523706	-2.45389807	-2.44834336
6	-5.26324579	-1.22753070	-1.78176300
6	-4.10097283	-0.56733731	-1.34445500
6	-2.83463065	-1.10396123	-1.57187220
1	-3.75145598	-3.96277669	-3.19914490
1	-6.01656904	-2.98530952	-2.78705862
6	-6.62394869	-0.61725477	-1.55640302
1	-4.19104595	0.38395698	-0.81587262
1	-1.93020491	-0.59508556	-1.22492330
1	1.27825176	7.48856050	1.39676498
1	3.02640741	7.69004338	1.57433078
1	2.32016421	7.52477313	-0.04648280
1	-6.84166026	0.14259472	-2.32321648
1	-7.41730022	-1.37406530	-1.60776188
1	-6.68298453	-0.11742460	-0.57998528
8	0.28502221	0.04589961	-0.86627204
1	1.00115686	0.38715842	0.68782258
6	0.35930236	1.23908925	-1.65418946
1	1.37934722	1.43618530	-2.03298603
1	0.05810112	2.10004819	-1.03609598
1	-0.32044820	1.18158693	-2.52120277

Energy = -8139.851357 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 12

Atomic N.	X	Y	Z
50	1.46814794	-2.15324866	0.31858550
7	1.22183733	-1.04925775	2.74626915
6	2.05026409	-1.99662575	3.52516941
1	1.93490998	-1.82990364	4.61193782
1	1.76868258	-3.03138147	3.29407062
1	3.10423779	-1.85799236	3.25458159
7	-0.33525676	-2.85095702	1.36767762
6	-0.21303891	-1.19978219	3.09937491
1	-0.36336841	-1.00751847	4.18017009
1	-0.77289024	-0.44633880	2.53130209
6	-0.76333349	-2.57971575	2.72874520
1	-1.86311785	-2.53576997	2.81290502
1	-0.42025273	-3.35324554	3.43730246
16	-1.04890183	-3.95701596	0.41050626
7	1.34832503	1.59176402	0.84003102
6	1.70215053	0.32632265	3.05080057
1	1.54629056	0.52205699	4.13212453
1	2.78686004	0.34007450	2.87729113
6	1.06964056	1.49280215	2.27711328
1	1.43527311	2.41025465	2.75894793
1	-0.02511190	1.49916019	2.37917735
16	2.96314038	1.86763545	0.41779240
8	3.59649657	0.60861713	-0.05172456
8	3.56939127	2.63081439	1.53298935
6	2.81849779	2.95628583	-1.01380779
6	2.35258993	4.26241199	-0.83740805
6	2.27947024	5.10885674	-1.94020942
6	2.67020373	4.67230311	-3.21943449
6	3.13737679	3.35859538	-3.36321560
6	3.21726795	2.49559616	-2.26692463
1	2.05718849	4.60738963	0.15294833
1	3.58835401	1.47695405	-2.37179589
1	3.44592872	3.00217548	-4.34751923
6	2.60808100	5.60919744	-4.39936203
1	1.91513614	6.12944084	-1.80893340
8	-0.14835920	-3.88880878	-0.80249138
8	-1.29772093	-5.27154716	1.04153418
6	-2.66495060	-3.29306460	-0.06445540
6	-3.79454164	-4.10601820	0.02894962
6	-5.03395947	-3.58951964	-0.35647785
6	-5.15559843	-2.27522134	-0.83119068
6	-3.99898754	-1.47844895	-0.90324048
6	-2.75275518	-1.97551989	-0.52472942
1	-3.69379401	-5.12476917	0.40142126
1	-5.92231811	-4.21978285	-0.28436827
6	-6.49092846	-1.73281814	-1.27558893
1	-4.07754953	-0.44998928	-1.26178440
1	-1.85358491	-1.35385753	-0.57298102
1	1.66528177	6.17356511	-4.41266376
1	3.42487234	6.34616828	-4.35631201
1	2.69966442	5.06604895	-5.34836688
1	-6.59733164	-1.80868274	-2.36908992
1	-7.32162948	-2.29071099	-0.82442766
1	-6.60079697	-0.67198694	-1.01264262

8	0.36051909	-0.60535166	-0.58148226
1	0.96019956	0.79342831	0.27169618
6	0.57282239	-0.39152017	-1.98110260
1	1.63061610	-0.52204851	-2.27599393
1	0.27651999	0.63791573	-2.23896275
1	-0.03615998	-1.08741528	-2.58272756

Energy = -8139.851352 Hartree
Number of imaginary frequencies = 0.

Compound 11a isomer 13

Atomic N.	X	Y	Z
50	1.64424850	-0.86059057	0.79814883
7	0.80583315	-0.19507997	3.08497981
6	1.74318988	-0.75940227	4.08265840
1	1.50374590	-0.40007758	5.09871030
1	1.67378725	-1.85471383	4.07062817
1	2.76345939	-0.46051354	3.81254803
7	-0.65791318	-1.28759057	1.01197498
6	-0.58906985	-0.68925123	3.32013622
1	-0.69036059	-1.01525421	4.36830077
1	-1.28236512	0.14550969	3.15798119
6	-0.95537808	-1.80559827	2.35034120
1	-2.02643115	-2.03986694	2.48231855
1	-0.40059715	-2.73443936	2.58483510
16	-1.20622552	-2.21087911	-0.23469411
7	1.01529964	1.55314714	0.68479164
6	0.86083571	1.29155171	3.12652679
1	0.34338195	1.66380460	4.02961471
1	1.92033701	1.57322375	3.18716188
6	0.23798238	1.94150682	1.89324761
1	0.25148469	3.03463930	2.02954887
1	-0.80035477	1.62239629	1.73700362
16	0.52458677	2.49974077	-0.72512641
8	0.87482274	3.90844609	-0.44862534
8	-0.86898966	2.11857229	-1.00899734
6	1.63241306	1.85072474	-1.97425849
6	1.31319920	0.64839844	-2.61226028
6	2.18891174	0.16184071	-3.58205892
6	3.36190228	0.85689943	-3.92140435
6	3.64752692	2.06238755	-3.25913356
6	2.79037347	2.56863148	-2.28249479
1	0.41021747	0.09309273	-2.35240122
1	3.00355918	3.50590509	-1.77026814
1	4.55627464	2.61199924	-3.50949720
6	4.28347374	0.32606172	-4.98922091
1	1.95607481	-0.78364154	-4.07392129
8	-0.47515201	-1.70674549	-1.43512087
8	-1.17416860	-3.66758474	0.06055964
6	-2.95445833	-1.76947517	-0.43713369
6	-3.93556688	-2.74322695	-0.25553107
6	-5.28034226	-2.39438061	-0.41641793
6	-5.65360774	-1.08777557	-0.75876384
6	-4.64119361	-0.12637544	-0.93438570
6	-3.29689310	-0.45561134	-0.77582110
1	-3.63783664	-3.75964012	0.00013238
1	-6.05158750	-3.15439105	-0.27614085
6	-7.10318737	-0.71648000	-0.95172160

1	-4.91147161	0.89729111	-1.20182826
1	-2.51957032	0.29666550	-0.91448567
1	4.36547302	-0.76776877	-4.93593116
1	3.89896070	0.57401616	-5.99073375
1	5.28900797	0.75714014	-4.90397101
1	-7.31746631	-0.50452610	-2.01043650
1	-7.77050912	-1.52631521	-0.63021122
1	-7.36268804	0.18914566	-0.38471192
8	3.23003136	0.54555201	1.51045946
1	2.04064573	1.71959697	0.85643549
6	4.56823656	0.19038958	1.21741839
1	4.63994996	-0.76763866	0.65875682
1	5.16379857	0.07265390	2.14215539
1	5.06035912	0.96390361	0.60033422

Energy = -8139.826427 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 14

Atomic N.	X	Y	Z
50	1.95489381	-2.00209236	-0.31873771
7	1.48602894	-1.49300511	2.14922898
6	2.59911288	-2.07842550	2.92837827
1	2.52386120	-1.80931257	3.99706103
1	2.57277759	-3.17206758	2.83875416
1	3.54735358	-1.70894740	2.51828790
7	-0.23246741	-2.52065148	0.26070698
6	0.17080619	-2.07514047	2.56649875
1	0.25411311	-2.47743384	3.58993689
1	-0.57291227	-1.26837860	2.58115637
6	-0.30634074	-3.14013144	1.58480922
1	-1.33725337	-3.42599609	1.85810165
1	0.30533620	-4.05912193	1.66558062
16	-0.88712747	-3.37708555	-0.98872086
7	1.22070388	0.41389557	-0.09430605
6	1.48858980	-0.01436560	2.30024124
1	1.11553327	0.26686188	3.30264945
1	2.53164551	0.31666753	2.20959929
6	0.64725056	0.69559789	1.23781461
1	0.65780790	1.77609479	1.46196724
1	-0.39598451	0.35514360	1.23815586
16	0.52640282	1.23323018	-1.44589994
8	-0.93780568	1.15504735	-1.29588188
8	1.24219276	0.67999894	-2.60613667
6	1.02072405	2.95549056	-1.23509624
6	2.31304223	3.34162746	-1.60516968
6	2.68923065	4.67303402	-1.44492536
6	1.79348834	5.62527308	-0.92562391
6	0.50352282	5.20646471	-0.56740709
6	0.10752726	3.87547178	-0.71867228
1	3.00203315	2.61009039	-2.02730401
1	-0.89978361	3.55060258	-0.46012187
1	-0.20609634	5.93351295	-0.16896707
6	2.20841901	7.06766827	-0.78587217
1	3.69471695	4.98310237	-1.73483965
8	-0.26674805	-2.76577252	-2.20008482
8	-0.80407726	-4.84707643	-0.78217787
6	-2.65210179	-2.96345419	-1.00784215

6	-3.59166597	-3.94344420	-0.68862625
6	-4.95067518	-3.61523350	-0.70307971
6	-5.37965634	-2.32350399	-1.03762391
6	-4.40845357	-1.35686309	-1.35604064
6	-3.04971055	-1.66505679	-1.34387041
1	-3.25239333	-4.95020343	-0.44694530
1	-5.68953933	-4.38020736	-0.45592559
6	-6.84779545	-1.97819773	-1.08202442
1	-4.72295289	-0.34551921	-1.62219186
1	-2.30559456	-0.90902373	-1.59576184
1	3.21738185	7.15330324	-0.35943153
1	2.23063983	7.56251443	-1.76898985
1	1.51287336	7.62630991	-0.14725855
1	-7.19887357	-1.89059858	-2.12194057
1	-7.45601249	-2.74770744	-0.58932239
1	-7.04755076	-1.01410695	-0.59317468
8	3.56084266	-0.46454315	0.20853902
1	2.28827814	0.51317854	-0.10014674
6	4.82897745	-0.65483058	-0.38916087
1	4.89022278	-1.61562499	-0.94333970
1	5.63003386	-0.66545817	0.37295143
1	5.06320811	0.14839952	-1.11177687

Energy = -8139.822729 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 15

Atomic N.	X	Y	Z
50	1.56983353	-0.88762625	0.10623285
7	0.62776339	0.17331341	2.44556477
6	1.73136575	0.10825503	3.42326628
1	1.45429970	0.59722607	4.37612245
1	1.97940275	-0.94038282	3.63326847
1	2.61076676	0.59928545	2.98933805
7	-0.05501152	-2.24319257	1.14001533
6	-0.54109904	-0.60927742	2.90759419
1	-0.68459946	-0.47391428	3.99712365
1	-1.43806806	-0.23790804	2.39671971
6	-0.39721150	-2.09374180	2.54904108
1	-1.33620577	-2.60670231	2.81379830
1	0.40133286	-2.56659259	3.14465102
16	-1.27650940	-2.30512734	0.05767028
7	0.35737291	1.33339930	-0.22675258
6	0.25785122	1.58489939	2.19717046
1	-0.35134836	1.98187131	3.03210133
1	1.19220827	2.16071663	2.15261699
6	-0.50460425	1.78410122	0.88610687
1	-0.75113741	2.85578229	0.79598091
1	-1.44439740	1.21793661	0.84911817
16	-0.14329198	1.74956987	-1.83397781
8	-1.59397640	1.53043623	-1.91667208
8	0.83362111	1.06267964	-2.69622994
6	0.16364627	3.52704320	-1.94057486
6	1.46776025	3.98475846	-2.15313924
6	1.69495467	5.35654879	-2.23771708
6	0.63891449	6.27779026	-2.11831834
6	-0.65836851	5.78673076	-1.90903788
6	-0.90607033	4.41489472	-1.81979847

1	2.28494667	3.27211750	-2.26580610
1	-1.91486333	4.02824444	-1.67731270
1	-1.49032380	6.48737884	-1.81960462
6	0.89720702	7.75784069	-2.24332849
1	2.70978519	5.72133549	-2.40614944
8	-2.54740189	-1.70628209	0.54621463
8	-0.64008887	-1.76032251	-1.19245598
6	-1.62799532	-4.05099098	-0.27269582
6	-0.63737922	-4.85391332	-0.84665734
6	-0.90921816	-6.19675605	-1.09272045
6	-2.16030139	-6.75624391	-0.77306322
6	-3.13362451	-5.92774065	-0.19928880
6	-2.87727937	-4.57617047	0.05225449
1	0.33120787	-4.42422354	-1.10288215
1	-0.13930742	-6.82526016	-1.54477890
6	-2.44277836	-8.21026448	-1.05884543
1	-4.11177472	-6.34245369	0.05168671
1	-3.63573044	-3.92501410	0.48519896
1	1.82135450	8.04780768	-1.72501759
1	1.01555787	8.04349637	-3.30005186
1	0.06795422	8.34676595	-1.83156878
1	-2.45961604	-8.40288393	-2.14235091
1	-1.66590773	-8.85941699	-0.62950338
1	-3.41239213	-8.51826889	-0.64752634
8	2.77667419	0.97972911	0.57468876
1	1.37036745	1.63329494	-0.08362955
6	4.11625217	0.97467861	0.12465250
1	4.38399283	0.03080419	-0.39888314
1	4.82438402	1.09155521	0.96676007
1	4.30710417	1.79838353	-0.58861800

Energy = -8139.823096 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 16

Atomic N.	X	Y	Z
50	1.46882748	0.43088246	0.62778236
7	-0.17272572	1.60019310	2.31346484
6	-0.09151972	0.81197964	3.56178322
1	-0.87914488	1.12157688	4.27299710
1	-0.17754979	-0.25692985	3.34261355
1	0.89059407	0.96886782	4.02478813
7	-0.56426394	-0.31658712	0.36496555
6	-1.51127186	1.46580634	1.68354938
1	-2.30895474	1.73200436	2.40414958
1	-1.55832049	2.16360136	0.83948423
6	-1.74145139	0.05348655	1.13920071
1	-2.64615113	0.07856184	0.50964920
1	-1.92764997	-0.66220212	1.96034638
16	-0.62931776	-1.40551026	-0.84806040
7	0.54778110	3.66445806	0.25739085
6	0.16968832	3.01050732	2.63366130
1	-0.40921165	3.34266617	3.51854655
1	1.23088340	3.01915978	2.92846422
6	-0.08038782	4.04668435	1.53501487
1	0.28029857	5.01883240	1.91289645
1	-1.15487674	4.15898318	1.34450397
16	-0.09012793	4.49957619	-1.12378800

8	0.58564259	5.80455592	-1.29333965
8	-1.55790904	4.42690021	-0.96358893
6	0.44163848	3.40428992	-2.44117322
6	-0.22867765	2.19236867	-2.63599135
6	0.20161252	1.34148413	-3.64922961
6	1.28972179	1.68651948	-4.47136139
6	1.93065218	2.91625249	-4.26015701
6	1.51562436	3.78309072	-3.24646611
1	-1.07026517	1.91152856	-2.00420617
1	2.00558711	4.74207669	-3.08279387
1	2.77091234	3.20131835	-4.89544843
6	1.75695807	0.73816483	-5.54508211
1	-0.30604792	0.38509608	-3.78069150
8	-1.71027265	-1.13674792	-1.82845996
8	0.79514143	-1.41188110	-1.32742498
6	-0.98761405	-3.02244198	-0.11760458
6	-0.21866652	-3.46678871	0.96324780
6	-0.49349910	-4.71933741	1.50966407
6	-1.51897542	-5.53322938	0.99545965
6	-2.27607731	-5.05328369	-0.08280269
6	-2.01871523	-3.79988324	-0.64420056
1	0.57302771	-2.83101168	1.37294428
1	0.09967890	-5.07400531	2.35524374
6	-1.78400729	-6.89596703	1.58531190
1	-3.08142512	-5.66732664	-0.49023400
1	-2.60527565	-3.41944555	-1.47962541
1	2.10803568	-0.20455181	-5.09991290
1	0.93611735	0.48178969	-6.23022112
1	2.57716319	1.16749750	-6.13383316
1	-0.99425939	-7.60706695	1.29758107
1	-1.79954879	-6.86028288	2.68374163
1	-2.74220885	-7.30404029	1.23934915
8	1.83210062	-1.05663671	2.02540655
1	1.55948616	3.82941734	0.26173971
6	3.16176548	-1.31330234	2.45718583
1	3.90823719	-0.62423340	2.01346951
1	3.46313876	-2.34001185	2.18475896
1	3.23605583	-1.21747316	3.55534078

Energy = -8139.845939 Hartree

Number of imaginary frequencies = 0.

Compound I1a isomer 17

Atomic N.	X	Y	Z
50	1.02562685	-0.42380669	1.68924398
7	-1.05615563	0.10915934	3.01457283
6	-0.76411820	-0.18481306	4.43611222
1	-1.59315903	0.14394293	5.08683685
1	-0.62274580	-1.26567808	4.56421536
1	0.15966267	0.33496671	4.71839237
7	-0.87970165	-1.36932911	0.68703762
6	-2.22963622	-0.68800193	2.53215476
1	-2.84632164	-0.99053025	3.39433555
1	-2.84220436	-0.04446387	1.88842380
6	-1.78550330	-1.89341341	1.71317653
1	-2.68431173	-2.36600845	1.27928565
1	-1.30940638	-2.65813967	2.35661251
16	-0.45770458	-2.44068669	-0.48823263

7	0.16211573	1.77052321	0.86565657
6	-1.29220242	1.56807660	2.84005404
1	-2.28288439	1.84217234	3.24658550
1	-0.51811191	2.09110709	3.41675956
6	-1.21381020	2.00980329	1.38055277
1	-1.46917905	3.08002659	1.32487268
1	-1.90941931	1.45170748	0.74099508
16	0.39460610	2.52378078	-0.71638307
8	0.27489330	3.98439821	-0.52681568
8	-0.50373400	1.81520957	-1.64310549
6	2.10670369	2.11042679	-1.04330887
6	2.42054593	0.84258251	-1.54070478
6	3.76002151	0.54227551	-1.78779695
6	4.77482368	1.48434430	-1.55224497
6	4.41946050	2.74868502	-1.05227987
6	3.08856882	3.07247644	-0.79275648
1	1.64354783	0.09743409	-1.72088651
1	2.80647801	4.05257598	-0.41049061
1	5.19705083	3.48969878	-0.86006034
6	6.21415825	1.15256041	-1.85139703
1	4.01613308	-0.45018244	-2.16114232
8	0.72337217	-1.82397168	-1.16242888
8	-0.34648169	-3.83726066	0.00918493
6	-1.82954993	-2.42934098	-1.67566899
6	-2.14400007	-1.24495958	-2.35136642
6	-3.19541564	-1.24631732	-3.26530598
6	-3.94223322	-2.41212389	-3.51676994
6	-3.60621113	-3.58209616	-2.82249813
6	-2.55240265	-3.59959035	-1.90317452
1	-1.57081174	-0.33630460	-2.16378182
1	-3.44145216	-0.32453584	-3.79659332
6	-5.06624481	-2.39851781	-4.52315152
1	-4.17403875	-4.49678304	-3.00424189
1	-2.27921010	-4.50827259	-1.36767552
1	6.41737888	0.08455255	-1.69967106
1	6.45405283	1.38538610	-2.90065990
1	6.90008087	1.73329891	-1.22117419
1	-5.75385823	-1.55964114	-4.34299189
1	-4.67702532	-2.28031916	-5.54602010
1	-5.64490122	-3.33049925	-4.49029290
8	1.66086010	1.33923629	2.90833959
1	0.86499854	2.17885351	1.53461523
6	2.96735458	1.29478464	3.45044053
1	3.50923925	0.36438575	3.17513115
1	2.94550219	1.34315128	4.55542994
1	3.57691028	2.14400470	3.09205500

Energy = -8139.826398 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 18

Atomic N.	X	Y	Z
50	1.91268285	0.25098880	-0.70943408
7	1.35779473	1.41170746	1.61728067
6	1.93375695	0.52298790	2.64963925
1	1.55984748	0.79240112	3.65488138
1	1.69892851	-0.52216713	2.42651579
1	3.02625775	0.61786213	2.63639084

7	0.00543210	-0.46500124	0.09596419
6	-0.12573947	1.37211740	1.64987799
1	-0.50174300	1.69219956	2.64198117
1	-0.49540773	2.07464512	0.89239443
6	-0.66917165	-0.01563133	1.30495346
1	-1.75630901	0.07535301	1.14673805
1	-0.51402666	-0.71725130	2.14459412
16	-0.69016385	-1.53021628	-0.92609060
7	1.59252745	3.68685535	-0.44219968
6	1.87959473	2.78249757	1.85715566
1	1.68331132	3.06830300	2.91034438
1	2.97389406	2.73107715	1.74396104
6	1.32848252	3.91150676	0.98527284
1	1.76871499	4.85375546	1.35266558
1	0.24338937	4.01235504	1.11762665
16	0.76855987	4.73042751	-1.54422855
8	1.66368180	4.78907300	-2.71600807
8	0.32332881	5.95414310	-0.84310886
6	-0.68655527	3.75310390	-1.93630174
6	-1.92648433	4.12528598	-1.41791162
6	-3.03870241	3.32543819	-1.69638309
6	-2.92292718	2.16469187	-2.47505275
6	-1.65957878	1.82811254	-2.99720870
6	-0.54236688	2.61455942	-2.73668615
1	-2.01241162	5.02893314	-0.81538897
1	0.43449319	2.35018145	-3.14068240
1	-1.54897543	0.92194486	-3.59379925
6	-4.10896301	1.27600607	-2.73887430
1	-4.01353998	3.60766343	-1.29499493
8	-2.12309291	-1.24842043	-1.19075259
8	0.27950226	-1.53255180	-2.07336688
6	-0.63180296	-3.16266994	-0.14324749
6	0.57667092	-3.61960998	0.39273047
6	0.61377706	-4.88367735	0.97929723
6	-0.53150106	-5.69782666	1.03726259
6	-1.72871217	-5.20567085	0.49810171
6	-1.78823925	-3.94066684	-0.09224385
1	1.46877109	-2.98571884	0.35982949
1	1.55237955	-5.24718050	1.40296854
6	-0.46376769	-7.07438713	1.65014606
1	-2.63036983	-5.81958718	0.54069673
1	-2.71619672	-3.55207468	-0.50972527
1	-5.02634992	1.68753534	-2.29968776
1	-4.27083909	1.14430598	-3.81860761
1	-3.92984720	0.27718054	-2.31383781
1	0.02774949	-7.78283946	0.96536874
1	0.11939570	-7.06983571	2.58155014
1	-1.46508605	-7.46599888	1.87047362
8	2.91080262	-1.25167148	0.30758441
1	2.58393809	3.75941787	-0.69037533
6	4.26958931	-1.53483807	-0.00302730
1	4.69570355	-0.85640820	-0.76878661
1	4.36875613	-2.56475903	-0.38797543
1	4.89715686	-1.44795673	0.90174045

Energy = -8139.846159 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 19

Atomic N.	X	Y	Z
50	2.70947179	-0.39843874	1.63909141
7	0.77768802	0.41295740	3.16866353
6	0.84935536	-0.38929762	4.41305739
1	-0.02544123	-0.17747454	5.05434183
1	0.90249321	-1.45545776	4.17572016
1	1.76978660	-0.13917558	4.95289214
7	0.79872104	-1.29335701	0.93030336
6	-0.46766751	0.10379979	2.41899346
1	-1.34757003	0.16859065	3.08702932
1	-0.57529897	0.84966266	1.62350864
6	-0.40906533	-1.27264014	1.75486607
1	-1.32286246	-1.37910147	1.14314581
1	-0.41627636	-2.08684212	2.49754507
16	1.21658668	-2.67244637	0.14628920
7	1.28700840	2.70482808	1.24558397
6	0.87617959	1.84865352	3.55530983
1	0.20198547	2.04360194	4.41195929
1	1.90294628	2.00711749	3.92062137
6	0.53552887	2.89682221	2.49463421
1	0.71314298	3.88765063	2.94544745
1	-0.53493983	2.85511570	2.24766390
16	0.91594648	3.81192746	-0.01673795
8	2.06693760	3.71700085	-0.93401397
8	0.48465666	5.11667457	0.53221411
6	-0.53009858	3.03048434	-0.75721604
6	-1.70596262	3.77006678	-0.88544582
6	-2.81047127	3.17919917	-1.50346093
6	-2.75248205	1.86425296	-1.98906403
6	-1.55444424	1.14273372	-1.83793141
6	-0.44047650	1.71745820	-1.22949667
1	-1.74464819	4.78962263	-0.50343038
1	0.48036182	1.14724888	-1.10836411
1	-1.49085704	0.11457732	-2.19888589
6	-3.93937204	1.24005066	-2.67833477
1	-3.73439129	3.75090136	-1.60620408
8	2.69792925	-2.48606681	-0.04960884
8	0.69331419	-3.90370868	0.77804919
6	0.47540301	-2.57941142	-1.50376061
6	-0.71165598	-3.26551927	-1.76191213
6	-1.29542721	-3.16338679	-3.02816198
6	-0.70374838	-2.39541347	-4.04143408
6	0.49768008	-1.72246785	-3.75417743
6	1.08896540	-1.80768506	-2.49534798
1	-1.15606734	-3.88593141	-0.98422869
1	-2.22259940	-3.70145369	-3.23442502
6	-1.32070739	-2.30874005	-5.41521230
1	0.97861037	-1.12539946	-4.53140267
1	2.02728649	-1.29651163	-2.28089928
1	-4.87514686	1.74320510	-2.40325430
1	-3.83398925	1.31229790	-3.77207436
1	-4.02938284	0.17374794	-2.43133473
1	-0.72269285	-2.86902912	-6.15001039
1	-2.33658048	-2.72364782	-5.42606078
1	-1.36757842	-1.26850729	-5.76762332
8	3.04422600	-1.76699302	3.13411924
1	2.30553942	2.74579190	1.36342050

6	4.26685072	-2.49648004	3.14780183
1	5.14988718	-1.86705820	2.91992240
1	4.25019296	-3.32838146	2.42252908
1	4.41322002	-2.92001793	4.15479119

Energy = -8139.840674 Hartree
Number of imaginary frequencies = 0.

Compound 11a isomer 20

Atomic N.	X	Y	Z
8	1.64622820	-1.52039888	-0.67936776
6	3.07366562	-1.59849954	-0.51538944
1	3.54793402	-0.68523518	-0.91114714
1	3.51801400	-2.46049088	-1.04783217
1	3.32202509	-1.70714529	0.55090351
50	0.85457474	-2.68763766	-2.22291837
7	-1.51815149	-2.98422871	-1.00648083
6	-2.13923688	-3.95261748	-1.93614025
1	-3.21569054	-4.08195038	-1.71942243
1	-2.02587472	-3.61580887	-2.97397133
1	-1.63844370	-4.92368498	-1.83508516
7	-0.55851475	-1.10912043	-2.77741663
6	-2.18685924	-1.66224630	-1.11044045
1	-3.26908210	-1.75867912	-0.89395572
1	-1.74008695	-1.00557045	-0.35454111
6	-1.97784335	-1.01245478	-2.48092650
1	-2.31096649	0.03713852	-2.40823073
1	-2.59988987	-1.49133521	-3.25643724
16	0.17961583	-0.20735551	-3.91747323
7	0.38938586	-2.71409088	1.55792624
6	-1.63696458	-3.54588670	0.36935362
1	-2.71147197	-3.72165953	0.58027747
1	-1.13493157	-4.52374716	0.36543998
6	-1.07500031	-2.71923718	1.52516584
1	-1.41649501	-3.21516681	2.44513160
1	-1.50667559	-1.70231301	1.53284229
16	1.09685896	-2.35458405	3.04888375
8	2.55240268	-2.42099941	2.82315527
8	0.42026619	-3.19378498	4.05877828
6	0.68026177	-0.63192928	3.42605607
6	-0.37133884	-0.35079199	4.29962344
6	-0.69648819	0.98135081	4.56796132
6	0.01622359	2.03544889	3.97818404
6	1.07108024	1.72164280	3.10318060
6	1.40861801	0.39864692	2.82373005
1	-0.90895768	-1.17050416	4.77520374
1	2.23771185	0.16154220	2.15733030
1	1.64354628	2.52885852	2.64161384
6	-0.31536609	3.47149331	4.29798107
1	-1.51507317	1.20444550	5.25478385
8	1.53804028	-0.87378885	-3.94666694
8	-0.57343164	-0.05341149	-5.18050486
6	0.40350841	1.44913555	-3.22709809
6	0.02760246	2.56269339	-3.97755470
6	0.22161153	3.83730798	-3.43915005
6	0.78390851	4.00816931	-2.16582430
6	1.14284772	2.86323874	-1.43166024
6	0.95918705	1.58301307	-1.95055134

1	-0.40927970	2.42338486	-4.96570358
1	-0.07046694	4.71383854	-4.02034389
6	1.02163543	5.38671909	-1.60232853
1	1.57523026	2.97821778	-0.43533026
1	1.23265724	0.69209591	-1.37726044
1	-1.33064843	3.56840171	4.70332892
1	0.38129371	3.87442614	5.04949954
1	-0.23497251	4.10991410	3.40751747
1	2.07527063	5.68152270	-1.72705725
1	0.40554533	6.14029817	-2.10932430
1	0.80100818	5.42409031	-0.52667304
1	0.86044264	-2.18067970	0.78635622

Energy = -8139.851270 Hartree
Number of imaginary frequencies = 0.

Compound 11a isomer 21

Atomic N.	X	Y	Z
8	3.93040391	-2.62904968	0.33033427
6	4.03204875	-3.12490680	1.66339323
1	3.04513879	-3.33710642	2.11376622
1	4.55645275	-2.42116847	2.33010061
1	4.60626297	-4.06525456	1.63511233
50	3.07478833	-0.86973969	-0.25605514
7	1.39854287	-2.46090490	-1.53384303
6	2.19648873	-3.53987489	-2.15723312
1	1.54731907	-4.37620420	-2.47506314
1	2.73253696	-3.15910863	-3.03419345
1	2.93742915	-3.89115270	-1.42807206
7	1.44231825	0.31831688	-3.31621353
6	0.43267334	-1.88645849	-2.50847240
1	-0.14167346	-2.72006747	-2.96066814
1	-0.28044373	-1.26168686	-1.95638165
6	1.04759229	-1.05217836	-3.64279994
1	0.31743627	-0.98251080	-4.46151519
1	1.92409637	-1.56090155	-4.07147035
16	0.38302771	1.60668720	-3.57999069
7	1.13996176	-0.96489666	0.83916935
6	0.67015010	-3.02589874	-0.36261347
1	-0.13362418	-3.70657421	-0.70501440
1	1.40423264	-3.61594357	0.20263015
6	0.09486962	-1.94738233	0.56086858
1	-0.24140689	-2.44512392	1.48522564
1	-0.78605432	-1.46146264	0.10690573
16	1.49245914	-0.50137803	2.36539274
8	2.92378176	-0.03914035	2.19932162
8	1.14992644	-1.50864124	3.39508415
6	0.54001800	0.98424378	2.76014680
6	-0.57827729	0.88005538	3.58710800
6	-1.32470951	2.02806661	3.86862916
6	-0.96486865	3.27678209	3.34161374
6	0.17496310	3.35171919	2.52013835
6	0.92770937	2.21715613	2.22605603
1	-0.84359082	-0.08496671	4.01735157
1	1.81991077	2.28512486	1.60374475
1	0.47876193	4.31578372	2.10797963
6	-1.76530436	4.51629614	3.65247983
1	-2.19807919	1.95117065	4.51877710

8	1.12401627	2.79206996	-3.11441979
8	-0.10861965	1.45629388	-4.96287942
6	-1.05463081	1.39610561	-2.50041977
6	-2.24693770	0.90003064	-3.03022113
6	-3.34485877	0.72505309	-2.18388426
6	-3.26804049	1.04169723	-0.81945111
6	-2.05501148	1.54452866	-0.31521085
6	-0.95027740	1.72416762	-1.14531325
1	-2.31026582	0.67447296	-4.09417351
1	-4.28056640	0.34153288	-2.59474834
6	-4.46194315	0.87396313	0.08646242
1	-1.97218948	1.79929208	0.74308468
1	-0.01814000	2.12542483	-0.74856453
1	-2.64278919	4.28369732	4.26857725
1	-1.15550363	5.25382473	4.19495836
1	-2.11287859	5.00522821	2.73063604
1	-4.91224337	1.85000209	0.32398463
1	-5.23771510	0.25451578	-0.38104765
1	-4.17567845	0.41122141	1.04116268
1	2.02100453	0.45515814	-2.48026232

Energy = -8139.843030 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 22

Atomic N.	X	Y	Z
8	1.63307226	-1.36447344	-0.93696432
6	3.06980041	-1.39537759	-0.86617361
1	3.51301227	-2.17020690	-1.51974883
1	3.38933469	-1.61291776	0.16400245
1	3.48238145	-0.42251561	-1.18066289
50	0.79111204	-2.40365213	-2.54463249
7	-1.49987057	-2.90563614	-1.23583633
6	-2.14248764	-3.80159444	-2.22180271
1	-3.20038576	-3.99036919	-1.96155618
1	-2.09872251	-3.36225700	-3.22600888
1	-1.60688514	-4.75898355	-2.24334525
7	-0.70289104	-0.83494061	-2.86492457
6	-2.21421293	-1.60501832	-1.17359320
1	-3.27881039	-1.76192072	-0.91006717
1	-1.74617942	-1.00863188	-0.38138253
6	-2.10464167	-0.81870407	-2.48266828
1	-2.46494525	0.20626722	-2.28903163
1	-2.75575042	-1.24276389	-3.26621849
16	-0.05682377	0.20693131	-3.93925919
7	0.55502245	-2.83649272	1.22353653
6	-1.52434101	-3.59987991	0.08282349
1	-2.58038294	-3.82274707	0.33803428
1	-1.00373970	-4.55940525	-0.04547734
6	-0.90808334	-2.87449234	1.27849339
1	-1.18277319	-3.46537500	2.16411980
1	-1.35665744	-1.87372764	1.41129943
16	1.35059337	-2.63754938	2.69975926
8	2.78946256	-2.64229322	2.37775744
8	0.75370945	-3.60545365	3.64255732
6	0.93205774	-0.98169679	3.30506565
6	-0.06943181	-0.82994655	4.26528626
6	-0.39600349	0.45299236	4.71217659

6	0.26564287	1.58518178	4.21493069
6	1.27028161	1.40140828	3.24864989
6	1.60872329	0.12905971	2.79150594
1	-0.56595565	-1.71203703	4.66840491
1	2.40037463	-0.00858742	2.05527986
1	1.80319727	2.27008574	2.85653746
6	-0.06505335	2.96473794	4.72666358
1	-1.17468684	0.57441190	5.46747776
8	1.31948711	-0.40044629	-4.10469070
8	-0.87963929	0.46084615	-5.14114277
6	0.14613312	1.79149184	-3.09124120
6	-0.30956154	2.96007634	-3.70073945
6	-0.13442879	4.17902906	-3.04082315
6	0.48779298	4.24056934	-1.78542479
6	0.92734600	3.04200850	-1.19487941
6	0.76366141	1.81580788	-1.83659618
1	-0.79335690	2.90549959	-4.67524169
1	-0.48929593	5.09793162	-3.51105491
6	0.70332225	5.56227231	-1.09183321
1	1.40689957	3.07097559	-0.21409726
1	1.09956590	0.88259080	-1.37450352
1	-1.05369144	2.99021381	5.20250908
1	0.67243082	3.28892954	5.47732861
1	-0.05032680	3.70757130	3.91736172
1	1.73188781	5.92196223	-1.25101781
1	0.02158056	6.33288533	-1.47388979
1	0.55573669	5.47486147	-0.00671844
1	0.96639338	-2.20650542	0.49168680

Energy = -8139.851265 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 23

Atomic N.	X	Y	Z
8	2.84001985	-1.98710059	2.44449434
6	3.19040366	-1.55108822	3.75467761
1	3.94170188	-0.74351427	3.73290251
1	3.62280698	-2.40582906	4.30103888
1	2.32328139	-1.17859675	4.33103384
50	1.82877890	-0.87606329	1.05225408
7	-0.15147900	-2.54690446	1.50991242
6	0.34817916	-3.93498926	1.49696177
1	-0.42638154	-4.64758750	1.83684490
1	0.66906601	-4.21516706	0.48641348
1	1.22420623	-3.99290280	2.15555891
7	-2.07671048	-2.15610658	-1.72873907
6	-1.29940294	-2.35000438	0.59843924
1	-2.15394939	-2.98103319	0.91324172
1	-1.61467842	-1.30149240	0.66806572
6	-0.97326281	-2.63447635	-0.87398961
1	-0.86480888	-3.71139043	-1.05935272
1	-0.01198250	-2.16159843	-1.14001877
16	-1.94128004	-0.60947585	-2.43481029
7	0.32029320	0.03284061	2.38408924
6	-0.51652327	-2.17137563	2.90230531
1	-1.40480935	-2.74245751	3.23556501
1	0.33763975	-2.45851293	3.53052881
6	-0.76345932	-0.66776788	3.06155363

1	-0.77857071	-0.43958768	4.14017692
1	-1.74673051	-0.38125114	2.64862185
16	0.97836100	1.40234022	2.96815857
8	2.26912784	1.44756376	2.17837890
8	1.04112576	1.48246618	4.44577597
6	-0.03937266	2.79233315	2.41828845
6	-0.23162147	3.87399145	3.27858545
6	-1.00232989	4.95509821	2.84567180
6	-1.58659068	4.96633228	1.57032569
6	-1.38596627	3.85600606	0.73223800
6	-0.61475155	2.77077719	1.14476071
1	0.21049575	3.85562620	4.27388857
1	-0.48518411	1.90890854	0.48976023
1	-1.84763212	3.83271467	-0.25650075
6	-2.40218905	6.14472845	1.10031184
1	-1.15761657	5.80285672	3.51558984
8	-3.17085779	-0.45426990	-3.23043325
8	-1.58213513	0.30230812	-1.33085702
6	-0.54222232	-0.66589287	-3.57405686
6	0.72625164	-0.27658091	-3.13870668
6	1.79753509	-0.34108507	-4.03231032
6	1.61857398	-0.78261868	-5.35161711
6	0.32630906	-1.15361968	-5.76463262
6	-0.75445107	-1.10073767	-4.88694435
1	0.87116791	0.08712918	-2.12140766
1	2.78920158	-0.03448201	-3.69563318
6	2.78291054	-0.86888376	-6.30519778
1	0.16352436	-1.47755221	-6.79418187
1	-1.75992045	-1.36103573	-5.21735111
1	-2.72365766	6.77179667	1.94176426
1	-1.81444349	6.77874829	0.41830797
1	-3.29462074	5.81859828	0.54880187
1	2.49389023	-0.56012444	-7.31890304
1	3.61923663	-0.24013749	-5.97500524
1	3.15308190	-1.90369232	-6.37406679
1	-2.36757808	-2.81617782	-2.45057218

Energy = -8139.845209 Hartree

Number of imaginary frequencies = 0.

Compound I1a isomer 24

Atomic N.	X	Y	Z
8	2.54208841	-3.40589636	0.96791987
6	3.81050692	-3.78142671	1.49608660
1	4.64918014	-3.22623043	1.03384925
1	3.97060248	-4.85276055	1.29336376
1	3.86043403	-3.62607423	2.58783654
50	2.04162214	-1.41872890	0.77831460
7	0.07443462	-2.48763946	-0.42132710
6	0.53180439	-3.44459613	-1.45267439
1	-0.31909409	-3.99697116	-1.89089186
1	1.07267242	-2.91815142	-2.24714159
1	1.22296620	-4.14658370	-0.97188880
7	0.80783118	-0.22520179	-2.28376152
6	-0.88191609	-1.48295822	-0.95052349
1	-1.87617165	-1.95292781	-1.08478331
1	-0.99763066	-0.70015312	-0.18546410
6	-0.52319440	-0.84279030	-2.29360332

1	-1.32684410	-0.12060006	-2.52788772
1	-0.51841658	-1.59738685	-3.09029488
16	1.48950081	0.21134498	-3.78494544
7	0.28349567	-1.49952386	2.17241546
6	-0.55401162	-3.24406446	0.70216738
1	-1.46863180	-3.75564384	0.34527576
1	0.18454124	-3.99498896	1.01275127
6	-0.87718691	-2.34547450	1.89853743
1	-1.10530099	-3.00015522	2.75486936
1	-1.77383645	-1.73061252	1.70390863
16	0.91853608	-1.45477828	3.68106551
8	2.35904166	-1.10630854	3.40770330
8	0.58500542	-2.63952695	4.50503788
6	0.21094632	-0.02112635	4.53214116
6	-0.70659383	-0.21957722	5.56340729
6	-1.26605230	0.89162280	6.20005554
6	-0.91548310	2.19620491	5.82494002
6	0.01547524	2.36489665	4.78440550
6	0.57985184	1.26792565	4.13718562
1	-0.96234584	-1.23433782	5.86622737
1	1.31268227	1.40380729	3.34170926
1	0.30642320	3.37309551	4.48268796
6	-1.49446356	3.39230799	6.53857988
1	-1.98325965	0.73951334	7.00889181
8	2.76935985	0.85248222	-3.44311085
8	1.39534051	-0.99675692	-4.62576286
6	0.41141491	1.46756793	-4.50960812
6	-0.59942441	1.08524404	-5.39403881
6	-1.43505788	2.06569266	-5.93233912
6	-1.27246044	3.42015696	-5.60303416
6	-0.24359683	3.77468293	-4.71313048
6	0.60028373	2.80971540	-4.16547696
1	-0.70924076	0.03713208	-5.67029932
1	-2.22363156	1.77321552	-6.62792557
6	-2.15512294	4.47737289	-6.21630643
1	-0.09577627	4.82442696	-4.45329347
1	1.41448067	3.08934055	-3.49698904
1	-2.41630008	3.13233728	7.07461509
1	-0.78155444	3.78873122	7.27834889
1	-1.71922139	4.20791935	5.83755624
1	-1.67201494	4.91999121	-7.10134814
1	-3.11669356	4.05962880	-6.54092081
1	-2.35069329	5.29540220	-5.51029405
1	0.92070005	0.54819330	-1.62278854

Energy = -8139.843635 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 25

Atomic N.	X	Y	Z
8	1.24217492	0.56875957	1.15990989
6	2.66657012	0.39486149	1.12621227
1	3.19382608	1.36325612	1.15920233
1	2.93443736	-0.10130063	0.17945583
1	3.03173696	-0.23685304	1.95505062
50	0.45651706	1.54092464	2.85993867
7	-1.93190339	0.45683939	2.56745458
6	-2.33181551	-0.34460983	3.74167252

8	4.33670312	-0.35510928	0.20814863
6	5.13027001	-1.52966869	0.34001490
1	5.38490119	-1.96372323	-0.64085073
1	4.63501108	-2.32217120	0.93134438
1	6.06787456	-1.25612902	0.85066518
50	2.43788948	-0.23784696	-0.49169728
7	1.49733811	-0.25583730	2.08295273
6	2.70589826	-0.38346401	2.92463940
1	2.43272238	-0.48726516	3.99178751
1	3.29321548	-1.25476213	2.61765374
1	3.33747560	0.50215119	2.79282823
7	1.64159162	-2.22999008	0.07337206
6	0.68458439	-1.49572852	2.15513301
1	0.49590612	-1.76514420	3.21361956
1	-0.28479549	-1.29060729	1.68140491
6	1.32278555	-2.67834409	1.42384186
1	0.58536341	-3.50018785	1.41735233
1	2.21304172	-3.05035869	1.95869543
16	2.18675204	-3.26805617	-1.06327848
7	-0.00171338	2.26899807	0.52797385
6	0.70805912	0.90469400	2.57731367
1	0.25372114	0.63438309	3.55255250
1	1.40158861	1.73329140	2.76772324
6	-0.40637915	1.41210935	1.64828033
1	-1.11318378	1.98586396	2.26337528
1	-0.98199705	0.57672743	1.22145480
16	0.36110743	3.90127389	0.84300057
8	1.38754668	4.26635018	-0.15195804
8	0.56924814	4.09498056	2.29629387
6	-1.17329463	4.75015877	0.41675180
6	-2.00871541	5.21344569	1.43270870
6	-3.18679525	5.88125625	1.08884302
6	-3.53370597	6.09650328	-0.25266256
6	-2.66669140	5.62241314	-1.25356829
6	-1.48877563	4.95366260	-0.92964481
1	-1.72626901	5.06395088	2.47408208
1	-0.81110271	4.60128315	-1.70671415
1	-2.91753122	5.78634611	-2.30317220
6	-4.78930563	6.84693711	-0.61862539
1	-3.84408831	6.24754480	1.87945475
8	2.75533287	-2.29715145	-2.07391643
8	3.03183102	-4.36581516	-0.54286929
6	0.74735938	-4.04336416	-1.83469339
6	0.53578091	-5.41188026	-1.67029957
6	-0.58827928	-6.00053655	-2.25644049
6	-1.49683851	-5.24175055	-3.00725524
6	-1.25568876	-3.86364800	-3.15631985
6	-0.14315023	-3.26033507	-2.57576635
1	1.25285821	-6.00103200	-1.09997606
1	-0.75728427	-7.07154143	-2.13089392
6	-2.69064268	-5.88604957	-3.66579075
1	-1.94997879	-3.25693866	-3.74079664
1	0.04378845	-2.19410292	-2.70390951
1	-5.50551192	6.86104793	0.21276751
1	-4.55707558	7.89247535	-0.87434898
1	-5.28156225	6.40195710	-1.49404820
1	-2.51340204	-6.02508958	-4.74358522
1	-2.90319562	-6.87263193	-3.23483535

1 -3.58951129 -5.26218140 -3.56505344
 1 0.72891918 1.87863728 -0.08305922
 Energy = -8139.840698 Hartree
 Number of imaginary frequencies = 0.

Compound 11a isomer 27

Atomic N.	X	Y	Z
8	1.48146897	0.29067126	-0.14816797
6	0.63764278	0.74728662	-1.19857518
1	-0.16402018	1.41320383	-0.83540806
1	0.16773317	-0.11862619	-1.69772775
1	1.22327722	1.29446313	-1.95756845
50	1.81560622	1.20318206	1.70313753
7	-0.02015890	-0.19932630	2.89355049
6	0.52612355	-0.92127406	4.06211145
1	-0.27026622	-1.45076645	4.61558012
1	1.28730109	-1.63974763	3.74008321
1	0.99953161	-0.19619314	4.73574441
7	1.42701670	-2.09308954	1.17524627
6	-0.71293387	-1.11266264	1.94872653
1	-1.68387316	-1.42666867	2.38083557
1	-0.92654287	-0.54232770	1.03472013
6	0.05429442	-2.39001728	1.58759323
1	-0.53284188	-2.89798245	0.79901894
1	0.10086777	-3.07172535	2.44674568
16	2.48893152	-3.38880459	0.97508436
7	-0.10503569	2.32457479	1.58225129
6	-0.94432201	0.86903184	3.35986886
1	-1.85584298	0.42002023	3.80070323
1	-0.41962073	1.42182765	4.15258982
6	-1.31665182	1.85988858	2.25602269
1	-1.85104301	2.69604915	2.73513713
1	-2.00874506	1.39984558	1.52907239
16	0.22506733	3.93588668	1.53403980
8	1.68040695	3.94772700	1.17347985
8	-0.25717929	4.65652209	2.73615761
6	-0.67256938	4.63879098	0.12857173
6	-1.89280792	5.28046381	0.34610900
6	-2.59206967	5.80134638	-0.74511744
6	-2.08418642	5.69970893	-2.04858762
6	-0.84755205	5.05787344	-2.23549829
6	-0.13971266	4.52701911	-1.15880241
1	-2.27310307	5.38801399	1.36132580
1	0.82716262	4.04695617	-1.30484177
1	-0.43024112	4.97845756	-3.24120934
6	-2.82611646	6.29190879	-3.22054276
1	-3.54562494	6.30566491	-0.57807961
8	3.79110093	-2.78219905	0.65257008
8	2.29614021	-4.27024020	2.14601267
6	1.92611725	-4.29503360	-0.48584808
6	1.15165417	-5.44558507	-0.33422570
6	0.71770578	-6.12701159	-1.47461983
6	1.04588466	-5.67326023	-2.76019762
6	1.83418723	-4.51459388	-2.88054210
6	2.27639044	-3.82262714	-1.75509101
1	0.91922646	-5.81082705	0.66560609
1	0.12142092	-7.03422487	-1.36135443

6	0.56346273	-6.40210430	-3.98915729
1	2.11456823	-4.15645541	-3.87297895
1	2.90573030	-2.93767069	-1.85016539
1	-3.87079603	6.51059209	-2.96531891
1	-2.35786691	7.23451476	-3.54367803
1	-2.81544976	5.61360555	-4.08493808
1	1.36925645	-6.51546648	-4.72767189
1	0.18125918	-7.39995891	-3.73965459
1	-0.24927723	-5.84573273	-4.48115562
1	1.50991441	-1.37289378	0.41902821

Energy = -8139.850067 Hartree
Number of imaginary frequencies = 0.

Compound 11a isomer 28

Atomic N.	X	Y	Z
8	4.11113060	1.41095880	-0.36038251
6	5.21940883	1.50588161	-1.25011426
1	5.46361389	0.54157511	-1.73569008
1	6.10455360	1.82039770	-0.67390170
1	5.04272465	2.25166999	-2.04453369
50	2.37475270	0.48132867	-0.95616066
7	1.85385192	0.85841072	1.50030499
6	2.94071477	0.34788935	2.36439078
1	2.77073355	0.61811146	3.42233089
1	3.01852985	-0.74141542	2.27426184
1	3.88011671	0.79105748	2.01394645
7	0.94262084	-1.98985397	1.08662531
6	0.51828447	0.33425694	1.88225249
1	0.16087754	0.85797295	2.79075393
1	-0.18107454	0.58604843	1.07046243
6	0.43638910	-1.16310891	2.18813282
1	-0.61891757	-1.38115223	2.43548470
1	1.03759998	-1.40853022	3.07269871
16	1.23440271	-3.63995764	1.40417145
7	1.07026909	2.29785192	-0.74983733
6	1.84772133	2.35049506	1.55296772
1	1.59861429	2.68918732	2.57708691
1	2.86935368	2.66691958	1.30403813
6	0.87987115	2.96379823	0.53795863
1	1.10753266	4.03960746	0.46910658
1	-0.16666489	2.86810024	0.87780571
16	1.35437739	3.19281790	-2.09141707
8	2.14129625	2.23563726	-2.94938113
8	1.88839434	4.54451046	-1.80592420
6	-0.22916676	3.43447093	-2.93676122
6	-0.81700400	4.69900756	-2.94341987
6	-2.04895739	4.87364798	-3.57971027
6	-2.69626885	3.80433503	-4.21459069
6	-2.07747344	2.54157838	-4.19420940
6	-0.85117617	2.34986194	-3.56161056
1	-0.30241866	5.53248120	-2.46662614
1	-0.36801486	1.37269919	-3.56226832
1	-2.56284772	1.69792963	-4.68897153
6	-4.00788940	4.00528055	-4.93181315
1	-2.51064116	5.86284901	-3.58859709
8	1.66800940	-4.19910084	0.11369578
8	2.07711818	-3.66477441	2.61425760

6	-0.35692636	-4.38362634	1.82806654
6	-0.74184650	-4.47966999	3.16617557
6	-1.98193199	-5.04386711	3.47599333
6	-2.83855245	-5.51314730	2.46958250
6	-2.41837332	-5.41119720	1.13103237
6	-1.18586733	-4.85124006	0.80257272
1	-0.06513067	-4.14140697	3.95012446
1	-2.28398608	-5.12988409	4.52114586
6	-4.17612781	-6.12217059	2.80596053
1	-3.06338196	-5.78823319	0.33514003
1	-0.84964369	-4.79969088	-0.23293364
1	-4.51390386	4.91894607	-4.59438785
1	-3.84933707	4.09605048	-6.01777250
1	-4.68599471	3.15518177	-4.77470855
1	-4.26786042	-7.13315492	2.38338525
1	-4.32490867	-6.19022763	3.89064442
1	-4.99852285	-5.52339711	2.38682945
1	0.42794767	-1.89999732	0.20633653

Energy = -8139.843608 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 29

Atomic N.	X	Y	Z
8	4.24420158	1.52411895	1.38336103
6	5.59843183	1.08493319	1.37945824
1	6.16966764	1.69689620	2.09646776
1	6.08583772	1.19016844	0.38991296
1	5.68162489	0.02756489	1.68493710
50	3.02174914	1.04135804	-0.19500478
7	1.44727123	2.84405555	0.80954238
6	2.16558502	3.45027987	1.95572729
1	1.49731898	4.13931180	2.50349907
1	2.54400955	2.67065226	2.62270028
1	3.03790205	4.00147090	1.58623590
7	1.45962132	0.03614519	1.03152691
6	0.25089118	2.09752206	1.27875321
1	-0.35679537	2.72723996	1.95615262
1	-0.35284652	1.84307948	0.40044952
6	0.62879866	0.78779246	1.97197893
1	-0.31207184	0.25582495	2.20057091
1	1.14514975	0.96462973	2.92937537
16	2.11556340	-1.39272266	1.50046724
7	0.49316793	2.45334113	-2.04481393
6	1.10638987	3.94326703	-0.13692409
1	0.68151113	4.79482219	0.42943244
1	2.05721530	4.29488405	-0.56719730
6	0.11263310	3.63581130	-1.25828038
1	0.02767536	4.54453254	-1.87761691
1	-0.88724349	3.44916874	-0.84102632
16	-0.60201651	2.01533709	-3.29581430
8	0.18887969	1.14152189	-4.18241833
8	-1.30383234	3.20472184	-3.82740992
6	-1.80906210	1.03765557	-2.38082017
6	-3.15820755	1.38424377	-2.45975582
6	-4.09726922	0.59648825	-1.79035124
6	-3.70380323	-0.52609940	-1.04618652
6	-2.33542347	-0.84440860	-0.98032871

6	-1.38449204	-0.07334072	-1.64601420
1	-3.45606187	2.25910224	-3.03670762
1	-0.32543329	-0.32212068	-1.58055546
1	-2.00615696	-1.70675812	-0.39777190
6	-4.72500404	-1.38862332	-0.34854527
1	-5.15432789	0.86219050	-1.84603218
8	3.29705591	-1.51523826	0.57481738
8	2.29400843	-1.51953638	2.96371399
6	0.95070072	-2.68811840	1.00482562
6	0.09485619	-3.24085884	1.95754954
6	-0.82481719	-4.21702435	1.56194071
6	-0.89255171	-4.65476535	0.23163097
6	-0.00722505	-4.08860107	-0.70398101
6	0.90980084	-3.10950787	-0.32808384
1	0.16702342	-2.92171509	2.99683472
1	-1.49351124	-4.65434730	2.30573155
6	-1.87963207	-5.71329037	-0.19306494
1	-0.03559339	-4.42399936	-1.74255532
1	1.60369284	-2.68358486	-1.05258555
1	-4.33003928	-1.79373212	0.59251120
1	-5.64354417	-0.82868579	-0.13068385
1	-5.00380564	-2.24606211	-0.98085627
1	-1.36349297	-6.59559749	-0.59933481
1	-2.50173939	-6.04259237	0.64862844
1	-2.54542784	-5.34000699	-0.98537193
1	1.41319302	2.53120583	-2.49264043

Energy = -8139.840678 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 30

Atomic N.	X	Y	Z
8	3.60820029	2.43438572	-0.09003312
6	4.69420880	2.84651900	-0.91437289
1	5.18786836	2.00002204	-1.42917930
1	5.45068341	3.33452264	-0.27871119
1	4.37114778	3.57006171	-1.68291390
50	2.19580224	1.12102358	-0.80621134
7	1.48655142	1.24602979	1.62838372
6	2.62689405	0.99351602	2.53641125
1	2.34403335	1.16549003	3.59070450
1	2.98685605	-0.03467481	2.41857989
1	3.43569068	1.67680631	2.25244743
7	1.37275243	-1.71741223	1.08200835
6	0.31543382	0.38023794	1.91699290
1	-0.20910653	0.75416440	2.81832289
1	-0.38508513	0.47894419	1.07377584
6	0.61010813	-1.09998026	2.17279663
1	-0.36350734	-1.59418269	2.34655791
1	1.20677990	-1.22085018	3.08572531
16	2.08086693	-3.24135194	1.37154172
7	0.46224337	2.53535792	-0.61559719
6	1.09374414	2.68306801	1.72694560
1	0.71935180	2.90100067	2.74569544
1	2.00984830	3.26068025	1.54533554
6	0.04833565	3.07353187	0.67929045
1	-0.00505939	4.17381071	0.65650794
1	-0.95284104	2.69925524	0.95754395

16	0.56431422	3.52872818	-1.91328130
8	1.60277015	2.83786460	-2.75882694
8	0.72644959	4.95823199	-1.56079814
6	-0.99325197	3.39797690	-2.82819690
6	-1.88945492	4.46632371	-2.81346589
6	-3.09968040	4.34918338	-3.50250278
6	-3.42200701	3.18301987	-4.21080779
6	-2.49662104	2.12400662	-4.21087970
6	-1.28740742	2.22325961	-3.52628110
1	-1.62795244	5.37904175	-2.27922170
1	-0.56651972	1.40576293	-3.54222967
1	-2.72652609	1.21034153	-4.76271922
6	-4.71325840	3.07417530	-4.98283121
1	-3.80241727	5.18455464	-3.49472780
8	2.72587388	-3.60297058	0.09909400
8	2.82537011	-3.09436162	2.63627852
6	0.73005247	-4.40561405	1.66268110
6	0.29789787	-4.65306193	2.96726528
6	-0.75855599	-5.54255380	3.17381056
6	-1.38475267	-6.18980163	2.09768516
6	-0.92442678	-5.92322696	0.79636616
6	0.12836936	-5.03829575	0.57036849
1	0.80118518	-4.17185794	3.80517887
1	-1.09681930	-5.74362972	4.19180503
6	-2.50105674	-7.17606689	2.32994747
1	-1.39245356	-6.42533009	-0.05230982
1	0.50153310	-4.85348213	-0.43687663
1	-5.44983235	3.81166014	-4.63897239
1	-4.54282446	3.25138201	-6.05622449
1	-5.15477929	2.07260924	-4.88714965
1	-2.11641115	-8.20769082	2.31449106
1	-2.98136557	-7.01751596	3.30383517
1	-3.26829955	-7.10489825	1.54730808
1	0.90105664	-1.72774022	0.17363985

Energy = -8139.843602 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 31

Atomic N.	X	Y	Z
8	4.19666405	1.53850092	1.50166644
6	5.56433350	1.14490078	1.46681370
1	5.68267468	0.07212418	1.69808526
1	6.11722757	1.72374851	2.22455694
1	6.04565865	1.33458953	0.48690246
50	2.98830392	1.12410230	-0.10684096
7	1.36596994	2.81877695	1.00466698
6	2.06287371	3.36216726	2.19471280
1	1.37494639	3.99600929	2.78329090
1	2.45623626	2.54810026	2.80987142
1	2.92368504	3.95780377	1.87001329
7	1.44928279	0.00486486	1.04692093
6	0.18485633	2.01451907	1.41295238
1	-0.44390484	2.58395527	2.12369504
1	-0.40516267	1.80318664	0.51407460
6	0.58967738	0.67228070	2.02406648
1	-0.33936404	0.10299712	2.20651818
1	1.09137875	0.79940058	2.99703591

16	2.13800924	-1.43437592	1.42832371
7	0.43981858	2.60090007	-1.87691462
6	1.00467979	3.97152511	0.13245517
1	0.55575193	4.77215976	0.75204177
1	1.94941138	4.37416466	-0.26529831
6	0.02565263	3.71760937	-1.01497827
1	-0.07757540	4.66412415	-1.57176507
1	-0.97191081	3.47910590	-0.61916786
16	-0.63704731	2.22138357	-3.16242428
8	0.18119889	1.43086025	-4.10088644
8	-1.36707898	3.42587250	-3.61628222
6	-1.82253932	1.15244176	-2.32466933
6	-3.17920659	1.47247967	-2.38236179
6	-4.10052631	0.61664014	-1.77451698
6	-3.68190769	-0.54718965	-1.11210173
6	-2.30645550	-0.83767373	-1.06529609
6	-1.37308236	0.00121203	-1.67084676
1	-3.49673607	2.37910030	-2.89634444
1	-0.30857389	-0.22699038	-1.62084900
1	-1.95788652	-1.73221236	-0.54595528
6	-4.68329011	-1.48146075	-0.48141165
1	-5.16345260	0.86092656	-1.81400657
8	3.32764161	-1.46767237	0.50565707
8	2.31029707	-1.65070371	2.88176391
6	1.01023415	-2.72466949	0.84150503
6	0.16177455	-3.35844376	1.74971869
6	-0.72838861	-4.33126786	1.28528535
6	-0.77337470	-4.68695287	-0.07051178
6	0.10099766	-4.03756107	-0.96082929
6	0.98934931	-3.06073659	-0.51560284
1	0.21655622	-3.10255642	2.80740767
1	-1.39208708	-4.83061775	1.99370776
6	-1.71459943	-5.75676028	-0.56526469
1	0.08714293	-4.30517245	-2.01915526
1	1.67522391	-2.57023039	-1.20609086
1	-5.62364046	-0.96572948	-0.24818827
1	-4.92225172	-2.31109619	-1.16496477
1	-4.28888379	-1.92553661	0.44225603
1	-1.16515225	-6.67689586	-0.81637542
1	-2.46509791	-6.01357819	0.19309057
1	-2.23845990	-5.43775001	-1.47745298
1	1.36012802	2.73130034	-2.31170264

Energy = -8139.840671 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 32

Atomic N.	X	Y	Z
8	4.28114478	-0.50089920	-0.75908190
6	4.63871757	-0.20182701	-2.10265798
1	4.87384381	0.86879283	-2.22638310
1	3.84283631	-0.44579325	-2.83074153
1	5.53806102	-0.78267695	-2.36872496
50	2.49795436	-0.15513995	0.16478172
7	1.74409520	-2.76467393	-0.50931108
6	2.87131244	-3.28647176	-1.30817577
1	2.64130273	-4.29163212	-1.71180683
1	3.09288772	-2.60990156	-2.13896357

1	3.77012596	-3.33776060	-0.68281239
7	1.13635997	-0.23638503	-1.60107273
6	0.55152300	-2.56360214	-1.36683375
1	0.31192532	-3.49669465	-1.91665141
1	-0.29767117	-2.32877823	-0.71127029
6	0.71452993	-1.40909982	-2.35665703
1	-0.26501782	-1.25102396	-2.84165201
1	1.42849361	-1.66473630	-3.15809033
16	1.16030904	1.24051122	-2.28913296
7	1.19081319	-2.36936397	2.60372797
6	1.44667680	-3.74816182	0.56000166
1	1.01173254	-4.66142988	0.10486915
1	2.40911436	-4.05224144	1.00051457
6	0.51171778	-3.30004327	1.68503997
1	0.15704297	-4.20334184	2.20759706
1	-0.37906089	-2.79555020	1.28536153
16	0.32772762	-1.94653853	4.03136855
8	1.38438308	-1.70631240	5.03421369
8	-0.76450948	-2.91514401	4.26953258
6	-0.42905346	-0.37198922	3.59497456
6	-1.81350764	-0.29311056	3.45183804
6	-2.39288856	0.94667880	3.16620696
6	-1.60719976	2.09972276	3.02528033
6	-0.21234088	1.98393061	3.16983165
6	0.38250332	0.75840820	3.45563968
1	-2.42137364	-1.18779554	3.58118090
1	1.46160580	0.67574514	3.57591606
1	0.41608152	2.86866548	3.05478887
6	-2.23251700	3.44218172	2.74249340
1	-3.47698413	1.01793118	3.06209291
8	1.93022279	2.02828107	-1.25768602
8	1.60781129	1.26487394	-3.70048606
6	-0.54269129	1.85848115	-2.28586248
6	-1.09962089	2.33492800	-3.47181128
6	-2.41488252	2.80820004	-3.46432994
6	-3.17914603	2.80874042	-2.28953175
6	-2.59185836	2.31639887	-1.10954327
6	-1.28154498	1.84412276	-1.09857534
1	-0.50230096	2.32888273	-4.38270909
1	-2.85405705	3.18144386	-4.39127487
6	-4.59206554	3.33620820	-2.27960692
1	-3.17377349	2.29970613	-0.18573049
1	-0.83635086	1.46196094	-0.17910007
1	-2.07756803	4.13185787	3.58563370
1	-1.77946444	3.91226602	1.85776077
1	-3.31328618	3.35547595	2.57328819
1	-4.64229266	4.31184705	-1.77198675
1	-4.97700833	3.47050028	-3.29830265
1	-5.26861650	2.65748711	-1.74140194
1	2.08579673	-2.73611116	2.94402405

Energy = -8139.838874 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 33

Atomic N.	X	Y	Z
8	3.95785595	-1.73833112	-0.52110637
6	5.34343802	-1.54235495	-0.25592354

1	5.92014979	-2.26264573	-0.85841156
1	5.58452636	-1.71366818	0.80764039
1	5.69246424	-0.52719414	-0.52627815
50	2.57248086	-0.35791122	0.11952957
7	1.10458243	-1.80012497	-1.37456750
6	1.70698694	-1.97499228	-2.71432818
1	1.13161177	-2.69851272	-3.31991816
1	1.75244452	-1.01466709	-3.24011292
1	2.73109010	-2.33960917	-2.57351498
7	0.29146657	0.99103519	-2.18346598
6	-0.29640675	-1.31259629	-1.43203663
1	-0.96700294	-2.14480735	-1.72409092
1	-0.58436116	-1.01060166	-0.41361320
6	-0.57856947	-0.16872576	-2.40940374
1	-1.65186608	0.07785128	-2.31250228
1	-0.40951173	-0.49649420	-3.44285612
16	0.36942231	2.17571530	-3.40747404
7	1.40523502	-1.79125317	1.39161658
6	1.16155999	-3.09931887	-0.64111260
1	0.53188483	-3.84995162	-1.15653038
1	2.21104366	-3.42084394	-0.67499481
6	0.73613134	-2.95991736	0.82247679
1	1.03196961	-3.88358574	1.34518453
1	-0.36091788	-2.86642260	0.91100859
16	2.25578112	-1.93850913	2.78304309
8	3.27468970	-0.83624587	2.64872299
8	2.69329943	-3.32364328	3.07197724
6	1.16731937	-1.44869546	4.14560867
6	0.70130508	-2.41725159	5.03412648
6	-0.15542729	-2.03498062	6.07000094
6	-0.54619266	-0.69844831	6.23320202
6	-0.05755915	0.25637558	5.32363845
6	0.79452582	-0.10866914	4.28371217
1	1.02191878	-3.45177172	4.91659500
1	1.18234488	0.63774366	3.59032971
1	-0.34575233	1.30328530	5.43791939
6	-1.44143539	-0.28429800	7.37436304
1	-0.52050926	-2.79058374	6.76823469
8	1.26694402	3.21110975	-2.87060589
8	0.64996449	1.43599855	-4.65233800
6	-1.28292597	2.89200473	-3.55572312
6	-2.17755295	2.38090265	-4.49806397
6	-3.45397210	2.93932091	-4.59310490
6	-3.84774914	3.99854037	-3.76126344
6	-2.92037069	4.49958397	-2.83090443
6	-1.64212483	3.95506689	-2.72115463
1	-1.86231243	1.57873186	-5.16445722
1	-4.15279741	2.55205946	-5.33661008
6	-5.23441142	4.58275388	-3.85372214
1	-3.20075413	5.33857374	-2.19148270
1	-0.91455638	4.36515486	-2.02083906
1	-2.00077234	-1.13896216	7.77617720
1	-0.85002062	0.14213669	8.19962405
1	-2.16083993	0.48485259	7.06138887
1	-5.21881393	5.67329599	-3.72423503
1	-5.70262186	4.35459531	-4.81957482
1	-5.88366535	4.17176450	-3.06495121
1	0.17733660	1.44813614	-1.27484773

Energy = -8139.843627 Hartree
 Number of imaginary frequencies = 0.

Compound 11a isomer 34

Atomic N.	X	Y	Z
8	4.34011124	-0.37731613	-0.61145318
6	4.74853662	-0.02455505	-1.92684850
1	5.54124626	-0.71830878	-2.25695977
1	5.16143685	0.99821701	-1.94846164
1	3.92758333	-0.06081707	-2.66612152
50	2.51468448	-0.11925241	0.25407779
7	1.82529873	-2.68090976	-0.63529525
6	2.99070355	-3.12998836	-1.42355734
1	2.79388956	-4.10865770	-1.90270628
1	3.23079722	-2.39529722	-2.19785213
1	3.86614354	-3.21005258	-0.76861840
7	1.23377917	-0.08924573	-1.57038188
6	0.66442866	-2.43229567	-1.52331691
1	0.45854770	-3.32642200	-2.14661052
1	-0.21255221	-2.25302471	-0.88714463
6	0.85169215	-1.20871562	-2.42189100
1	-0.11076609	-1.02347264	-2.93076448
1	1.59718261	-1.40125055	-3.21217793
16	1.24139329	1.43660361	-2.14287331
7	1.13036816	-2.51166513	2.46786387
6	1.50209630	-3.74247858	0.34839382
1	1.10453816	-4.62822985	-0.18813677
1	2.45098014	-4.06124561	0.80763621
6	0.51204555	-3.39176032	1.46072843
1	0.15869078	-4.33622252	1.90569778
1	-0.37405667	-2.88069865	1.05899221
16	0.20089363	-2.20895026	3.88440663
8	1.21044150	-2.01334847	4.94380994
8	-0.87369589	-3.21741904	4.01146327
6	-0.57969127	-0.62655293	3.52510059
6	-1.96028808	-0.57017508	3.34007742
6	-2.56142363	0.67237744	3.11869347
6	-1.80108444	1.85020247	3.08249093
6	-0.40899733	1.75703989	3.26554279
6	0.20714555	0.52907321	3.48911198
1	-2.54906230	-1.48544190	3.38816695
1	1.28358357	0.46356618	3.64014828
1	0.20025346	2.66174695	3.23081845
6	-2.45121872	3.19412038	2.87199825
1	-3.64302507	0.72532187	2.98243201
8	1.95353439	2.16186338	-1.02861114
8	1.73660899	1.57834077	-3.53138119
6	-0.47725197	2.00976584	-2.15693990
6	-0.99701925	2.58553073	-3.31583067
6	-2.32315442	3.02632063	-3.32125629
6	-3.13543725	2.89698445	-2.18591505
6	-2.58556033	2.30531022	-1.03444079
6	-1.26425368	1.86409498	-1.01060260
1	-0.36295885	2.67863497	-4.19667117
1	-2.73339460	3.47594966	-4.22734811
6	-4.55863348	3.39595192	-2.18760251
1	-3.20539586	2.18479672	-0.14368750

1	-0.84823403	1.40401436	-0.11341761
1	-2.35637409	3.81996568	3.77201352
1	-1.97125441	3.74270857	2.04894467
1	-3.51993250	3.09334728	2.64404342
1	-4.62782773	4.37917547	-1.69649095
1	-4.94282700	3.50980724	-3.20927420
1	-5.22366087	2.71344424	-1.64084601
1	2.02039687	-2.88050580	2.81883444

Energy = -8139.838885 Hartree
Number of imaginary frequencies = 0.

Compound I1a isomer 35

Atomic N.	X	Y	Z
8	4.02002025	-1.58412888	-0.45054558
6	5.38154931	-1.38762199	-0.08118671
1	5.55833114	-1.64447337	0.97771138
1	5.72391994	-0.34726347	-0.24152616
1	6.01114741	-2.04346145	-0.70405329
50	2.56934818	-0.26702590	0.17729293
7	1.20615517	-1.70314403	-1.41206448
6	1.86512767	-1.81883838	-2.73156004
1	1.33493316	-2.53846194	-3.38132983
1	1.90283928	-0.84128386	-3.22519367
1	2.89314535	-2.15906800	-2.56114876
7	0.34108240	1.08645128	-2.17307704
6	-0.20556158	-1.25383577	-1.50947293
1	-0.83971232	-2.09598439	-1.85013059
1	-0.54031405	-0.99014196	-0.49463734
6	-0.48510594	-0.09068599	-2.46426151
1	-1.56823648	0.12175096	-2.40094845
1	-0.26827658	-0.38281032	-3.49952989
16	0.40635339	2.31962380	-3.34937904
7	1.40109585	-1.77330470	1.36542947
6	1.27247106	-3.02253758	-0.71629271
1	0.68425107	-3.77331961	-1.27833700
1	2.33118088	-3.31400052	-0.71933584
6	0.78763859	-2.94042452	0.73318975
1	1.08844035	-3.87247118	1.23790438
1	-0.31402175	-2.87853995	0.78165956
16	2.22213838	-1.95060989	2.77112636
8	3.20489430	-0.80974068	2.70947441
8	2.70155242	-3.33116363	3.01235597
6	1.08542763	-1.55784765	4.12538375
6	0.62325047	-2.58174547	4.95156926
6	-0.27069047	-2.27469262	5.98098110
6	-0.70262965	-0.95885332	6.19912787
6	-0.21693171	0.05300875	5.35171532
6	0.67216736	-0.23668035	4.31908555
1	0.97573172	-3.60020979	4.79247906
1	1.05796214	0.55340380	3.67474398
1	-0.53671659	1.08495807	5.50975514
6	-1.63894485	-0.62624817	7.33400162
1	-0.63241235	-3.07359985	6.63109744
8	1.25442935	3.36310618	-2.75127104
8	0.74117531	1.63858537	-4.61404149
6	-1.26666905	2.98343660	-3.51004612
6	-2.11995400	2.48011825	-4.49365223

6	-3.41413367	2.99531797	-4.59635683
6	-3.86546043	4.00422523	-3.73234587
6	-2.97867056	4.49901710	-2.75955221
6	-1.68417656	3.99708241	-2.64136642
1	-1.76054156	1.71747625	-5.18365871
1	-4.08159624	2.61342345	-5.37076891
6	-5.26848860	4.54608694	-3.83604617
1	-3.30445730	5.29981059	-2.09317645
1	-0.98856978	4.40291201	-1.90690502
1	-2.17440534	-1.51711237	7.68665230
1	-1.08357188	-0.21286217	8.19036106
1	-2.37989896	0.12807709	7.03541134
1	-5.28009239	5.64151111	-3.75233515
1	-5.73761809	4.26680862	-4.78772028
1	-5.89995429	4.15336652	-3.02415376
1	0.19005352	1.50463540	-1.25110151

Energy = -8139.843611 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 36

Atomic N.	X	Y	Z
8	0.63061157	-0.65206445	-0.05870747
6	1.84248805	-0.70766884	0.70188081
1	2.72467844	-0.64177869	0.04273625
1	1.92960078	-1.63596366	1.29644281
1	1.86991111	0.14327517	1.40125089
50	-0.03075035	-2.45500280	-0.92197797
7	-2.55927676	-1.57948800	-1.04767995
6	-3.20964487	-2.80150107	-1.57126365
1	-4.25184352	-2.59981988	-1.88003033
1	-2.65446873	-3.19172967	-2.43318751
1	-3.21369660	-3.56942479	-0.78796039
7	-0.45373702	-1.40966449	-2.81097338
6	-2.55055345	-0.51082181	-2.07915506
1	-3.58690382	-0.26484089	-2.38442272
1	-2.10100661	0.38128301	-1.62538719
6	-1.71687178	-0.89100802	-3.30582660
1	-1.57767949	0.02076629	-3.91234555
1	-2.24753898	-1.61947731	-3.94287611
16	0.89210484	-1.50149744	-3.72156499
7	-1.50342345	-0.12814418	1.67221598
6	-3.31590345	-1.14695676	0.15890249
1	-4.35318144	-0.89716107	-0.14674540
1	-3.38120135	-2.01266688	0.83211640
6	-2.77089484	0.04860086	0.95460185
1	-3.54644578	0.30235129	1.69060182
1	-2.64186245	0.93430367	0.31600617
16	-1.51589044	-1.26865927	2.92166742
8	-0.87394400	-2.53216582	2.47622829
8	-2.89438847	-1.29021024	3.46285175
6	-0.42492768	-0.52197671	4.14961440
6	-0.82745984	0.64518623	4.80571862
6	0.00109391	1.19225443	5.78124842
6	1.22686831	0.58802626	6.11709854
6	1.60002096	-0.58399112	5.44539366
6	0.78030547	-1.14663636	4.46295264
1	-1.77951131	1.11180131	4.55485439

1	1.06169766	-2.06201346	3.94405937
1	2.54610405	-1.06813696	5.69352964
6	2.10455090	1.18529234	7.18802528
1	-0.30733169	2.10404510	6.29613976
8	1.82641472	-2.19661911	-2.75679494
8	0.70261962	-2.07635504	-5.07127292
6	1.49861037	0.18825828	-3.95563515
6	1.85999073	0.61620356	-5.23295254
6	2.34324252	1.91637818	-5.39975735
6	2.46768241	2.78892749	-4.30874617
6	2.08441365	2.32991426	-3.03572353
6	1.60099971	1.03600518	-2.84809579
1	1.75848147	-0.06551224	-6.07657222
1	2.62693048	2.25815547	-6.39690185
6	3.01913076	4.18113052	-4.48881782
1	2.16604556	2.99950065	-2.17696043
1	1.29471753	0.68073510	-1.85954060
1	1.63775337	1.08378931	8.17961311
1	3.08359759	0.69156853	7.22567617
1	2.26638795	2.25920211	7.01749279
1	4.08275869	4.21811029	-4.20592526
1	2.94363765	4.51140644	-5.53282103
1	2.49090133	4.90702273	-3.85563969
1	-0.67401396	-0.29453707	1.04334188

Energy = -8139.851356 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 37

Atomic N.	X	Y	Z
8	4.26314531	-2.03055071	0.49136387
6	4.58390821	-2.02592832	1.88058584
1	5.07286544	-1.08837756	2.19110176
1	5.27997336	-2.85838772	2.07347108
1	3.69444133	-2.16533133	2.52234721
50	3.09963075	-0.67383659	-0.49585860
7	1.47426355	-2.73820921	-0.82045855
6	2.31092491	-3.90734198	-1.16988603
1	1.74207563	-4.84802808	-1.05356201
1	2.65583577	-3.83223820	-2.20759656
1	3.19180702	-3.91405201	-0.51552856
7	0.88725449	-0.79390744	-3.41941160
6	0.30846018	-2.62863662	-1.73753475
1	-0.20693159	-3.61001913	-1.76371427
1	-0.39527161	-1.90259915	-1.31174272
6	0.63353631	-2.21490915	-3.18106627
1	-0.21190765	-2.49628112	-3.82482088
1	1.49696173	-2.77914069	-3.56462113
16	-0.35961144	0.23574721	-3.90585490
7	1.37508652	-0.50961462	0.89992660
6	1.00671710	-2.89213968	0.58613932
1	0.25775780	-3.70544113	0.65245616
1	1.88634658	-3.18593740	1.17476419
6	0.43733304	-1.59619285	1.17247317
1	0.30824671	-1.74926968	2.25656636
1	-0.55654796	-1.36948443	0.74906565
16	1.87646765	0.50480666	2.07805777
8	3.19714758	0.97304260	1.50618933

8	1.81756721	-0.07561275	3.43872261
6	0.80487491	1.96145280	2.09184119
6	-0.16003853	2.09141344	3.09060462
6	-0.99983721	3.20888674	3.08295067
6	-0.88461532	4.19839984	2.09576688
6	0.10733352	4.04586348	1.10977528
6	0.95008429	2.93667166	1.10027269
1	-0.23224287	1.33671167	3.87288423
1	1.72910817	2.83429747	0.34491578
1	0.22376179	4.81162796	0.34060386
6	-1.79690738	5.39890370	2.08299960
1	-1.75141202	3.31748529	3.86698883
8	0.27862099	1.55967913	-4.01110009
8	-1.02201224	-0.43094548	-5.04308171
6	-1.58464637	0.31846686	-2.57581635
6	-2.76543142	-0.41925672	-2.67898860
6	-3.69804025	-0.35598927	-1.64080509
6	-3.46657590	0.43235440	-0.50338641
6	-2.27366601	1.17378864	-0.43307268
6	-1.33243420	1.12130368	-1.45963514
1	-2.95324157	-1.01146338	-3.57394276
1	-4.62755439	-0.92242445	-1.72216722
6	-4.46441498	0.47722102	0.62643768
1	-2.07822173	1.80463486	0.43612874
1	-0.41777264	1.71087966	-1.40424822
1	-2.41528164	5.44309990	2.98820372
1	-1.22304580	6.33373726	2.01253387
1	-2.47109601	5.37106249	1.21341643
1	-4.55615505	1.49127452	1.03826253
1	-5.45750462	0.14371902	0.29953936
1	-4.14839872	-0.17923977	1.45225316
1	1.55927927	-0.32574532	-2.80170892

Energy = -8139.843032 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 38

Atomic N.	X	Y	Z
8	0.94858030	0.03687776	0.71711122
6	2.23785574	-0.58121194	0.76329138
1	2.79868072	-0.15708873	1.61078466
1	2.80561113	-0.39087887	-0.16082845
1	2.17586525	-1.67568687	0.91025451
50	-0.50605251	-0.66447607	-0.62050237
7	-1.92565549	1.28697443	0.28496784
6	-3.14455917	1.20562864	-0.55571757
1	-3.75712532	2.11942222	-0.45626181
1	-2.87294392	1.06721613	-1.60871219
1	-3.74079737	0.34337364	-0.23249685
7	-0.32343614	1.12825932	-1.95304251
6	-1.10075893	2.47262340	-0.07705167
1	-1.64234231	3.40524535	0.17518119
1	-0.18067791	2.42052725	0.51893276
6	-0.72077706	2.47867925	-1.56204137
1	0.10696096	3.19348087	-1.69495154
1	-1.56759769	2.83285529	-2.17562055
16	1.03503860	0.88829503	-2.82750731
7	-0.43631300	0.33499017	3.04261953

6	-2.38387135	1.36032821	1.70414411
1	-3.05232033	2.24017529	1.79937623
1	-2.99774880	0.46838496	1.89071027
6	-1.32936741	1.47766761	2.81552079
1	-1.89349917	1.66333005	3.74045060
1	-0.67825185	2.34948083	2.66076816
16	-1.20665425	-1.09866580	3.49762950
8	-1.49784120	-1.94234170	2.30589981
8	-2.31144627	-0.72494540	4.41047894
6	0.08597809	-1.93174489	4.43829028
6	0.36442456	-1.50736850	5.74051872
6	1.35045115	-2.16753118	6.46903685
6	2.06203276	-3.24823077	5.91691166
6	1.75590796	-3.65296469	4.61003155
6	0.76831505	-3.00324673	3.86511704
1	-0.19271089	-0.67658320	6.17225250
1	0.51728596	-3.32356744	2.85465280
1	2.29565080	-4.49133888	4.16638607
6	3.11361711	-3.96454865	6.72631464
1	1.57317667	-1.84141523	7.48669272
8	2.06419935	1.93727545	-2.64529364
8	1.36041494	-0.54769060	-2.49249596
6	0.58030105	0.90816774	-4.57899627
6	-0.24266552	-0.10066931	-5.08916811
6	-0.60536993	-0.06670459	-6.43312398
6	-0.15880005	0.96308790	-7.28144037
6	0.66553266	1.96014751	-6.74227617
6	1.04120614	1.93953423	-5.39593229
1	-0.58300851	-0.90755358	-4.43996576
1	-1.24429792	-0.85514959	-6.83573565
6	-0.54342951	0.97403669	-8.73976011
1	1.02555724	2.76535770	-7.38533876
1	1.69403770	2.70462526	-4.97747276
1	3.78381691	-3.25308643	7.22879988
1	2.65029562	-4.58135963	7.51169629
1	3.72206276	-4.62643372	6.09733203
1	-0.00747772	0.18704581	-9.29235256
1	-1.61810241	0.78442871	-8.87103246
1	-0.30281041	1.93547115	-9.21080125
1	0.18585317	0.14948914	2.20376573

Energy = -8139.851850 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 39

Atomic N.	X	Y	Z
8	4.81239037	-1.68751757	-0.40397412
6	5.61387490	-1.73512632	0.77028290
1	5.03016755	-1.98047584	1.67860347
1	6.12842031	-0.77816633	0.96216453
1	6.38268411	-2.51537529	0.64092290
50	3.25125715	-0.38852862	-0.75894755
7	1.77777776	-2.64676706	-0.61417934
6	2.40574360	-3.58755724	-1.56212397
1	2.06292121	-4.62481950	-1.38676286
1	2.15360043	-3.30344311	-2.59206629
1	3.49581408	-3.53151579	-1.44207999
7	0.01346493	-0.25321866	-1.45928777

6	0.31180685	-2.60302037	-0.80811975
1	-0.06375868	-3.61757526	-1.04381119
1	-0.15551896	-2.31191905	0.14394991
6	-0.17686499	-1.64423238	-1.89458297
1	-1.23747446	-1.88044029	-2.09945198
1	0.38259743	-1.77868397	-2.83014089
16	-0.49600489	0.99667418	-2.49688718
7	2.25969361	-0.64553296	1.23771097
6	2.11790023	-3.02685283	0.78119066
1	1.60886839	-3.96747290	1.07113245
1	3.20195183	-3.20026348	0.79335385
6	1.78174954	-1.91324906	1.78115634
1	2.27603026	-2.15501355	2.73668638
1	0.69379879	-1.87990287	1.98275608
16	2.91488849	0.48976403	2.21152060
8	3.79275100	1.24487587	1.24242215
8	3.49173014	-0.04723097	3.46596136
6	1.59596907	1.63463381	2.68837553
6	1.21343320	1.72516622	4.02637633
6	0.18107959	2.59830538	4.38072787
6	-0.46896063	3.38249437	3.41712054
6	-0.06254349	3.26750613	2.07542822
6	0.96451494	2.40208111	1.70412776
1	1.73107500	1.12504889	4.77388578
1	1.27301581	2.33530326	0.66018219
1	-0.55065979	3.87002423	1.30688034
6	-1.55521827	4.35250461	3.81022903
1	-0.11860933	2.67469807	5.42770450
8	-0.22197135	2.23546624	-1.74586821
8	0.10397773	0.70378681	-3.80941774
6	-2.28929816	0.83696747	-2.66283209
6	-2.82435654	0.16590100	-3.76371304
6	-4.21123113	0.03647212	-3.87044988
6	-5.06806830	0.56978204	-2.89632515
6	-4.49931887	1.24337110	-1.80047135
6	-3.11850822	1.38247451	-1.67711459
1	-2.15935576	-0.22762959	-4.53178328
1	-4.63485692	-0.48290617	-4.73178123
6	-6.56513427	0.45424425	-3.03160428
1	-5.15096318	1.67321829	-1.03749074
1	-2.68205866	1.92655954	-0.83939370
1	-2.00103580	4.08661975	4.77745596
1	-1.15155845	5.37301369	3.90140722
1	-2.35381350	4.38846854	3.05662755
1	-6.99832435	1.40354735	-3.38273181
1	-6.84455282	-0.32443888	-3.75234250
1	-7.03738164	0.22132233	-2.06739492
1	-0.32754687	-0.06141927	-0.51321304

Energy = -8139.841300 Hartree

Number of imaginary frequencies = 0.

Compound I1a isomer 40

Atomic N.	X	Y	Z
8	3.59981462	3.14426171	-1.46075082
6	3.05614225	3.75380429	-2.62900325
1	1.95237619	3.81446103	-2.60208407
1	3.33422682	3.21226679	-3.54824513

1	3.45415404	4.77903809	-2.70065094
50	3.35255600	1.20702413	-0.85624628
7	1.94452158	2.29829338	1.18424557
6	2.85198483	3.32925893	1.72535610
1	2.31225486	4.03327173	2.38576089
1	3.65135998	2.84957594	2.30583428
1	3.30753189	3.87862349	0.89056562
7	1.90160328	-0.93277372	1.62784799
6	1.39243759	1.45889433	2.28424499
1	1.35288986	2.06412247	3.20830516
1	0.35779400	1.18539962	2.03940876
6	2.19179889	0.17765731	2.54810512
1	2.00230220	-0.18695267	3.56708613
1	3.27178741	0.39009066	2.49043850
16	0.89984587	-2.20073207	2.13732760
7	1.11739310	1.02244872	-1.12973018
6	0.87080070	2.92512700	0.37720763
1	0.15266332	3.47002130	1.02090379
1	1.36284666	3.65227604	-0.28321824
6	0.13050221	1.89145965	-0.47994386
1	-0.47323770	2.43582715	-1.22408309
1	-0.56627781	1.29690127	0.13703007
16	0.96349151	0.65991518	-2.72212949
8	2.40686870	0.37834257	-3.08865054
8	0.19745756	1.65866442	-3.50183953
6	0.08061578	-0.90897790	-2.86753991
6	-1.15463690	-0.93785733	-3.51446339
6	-1.84851664	-2.14859271	-3.59509886
6	-1.32593676	-3.32432620	-3.03732058
6	-0.07745770	-3.26261368	-2.39182340
6	0.62949489	-2.06625558	-2.30639564
1	-1.55414587	-0.02378948	-3.95182776
1	1.59630182	-2.03719848	-1.80419413
1	0.34211213	-4.15893358	-1.93303630
6	-2.07096800	-4.63163876	-3.13309185
1	-2.81394073	-2.17778719	-4.10362459
8	0.93517218	-3.17295218	1.02993786
8	1.32792068	-2.53516059	3.50872187
6	-0.79504101	-1.57396965	2.24509814
6	-1.30788170	-1.18253713	3.48313748
6	-2.60964611	-0.68011562	3.55088943
6	-3.40589139	-0.56770327	2.40122294
6	-2.86375162	-0.97582825	1.16958610
6	-1.56718933	-1.48040108	1.08233880
1	-0.69781085	-1.29302399	4.37911919
1	-3.01638186	-0.37760426	4.51755664
6	-4.82056769	-0.05224307	2.48297945
1	-3.46866686	-0.90098430	0.26382992
1	-1.15752078	-1.80755572	0.12622771
1	-3.09293605	-4.48599319	-3.50512969
1	-1.55899641	-5.32442962	-3.81814097
1	-2.12464012	-5.13049791	-2.15515928
1	-5.54102775	-0.88356256	2.43853850
1	-4.99766798	0.48971429	3.42056528
1	-5.05075812	0.61882827	1.64410336
1	1.66047036	-0.65257803	0.66990091

Energy = -8139.841921 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 41

Atomic N.	X	Y	Z
8	1.63921283	0.40947656	-0.62139011
6	0.97661705	-0.83610143	-0.42984826
1	0.12419365	-0.92122814	-1.12752106
1	0.59236186	-0.95288914	0.59760009
1	1.66901423	-1.66923658	-0.63917514
50	2.20240546	1.80515420	0.81542076
7	-0.11372898	3.00726832	0.85249779
6	0.13012558	4.11914657	1.79771019
1	-0.81264051	4.63020957	2.06483344
1	0.60316280	3.74714565	2.71460588
1	0.80830287	4.84425388	1.33139293
7	0.91225030	0.87239909	2.36875064
6	-1.02658968	2.00158688	1.45253291
1	-1.99718092	2.47022818	1.70820497
1	-1.21140544	1.22933790	0.69478931
6	-0.43323485	1.34126524	2.69788588
1	-1.09697979	0.50045583	2.97071745
1	-0.42774706	2.03745918	3.55315025
16	1.88873279	0.36324867	3.59368565
7	0.50320440	2.37000671	-2.20515625
6	-0.69581930	3.57851007	-0.39607198
1	-1.70550274	3.97114828	-0.16125432
1	-0.06605974	4.42904663	-0.68937515
6	-0.80484543	2.64771880	-1.60675819
1	-1.40814057	3.19100759	-2.34833578
1	-1.34889592	1.72029888	-1.36053628
16	0.62945632	2.41169042	-3.88994342
8	2.06342566	2.24335931	-4.17717538
8	-0.13738883	3.59059914	-4.34569439
6	-0.22611402	0.94218833	-4.51220350
6	-1.51576670	1.05800687	-5.03098054
6	-2.16751382	-0.08817117	-5.49520687
6	-1.54837476	-1.34501980	-5.44681883
6	-0.24471067	-1.42919039	-4.92500823
6	0.42055679	-0.29743678	-4.45904875
1	-1.98524343	2.03933247	-5.09194860
1	1.43803170	-0.36300354	-4.07303875
1	0.25962886	-2.39699218	-4.89290703
6	-2.25408024	-2.58166554	-5.94445511
1	-3.17274165	-0.00050982	-5.91154478
8	3.22749227	0.29868428	2.92030741
8	1.71830153	1.15629773	4.83389103
6	1.40275082	-1.33220487	3.98957584
6	0.60413152	-1.57388647	5.10783825
6	0.21804165	-2.88545231	5.39643108
6	0.62667556	-3.95662579	4.58913439
6	1.43808473	-3.68243991	3.47353687
6	1.82752696	-2.38050762	3.16734582
1	0.31121537	-0.74431306	5.75048556
1	-0.40441868	-3.07947722	6.27176471
6	0.23352003	-5.37456252	4.91950123
1	1.77431742	-4.50477124	2.83905965
1	2.47076784	-2.17350637	2.31272878
1	-3.21815562	-2.33451106	-6.40632047

1	-1.64438805	-3.11425530	-6.68854630
1	-2.44393614	-3.28641353	-5.12083751
1	1.09337816	-5.93633457	5.31559654
1	-0.56173725	-5.40519524	5.67488665
1	-0.11694888	-5.91044726	4.02625058
1	0.98340269	1.52981763	-1.80501155

Energy = -8139.850011 Hartree
Number of imaginary frequencies = 0.

Compound 11a isomer 42

Atomic N.	X	Y	Z
8	3.57108684	3.26159081	-1.25465468
6	3.04066782	3.92402373	-2.40005979
1	3.34919338	3.43892986	-3.34088659
1	3.41980574	4.95887574	-2.40689657
1	1.93572419	3.96214983	-2.39467043
50	3.35263835	1.28961261	-0.76007052
7	1.91522311	2.25089662	1.32386301
6	2.80265919	3.26646193	1.92435643
1	2.24614214	3.92992656	2.61225391
1	3.60110986	2.76880527	2.49072356
1	3.25916653	3.86225876	1.12259815
7	1.88130836	-0.99632969	1.55237595
6	1.37385233	1.34299118	2.37452282
1	1.34609851	1.88739296	3.33571407
1	0.33582067	1.08634516	2.12530709
6	2.17544521	0.04772013	2.54642387
1	1.99162620	-0.38587435	3.53909322
1	3.25469117	0.26656928	2.49774479
16	0.90111023	-2.30837064	1.98467337
7	1.11863448	1.08160551	-1.05785114
6	0.83554625	2.90134364	0.54423065
1	0.10583045	3.40132816	1.21093311
1	1.31920531	3.66872848	-0.07568732
6	0.11596539	1.90133078	-0.36845091
1	-0.49366543	2.47351743	-1.08638350
1	-0.57331283	1.26475565	0.21404327
16	0.98455084	0.82062404	-2.67259533
8	2.43428213	0.57504109	-3.04019934
8	0.21999509	1.86279069	-3.39507832
6	0.11457375	-0.74076593	-2.93060445
6	-1.10452227	-0.73564321	-3.60846999
6	-1.78953055	-1.94189538	-3.77860449
6	-1.27402871	-3.14692037	-3.27950535
6	-0.04259234	-3.11886519	-2.60034085
6	0.65583822	-1.92699975	-2.42583447
1	-1.49868113	0.20170007	-3.99880368
1	1.60882205	-1.92469576	-1.89721171
1	0.37000285	-4.03905316	-2.18456719
6	-2.00784287	-4.44936055	-3.47567103
1	-2.74255662	-1.94415321	-4.31081928
8	0.93177560	-3.20103438	0.81204680
8	1.35069935	-2.73288449	3.32388013
6	-0.79869432	-1.71025583	2.15749636
6	-1.29792224	-1.40988986	3.42643450
6	-2.60330569	-0.92774780	3.54607945
6	-3.41707663	-0.74549664	2.41751340

6	-2.88834143	-1.06174285	1.15378934
6	-1.58806998	-1.54546438	1.01462060
1	-0.67395068	-1.57453030	4.30433556
1	-2.99912541	-0.69625668	4.53662999
6	-4.83629864	-0.25522510	2.55585589
1	-3.50679048	-0.93094723	0.26372534
1	-1.18853438	-1.80174460	0.03292006
1	-3.03926746	-4.28353356	-3.81165079
1	-1.50491937	-5.07064183	-4.23256064
1	-2.03374374	-5.03512058	-2.54628948
1	-5.54219153	-1.10025981	2.54678979
1	-4.98405625	0.28728478	3.49841336
1	-5.11400761	0.40752562	1.72520357
1	1.62393698	-0.65042327	0.61982644

Energy = -8139.841922 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 43

Atomic N.	X	Y	Z
8	0.83023872	-0.07645997	-0.34708330
6	1.22614903	-1.00126017	-1.36587871
1	1.98137105	-1.70886185	-0.98376593
1	1.64888666	-0.49899876	-2.25574869
1	0.34613977	-1.57848258	-1.69203315
50	2.07627681	1.59430992	-0.04749238
7	0.08244356	3.00721545	1.04790618
6	0.78401623	4.29486927	1.24860081
1	0.18485023	4.98487011	1.87074155
1	1.75351485	4.13111400	1.73507265
1	0.96315566	4.76180080	0.27229014
7	1.95649445	1.30856549	2.13069113
6	-0.18858969	2.35230036	2.35321902
1	-0.81480912	3.00955701	2.98845977
1	-0.74787154	1.43060730	2.14943666
6	1.09699102	1.97393440	3.09392453
1	0.81933470	1.30586445	3.92768556
1	1.57848541	2.85999915	3.54244849
16	3.19527210	0.34266492	2.55648910
7	-1.52272799	1.20728826	-1.14456421
6	-1.18592139	3.29247365	0.32306672
1	-1.81623869	3.94671101	0.96067385
1	-0.92720805	3.87360720	-0.57264542
6	-2.05072616	2.09709396	-0.10413489
1	-2.99709008	2.52145320	-0.46732963
1	-2.30242568	1.45405425	0.75148724
16	-1.29833048	1.90745807	-2.66821167
8	0.13680128	2.22302140	-2.88788358
8	-2.31761765	2.97400885	-2.79910685
6	-1.72419834	0.55908580	-3.78881462
6	-3.04550543	0.10586671	-3.84663077
6	-3.37443854	-0.90583372	-4.74429878
6	-2.40324126	-1.47068247	-5.59166510
6	-1.08848302	-0.99166243	-5.51343309
6	-0.74071932	0.02309358	-4.61740849
1	-3.80240858	0.54572422	-3.19803936
1	0.27787637	0.40425812	-4.55786499
1	-0.32162279	-1.41668067	-6.16330815

6	-2.78088730	-2.55310998	-6.57130239
1	-4.40409808	-1.26508021	-4.79273332
8	3.77859920	0.03242643	1.19621651
8	4.08438774	0.88314693	3.60791583
6	2.48262083	-1.18700886	3.21259051
6	2.96804484	-1.71067690	4.41065337
6	2.42372511	-2.90116195	4.89882532
6	1.40386929	-3.56963559	4.20590605
6	0.92933301	-3.00934575	3.00627856
6	1.46025806	-1.82337523	2.50154433
1	3.75809585	-1.18500577	4.94565587
1	2.79840649	-3.31617878	5.83635185
6	0.84070198	-4.87052743	4.72098402
1	0.12919490	-3.51209514	2.45899009
1	1.08672739	-1.38269856	1.57223983
1	-3.36639223	-3.34544209	-6.08373768
1	-3.40271831	-2.14659110	-7.38351854
1	-1.89312980	-3.01055307	-7.02559806
1	1.28792024	-5.72559443	4.19037645
1	1.04622121	-5.00171217	5.79114248
1	-0.24553575	-4.92685478	4.56641678
1	-0.65346878	0.68312612	-0.86004952

Energy = -8139.851360 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 44

Atomic N.	X	Y	Z
8	4.82051393	1.22696097	1.06762153
6	5.71309653	1.53688390	0.00427379
1	5.21008052	2.03408936	-0.84756304
1	6.21463476	0.63785270	-0.39288068
1	6.49060929	2.22069741	0.38450174
50	3.18192214	-0.01913335	0.95567458
7	1.82681646	2.28588998	1.33727477
6	2.42749929	2.90257814	2.53610025
1	2.14518043	3.96871429	2.62473725
1	2.09016006	2.37365378	3.43693413
1	3.51962688	2.81157263	2.46737823
7	-0.11181421	-0.12935166	1.42569377
6	0.35060406	2.28350497	1.43011304
1	0.00484316	3.22523614	1.89895625
1	-0.06118601	2.27426028	0.41037596
6	-0.25399632	1.11008710	2.20280992
1	-1.31087465	1.35476571	2.41654485
1	0.25563467	0.95824770	3.16378927
16	-0.69851579	-1.57918240	2.09959389
7	2.36257198	0.82328826	-0.95407878
6	2.28091192	3.00074815	0.11656595
1	1.83294904	4.01282008	0.06046434
1	3.36930907	3.10743060	0.21373542
6	1.97197954	2.21365848	-1.16314221
1	2.54011596	2.67304340	-1.98901109
1	0.90004494	2.29543064	-1.42709794
16	3.03716193	-0.05023656	-2.15659488
8	3.80743491	-1.08835083	-1.37632344
8	3.72729652	0.76375713	-3.18415678
6	1.70832571	-0.94390242	-3.00137457

6	1.42554814	-0.65642965	-4.33636695
6	0.38550114	-1.33918432	-4.97340465
6	-0.37043237	-2.30599191	-4.29524667
6	-0.06291312	-2.57266794	-2.94888238
6	0.96985600	-1.90103082	-2.29779615
1	2.02492948	0.08484697	-4.86372212
1	1.19977228	-2.12901604	-1.25630617
1	-0.63484373	-3.32367084	-2.40038992
6	-1.46557783	-3.06834385	-4.99871161
1	0.16333828	-1.11916941	-6.01938540
8	-0.46347232	-2.59352099	1.05581753
8	-0.11394618	-1.66272448	3.44856591
6	-2.48602515	-1.38260778	2.28676733
6	-3.01026802	-0.97552050	3.51513065
6	-4.39145190	-0.81160034	3.64188032
6	-5.25404119	-1.05170361	2.56165666
6	-4.69651694	-1.46345967	1.33828879
6	-3.32078644	-1.63226083	1.19293533
1	-2.34225227	-0.81262051	4.36021794
1	-4.80673074	-0.49807345	4.60126846
6	-6.74680644	-0.90685410	2.71479957
1	-5.35299695	-1.66353422	0.48949171
1	-2.89395765	-1.97551470	0.25050074
1	-1.09899293	-4.04819628	-5.34255868
1	-2.31572469	-3.25924624	-4.32963513
1	-1.83115704	-2.52553506	-5.88003210
1	-7.21343498	-1.88506099	2.90934095
1	-7.00261124	-0.24709705	3.55360984
1	-7.20641989	-0.50434865	1.80217196
1	-0.44052203	-0.05487734	0.45907869

Energy = -8139.841328 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 45

Atomic N.	X	Y	Z
8	4.10879748	-1.09385817	0.86477526
6	4.67568944	-1.56697175	2.08188418
1	4.62489048	-2.66568297	2.15678804
1	4.17997495	-1.15317692	2.97969620
1	5.73610964	-1.26764317	2.10708649
50	2.16020258	-1.17180819	0.31227870
7	1.83623125	1.42105507	1.14692605
6	3.15544131	1.80620021	1.69172299
1	3.11612344	2.81748121	2.13893945
1	3.47674337	1.08872040	2.45349691
1	3.90084642	1.78933037	0.88882621
7	1.14059185	-1.06703552	2.28075660
6	0.83600801	1.31958413	2.23864122
1	0.84087825	2.24676540	2.84606079
1	-0.15628349	1.22356860	1.77782187
6	1.05187866	0.10505629	3.14384280
1	0.18653915	0.04408658	3.82701907
1	1.94977953	0.22582387	3.77324090
16	1.21268395	-2.57681830	2.89883824
7	0.54258981	1.22390018	-1.90237125
6	1.42005022	2.45746936	0.16376889
1	1.15492929	3.38282458	0.71520953

1	2.28617329	2.69844915	-0.46525997
6	0.24461581	2.08879562	-0.75520287
1	-0.17243040	3.02595666	-1.14849343
1	-0.56772426	1.60558004	-0.19130882
16	1.28298513	1.91238149	-3.27104486
8	2.13203587	0.84272368	-3.82980194
8	1.82227737	3.24710205	-2.92420508
6	-0.10217032	2.18316304	-4.39555548
6	-0.60722102	3.47151341	-4.56799205
6	-1.67182879	3.66881017	-5.45104322
6	-2.22951078	2.59905085	-6.16581789
6	-1.69263767	1.31313504	-5.97493924
6	-0.63248067	1.09730209	-5.09794961
1	-0.15822318	4.30434014	-4.02818819
1	-0.20796420	0.10280303	-4.96380090
1	-2.10944218	0.46948112	-6.52814801
6	-3.35743715	2.82132153	-7.14154500
1	-2.07067898	4.67502934	-5.59139614
8	1.72183451	-3.34304187	1.69806130
8	1.92339900	-2.68061431	4.19276703
6	-0.48209915	-3.13314710	3.19276362
6	-0.91589236	-3.34699059	4.50063849
6	-2.23287307	-3.76075966	4.72031327
6	-3.11638267	-3.96824583	3.65214056
6	-2.64886026	-3.74601029	2.34375667
6	-1.34149137	-3.32971408	2.10723395
1	-0.22137404	-3.20164943	5.32712723
1	-2.57610253	-3.93065833	5.74240380
6	-4.52754631	-4.44372942	3.89015266
1	-3.32082621	-3.90690382	1.49855092
1	-0.98196523	-3.17016853	1.09063776
1	-3.86432988	3.77724917	-6.95841242
1	-2.98014825	2.83813590	-8.17584124
1	-4.10246053	2.01610432	-7.08275395
1	-4.63126840	-5.50702808	3.62420888
1	-4.81555988	-4.33434808	4.94332383
1	-5.24705892	-3.88603628	3.27457298
1	1.02197207	0.34174656	-1.67520174

Energy = -8139.840710 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 46

Atomic N.	X	Y	Z
8	3.75635724	2.25217635	-1.21236885
6	4.65757925	2.24484106	-2.31759604
1	5.49817819	1.53859055	-2.17876562
1	5.08453416	3.25481542	-2.42237124
1	4.14602690	1.98636596	-3.26022032
50	2.99276411	0.49016377	-0.48504726
7	2.06039295	2.10758723	1.25855652
6	3.14989500	3.00713605	1.70585628
1	2.74076871	3.85261384	2.28725471
1	3.86214324	2.45947669	2.33377620
1	3.68095231	3.37555526	0.82031388
7	2.18094518	-0.85698590	2.77565369
6	1.33649262	1.53519379	2.42934298
1	1.03443056	2.37493358	3.08556531

1	0.41801531	1.06041686	2.06343535
6	2.11872213	0.51664373	3.27465945
1	1.65774121	0.46528795	4.27123125
1	3.15107388	0.85783168	3.44405322
16	1.03824867	-2.00572012	3.25371604
7	0.86732359	0.90694370	-0.98038066
6	1.11499805	2.89354038	0.40770035
1	0.57228094	3.63034277	1.03004503
1	1.73507771	3.42967460	-0.32319132
6	0.12856155	2.00075197	-0.35078932
1	-0.37244258	2.62807881	-1.10552493
1	-0.65206917	1.60256662	0.31991256
16	0.76187365	0.65655779	-2.59550039
8	2.09348151	0.00486760	-2.88720731
8	0.33018120	1.84802255	-3.35960737
6	-0.48388665	-0.62398271	-2.88343973
6	-1.75146867	-0.25532980	-3.33430482
6	-2.71874414	-1.24531397	-3.52867359
6	-2.43485550	-2.59710598	-3.28446452
6	-1.14287981	-2.93930385	-2.84597693
6	-0.16818336	-1.96436962	-2.64276626
1	-1.96407774	0.79119832	-3.55003683
1	0.83669593	-2.23703405	-2.32079647
1	-0.89597187	-3.98743822	-2.66691269
6	-3.48552811	-3.66142681	-3.47778140
1	-3.70928484	-0.96121339	-3.88873492
8	1.44750284	-3.23942028	2.56036070
8	0.94452722	-1.90059409	4.72255843
6	-0.57710548	-1.51722836	2.59955317
6	-1.51197560	-0.92333019	3.44912236
6	-2.75091913	-0.53742727	2.93115231
6	-3.06777822	-0.73921893	1.57955181
6	-2.10730672	-1.34378594	0.74873942
6	-0.86686192	-1.73441064	1.24890383
1	-1.27076102	-0.78612139	4.50262687
1	-3.48681643	-0.07700615	3.59288876
6	-4.41427809	-0.34268923	1.02842000
1	-2.33162386	-1.51081194	-0.30640643
1	-0.13373343	-2.21345801	0.60041539
1	-4.33946068	-3.28293196	-4.05362486
1	-3.07602960	-4.53637808	-4.00120138
1	-3.86672330	-4.01668307	-2.50779151
1	-5.04374650	-1.22978096	0.85909881
1	-4.95178232	0.32035458	1.71803587
1	-4.31378386	0.16926023	0.06126064
1	2.49231282	-0.99528878	1.80772181

Energy = -8139.844004 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 47

Atomic N.	X	Y	Z
8	4.14649169	-1.01222341	0.88098883
6	4.71244581	-1.48480691	2.09877117
1	4.20474956	-1.08392647	2.99579304
1	5.76804170	-1.16978473	2.13278230
1	4.67773328	-2.58458484	2.16684252
50	2.20584192	-1.13632845	0.30890798

7	1.79979445	1.43998732	1.16476402
6	3.10285621	1.85697789	1.72463176
1	3.03010482	2.86055381	2.18490579
1	3.44008112	1.13911052	2.47912517
1	3.85411292	1.87344662	0.92720620
7	1.16908847	-1.07765511	2.26978675
6	0.79402920	1.29910986	2.24694344
1	0.76690243	2.22032311	2.86285539
1	-0.19127291	1.17844877	1.77705774
6	1.03803948	0.08295168	3.14275236
1	0.16908649	-0.01043143	3.81762848
1	1.92651036	0.22433951	3.78119869
16	1.27001741	-2.59197939	2.87164659
7	0.52961606	1.23353515	-1.89292688
6	1.36250185	2.47389370	0.18823337
1	1.06908254	3.38681673	0.74614304
1	2.22578208	2.74353991	-0.43299608
6	0.20306319	2.08265620	-0.74157013
1	-0.23435843	3.01223039	-1.13115791
1	-0.60133312	1.57627261	-0.18671692
16	1.25710785	1.95299962	-3.25250568
8	2.10898108	0.89890383	-3.83577049
8	1.79210956	3.28464974	-2.88726582
6	-0.13927478	2.23551082	-4.36016485
6	-0.64209140	3.52625419	-4.51911950
6	-1.71465620	3.73250145	-5.39083883
6	-2.28232019	2.66924980	-6.10698843
6	-1.74729984	1.38030596	-5.92988364
6	-0.67969050	1.15569008	-5.06463331
1	-0.18537467	4.35399476	-3.97796733
1	-0.25682297	0.15911526	-4.94106167
1	-2.17178442	0.54155532	-6.48472990
6	-3.42097358	2.89949612	-7.06830241
1	-2.11170901	4.74079615	-5.52090620
8	1.80805700	-3.33192091	1.66698678
8	1.97051768	-2.69550168	4.17108330
6	-0.41420771	-3.19057527	3.14193298
6	-0.85285881	-3.43904666	4.44209643
6	-2.16147147	-3.88699756	4.64345638
6	-3.03171156	-4.09497671	3.56443513
6	-2.55980785	-3.83679730	2.26432257
6	-1.26059891	-3.38613741	2.04612614
1	-0.16830540	-3.29257663	5.27666251
1	-2.50858235	-4.08355524	5.65944840
6	-4.43256359	-4.60882935	3.78261765
1	-3.22157053	-3.99682375	1.41097889
1	-0.89756657	-3.19832493	1.03564247
1	-3.88958397	3.87878666	-6.90875326
1	-3.06526271	2.86542224	-8.10965948
1	-4.19334990	2.12460751	-6.96631474
1	-4.50140625	-5.67655403	3.52280303
1	-4.74075997	-4.50149813	4.83032687
1	-5.15745482	-4.07618643	3.15158911
1	1.03327816	0.36398944	-1.66923983

Energy = -8139.840701 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 48

Atomic N.	X	Y	Z
8	4.35180871	-0.17114650	-0.55443033
6	4.73347879	-0.72943657	-1.80493979
1	3.91799932	-1.28030877	-2.30783814
1	5.57649676	-1.42563629	-1.64991696
1	5.06962917	0.06080722	-2.49741203
50	2.49277301	0.36679161	0.07895460
7	2.18217208	-2.21335449	1.10700004
6	3.41775713	-2.92374913	0.71969166
1	3.36912765	-3.99204078	1.00678531
1	3.57375562	-2.85151497	-0.36077478
1	4.27927721	-2.45084812	1.20544263
7	1.25800173	-0.94368616	-1.23326717
6	1.02174830	-2.74500172	0.35259130
1	0.95916643	-3.84621379	0.46960995
1	0.11185005	-2.30580571	0.78292522
6	1.06034044	-2.38421141	-1.13317178
1	0.09575230	-2.69427214	-1.57245028
1	1.84665645	-2.94808680	-1.66347075
16	1.04761743	-0.16513093	-2.65018522
7	1.41167721	-0.14946659	3.41444786
6	1.97991498	-2.40704962	2.56344113
1	1.71381537	-3.46638395	2.75660526
1	2.95215480	-2.23992261	3.05295849
6	0.92831347	-1.53164625	3.24800496
1	0.68145800	-1.99682844	4.21618616
1	-0.00314559	-1.49952975	2.66571019
16	0.41843696	0.89354764	4.35708224
8	1.37183335	1.83093174	4.98335028
8	-0.53176809	0.09683460	5.16342812
6	-0.53523873	1.77779529	3.11185207
6	-1.90740753	1.55264293	3.01261430
6	-2.64566175	2.28507204	2.07832371
6	-2.02964427	3.23364102	1.24921080
6	-0.64188109	3.43202048	1.37108020
6	0.10944952	2.71379103	2.29683313
1	-2.38446798	0.82809542	3.67149253
1	1.18156862	2.87793159	2.39384568
1	-0.14373764	4.15975635	0.72834553
6	-2.82759955	4.03967056	0.25590209
1	-3.72202658	2.12125694	2.00182895
8	1.62084083	1.19100921	-2.32676989
8	1.54149639	-0.89722026	-3.83912763
6	-0.73749161	0.03735152	-2.88500444
6	-1.32387617	-0.38792193	-4.07647637
6	-2.70190564	-0.23236482	-4.25061372
6	-3.49968154	0.33988220	-3.25011584
6	-2.88070154	0.75351178	-2.05646001
6	-1.50811112	0.60870583	-1.86770575
1	-0.69954188	-0.83473371	-4.84924051
1	-3.16408712	-0.56526727	-5.18176404
6	-4.98266466	0.52783447	-3.45009321
1	-3.48614296	1.19256122	-1.26088018
1	-1.03850183	0.93106462	-0.93751442
1	-2.80123301	5.11022862	0.50799326
1	-2.41431162	3.93965642	-0.75817203
1	-3.87857165	3.72475060	0.23326212

1	-5.21368699	1.57568627	-3.69737168
1	-5.35924993	-0.09653266	-4.27019215
1	-5.54449131	0.27929990	-2.53908499
1	2.33046132	-0.10681699	3.86764434

Energy = -8139.838891 Hartree
Number of imaginary frequencies = 0.

Compound 11a isomer 49

Atomic N.	X	Y	Z
8	3.99586451	-1.57804390	0.62500417
6	5.37359996	-1.22118854	0.68325959
1	5.97445428	-2.14500375	0.68270012
1	5.61077498	-0.65646158	1.60159374
1	5.69644297	-0.61362925	-0.18387477
50	2.56889293	-0.15579361	0.20743897
7	1.13555088	-2.25243266	0.15174231
6	1.72492646	-3.28348893	-0.73043431
1	1.16765289	-4.23520784	-0.66058662
1	1.72764537	-2.93824738	-1.77039444
1	2.76359057	-3.43670086	-0.41518823
7	0.21249355	-0.77620738	-2.30950582
6	-0.28304883	-1.95834760	-0.17248659
1	-0.92703600	-2.77743447	0.20407647
1	-0.56689401	-1.04815208	0.37750921
6	-0.62117443	-1.79114273	-1.65610558
1	-1.70068763	-1.55941085	-1.71382491
1	-0.45846354	-2.73236659	-2.19616993
16	0.21402984	-0.72307863	-4.01464949
7	1.47824169	-0.35398898	2.16124450
6	1.25008865	-2.70131537	1.57105519
1	0.63993708	-3.61170065	1.72732092
1	2.30964881	-2.94321829	1.72836702
6	0.84161969	-1.60814219	2.56151835
1	1.17617805	-1.92445761	3.56250475
1	-0.25635614	-1.49536883	2.59984613
16	2.37581685	0.48232168	3.24593163
8	3.34345406	1.21799766	2.35479238
8	2.88078418	-0.34343640	4.36704513
6	1.30993417	1.74934009	3.97980922
6	0.91160137	1.62390315	5.30967727
6	0.07380163	2.59636852	5.86404807
6	-0.36626361	3.69158740	5.10865679
6	0.05921420	3.79561514	3.77150527
6	0.89108670	2.83430219	3.20335049
1	1.27229896	0.78311779	5.90109557
1	1.23241907	2.92839239	2.17237465
1	-0.26088714	4.64956416	3.17097588
6	-1.26810392	4.74179866	5.70801378
1	-0.23510741	2.50444045	6.90698097
8	1.09619921	0.40563202	-4.35184700
8	0.47883105	-2.10753418	-4.44897684
6	-1.46170154	-0.29529809	-4.53495211
6	-2.37184959	-1.30890615	-4.83912427
6	-3.66913123	-0.96181767	-5.22450456
6	-4.06692610	0.38032286	-5.31086587
6	-3.12419957	1.37922311	-5.00746399
6	-1.82630686	1.05269651	-4.62088311

1	-2.05560560	-2.35071853	-4.79969783
1	-4.38209798	-1.74997807	-5.47241575
6	-5.46825306	0.75258020	-5.72421088
1	-3.40979513	2.42976102	-5.08757258
1	-1.08894041	1.82818303	-4.41383182
1	-1.46217213	4.54444298	6.76975907
1	-0.82158015	5.74334481	5.62301167
1	-2.23672025	4.77696339	5.18705891
1	-5.45835013	1.45114636	-6.57318049
1	-6.04934634	-0.13129787	-6.01482104
1	-6.00106895	1.25369698	-4.90215776
1	0.11099306	0.17277497	-1.93954160

Energy = -8139.843575 Hartree
Number of imaginary frequencies = 0.

Compound 11a isomer 50

Atomic N.	X	Y	Z
8	4.36166768	0.18840760	-0.53450347
6	4.78805016	-0.25076447	-1.81755986
1	5.66127148	-0.91717464	-1.70302202
1	5.09625283	0.60738988	-2.43851048
1	4.00732158	-0.79679120	-2.37751010
50	2.46745329	0.54375617	0.12226328
7	2.33814286	-2.12576252	0.94419549
6	3.61956270	-2.71590711	0.50710547
1	3.64621451	-3.80409844	0.71013378
1	3.76782793	-2.54926106	-0.56394037
1	4.44689383	-2.22324922	1.03115282
7	1.33045499	-0.74445215	-1.29636085
6	1.21644246	-2.67474296	0.14515638
1	1.22849576	-3.78343009	0.17639467
1	0.27889592	-2.33257456	0.60337653
6	1.23044080	-2.19846003	-1.30822279
1	0.28879916	-2.53783422	-1.77482132
1	2.05279029	-2.66562142	-1.87647272
16	1.07083540	0.12489428	-2.65090120
7	1.42245531	-0.30769904	3.39544997
6	2.15230593	-2.44768246	2.37993461
1	1.96226624	-3.53513779	2.48810069
1	3.11107612	-2.25108851	2.88489381
6	1.04246869	-1.70592633	3.12736201
1	0.83665993	-2.25866821	4.05844360
1	0.10773973	-1.70073523	2.54937870
16	0.36198326	0.58461115	4.41608478
8	1.24655931	1.54727666	5.10202122
8	-0.51444231	-0.33929814	5.16850912
6	-0.67078235	1.47833844	3.24265908
6	-2.02166962	1.15251188	3.13162929
6	-2.82450660	1.89137248	2.25763351
6	-2.29367271	2.94578454	1.50056473
6	-0.92468051	3.24387427	1.63124386
6	-0.10995903	2.52056800	2.49758407
1	-2.43370310	0.34541139	3.73619402
1	0.94677585	2.76166925	2.60251120
1	-0.49175157	4.05487759	1.04327597
6	-3.16370012	3.76118338	0.57792695
1	-3.88513296	1.64827515	2.17272363

8	1.54601172	1.48852644	-2.21856321
8	1.61972394	-0.47566352	-3.88849792
6	-0.72312366	0.21874864	-2.88644856
6	-1.27174052	-0.14757869	-4.11466914
6	-2.65661872	-0.07538020	-4.29053597
6	-3.49792582	0.35514282	-3.25563992
6	-2.91580113	0.71322717	-2.02578184
6	-1.53750748	0.65019926	-1.83455746
1	-0.61346454	-0.48427299	-4.91459629
1	-3.08926056	-0.36167213	-5.25087625
6	-4.99025364	0.44884096	-3.45271767
1	-3.55475567	1.04357009	-1.20428350
1	-1.09654696	0.92862727	-0.87652997
1	-3.23785038	4.80162694	0.92803082
1	-2.74323923	3.79478457	-0.43745519
1	-4.18080904	3.35364067	0.51828636
1	-5.31137097	1.49977235	-3.51910537
1	-5.30521012	-0.05509786	-4.37505827
1	-5.53397030	-0.00153148	-2.61025120
1	2.33960994	-0.22935257	3.84717250

Energy = -8139.838873 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 51

Atomic N.	X	Y	Z
8	5.03193017	-0.02384307	0.71222421
6	6.26784078	0.59727405	0.38283286
1	6.65601908	1.17151945	1.24178405
1	6.19337676	1.29499867	-0.47581787
1	7.01649134	-0.17018674	0.11879829
50	3.26607995	0.75531693	-0.04878972
7	2.67666781	-1.81873288	-0.11547274
6	3.70558338	-2.47613367	-0.94467700
1	3.68184933	-3.57412225	-0.81571132
1	3.54060379	-2.24089151	-2.00408816
1	4.68857835	-2.08965603	-0.64794637
7	0.40877535	-0.11229406	-1.33110645
6	1.31903163	-2.24592273	-0.52519327
1	1.32719979	-3.32708998	-0.76204430
1	0.64506480	-2.11870086	0.33388093
6	0.72350079	-1.49565913	-1.71621946
1	-0.17064841	-2.05413497	-2.04957938
1	1.42422116	-1.45434081	-2.56091535
16	-0.32018643	0.90020612	-2.49209714
7	2.09760268	0.12284064	1.73031215
6	2.91206471	-2.12742646	1.32366300
1	2.72113785	-3.19843171	1.53035157
1	3.97149805	-1.90752910	1.51248273
6	2.05551515	-1.24632260	2.23949709
1	2.47285064	-1.30905706	3.25722036
1	1.01571445	-1.62255595	2.29485660
16	2.05287831	1.38346611	2.78002535
8	2.72012514	2.47892279	1.99859298
8	2.52641209	1.03482589	4.13867453
6	0.31257767	1.86486930	2.94002414
6	-0.36409618	1.61770214	4.13365725
6	-1.71246059	1.97324885	4.23862083

6	-2.38946287	2.57519104	3.16910520
6	-1.68002533	2.81346692	1.97754461
6	-0.33660172	2.46476501	1.85529321
1	0.16961015	1.16649589	4.96953690
1	0.20282511	2.67061311	0.93007840
1	-2.18236588	3.29082223	1.13354762
6	-3.83520470	2.98740989	3.29536000
1	-2.24402311	1.78505209	5.17347504
8	-0.55685165	2.16958252	-1.78203081
8	0.51906877	0.79818752	-3.69814960
6	-1.92910546	0.17108073	-2.87647182
6	-2.06907870	-0.63723287	-4.00593903
6	-3.31488413	-1.20528816	-4.28269981
6	-4.41984326	-0.97491828	-3.44969650
6	-4.24789203	-0.15442615	-2.32052764
6	-3.01311341	0.42139820	-2.02866377
1	-1.21609540	-0.79682628	-4.66467320
1	-3.43112553	-1.83383331	-5.16731328
6	-5.76990417	-1.56372559	-3.77111954
1	-5.09861043	0.04255767	-1.66557290
1	-2.88928184	1.07571591	-1.16546817
1	-4.29396008	2.57051519	4.20092820
1	-3.92654281	4.08315461	3.34742124
1	-4.42361740	2.65811537	2.42699158
1	-6.41642711	-0.81295827	-4.25137738
1	-5.68367802	-2.41455096	-4.45867492
1	-6.28659188	-1.90128299	-2.86246202
1	-0.10101651	-0.03124045	-0.44628200

Energy = -8139.842014 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 52

Atomic N.	X	Y	Z
8	2.40742892	0.62331720	0.03105738
6	3.54473928	1.02635052	0.79900171
1	3.68222795	2.11790106	0.71848271
1	4.48632887	0.55066969	0.46149082
1	3.40316856	0.76214751	1.85909787
50	2.69425670	-0.67620366	-1.54305072
7	1.06193978	-2.96893215	-1.39126327
6	1.26222747	-3.49181919	-2.75308834
1	0.52713088	-4.28177775	-3.00105518
1	1.17649798	-2.68556739	-3.49162624
1	2.27189296	-3.91631772	-2.83098811
7	0.59766213	-0.32849509	-2.15384727
6	-0.28323442	-2.38819920	-1.21743602
1	-1.07552454	-3.15494116	-1.34475032
1	-0.34447687	-1.99664791	-0.19387266
6	-0.54531246	-1.23664517	-2.19167880
1	-1.47275290	-0.73448292	-1.86307856
1	-0.72780294	-1.61312265	-3.21165602
16	0.69303774	0.89512666	-3.23339595
7	1.87783111	-2.58801492	1.49345777
6	1.34239769	-4.05867262	-0.43348139
1	0.72611757	-4.94905778	-0.67977622
1	2.39377191	-4.35353721	-0.58307223
6	1.10629065	-3.75799722	1.04516598

1	1.35351446	-4.66919810	1.61519409
1	0.04356022	-3.54921549	1.23282503
16	1.64305343	-2.15866042	3.14452047
8	2.79574955	-1.29397346	3.46479255
8	1.35493497	-3.35550774	3.96716280
6	0.12821690	-1.18756948	3.04838764
6	-0.92355670	-1.51207435	3.90656330
6	-2.08210574	-0.73336405	3.87633351
6	-2.19934356	0.35550426	2.99925692
6	-1.12355442	0.64710865	2.14171443
6	0.04733684	-0.11067332	2.15938353
1	-0.82844556	-2.36382104	4.57902187
1	0.87231807	0.12317776	1.47680868
1	-1.20355889	1.48019560	1.44013134
6	-3.44250400	1.20886759	2.98728788
1	-2.91014492	-0.98032491	4.54303910
8	2.16792258	1.22856120	-3.15769604
8	0.08773016	0.59075600	-4.54951113
6	-0.19543122	2.31332317	-2.55054999
6	-1.22189685	2.90232741	-3.28750372
6	-1.89406413	4.00321894	-2.74942204
6	-1.54912031	4.51864185	-1.49190236
6	-0.51293029	3.89558866	-0.77195281
6	0.16878292	2.79566612	-1.28905857
1	-1.48010843	2.50151098	-4.26699635
1	-2.69857135	4.47049946	-3.32031529
6	-2.25197774	5.72942974	-0.93087459
1	-0.23427457	4.28271301	0.21055230
1	0.96998818	2.30511465	-0.72804764
1	-4.30171979	0.67482561	3.41294531
1	-3.29130336	2.12195731	3.58395946
1	-3.69875510	1.52738184	1.96785046
1	-1.64324479	6.63534350	-1.07679416
1	-3.21822229	5.89756969	-1.42355202
1	-2.42513616	5.62859739	0.14940139
1	2.89101790	-2.71857894	1.39640771

Energy = -8139.843081 Hartree

Number of imaginary frequencies = 0.

Compound I1a isomer 53

Atomic N.	X	Y	Z
8	4.53881983	-2.25019664	0.30898306
6	4.96587854	-2.80672830	1.54638935
1	4.12852022	-3.21121658	2.14728085
1	5.49083302	-2.06749671	2.17525248
1	5.66456904	-3.63453190	1.33839366
50	3.23818422	-0.66939831	0.06799674
7	1.63054051	-2.58954264	-0.95170692
6	2.44278197	-3.28180810	-1.97121097
1	1.99224208	-4.25197188	-2.25413464
1	2.52496308	-2.65720874	-2.87023542
1	3.45062712	-3.44326136	-1.56631048
7	0.34726433	0.20568237	-1.35451044
6	0.29534407	-2.24664526	-1.48757352
1	-0.06601995	-3.06491529	-2.14029413
1	-0.41107871	-2.18491671	-0.64689335
6	0.22375013	-0.93559213	-2.27244887

1	-0.73077359	-0.92633090	-2.83038605
1	1.04008975	-0.86197219	-3.00356728
16	0.32383754	1.77837313	-2.00810651
7	1.70747682	-1.37980159	1.54280204
6	1.51450280	-3.43438210	0.26485666
1	0.87247638	-4.31727340	0.07406695
1	2.53000478	-3.78591103	0.48970185
6	0.98548447	-2.64543924	1.46901905
1	1.14826193	-3.25639629	2.37244572
1	-0.10616708	-2.48225182	1.38467123
16	2.13506967	-0.73561453	2.97980383
8	3.31196008	0.12329707	2.58264294
8	2.27972206	-1.72715252	4.07099539
6	0.82710592	0.41056668	3.48340544
6	0.09748372	0.15577590	4.64420912
6	-0.92037539	1.03896407	5.01511019
6	-1.21416829	2.17265496	4.24409819
6	-0.46310603	2.40136361	3.07707980
6	0.55462470	1.53108900	2.69183465
1	0.33867222	-0.71844005	5.24788016
1	1.13239723	1.73115883	1.78867166
1	-0.67091955	3.27856950	2.46126962
6	-2.28625526	3.14438323	4.67043192
1	-1.49155644	0.84447908	5.92492473
8	0.38788898	2.66618949	-0.83261709
8	1.33524758	1.78706805	-3.07826096
6	-1.29576343	1.99938971	-2.78060968
6	-1.44369987	1.77067422	-4.14993487
6	-2.70365868	1.92935797	-4.73141007
6	-3.81401172	2.31592802	-3.96587338
6	-3.63282528	2.54186450	-2.58987518
6	-2.38332626	2.38841992	-1.99213850
1	-0.57624962	1.49444146	-4.74843957
1	-2.82374862	1.75657137	-5.80233095
6	-5.16389365	2.51933382	-4.60552560
1	-4.48345249	2.85202843	-1.98019035
1	-2.24063379	2.58869556	-0.93021404
1	-3.00875212	2.67361285	5.34970418
1	-1.84488994	4.00277933	5.20062245
1	-2.83165082	3.54579509	3.80541677
1	-5.34273078	3.58777761	-4.80264927
1	-5.23843900	1.98984758	-5.56379623
1	-5.97452713	2.17099502	-3.95133547
1	-0.29395130	0.16926878	-0.55738087

Energy = -8139.841298 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 54

Atomic N.	X	Y	Z
8	2.35431390	0.78591776	0.02392919
6	3.47852949	1.22282107	0.79260922
1	3.38120280	0.88672287	1.83723420
1	3.53721721	2.32425059	0.77595093
1	4.44280705	0.83638505	0.40846374
50	2.69328095	-0.39413867	-1.63185152
7	1.22112035	-2.79901047	-1.59525782
6	1.42307617	-3.22188576	-2.99111962

1	0.73630354	-4.04295474	-3.27413919
1	1.26646466	-2.37915476	-3.67528695
1	2.45653252	-3.57141168	-3.11554524
7	0.56462648	-0.15422944	-2.18132792
6	-0.15500796	-2.32237890	-1.35858075
1	-0.89752320	-3.13171229	-1.51823425
1	-0.21748700	-1.99948690	-0.31139147
6	-0.51617133	-1.13368193	-2.25327951
1	-1.46679817	-0.71645553	-1.87577453
1	-0.69744344	-1.45865010	-3.29103098
16	0.55492051	1.13426502	-3.18698764
7	2.08365205	-2.54205797	1.28920530
6	1.59571804	-3.92437218	-0.71407982
1	1.03255389	-4.83698344	-1.00265118
1	2.65989712	-4.13914594	-0.90415669
6	1.37830701	-3.73101527	0.78519042
1	1.69861153	-4.65694286	1.29156623
1	0.30941833	-3.60501989	1.00842655
16	1.86658903	-2.23313165	2.96950125
8	2.96800582	-1.31379954	3.31690902
8	1.68164450	-3.49574652	3.72040395
6	0.28868948	-1.36309077	2.97144699
6	-0.71472746	-1.81033242	3.83254427
6	-1.92248190	-1.11159576	3.87953826
6	-2.13613422	0.01884094	3.07609974
6	-1.10685544	0.43466667	2.21298441
6	0.11174388	-0.24171345	2.15455154
1	-0.54450975	-2.69347308	4.44720580
1	0.89979566	0.08912793	1.46851686
1	-1.26157435	1.30200369	1.56769492
6	-3.43239757	0.78567900	3.14996517
1	-2.71329764	-1.45462146	4.54894396
8	2.00558213	1.56221019	-3.11689442
8	-0.05526504	0.86677689	-4.50886162
6	-0.41220784	2.44562789	-2.40511543
6	-1.49005692	3.00686274	-3.08841315
6	-2.22352735	4.02514648	-2.47332267
6	-1.88928202	4.48590043	-1.19190225
6	-0.79979366	3.89240579	-0.52782597
6	-0.05620291	2.87468400	-1.12221182
1	-1.74024852	2.64904494	-4.08646603
1	-3.06856122	4.47026306	-3.00180716
6	-2.66027558	5.61016722	-0.54664361
1	-0.52850391	4.23754579	0.47223033
1	0.78688361	2.40664467	-0.60506537
1	-4.25044281	0.15859515	3.52732333
1	-3.33486340	1.64599704	3.83046201
1	-3.71957688	1.18124011	2.16653976
1	-2.11833718	6.56316137	-0.64990330
1	-3.64675978	5.73909651	-1.01019088
1	-2.80140291	5.43492777	0.52876221
1	3.10022970	-2.59878526	1.16111918

Energy = -8139.843075 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 55

Atomic N. X Y Z

8	4.75702851	-1.59974215	0.55814553
6	5.18327232	-2.12378759	1.80978844
1	4.38260980	-2.67557380	2.33923757
1	5.53996697	-1.33320173	2.49182455
1	6.01751558	-2.82358576	1.63320332
50	3.25650085	-0.21601904	0.25839530
7	2.03150191	-2.30448878	-0.90897183
6	3.00276976	-2.83373099	-1.88685967
1	2.71905596	-3.84747520	-2.22697718
1	3.05169362	-2.17060203	-2.76038191
1	3.99389903	-2.86232003	-1.41515944
7	0.38576054	0.28865290	-1.31729645
6	0.69884073	-2.13765303	-1.52949793
1	0.50745163	-2.97184836	-2.23187362
1	-0.06367113	-2.21355677	-0.74064722
6	0.48824066	-0.81939993	-2.27678775
1	-0.41866207	-0.92338197	-2.90054911
1	1.33177940	-0.60038127	-2.94532432
16	0.21613969	1.87376785	-1.91736930
7	1.76317028	-1.18837845	1.61632037
6	1.95994752	-3.20249950	0.27324101
1	1.46744608	-4.16027413	0.01264634
1	2.99890084	-3.41221674	0.55941142
6	1.24291589	-2.54234953	1.45743994
1	1.43421399	-3.15577564	2.35356564
1	0.14703714	-2.53630498	1.30077848
16	2.01110609	-0.55215101	3.09918920
8	3.06267212	0.49050845	2.80823531
8	2.24461289	-1.56057065	4.15933882
6	0.51491467	0.35587114	3.56359457
6	-0.23803332	-0.07282560	4.65626963
6	-1.40293395	0.62175805	4.99421675
6	-1.82067546	1.73933595	4.25773976
6	-1.04137464	2.14678748	3.15997783
6	0.12198740	1.46537551	2.80789984
1	0.09786695	-0.93309361	5.23413349
1	0.71775714	1.80159727	1.95844997
1	-1.34424481	3.01630871	2.57331811
6	-3.05716701	2.50915474	4.65005925
1	-1.99344975	0.29051801	5.85062141
8	0.07252291	2.70911370	-0.71098696
8	1.30194081	2.05382833	-2.89563007
6	-1.34981292	1.93034557	-2.81898558
6	-1.35445600	1.75465994	-4.20396582
6	-2.57196028	1.78963935	-4.88749803
6	-3.78110950	2.00100412	-4.20811592
6	-3.74380967	2.17699310	-2.81350739
6	-2.53865432	2.14523400	-2.11451862
1	-0.41288165	1.61558662	-4.73411069
1	-2.58067094	1.65837085	-5.97093282
6	-5.08826153	2.07361555	-4.95564894
1	-4.67379398	2.35168287	-2.26935844
1	-2.51033602	2.30836988	-1.03715078
1	-3.73590197	1.89695657	5.25798614
1	-2.79085651	3.39710029	5.24449235
1	-3.60575778	2.86508346	3.76728835
1	-5.38486766	3.12163132	-5.11718719
1	-5.01521836	1.59540429	-5.94059355

1 -5.89922705 1.59111169 -4.39350824
 1 -0.30525145 0.13782077 -0.57741396
 Energy = -8139.841364 Hartree
 Number of imaginary frequencies = 0.

Compound 11a isomer 56

Atomic N.	X	Y	Z
8	3.86178352	1.05639803	3.13234457
6	4.62829050	2.23615810	2.92194944
1	4.02507697	3.07430656	2.52250762
1	5.46210332	2.07061267	2.21858477
1	5.05518326	2.55599924	3.88740981
50	2.85924204	-0.01595066	1.68480309
7	0.68372242	0.86648349	3.02207165
6	0.91871800	0.50904794	4.43465027
1	0.23498150	1.05954298	5.10819224
1	0.76145341	-0.56789067	4.57819872
1	1.96069525	0.74569442	4.68773212
7	-0.15011353	-1.15592239	0.82573796
6	-0.67449127	0.46347692	2.59699056
1	-1.38981247	0.63040572	3.42552101
1	-0.99132113	1.12248012	1.77543083
6	-0.80890179	-0.98647811	2.12860951
1	-1.88647120	-1.23141669	2.09110713
1	-0.33187947	-1.68061599	2.83362365
16	-0.16204756	-2.69850217	0.10455948
7	1.89718596	1.74877335	0.69068884
6	0.89316754	2.32413874	2.82501076
1	0.08683804	2.90940792	3.31006963
1	1.84307488	2.56455341	3.32029411
6	0.99960981	2.69756131	1.34124292
1	1.38670177	3.72814205	1.27814417
1	0.00129284	2.70031717	0.86289281
16	2.94149747	2.23478652	-0.46557742
8	4.00816914	1.16991097	-0.37028598
8	3.31767244	3.66528565	-0.38231797
6	2.13921798	1.99672699	-2.07105983
6	1.87208642	3.10238519	-2.87784545
6	1.23807194	2.90881716	-4.10836477
6	0.87270807	1.62666864	-4.54267128
6	1.15277832	0.53139029	-3.70584237
6	1.78360475	0.70591627	-2.47573958
1	2.17030765	4.09513395	-2.54266106
1	2.00083894	-0.15736413	-1.84558048
1	0.88071793	-0.47729287	-4.02276556
6	0.22487277	1.41894171	-5.88898055
1	1.03005657	3.77158899	-4.74411884
8	0.50344638	-2.50184563	-1.19642809
8	0.33772730	-3.62937599	1.13023875
6	-1.89242913	-3.11209131	-0.21685351
6	-2.59476478	-3.89874100	0.69722556
6	-3.93534635	-4.19981657	0.44306905
6	-4.58013195	-3.72863768	-0.70973998
6	-3.84451583	-2.94161040	-1.61436907
6	-2.50726395	-2.63123201	-1.37795582
1	-2.08669339	-4.28501949	1.58018785
1	-4.48749701	-4.81980841	1.15141135

6	-6.02021342	-4.07386188	-0.99258432
1	-4.32632044	-2.57588356	-2.52308515
1	-1.93256338	-2.04324599	-2.09364662
1	0.97302701	1.11688060	-6.63849142
1	-0.53285929	0.62436506	-5.85194263
1	-0.25245624	2.33852978	-6.25167594
1	-6.09548481	-4.77003218	-1.84168611
1	-6.49705905	-4.54870086	-0.12619981
1	-6.59997914	-3.17867442	-1.25848514
1	-0.42530553	-0.46081684	0.12645452

Energy = -8139.841307 Hartree
Number of imaginary frequencies = 0.

Compound 11a isomer 57

Atomic N.	X	Y	Z
8	4.03431106	2.16114076	0.24576016
6	4.19253158	1.87777586	-1.14045611
1	3.27911685	2.10505987	-1.71336462
1	4.44468109	0.81973583	-1.30519872
1	5.01242522	2.50648006	-1.52441061
50	2.61224299	1.91665133	1.63529268
7	-0.12230000	0.94907496	3.37287418
6	0.28920956	1.55290200	4.63803928
1	-0.31993693	1.19902749	5.49690103
1	1.34227690	1.31674482	4.84271129
1	0.20204075	2.64621456	4.57275617
7	1.65872279	-0.19614433	1.41137734
6	0.14504538	-0.49788765	3.34051935
1	0.04634054	-0.95154301	4.34783968
1	-0.59471861	-0.99319610	2.69667650
6	1.53801727	-0.78926770	2.76817460
1	1.70167443	-1.87745801	2.74876375
1	2.31499148	-0.38268797	3.44081892
16	2.21105166	-1.24317703	0.23474554
7	-0.86648556	1.04074017	0.57041662
6	-1.48913055	1.33269217	3.02097177
1	-2.24569945	0.92644368	3.73110277
1	-1.54246135	2.42920298	3.08572694
6	-1.90610592	0.90102198	1.60174956
1	-2.79334292	1.47625476	1.30658316
1	-2.19768046	-0.15966766	1.58259426
16	-0.52282497	2.55679363	-0.03298801
8	0.97837219	2.72004419	0.05328410
8	-1.40397286	3.57403281	0.57161041
6	-0.86690141	2.46977893	-1.79408990
6	-1.89116097	3.25609504	-2.31903383
6	-2.14964589	3.19169307	-3.69045044
6	-1.39896901	2.35739770	-4.53099225
6	-0.37427337	1.57720589	-3.96428611
6	-0.09591286	1.62541342	-2.60060918
1	-2.46551460	3.90940369	-1.66360956
1	0.70206043	1.01641128	-2.17099386
1	0.22031385	0.92198080	-4.60336866
6	-1.66355499	2.30902682	-6.01439349
1	-2.94765340	3.80473888	-4.11257757
8	2.10153149	-0.48816563	-1.03909838
8	3.50113656	-1.87666129	0.59901578

6	0.98793720	-2.58851109	0.17601693
6	1.33241849	-3.84843175	0.66758165
6	0.39943403	-4.88657301	0.60217098
6	-0.87144594	-4.68608934	0.04391195
6	-1.18934773	-3.40857511	-0.44970834
6	-0.27053606	-2.36144200	-0.38988433
1	2.32873721	-4.00587092	1.07999056
1	0.66787966	-5.87242293	0.98666273
6	-1.86203850	-5.81889251	-0.05782862
1	-2.17113462	-3.23437765	-0.89476467
1	-0.52308280	-1.37778202	-0.78626151
1	-2.62108462	2.78088857	-6.26817525
1	-0.87219102	2.83739132	-6.56796626
1	-1.67726342	1.27410085	-6.38341784
1	-1.82291021	-6.28242833	-1.05597989
1	-1.64963682	-6.60500280	0.67821467
1	-2.89132558	-5.46757314	0.09606693
1	0.03574272	0.56026882	0.82698576

Energy = -8139.827964 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 58

Atomic N.	X	Y	Z
8	3.09658835	3.20032980	1.62412660
6	2.62318307	4.49912591	1.27468657
1	3.01609306	5.21616915	2.01377331
1	1.51981417	4.56568190	1.28287915
1	2.96680630	4.81159655	0.27517782
50	2.78342772	1.46702549	0.59072097
7	1.46535158	0.75857624	2.76774706
6	2.26210447	1.19968784	3.93403584
1	1.65425463	1.17827424	4.85704941
1	3.13117369	0.54604040	4.07102814
1	2.62535049	2.21732549	3.74288747
7	2.58484054	-2.07853521	1.50657758
6	1.01753885	-0.65016431	2.93412574
1	0.52219939	-0.74292228	3.92173724
1	0.26012983	-0.86117849	2.16889121
6	2.12128218	-1.71529638	2.84601838
1	1.75304191	-2.63987005	3.31276270
1	3.00078605	-1.41700814	3.43620924
16	1.90878470	-3.39176850	0.68780952
7	0.59285373	1.59277287	0.22148705
6	0.28503308	1.65861355	2.63265038
1	-0.43299299	1.47249907	3.45510939
1	0.66519350	2.68428361	2.73258856
6	-0.41567034	1.52706905	1.27669430
1	-1.13629239	2.35703833	1.19229896
1	-0.98657202	0.58467458	1.21212507
16	0.43279480	2.60339867	-1.05192689
8	1.87855083	2.77215476	-1.46529302
8	-0.40689942	3.79115056	-0.77564785
6	-0.36476262	1.71309807	-2.40894899
6	-1.71228543	1.94817313	-2.68209530
6	-2.32930301	1.24072016	-3.71782699
6	-1.61740989	0.30835210	-4.48645433
6	-0.25614418	0.10363341	-4.19604227

6	0.37334745	0.79668015	-3.16439627
1	-2.25879436	2.69195561	-2.10340341
1	1.43284473	0.64772036	-2.95673961
1	0.32017040	-0.60678691	-4.79162812
6	-2.28583439	-0.45999834	-5.59845526
1	-3.38194146	1.42666170	-3.93866174
8	2.61324646	-3.41998527	-0.60590420
8	1.92588716	-4.51986040	1.63857241
6	0.16642908	-3.02754741	0.35863288
6	-0.82046051	-3.60201061	1.16167825
6	-2.16127277	-3.30236523	0.90824155
6	-2.52819929	-2.44130156	-0.13684137
6	-1.51221537	-1.88051309	-0.93139540
6	-0.16985942	-2.16829241	-0.69162895
1	-0.53401235	-4.28689953	1.95901855
1	-2.93645903	-3.75276351	1.53090694
6	-3.97806474	-2.14308848	-0.42509519
1	-1.77406449	-1.20797801	-1.75040514
1	0.61011736	-1.73965887	-1.32034696
1	-1.71613075	-0.37997098	-6.53513912
1	-2.34970758	-1.53111693	-5.35341474
1	-3.30366796	-0.09473218	-5.78365669
1	-4.12633455	-1.08276581	-0.67174332
1	-4.33233472	-2.72909349	-1.28740082
1	-4.61807244	-2.39433510	0.43023365
1	2.83653891	-1.31267525	0.87201006

Energy = -8139.843036 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 59

Atomic N.	X	Y	Z
8	3.69595167	1.85946967	2.26613886
6	4.83945311	1.42649334	2.99539370
1	5.26157900	2.28931854	3.53608332
1	5.63881312	1.01676181	2.34653092
1	4.57624868	0.65036875	3.73471448
50	3.03049026	0.73628861	0.68048025
7	1.64026045	2.84925248	0.10032122
6	2.01146550	3.89107658	1.08731795
1	1.35926353	4.77575758	0.97166002
1	1.94303081	3.49380416	2.10384217
1	3.05645956	4.18220057	0.93114690
7	0.95587927	0.47017943	1.43987678
6	0.22246032	2.44147876	0.27944841
1	-0.43494916	3.33118361	0.31080355
1	-0.06142146	1.82546632	-0.58123290
6	0.02516782	1.59409125	1.53712300
1	-1.02610938	1.25442714	1.54047358
1	0.18146212	2.18176604	2.45622707
16	1.06537608	-0.59586597	2.68197835
7	1.72378680	1.22256081	-2.46208974
6	1.91363509	3.40095342	-1.25656566
1	1.51054152	4.43044801	-1.32034514
1	3.00786662	3.48544797	-1.34803850
6	1.34988248	2.64447657	-2.46040055
1	1.69240287	3.17144681	-3.36678945
1	0.25188118	2.69918320	-2.46520158

16	1.08560651	0.29278770	-3.76019063
8	1.93989982	-0.90872769	-3.80123879
8	0.88854002	1.12920114	-4.96489964
6	-0.54598793	-0.13091517	-3.12130046
6	-1.67178967	0.18232358	-3.88269704
6	-2.93192648	-0.19121355	-3.40891719
6	-3.07658892	-0.86757649	-2.18870929
6	-1.92179947	-1.16275357	-1.44111695
6	-0.65663367	-0.80354237	-1.90017659
1	-1.55222508	0.71036799	-4.82812660
1	0.23148405	-1.02861044	-1.30996786
1	-2.01193559	-1.67968168	-0.48395813
6	-4.43624185	-1.28841878	-1.69092881
1	-3.81769600	0.05091236	-3.99862158
8	2.44100417	-1.17358265	2.48096136
8	0.67311870	-0.03137082	3.99214993
6	-0.10158956	-1.93395113	2.32304265
6	-1.34582350	-1.94550548	2.95377072
6	-2.25415862	-2.96395663	2.64952536
6	-1.93190683	-3.97485962	1.73275286
6	-0.66366366	-3.94551195	1.12437474
6	0.25013998	-2.93331469	1.41031361
1	-1.58460771	-1.17770379	3.68906416
1	-3.22643457	-2.97893997	3.14557277
6	-2.91437907	-5.07049622	1.40185853
1	-0.38725533	-4.73182743	0.41923578
1	1.23741762	-2.92232465	0.94886198
1	-4.54114010	-1.10331025	-0.61314368
1	-5.23952403	-0.75632879	-2.21596733
1	-4.59106086	-2.36682746	-1.85022934
1	-2.45708416	-6.06352024	1.51730185
1	-3.79960882	-5.02426686	2.04851436
1	-3.25395096	-4.99464076	0.35744655
1	2.73692373	1.06005089	-2.47345428

Energy = -8139.840687 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 60

Atomic N.	X	Y	Z
8	3.90491666	1.95715162	0.31061741
6	5.27895872	1.84106090	-0.04616872
1	5.85439368	2.58321776	0.53049039
1	5.43964314	2.03937504	-1.12014400
1	5.69939050	0.84304383	0.18296354
50	2.56541822	0.48404325	-0.20793247
7	1.09512134	1.90579783	1.29659839
6	1.74680146	2.16150805	2.59979890
1	1.16172439	2.87653012	3.20601660
1	1.86626313	1.22457211	3.15533320
1	2.74286786	2.57264899	2.39852099
7	0.46205519	-0.88819803	2.24781595
6	-0.27487179	1.35058700	1.43513787
1	-0.97479809	2.15921643	1.72420342
1	-0.58943941	0.99330318	0.44269699
6	-0.45669917	0.23482195	2.46684493
1	-1.51919624	-0.06815747	2.42447302
1	-0.26346970	0.61132343	3.47925495

16	0.60695424	-2.04576172	3.49217379
7	1.26816688	1.80307241	-1.47797821
6	1.05117620	3.17696457	0.51457332
1	0.40681628	3.91389217	1.03156512
1	2.08285636	3.55212480	0.48756485
6	0.56732683	2.95911519	-0.92121239
1	0.79185517	3.87498960	-1.49100868
1	-0.52642483	2.80865784	-0.95400633
16	2.04775833	1.93830837	-2.91183884
8	3.12605526	0.89328018	-2.78554502
8	2.40164820	3.33131217	-3.26934654
6	0.92467080	1.34477805	-4.20281885
6	0.35359315	2.25836567	-5.08835057
6	-0.53115126	1.79639923	-6.06648980
6	-0.84631853	0.43461353	-6.17563149
6	-0.25163057	-0.46337053	-5.27136899
6	0.62969189	-0.01879335	-4.28824141
1	0.61541030	3.31326597	-5.01425433
1	1.10016541	-0.72068780	-3.59956983
1	-0.47921445	-1.52870788	-5.34488934
6	-1.77346191	-0.06429186	-7.25575757
1	-0.97850419	2.50885565	-6.76220807
8	1.54090494	-3.05197176	2.96192889
8	0.87138905	-1.27232596	4.71977300
6	-1.01151034	-2.82852814	3.67419958
6	-1.91898886	-2.33344861	4.61233147
6	-3.17235494	-2.93926087	4.72811454
6	-3.52853907	-4.03178562	3.92360688
6	-2.59088580	-4.51097929	2.99141961
6	-1.33596997	-3.91975419	2.86140328
1	-1.63339926	-1.50208261	5.25592689
1	-3.88337928	-2.56024233	5.46421726
6	-4.87207299	-4.70000228	4.06990077
1	-2.84570085	-5.36795039	2.36513668
1	-0.60068545	-4.30981799	2.15770759
1	-2.40296047	0.74415034	-7.64932239
1	-1.20158233	-0.47962583	-8.10022164
1	-2.42837991	-0.86450600	-6.88451417
1	-5.56244511	-4.08872334	4.66437894
1	-5.33247135	-4.88942026	3.09024439
1	-4.77009903	-5.67430856	4.57195073
1	0.35261160	-1.36764455	1.34993554

Energy = -8139.843610 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 61

Atomic N.	X	Y	Z
8	3.57400050	1.90497004	2.41690930
6	4.71212637	1.48388429	3.16126265
1	4.46622960	0.64663855	3.83717801
1	5.06529917	2.32934814	3.77394117
1	5.55614847	1.16267355	2.51919402
50	2.99287454	0.83158914	0.76508932
7	1.51794916	2.90750013	0.25948992
6	1.83230986	3.92042706	1.29517510
1	1.14250861	4.77967449	1.21014644
1	1.77230884	3.47622853	2.29265066

1	2.86466297	4.26432169	1.16383155
7	0.91906760	0.43617136	1.47085677
6	0.11695271	2.43222837	0.40211691
1	-0.57775233	3.29108948	0.46902468
1	-0.13261904	1.84770506	-0.49048857
6	-0.05652758	1.51646411	1.61460683
1	-1.09343288	1.13611388	1.59098539
1	0.06934110	2.06373241	2.56286237
16	1.06085452	-0.68551375	2.65950865
7	1.69846590	1.39864679	-2.36799053
6	1.78290726	3.52917554	-1.06853911
1	1.33657853	4.54239756	-1.09334512
1	2.87345446	3.66415243	-1.14145726
6	1.26653116	2.80286252	-2.31159718
1	1.59885479	3.38174708	-3.18969797
1	0.16733710	2.81298370	-2.33014366
16	1.11704393	0.50141842	-3.71451849
8	2.01342439	-0.66745675	-3.78741712
8	0.91331452	1.37853087	-4.88896057
6	-0.51092972	-0.00129772	-3.12498846
6	-1.63290382	0.29868196	-3.90081725
6	-2.88643549	-0.13525946	-3.46922582
6	-3.03214912	-0.85849590	-2.27370114
6	-1.88457391	-1.14143876	-1.51461004
6	-0.62191812	-0.72078379	-1.93318711
1	-1.51182095	0.86160427	-4.82573104
1	0.26119039	-0.93814771	-1.33266404
1	-1.97590076	-1.69893397	-0.58088072
6	-4.39425321	-1.31997583	-1.81957152
1	-3.76752238	0.09377149	-4.07157171
8	2.46549645	-1.18753658	2.45237196
8	0.62457625	-0.20827475	3.99030282
6	-0.03421830	-2.05828504	2.21538352
6	-1.28036686	-2.16831157	2.83276170
6	-2.13342600	-3.21257097	2.46329138
6	-1.75339201	-4.15332582	1.49522269
6	-0.48677432	-4.02213507	0.89725341
6	0.37261258	-2.98331423	1.24884713
1	-1.56410766	-1.45429045	3.60531573
1	-3.10816997	-3.30304849	2.94639438
6	-2.66409613	-5.29464941	1.11678423
1	-0.16856741	-4.74848401	0.14691840
1	1.35887141	-2.89357603	0.79382420
1	-5.07942584	-0.46860144	-1.69437222
1	-4.85005294	-1.99214666	-2.56149849
1	-4.33674175	-1.85505920	-0.86373447
1	-2.27332401	-6.25100135	1.49633461
1	-3.67170199	-5.15816663	1.52951238
1	-2.74767920	-5.39431166	0.02515955
1	2.71749057	1.27766009	-2.36979822

Energy = -8139.840604 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 62

Atomic N.	X	Y	Z
8	4.36842939	0.24472216	0.22733865
6	4.97396822	0.53060484	-1.02696061

1	4.33708816	0.26847648	-1.89162405
1	5.91753038	-0.03637502	-1.10878810
1	5.21369211	1.60401429	-1.11273321
50	2.39064904	0.29555851	0.71144358
7	2.24794415	-2.41947963	0.05322587
6	3.59673626	-2.75672877	-0.44495939
1	3.63366448	-3.79811395	-0.81948493
1	3.88378161	-2.07660755	-1.25245206
1	4.32736574	-2.62964587	0.36234205
7	1.50199451	-0.06351982	-1.30161805
6	1.26413465	-2.45072411	-1.05546625
1	1.31196851	-3.42448803	-1.58448062
1	0.26186050	-2.35169738	-0.61765073
6	1.45545664	-1.30977460	-2.05594740
1	0.59730496	-1.33381931	-2.75062343
1	2.36255523	-1.45855630	-2.66621047
16	1.41280996	1.37790856	-2.05681182
7	0.94786253	-2.05132973	2.94114976
6	1.88196919	-3.41234527	1.09232774
1	1.71808742	-4.39887206	0.61243266
1	2.75626022	-3.53207027	1.75117494
6	0.65555981	-3.10565158	1.95414111
1	0.34201612	-4.04395857	2.43995676
1	-0.19029435	-2.77084418	1.33758071
16	-0.27606459	-1.74626818	4.11200700
8	0.46993029	-1.30814860	5.30837848
8	-1.22582838	-2.87919811	4.15931232
6	-1.15209499	-0.33238557	3.42244055
6	-2.45822747	-0.49311410	2.96238723
6	-3.14567747	0.62393544	2.47859624
6	-2.54449585	1.89064987	2.45177150
6	-1.22273863	2.01676392	2.91762110
6	-0.52284251	0.91649078	3.40439753
1	-2.92807795	-1.47506709	3.00348521
1	0.49644408	1.02122386	3.77298584
1	-0.73544389	2.99293694	2.89632654
6	-3.29199769	3.10066856	1.95167679
1	-4.17199601	0.50752256	2.12593374
8	1.78601570	2.31697909	-0.93723196
8	2.14648109	1.45435189	-3.34102013
6	-0.33174191	1.66549549	-2.45254660
6	-0.68940419	2.01406350	-3.75435903
6	-2.03667507	2.23339327	-4.05483791
6	-3.02903711	2.10681236	-3.07307014
6	-2.63843268	1.74771081	-1.77013570
6	-1.29984123	1.52869580	-1.45281992
1	0.08539550	2.10700525	-4.51437717
1	-2.31986292	2.50547744	-5.07327737
6	-4.47968840	2.36486015	-3.39487756
1	-3.39725125	1.63441497	-0.99318102
1	-1.00786116	1.24882153	-0.43983439
1	-3.43179142	3.83613784	2.75781150
1	-2.73503378	3.60685961	1.14996315
1	-4.28345341	2.83086568	1.56640644
1	-4.79987339	3.34164312	-3.00026138
1	-4.65534101	2.37084910	-4.47800951
1	-5.13184170	1.60467780	-2.94265723
1	1.78795395	-2.25180780	3.49369315

Energy = -8139.838880 Hartree
 Number of imaginary frequencies = 0.

Compound 11a isomer 63

Atomic N.	X	Y	Z
8	4.14869012	-1.31127187	0.29924398
6	5.40883750	-1.01025852	0.89117616
1	6.17817384	-1.63922423	0.41475225
1	5.41230063	-1.22271119	1.97438583
1	5.70793718	0.04604161	0.74964239
50	2.52791843	-0.08489361	0.62099835
7	1.55903214	-1.65049540	-1.12829590
6	2.44328108	-1.74714506	-2.31036241
1	2.08367005	-2.51714805	-3.01672873
1	2.50009162	-0.78032052	-2.82302891
1	3.44671841	-2.00843736	-1.95470629
7	0.64569512	1.05349483	-2.11405950
6	0.15850089	-1.30794086	-1.48227522
1	-0.34711916	-2.20119502	-1.89925187
1	-0.36525842	-1.04888111	-0.54949018
6	-0.03022495	-0.18785394	-2.50806126
1	-1.12003622	-0.05690049	-2.64068264
1	0.38520316	-0.48206774	-3.48012353
16	0.81933823	2.27075261	-3.29601557
7	1.27064474	-1.64181258	1.64088313
6	1.59270798	-2.94534816	-0.38574771
1	1.16348666	-3.74974693	-1.01368714
1	2.65309302	-3.15889333	-0.19653345
6	0.85842254	-2.86564705	0.95500665
1	1.13015726	-3.76084928	1.53699385
1	-0.23644683	-2.88454867	0.81085647
16	1.83828579	-1.72368813	3.17480110
8	2.74445815	-0.52121330	3.24139063
8	2.35118901	-3.06123863	3.55104608
6	0.45641653	-1.36978342	4.29076538
6	-0.07948114	-2.39676133	5.06617286
6	-1.15810672	-2.11972061	5.91154628
6	-1.70333151	-0.83142736	5.99441188
6	-1.13555619	0.18656260	5.20645800
6	-0.06322326	-0.07327383	4.35691984
1	0.36000642	-3.39234959	5.01651759
1	0.38500713	0.72255252	3.76191459
1	-1.53636197	1.20037327	5.26844233
6	-2.86645817	-0.53309111	6.90744874
1	-1.57616889	-2.92026716	6.52468061
8	1.47252672	3.38618430	-2.59243076
8	1.41512213	1.60007823	-4.46670026
6	-0.84640707	2.79959525	-3.75563217
6	-1.48081789	2.21430587	-4.85322478
6	-2.77209937	2.62669586	-5.18875575
6	-3.43663725	3.61324143	-4.44432259
6	-2.76690761	4.19257351	-3.35236412
6	-1.47811543	3.79392316	-3.00210143
1	-0.95415577	1.46991098	-5.44942293
1	-3.26780140	2.18121677	-6.05303214
6	-4.83894024	4.03842096	-4.79861933
1	-3.25852352	4.97848629	-2.77614412

1	-0.94902101	4.26584654	-2.17424803
1	-3.14214186	-1.41129592	7.50469904
1	-2.62820939	0.28878986	7.59829403
1	-3.75208825	-0.22276868	6.33266826
1	-4.97904960	5.11774594	-4.65192818
1	-5.08077308	3.79544498	-5.84104130
1	-5.57475059	3.52577659	-4.15957324
1	0.30730027	1.47245609	-1.24352485

Energy = -8139.843596 Hartree

Number of imaginary frequencies = 0.

Compound I1a isomer 64

Atomic N.	X	Y	Z
8	4.33778203	0.39963746	0.41952374
6	4.98448571	0.76332694	-0.79318205
1	4.35114873	0.62475122	-1.68813775
1	5.89616558	0.15251217	-0.91681701
1	5.28796503	1.82366005	-0.76855824
50	2.34308332	0.33666616	0.82448540
7	2.33702044	-2.32591026	-0.01868689
6	3.71747455	-2.57745298	-0.47981232
1	3.81252287	-3.59050212	-0.91650588
1	4.00705537	-1.83672269	-1.23106756
1	4.40968069	-2.47359261	0.36389238
7	1.54714904	0.08701710	-1.24176347
6	1.40098265	-2.31906528	-1.16855457
1	1.51106502	-3.25143341	-1.75919996
1	0.37852302	-2.28935359	-0.76891137
6	1.58489971	-1.10479476	-2.08019402
1	0.75782718	-1.11408151	-2.81191944
1	2.52171353	-1.17461216	-2.65890669
16	1.41579047	1.57132423	-1.90373742
7	0.91500316	-2.20795325	2.83483466
6	1.96986705	-3.40047582	0.93533911
1	1.86285866	-4.35660241	0.38340151
1	2.82198110	-3.53403288	1.62006082
6	0.70014274	-3.19792353	1.76467357
1	0.40206390	-4.17865555	2.16963426
1	-0.13252209	-2.84810503	1.13859279
16	-0.36643968	-2.02678702	3.96993822
8	0.31427084	-1.65938918	5.22751158
8	-1.28071500	-3.18672005	3.89016366
6	-1.25662368	-0.59015866	3.34914694
6	-2.53498732	-0.75274123	2.81756954
6	-3.23546903	0.37781600	2.38682384
6	-2.67411775	1.65942466	2.48173643
6	-1.37934524	1.78748588	3.01763767
6	-0.66725248	0.67385946	3.45357043
1	-2.97471180	-1.74793634	2.76360443
1	0.33038469	0.77924836	3.87711095
1	-0.92295083	2.77593156	3.09181478
6	-3.43497185	2.88172780	2.03444009
1	-4.24100672	0.25935169	1.97925313
8	1.69920175	2.45020243	-0.71258776
8	2.19305457	1.76367113	-3.14973517
6	-0.32462768	1.80182530	-2.35147041
6	-0.65216914	2.18407429	-3.65194346

6	-1.99643419	2.35754851	-3.99247028
6	-3.01547371	2.15325688	-3.05167598
6	-2.65457352	1.76231957	-1.74960671
6	-1.31931460	1.58709299	-1.39266087
1	0.14370333	2.33913943	-4.37935760
1	-2.25609398	2.65519624	-5.01005930
6	-4.46328504	2.36755400	-3.41547680
1	-3.43406950	1.58858653	-1.00498432
1	-1.05060099	1.28173227	-0.38061206
1	-3.60781285	3.56726212	2.87716076
1	-2.87007170	3.44347887	1.27626767
1	-4.41119775	2.61548002	1.60989686
1	-4.81101360	3.35294483	-3.06787288
1	-4.61408340	2.32898251	-4.50183987
1	-5.11042479	1.61264523	-2.94825554
1	1.73749319	-2.42173156	3.40847840

Energy = -8139.838945 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 65

Atomic N.	X	Y	Z
8	4.17681202	-1.17385599	0.23330816
6	5.43507608	-0.84747654	0.81559951
1	5.46529272	-1.09870554	1.89011416
1	5.69272474	0.22368366	0.70813266
1	6.21874564	-1.42974869	0.30441298
50	2.51723716	-0.02214436	0.62714251
7	1.58912195	-1.53484964	-1.19100508
6	2.46702981	-1.54125222	-2.38172969
1	2.12873482	-2.28709044	-3.12372018
1	2.48682942	-0.54871384	-2.84577052
1	3.48154652	-1.78480676	-2.04552307
7	0.57143418	1.18151807	-2.02958653
6	0.17477454	-1.22596631	-1.51957463
1	-0.30124130	-2.11423134	-1.97991465
1	-0.35170446	-1.03428115	-0.57217767
6	-0.06021363	-0.06189431	-2.48531607
1	-1.15443092	0.03598190	-2.60877656
1	0.36178618	-0.29044271	-3.47212808
16	0.72435764	2.45364207	-3.15468313
7	1.32614881	-1.67245896	1.57748360
6	1.67528451	-2.86253132	-0.51358678
1	1.26888587	-3.65002057	-1.17715788
1	2.74429474	-3.04702401	-0.34335397
6	0.95160500	-2.87528012	0.83523171
1	1.26076751	-3.78755399	1.37012526
1	-0.14327348	-2.92674741	0.69894246
16	1.91076602	-1.80877026	3.10120225
8	2.77221663	-0.57796096	3.22112619
8	2.47615362	-3.14314356	3.40694481
6	0.52662397	-1.56249474	4.24300977
6	0.02950123	-2.64797032	4.96270160
6	-1.05154681	-2.45370468	5.82773644
6	-1.63758455	-1.19045055	5.98508670
6	-1.10808841	-0.11217002	5.25278251
6	-0.03388120	-0.28927218	4.38443108
1	0.50073479	-3.62436203	4.85576392

1	0.38480571	0.55265100	3.83296752
1	-1.54056890	0.88313180	5.37382387
6	-2.80524837	-0.98222323	6.91714367
1	-1.43901030	-3.30020074	6.39774863
8	1.32449430	3.55906897	-2.39059946
8	1.36592462	1.85518795	-4.34031550
6	-0.94905450	2.94484084	-3.62796191
6	-1.53611410	2.39144777	-4.76728687
6	-2.83367259	2.77379369	-5.11453292
6	-3.55043427	3.69878953	-4.34055934
6	-2.92809588	4.24790470	-3.20543760
6	-1.63412341	3.87827184	-2.84322934
1	-0.96916509	1.69572379	-5.38489209
1	-3.29311435	2.35349861	-6.01083265
6	-4.95795038	4.09408266	-4.70867960
1	-3.46147401	4.98660554	-2.60443743
1	-1.14187818	4.32784658	-1.98093342
1	-3.03050513	-1.89279041	7.48645718
1	-2.60301025	-0.17226336	7.63290324
1	-3.71108582	-0.69948297	6.35965957
1	-5.12007324	5.17133723	-4.56752874
1	-5.18594853	3.84293861	-5.75216771
1	-5.68898448	3.57084211	-4.07288658
1	0.21176581	1.55154734	-1.14569632

Energy = -8139.843615 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 66

Atomic N.	X	Y	Z
8	1.89611730	-0.63231973	-1.20080777
6	3.30954028	-0.55069616	-0.94507064
1	3.59092303	0.49165306	-0.72172778
1	3.91934849	-0.88087734	-1.80707934
1	3.57357347	-1.19219922	-0.09090190
50	1.35964639	-0.89529805	-3.20472952
7	-0.92920212	-2.16310157	-2.59501624
6	-1.33996454	-2.57282837	-3.95558507
1	-2.37378089	-2.96489586	-3.96088048
1	-1.28119264	-1.72309002	-4.64686076
1	-0.66233202	-3.35599913	-4.31805497
7	-0.32458625	0.48969785	-3.01136618
6	-1.83900022	-1.11136283	-2.07314581
1	-2.88504570	-1.47622815	-2.06412725
1	-1.53851746	-0.89696590	-1.04065840
6	-1.73998544	0.19059596	-2.87248830
1	-2.27108988	0.97487319	-2.30607971
1	-2.24607459	0.10634077	-3.84941303
16	0.24270821	1.96799128	-3.39877178
7	0.87375027	-3.01833567	-0.08342632
6	-0.95762707	-3.37937597	-1.73356322
1	-1.98425660	-3.79815326	-1.75911497
1	-0.28568067	-4.11838930	-2.19234783
6	-0.56568177	-3.21855611	-0.26515914
1	-0.82329230	-4.16999288	0.22193932
1	-1.17136689	-2.43530234	0.22484325
16	1.49804416	-3.42859624	1.43112891
8	2.94560888	-3.16068090	1.34845619

8	0.96454189	-4.76440814	1.76713488
6	0.79500760	-2.26068014	2.62474860
6	-0.31364096	-2.63374941	3.38632523
6	-0.85900064	-1.71777580	4.28961408
6	-0.31039152	-0.43639052	4.44444790
6	0.80687408	-0.08923117	3.66474007
6	1.36314389	-0.98995748	2.75834961
1	-0.72360522	-3.63803382	3.28390714
1	2.23989312	-0.72181745	2.16930482
1	1.25431522	0.90031774	3.77860022
6	-0.88049178	0.53693639	5.44555621
1	-1.72234339	-2.00859956	4.89095152
8	1.70540425	1.64405755	-3.61299160
8	-0.50356805	2.66615750	-4.46718558
6	0.12290853	2.99162822	-1.91251649
6	-0.45772007	4.25645467	-1.99510175
6	-0.53199028	5.04265099	-0.84204653
6	-0.03517093	4.57895952	0.38429837
6	0.53734943	3.29462686	0.43418160
6	0.62243225	2.49525318	-0.70369956
1	-0.84274378	4.61063396	-2.95064048
1	-0.98510391	6.03403265	-0.89857039
6	-0.09462346	5.43924581	1.62161411
1	0.92377458	2.91502412	1.38258850
1	1.06160771	1.49386567	-0.66403057
1	-1.90436535	0.26483167	5.73201675
1	-0.27242239	0.55326268	6.36335762
1	-0.89217964	1.56079026	5.04721844
1	0.90393482	5.82652874	1.87640069
1	-0.76010159	6.30028923	1.48094758
1	-0.44896415	4.86669777	2.49039324
1	1.24665629	-2.08950876	-0.39990549

Energy = -8139.851271 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 67

Atomic N.	X	Y	Z
8	4.18618550	-1.80762350	-1.31439106
6	4.60908412	-2.72720738	-0.31001699
1	5.19217674	-2.23449908	0.48499548
1	5.25063174	-3.48484833	-0.78870846
1	3.76236066	-3.24846055	0.17292626
50	3.03332360	-0.14491511	-1.03699545
7	1.31130176	-1.45038507	-2.55834017
6	2.07578921	-2.06740943	-3.66493173
1	1.47274807	-2.83869650	-4.17810229
1	2.36777709	-1.30583952	-4.39713787
1	2.98902019	-2.51351733	-3.25129015
7	0.66891354	1.73840660	-3.11064935
6	0.10269773	-0.75321514	-3.07410587
1	-0.45717601	-1.45988037	-3.71945372
1	-0.54276808	-0.51012074	-2.22085419
6	0.36593510	0.52978497	-3.87744997
1	-0.52545070	0.75445154	-4.48014263
1	1.18083763	0.37777635	-4.60110360
16	-0.55572193	2.82170358	-2.68902088
7	1.39811262	-0.98164578	0.21806006

6	0.91574220	-2.52154971	-1.60038500
1	0.13845247	-3.16902940	-2.05115792
1	1.81401079	-3.12995794	-1.42870211
6	0.43332040	-1.97207027	-0.25407649
1	0.35860027	-2.82125019	0.44493322
1	-0.57238122	-1.52588142	-0.34233359
16	2.00729628	-1.03370629	1.73279986
8	3.31043335	-0.28898877	1.54046069
8	2.00282007	-2.38472702	2.33852187
6	0.99709478	0.01378548	2.80650498
6	0.09447888	-0.58080055	3.68804957
6	-0.70090882	0.23419486	4.49883586
6	-0.60147451	1.63194689	4.44509630
6	0.32715510	2.20173505	3.55477815
6	1.12459973	1.40463808	2.73672709
1	0.03512786	-1.66685700	3.74891867
1	1.85507142	1.85178157	2.06263883
1	0.42930917	3.28742263	3.50582381
6	-1.45861110	2.51040726	5.32105675
1	-1.40464487	-0.22773798	5.19363806
8	0.13301865	3.87246621	-1.91929644
8	-1.30744579	3.09387047	-3.92901307
6	-1.70316960	1.98089812	-1.57004732
6	-2.92328449	1.51216059	-2.05932072
6	-3.79448625	0.85054389	-1.18987822
6	-3.46440062	0.65466688	0.15919824
6	-2.23002891	1.14273586	0.62513061
6	-1.34946234	1.80366718	-0.22875918
1	-3.18623176	1.68390576	-3.10252178
1	-4.75206619	0.48679302	-1.56696139
6	-4.41560892	-0.04119833	1.10006712
1	-1.95252813	1.00393297	1.67179792
1	-0.40084982	2.18928919	0.14373261
1	-2.10414378	1.91448578	5.97814780
1	-0.83954546	3.16424215	5.95240007
1	-2.10086732	3.16647127	4.71482841
1	-4.86084709	0.67546282	1.80691320
1	-5.23520256	-0.52736433	0.55614557
1	-3.89727692	-0.80288297	1.69946854
1	1.39315649	1.66863896	-2.38744797

Energy = -8139.843066 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 68

Atomic N.	X	Y	Z
8	1.75688812	-0.32492718	0.11774533
6	0.93967971	0.67538475	0.71703505
1	0.25507565	0.21204459	1.44971780
1	0.33159017	1.21989476	-0.02499043
1	1.56757873	1.40554437	1.25552920
50	2.17683306	-0.60431451	-1.90051559
7	0.04951380	-2.05484228	-2.36175458
6	0.23768546	-2.42817939	-3.78143819
1	-0.67266968	-2.89919269	-4.19452548
1	0.48202332	-1.54353721	-4.38211126
1	1.07134633	-3.13667257	-3.85843463
7	0.50257215	0.71725481	-2.53507668

6	-1.07373538	-1.09515852	-2.21831491
1	-2.01233461	-1.54562659	-2.59684602
1	-1.20187223	-0.89347494	-1.14688658
6	-0.81270861	0.22573903	-2.94309591
1	-1.61400673	0.92670409	-2.64561238
1	-0.88420020	0.10068258	-4.03652062
16	1.15702511	1.98618307	-3.35608270
7	1.18445314	-3.00837081	0.45002557
6	-0.21051388	-3.29872312	-1.58353188
1	-1.19769548	-3.70112763	-1.88764282
1	0.55338683	-4.03181455	-1.87506821
6	-0.17867755	-3.18540436	-0.05674746
1	-0.56090026	-4.14363038	0.32359396
1	-0.85659335	-2.39545219	0.30800366
16	1.65748883	-3.91412282	1.79593026
8	3.09654456	-3.64929137	1.95794421
8	1.11865763	-5.27725650	1.60252978
6	0.81134132	-3.20096006	3.22910345
6	-0.32925751	-3.82076131	3.74122308
6	-0.97837919	-3.24990236	4.83891892
6	-0.50229556	-2.07117191	5.43152757
6	0.64958859	-1.47016183	4.89404800
6	1.31091077	-2.02630104	3.80059750
1	-0.68350632	-4.74941057	3.29482157
1	2.21366586	-1.56707225	3.39728064
1	1.03816668	-0.55512447	5.34522361
6	-1.18564968	-1.47816886	6.63818688
1	-1.86717151	-3.73505767	5.24678480
8	2.57982240	1.96391254	-2.88048888
8	0.85914699	1.95012583	-4.80720772
6	0.39399052	3.48995518	-2.70546234
6	-0.63465389	4.10270150	-3.42261594
6	-1.23366341	5.25265594	-2.90289004
6	-0.81214677	5.80292650	-1.68354288
6	0.23134423	5.16739382	-0.98779519
6	0.83607268	4.01600948	-1.48802211
1	-0.94216603	3.69047598	-4.38313025
1	-2.03756227	5.73600845	-3.46101952
6	-1.43686832	7.06527838	-1.14451380
1	0.57822969	5.58587277	-0.04108179
1	1.65517924	3.53503003	-0.95454989
1	-2.22130909	-1.83049415	6.72730233
1	-0.65881242	-1.76202337	7.56254479
1	-1.19416397	-0.38053956	6.59533045
1	-0.80507893	7.93897489	-1.36804589
1	-2.42284798	7.24771570	-1.59069682
1	-1.55221356	7.02085685	-0.05296354
1	1.47785282	-2.00705688	0.53827453

Energy = -8139.850028 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 69

Atomic N.	X	Y	Z
8	2.80894928	-3.68045325	0.53607326
6	3.69870247	-4.16874182	1.53547183
1	3.81052228	-5.25728786	1.40492173
1	3.31179793	-3.98087174	2.55174196

1	4.70875327	-3.71928892	1.46877581
50	2.70401133	-1.65504030	0.15673167
7	1.25244333	-2.54714196	-1.74681770
6	1.99606892	-3.64116507	-2.41436078
1	1.32859321	-4.21222946	-3.08390277
1	2.81950733	-3.22791507	-3.01039060
1	2.41699068	-4.29785060	-1.64365651
7	2.04883938	0.51574491	-2.39197575
6	0.74518828	-1.58061457	-2.75844886
1	0.30106119	-2.15227801	-3.59570751
1	-0.05768641	-0.99007019	-2.30031622
6	1.79112018	-0.60700468	-3.31090337
1	1.43378054	-0.21098906	-4.27383253
1	2.74054848	-1.11819884	-3.52352049
16	1.56323261	2.08493739	-2.87361249
7	0.56528724	-1.44197429	0.74310916
6	0.12273882	-3.13194398	-0.96469026
1	-0.64578222	-3.53624534	-1.65089540
1	0.55023939	-3.95649619	-0.37847619
6	-0.49914377	-2.11686270	-0.00088942
1	-1.16671581	-2.67173335	0.67771801
1	-1.11639501	-1.37791776	-0.54109544
16	0.56145868	-1.47595021	2.38261394
8	2.02821992	-1.33660672	2.70187570
8	-0.22623413	-2.59101408	2.95517338
6	-0.21677181	0.05382818	2.96081722
6	-1.52962578	0.01926285	3.43071383
6	-2.13481385	1.20830802	3.84815693
6	-1.44385838	2.42804165	3.80974597
6	-0.11819842	2.42985229	3.33937778
6	0.49870614	1.25439597	2.91664549
1	-2.05836319	-0.93189328	3.48303373
1	1.53126797	1.25967397	2.56776477
1	0.43984786	3.36752110	3.30778914
6	-2.09058302	3.70665115	4.28040961
1	-3.16105278	1.18393551	4.21953049
8	2.44556055	2.98337662	-2.10377358
8	1.46941597	2.17953573	-4.34770549
6	-0.11781369	2.19474396	-2.22958455
6	-1.13366293	2.64042921	-3.07572138
6	-2.42470378	2.78457603	-2.56272293
6	-2.70976613	2.49014736	-1.22101273
6	-1.66532389	2.03566605	-0.39591496
6	-0.37047726	1.88882392	-0.88939564
1	-0.90830069	2.86350011	-4.11781896
1	-3.22485494	3.12955087	-3.21992022
6	-4.09977210	2.67381670	-0.66622389
1	-1.86728447	1.78682216	0.64751529
1	0.42755594	1.51988860	-0.24569167
1	-3.16461471	3.57106116	4.45978120
1	-1.63461320	4.05422377	5.21986845
1	-1.96181539	4.51319245	3.54460938
1	-4.18710288	3.64428777	-0.15317265
1	-4.85633862	2.65227682	-1.46105351
1	-4.34271098	1.89547251	0.06937627
1	3.01397108	0.60223455	-2.06613752

Energy = -8139.844267 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 70

Atomic N.	X	Y	Z
8	4.06248552	1.56276863	0.35338614
6	5.30063020	1.70493799	-0.33630597
1	5.23801240	2.46466740	-1.13468232
1	5.64900554	0.75851065	-0.79257965
1	6.06838884	2.02707799	0.38566830
50	2.48318994	0.58660371	-0.53351209
7	1.54725284	0.90715434	1.80527271
6	2.49218787	0.41974909	2.83384173
1	2.13873727	0.66779679	3.85103602
1	2.62213510	-0.66488230	2.74747370
1	3.46075514	0.89893964	2.64965752
7	0.82194681	-1.96164164	1.21302119
6	0.18638965	0.33253863	1.95389601
1	-0.33487427	0.82769211	2.79679858
1	-0.37737419	0.57568809	1.04036596
6	0.10828774	-1.17218510	2.22320121
1	-0.96511345	-1.42955658	2.28625645
1	0.56059373	-1.41351220	3.19340142
16	1.11507177	-3.60645722	1.55570199
7	1.09883374	2.35407499	-0.52937523
6	1.47927675	2.39722248	1.87098900
1	1.05104740	2.71122814	2.84237504
1	2.51620155	2.75151026	1.79960359
6	0.67288924	2.99359453	0.71464085
1	0.87052913	4.07730439	0.69468734
1	-0.41157208	2.85785193	0.87428392
16	1.56469525	3.27806742	-1.79866393
8	2.52121050	2.36468651	-2.52114012
8	1.98800747	4.64529308	-1.41763181
6	0.13432011	3.46880587	-2.89315861
6	-0.50767095	4.70415484	-2.97455839
6	-1.62459892	4.83751914	-3.80385319
6	-2.10311535	3.75605074	-4.55693270
6	-1.43279203	2.52381390	-4.45718561
6	-0.31994742	2.37319731	-3.63274527
1	-0.12183613	5.54831900	-2.40414151
1	0.20585910	1.42033115	-3.57097025
1	-1.78616508	1.67168323	-5.04127264
6	-3.28682332	3.91384298	-5.47845516
1	-2.12799739	5.80383353	-3.87152382
8	1.78649887	-4.12643079	0.35383784
8	1.73517484	-3.62478844	2.89381809
6	-0.49641936	-4.41360842	1.68694706
6	-1.10384264	-4.54912918	2.93690935
6	-2.35676117	-5.16032573	3.01868728
6	-3.00759097	-5.64025395	1.87190850
6	-2.36867056	-5.49292172	0.62829840
6	-1.11830079	-4.88562698	0.52678462
1	-0.58744454	-4.20035719	3.83057504
1	-2.83377209	-5.27340985	3.99380589
6	-4.34410325	-6.33071018	1.97105133
1	-2.85519682	-5.86930608	-0.27339416
1	-0.61272256	-4.79709772	-0.43475425
1	-3.88968975	4.79111582	-5.21077174

1	-2.95588677	4.04473143	-6.52057638
1	-3.93507490	3.02708184	-5.45458546
1	-4.21635840	-7.42439415	1.97238284
1	-4.86959998	-6.05876699	2.89528503
1	-4.98856385	-6.08118583	1.11743753
1	0.46026467	-1.87289135	0.25948279

Energy = -8139.843619 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 71

Atomic N.	X	Y	Z
8	3.87016405	0.23421956	1.97132257
6	5.21774986	-0.22373736	1.91516906
1	5.77609186	0.25122650	1.08984854
1	5.29337387	-1.32109042	1.79114546
1	5.71589718	0.03768720	2.86280234
50	2.49279545	-0.41158985	0.58578141
7	0.96688012	0.85644402	2.17114335
6	1.16675310	0.42286962	3.57139566
1	0.59166948	1.05538397	4.27165399
1	0.86428541	-0.62333731	3.69269244
1	2.23733903	0.50020334	3.79388304
7	-0.58884260	-1.68360129	1.68263618
6	-0.45547789	0.80487717	1.74866671
1	-1.00306333	1.66329701	2.18533042
1	-0.48140816	0.93020943	0.65543553
6	-1.23729915	-0.45046447	2.14312151
1	-2.25985485	-0.32970586	1.74047891
1	-1.32141218	-0.52364515	3.23471263
16	-1.14032541	-3.15962010	2.33558266
7	2.06796899	1.62156177	-0.26971056
6	1.49495499	2.24357763	2.00968181
1	0.90152994	2.94557887	2.62665961
1	2.52861475	2.21943417	2.37954227
6	1.50462630	2.69547226	0.54726679
1	2.11800133	3.60862730	0.48535603
1	0.48750582	2.95604308	0.20458813
16	3.32010710	1.93989406	-1.27593010
8	4.00674860	0.60084378	-1.35950194
8	4.09248423	3.14805660	-0.90492378
6	2.63617207	2.25312209	-2.92347586
6	2.65978167	3.54778358	-3.44143733
6	2.11090808	3.78568755	-4.70435757
6	1.54608870	2.74700349	-5.45803484
6	1.53951492	1.45160310	-4.91085198
6	2.07974085	1.19803602	-3.65194981
1	3.11719868	4.34921583	-2.86237636
1	2.08645883	0.18930751	-3.23882507
1	1.10985129	0.62847771	-5.48528179
6	0.98932033	3.00159370	-6.83656708
1	2.12982577	4.79759823	-5.11352385
8	-0.34830343	-4.19271764	1.64906286
8	-1.12201215	-2.97331685	3.79849976
6	-2.86421944	-3.34900570	1.82796151
6	-3.88680986	-2.91808970	2.67451992
6	-5.21385769	-3.06079316	2.26158590
6	-5.53118712	-3.62735043	1.01841851

6	-4.47899162	-4.06141662	0.19202797
6	-3.14965261	-3.92719504	0.58641233
1	-3.64230314	-2.50426662	3.65222235
1	-6.01757023	-2.73470609	2.92391123
6	-6.96379693	-3.77461452	0.57225905
1	-4.70707901	-4.52349557	-0.77028871
1	-2.33706880	-4.29138402	-0.04214997
1	0.74118324	4.06119741	-6.97976344
1	1.72267205	2.72612078	-7.61055728
1	0.08521373	2.40533879	-7.02098284
1	-7.17407232	-4.80314793	0.24622524
1	-7.66347639	-3.51978520	1.37781418
1	-7.17846751	-3.11599812	-0.28291093
1	-0.50291983	-1.77351813	0.66658326

Energy = -8139.843607 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 72

Atomic N.	X	Y	Z
8	0.83686575	-0.26654218	-0.09752412
6	1.60721111	-0.21468434	-1.30328285
1	1.88071734	-1.22899835	-1.64008305
1	2.53947309	0.36896516	-1.18837182
1	1.00786123	0.26222217	-2.09529143
50	1.91063072	-0.44660012	1.70493967
7	-0.11304082	0.58824853	3.12312169
6	0.52557200	0.62530142	4.45781518
1	-0.21195745	0.85502698	5.24868352
1	0.99761092	-0.33887830	4.68352574
1	1.30330565	1.39886336	4.46190086
7	0.50990745	-1.99369516	2.40181902
6	-1.18245923	-0.44185413	3.08539537
1	-1.95376847	-0.22074733	3.84952403
1	-1.65112974	-0.39377716	2.09448935
6	-0.63591286	-1.85832044	3.28378776
1	-1.44089466	-2.56761711	3.02393580
1	-0.37573872	-2.04480237	4.34004865
16	1.11105066	-3.43129320	1.93197522
7	-0.39522303	2.20998255	0.30822562
6	-0.67077555	1.94140811	2.85216177
1	-1.45041150	2.15918493	3.61148286
1	0.13928936	2.66648258	3.01015323
6	-1.29169064	2.19650660	1.47046814
1	-1.78101720	3.17843564	1.53390622
1	-2.08067551	1.46608292	1.24067806
16	0.77482272	3.43205747	0.30113480
8	2.08941063	2.89897849	0.74404982
8	0.17858842	4.59357153	1.00029605
6	0.92326154	3.82256064	-1.45396029
6	-0.16219255	4.39189419	-2.12646472
6	-0.02200284	4.73246924	-3.46888931
6	1.18975052	4.51777317	-4.15139081
6	2.26081664	3.94913659	-3.44885650
6	2.13703570	3.60070276	-2.10094181
1	-1.10014193	4.56624765	-1.60029550
1	2.96819718	3.16490073	-1.54807711
1	3.20881938	3.77571961	-3.96084922

6	1.32903300	4.90847542	-5.60132631
1	-0.86641422	5.17569734	-4.00006406
8	2.31799943	-2.97652957	1.14244423
8	1.29877633	-4.42146007	3.01475247
6	-0.07247182	-4.15144450	0.76650754
6	-0.45461518	-5.48417231	0.91343682
6	-1.35233504	-6.03618305	-0.00462603
6	-1.87174521	-5.27230694	-1.05923738
6	-1.46917251	-3.92917227	-1.17670546
6	-0.57416889	-3.36054587	-0.27277284
1	-0.04814868	-6.07219538	1.73549821
1	-1.65289149	-7.08009131	0.10201351
6	-2.84943284	-5.86608498	-2.04248975
1	-1.86349349	-3.32011177	-1.99294880
1	-0.26469444	-2.31462483	-0.35959452
1	0.49995042	4.50962658	-6.20303097
1	1.31223844	6.00304429	-5.71551857
1	2.27103937	4.54081801	-6.02695358
1	-2.52838183	-5.68801196	-3.07882007
1	-2.95638740	-6.94848389	-1.89784367
1	-3.84541445	-5.41083290	-1.93172092
1	0.05956524	1.27967716	0.10976024

Energy = -8139.851363 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 73

Atomic N.	X	Y	Z
8	3.15595073	2.87887809	-2.39384084
6	2.45447733	3.53326060	-3.44690313
1	2.43059913	2.92885177	-4.36869607
1	2.97241130	4.48053831	-3.67040242
1	1.40773304	3.76972480	-3.17962316
50	2.73471213	1.04423655	-1.58336824
7	2.20727590	2.45915161	0.56723956
6	3.29873127	3.44797242	0.70858858
1	3.01558662	4.24939321	1.41494396
1	4.20521089	2.95693841	1.08418277
1	3.51811271	3.87234119	-0.27955625
7	2.70404222	-0.58804719	1.47950926
6	1.96720121	1.76557805	1.85903096
1	1.96177565	2.51945146	2.67062602
1	0.97023474	1.30846835	1.82775321
6	2.97841987	0.66623347	2.20021094
1	2.93906808	0.47135466	3.28260096
1	4.00728676	0.98905334	1.98668309
16	2.28005797	-1.97198728	2.38418511
7	0.53139600	1.24388306	-1.33489094
6	0.97524005	3.15618931	0.10549379
1	0.56261758	3.78780198	0.91616682
1	1.28167156	3.81160654	-0.72094130
6	-0.09308299	2.18497240	-0.40754418
1	-0.87329464	2.78076347	-0.90913874
1	-0.57330923	1.64689174	0.42884436
16	-0.12375192	0.93939386	-2.80134705
8	1.08350164	0.46093525	-3.57070464
8	-0.95435282	2.04704447	-3.32768415
6	-1.21745267	-0.49457166	-2.65074577

6	-2.59891980	-0.30340047	-2.62888026
6	-3.43693476	-1.41328390	-2.48594045
6	-2.91373776	-2.70911828	-2.37046830
6	-1.51668579	-2.87097428	-2.40539239
6	-0.66717109	-1.77592461	-2.54454341
1	-3.00612397	0.70059131	-2.74295467
1	0.41363089	-1.91004161	-2.58686026
1	-1.08879000	-3.87195642	-2.32507616
6	-3.81852397	-3.90702792	-2.22689297
1	-4.51870444	-1.26770515	-2.47292942
8	2.62747813	-3.10041067	1.49849317
8	2.80854791	-1.88812235	3.76393750
6	0.48515477	-1.82876859	2.49934865
6	-0.12351535	-1.95595495	3.74797338
6	-1.51701210	-1.90080064	3.82870877
6	-2.30421030	-1.72213503	2.68147478
6	-1.65979174	-1.59120370	1.43800445
6	-0.27107679	-1.64604059	1.33826656
1	0.49227791	-2.09095572	4.63632094
1	-1.99975431	-1.99603827	4.80292662
6	-3.80907625	-1.69046225	2.77197634
1	-2.25187210	-1.43986527	0.53337081
1	0.21938713	-1.52999162	0.37217187
1	-4.87132178	-3.60794387	-2.14916757
1	-3.72095721	-4.58062592	-3.09129143
1	-3.56079766	-4.49461993	-1.33368968
1	-4.23329871	-2.67591838	2.52387276
1	-4.14576225	-1.43218966	3.78413021
1	-4.23725150	-0.96651467	2.06579414
1	3.41674278	-0.87889883	0.80664349

Energy = -8139.843154 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 74

Atomic N.	X	Y	Z
8	2.99206159	0.69761698	-0.74826079
6	3.83769082	-0.24145659	-1.40221489
1	4.68683955	0.30002478	-1.85108084
1	3.32791248	-0.79176984	-2.21869061
1	4.23805912	-0.98819510	-0.69470675
50	1.05193246	0.15899815	-0.32689700
7	0.90241171	2.68599093	0.39440015
6	2.28280818	3.22608876	0.42296478
1	2.29066051	4.23878104	0.86768873
1	2.93710829	2.56070833	0.99265778
1	2.67725933	3.25889229	-0.59760543
7	1.11338623	0.33352303	1.89884990
6	0.36102004	2.60945791	1.77834243
1	0.40795852	3.60757075	2.25527896
1	-0.69433333	2.31092583	1.71195215
6	1.10004119	1.58605598	2.64151727
1	0.54527453	1.49657337	3.59311972
1	2.11687867	1.93263859	2.88973472
16	1.98166145	-0.93987442	2.43842322
7	-1.19456005	2.21497338	-2.04117765
6	0.06926463	3.60508422	-0.42529926
1	-0.07130864	4.55072685	0.13413476

1	0.65250131	3.85656949	-1.32345982
6	-1.30781213	3.09073000	-0.85173153
1	-1.95530086	3.96313798	-1.04445312
1	-1.78336943	2.50015828	-0.05824905
16	-2.72095636	1.51926468	-2.48418033
8	-3.58779484	2.54016640	-3.11688101
8	-3.17891345	0.79386638	-1.28333516
6	-2.20152436	0.35873809	-3.75543722
6	-1.53971984	-0.81488303	-3.38498908
6	-1.17349552	-1.71983141	-4.37835428
6	-1.46025980	-1.47031063	-5.73223966
6	-2.13573004	-0.28717027	-6.06884494
6	-2.51007661	0.63361919	-5.08837089
1	-1.31575608	-1.01016033	-2.33641997
1	-3.04927832	1.54591062	-5.34110760
1	-2.37845483	-0.08469918	-7.11331455
6	-1.03267546	-2.44713825	-6.79770923
1	-0.65500617	-2.63838827	-4.09825143
8	2.04774536	-1.80324197	1.20469631
8	3.23159930	-0.57454470	3.14359430
6	0.94732955	-1.81550246	3.63955590
6	1.41408644	-2.00608442	4.93875906
6	0.60703191	-2.68252296	5.85886732
6	-0.65608417	-3.16865936	5.49620655
6	-1.09988223	-2.96183338	4.17669422
6	-0.30932432	-2.28936252	3.24898886
1	2.39961150	-1.63189991	5.21343826
1	0.96964398	-2.83601390	6.87695197
6	-1.52695331	-3.89718951	6.48914410
1	-2.08026586	-3.33528002	3.87439227
1	-0.65832063	-2.13349035	2.22796352
1	0.02930241	-2.30337206	-7.05091987
1	-1.14624736	-3.48513554	-6.45758632
1	-1.61351692	-2.31677585	-7.71958581
1	-1.77863139	-4.90596939	6.13009754
1	-1.02888357	-3.99637086	7.46174701
1	-2.47770681	-3.36630160	6.64625616
1	-0.89693838	2.76663580	-2.85506383

Energy = -8139.837970 Hartree

Number of imaginary frequencies = 0.

Compound I1a isomer 75

Atomic N.	X	Y	Z
8	3.02431392	0.63620683	-0.75461098
6	3.84573518	-0.32720781	-1.40413388
1	4.70385104	0.19115942	-1.86316680
1	3.31949515	-0.87452682	-2.21209805
1	4.23357894	-1.07541016	-0.69124622
50	1.06978233	0.14826607	-0.33768234
7	0.98581232	2.67714393	0.37906247
6	2.38239074	3.17199185	0.43498492
1	2.41427184	4.18517238	0.87744524
1	3.00237907	2.48711069	1.01976523
1	2.79876609	3.18812583	-0.57720944
7	1.11752186	0.32805359	1.88841334
6	0.41496941	2.61904862	1.75183622
1	0.47714194	3.61700484	2.22736294

1	-0.64576146	2.34617830	1.66512535
6	1.11160409	1.57987565	2.63207184
1	0.53178561	1.50130940	3.56959595
1	2.12893690	1.90546532	2.90539324
16	1.95074772	-0.96271196	2.44028638
7	-1.10368792	2.25622391	-2.06403631
6	0.20211480	3.62243033	-0.45938520
1	0.09504980	4.57866371	0.08955040
1	0.80715262	3.84016456	-1.35200540
6	-1.19102083	3.16640192	-0.89882660
1	-1.78873669	4.06612681	-1.12432017
1	-1.71068255	2.62180674	-0.10026172
16	-2.65589432	1.62688076	-2.51608374
8	-3.45698035	2.67165715	-3.19473028
8	-3.17209327	0.96196405	-1.30382346
6	-2.17650370	0.40400339	-3.74371391
6	-1.59492359	-0.79667309	-3.32771141
6	-1.25920253	-1.74718352	-4.28859898
6	-1.49721386	-1.51634163	-5.65531887
6	-2.09257277	-0.30475249	-6.03811418
6	-2.43550982	0.66166445	-5.09045919
1	-1.40807655	-0.97734385	-2.26948229
1	-2.91330173	1.59702930	-5.37973287
1	-2.29672451	-0.11523321	-7.09318502
6	-1.10307258	-2.54468375	-6.68455186
1	-0.80257039	-2.68672046	-3.97270069
8	2.01332168	-1.82846263	1.20794282
8	3.19996727	-0.62480192	3.16027881
6	0.88267563	-1.81458801	3.62899264
6	1.33806250	-2.03746477	4.92707174
6	0.50523959	-2.69752850	5.83611837
6	-0.77268191	-3.13532391	5.46368474
6	-1.20410239	-2.89788546	4.14529922
6	-0.38777281	-2.24103289	3.22867319
1	2.33468523	-1.70028129	5.20959351
1	0.85919549	-2.87657756	6.85307845
6	-1.67398508	-3.83879552	6.44745866
1	-2.19514779	-3.23479466	3.83497522
1	-0.72762367	-2.06076285	2.20854865
1	-0.01993607	-2.50335283	-6.87822786
1	-1.33044814	-3.56265140	-6.34032826
1	-1.61812803	-2.37671635	-7.63876519
1	-2.02883201	-4.79874279	6.04526409
1	-1.15684952	-4.03493341	7.39509656
1	-2.56627982	-3.23349225	6.66789282
1	-0.76423208	2.76984796	-2.88635185

Energy = -8139.837990 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 76

Atomic N.	X	Y	Z
8	4.46383852	1.31301922	-0.77228733
6	5.75006809	0.71950341	-0.91452466
1	6.51546673	1.50365875	-0.79543124
1	5.90471585	0.25161390	-1.90701904
1	5.92568604	-0.05384380	-0.14679413
50	2.81255855	0.32441235	-1.48962363

7	1.62677568	2.61076999	-1.17201689
6	2.66309232	3.57482448	-0.73128305
1	2.19613862	4.53854868	-0.45823745
1	3.22642173	3.16792163	0.11308313
1	3.38103217	3.73203625	-1.54434971
7	1.70526716	0.30396291	0.44088311
6	0.63059785	2.38521512	-0.09246801
1	0.25990355	3.35134132	0.29980807
1	-0.21310655	1.83431456	-0.52297341
6	1.20137165	1.53706296	1.04496324
1	0.37475129	1.33781434	1.75030799
1	1.98521476	2.07390634	1.60345203
16	2.47059211	-0.80043105	1.38221824
7	-0.15967074	1.04258878	-3.06001407
6	1.01397651	3.15121246	-2.41816752
1	0.78607414	4.22571446	-2.27705837
1	1.78720629	3.09381687	-3.20025387
6	-0.27735453	2.50113734	-2.91756162
1	-0.54710483	2.99682175	-3.86522451
1	-1.10076066	2.70072469	-2.21691881
16	-1.58913609	0.23289284	-3.56733403
8	-1.11186766	-1.07134786	-4.06364423
8	-2.42422294	1.11184333	-4.41570278
6	-2.44909685	0.01936975	-1.99729623
6	-3.75493353	0.49353376	-1.87262601
6	-4.43718366	0.28330023	-0.67181945
6	-3.83020076	-0.38962090	0.39887513
6	-2.50977433	-0.84961783	0.24365385
6	-1.81552637	-0.65402217	-0.94823019
1	-4.21938207	1.01704750	-2.70757836
1	-0.78958106	-1.00560053	-1.05570038
1	-2.01454953	-1.36688899	1.06746141
6	-4.57797472	-0.63432958	1.68515652
1	-5.45885121	0.65211566	-0.56619791
8	3.31160567	-1.54202134	0.37720581
8	3.08773731	-0.22666064	2.59833023
6	1.20681693	-1.97050701	1.94325956
6	0.67710418	-1.84348978	3.22782343
6	-0.31937855	-2.73103360	3.64427236
6	-0.78640694	-3.74787335	2.79863039
6	-0.22155042	-3.86146163	1.51546958
6	0.76716952	-2.98025541	1.08191787
1	1.06184658	-1.07339194	3.89573852
1	-0.73075445	-2.63880270	4.65122409
6	-1.87294768	-4.69431812	3.24446024
1	-0.55854796	-4.65711750	0.84828090
1	1.21384670	-3.08139140	0.09297630
1	-5.44743200	0.02871096	1.77777539
1	-4.94464612	-1.67167565	1.72931771
1	-3.92915671	-0.48389401	2.55869893
1	-1.63478724	-5.73218572	2.97352714
1	-2.02571823	-4.64754326	4.33013692
1	-2.83130527	-4.44835644	2.76081671
1	0.57603316	0.74692560	-3.71138789

Energy = -8139.840671 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 77

Atomic N.	X	Y	Z
8	3.06554292	3.05578482	-2.28723127
6	2.34172899	3.70967545	-3.32530361
1	2.81986321	4.68404991	-3.51897674
1	1.28456924	3.89385036	-3.05770050
1	2.34786667	3.13088811	-4.26363901
50	2.71416920	1.18460562	-1.52871813
7	2.10467445	2.51845263	0.65299314
6	3.15201169	3.54812838	0.83124035
1	2.82884370	4.31778733	1.55552112
1	4.07483808	3.08552582	1.20325314
1	3.36243350	4.00759467	-0.14305918
7	2.70158029	-0.53511841	1.48724043
6	1.88363281	1.78126736	1.92381610
1	1.84715230	2.51155466	2.75582947
1	0.90398065	1.28966888	1.87460814
6	2.93269292	0.70988326	2.23907081
1	2.90208989	0.48793757	3.31658243
1	3.94921591	1.07320763	2.03176476
16	2.30529349	-1.94928312	2.35817239
7	0.50262181	1.28561259	-1.30023257
6	0.84821627	3.17409319	0.19666248
1	0.40048473	3.76502869	1.01929965
1	1.13394636	3.86439338	-0.60851430
6	-0.17153278	2.17159815	-0.35380161
1	-0.97282879	2.74622139	-0.84683442
1	-0.63523439	1.59000602	0.46256006
16	-0.12509868	0.99035674	-2.78020557
8	1.10962982	0.58712055	-3.54926813
8	-1.00095104	2.07211522	-3.28668511
6	-1.15358060	-0.49535252	-2.67833633
6	-2.54263381	-0.36891191	-2.67867342
6	-3.33030569	-1.51926064	-2.57442213
6	-2.74932533	-2.79167303	-2.47569801
6	-1.34583358	-2.88787368	-2.48697973
6	-0.54618991	-1.75184522	-2.58786808
1	-2.99397317	0.61745868	-2.77968017
1	0.54030914	-1.83500428	-2.61254138
1	-0.87300398	-3.86932984	-2.41853298
6	-3.59976709	-4.03319120	-2.37786048
1	-4.41776621	-1.42427329	-2.57886451
8	2.68762200	-3.04865483	1.45058362
8	2.82079980	-1.88296849	3.74383711
6	0.50659961	-1.85251102	2.46125232
6	-0.10828108	-1.99493949	3.70508843
6	-1.50333398	-1.97277895	3.77519355
6	-2.28576483	-1.81258289	2.62201287
6	-1.63515514	-1.66672835	1.38334586
6	-0.24485702	-1.68821298	1.29432326
1	0.50387480	-2.11641344	4.59788492
1	-1.99094927	-2.08013040	4.74570328
6	-3.79161203	-1.81679546	2.70078725
1	-2.22368118	-1.52989378	0.47408284
1	0.24990229	-1.56136385	0.33185097
1	-4.66427020	-3.78430371	-2.28409859
1	-3.47789329	-4.66493878	-3.27043801
1	-3.31105391	-4.64550473	-1.51133125

1	-4.19029847	-2.81226348	2.45039392
1	-4.14229666	-1.56563354	3.70996487
1	-4.23121255	-1.10388428	1.99040286
1	3.43249811	-0.79224747	0.82017282

Energy = -8139.843159 Hartree
Number of imaginary frequencies = 0.

Compound 11a isomer 78

Atomic N.	X	Y	Z
8	4.43747378	1.46248800	-0.66679196
6	5.73801474	0.91834994	-0.86454265
1	5.94159738	0.09204164	-0.16160112
1	6.48296530	1.71158513	-0.68908240
1	5.89639780	0.53461626	-1.89196480
50	2.80807274	0.49424660	-1.45770792
7	1.57075009	2.72352252	-0.96916272
6	2.58630995	3.67551032	-0.45941967
1	2.09853528	4.60546648	-0.11497166
1	3.16125795	3.22006675	0.35168230
1	3.29802825	3.90901421	-1.25953629
7	1.70490161	0.30455710	0.46534922
6	0.58324859	2.39560666	0.09194625
1	0.19254227	3.32106587	0.55623729
1	-0.24939903	1.85962473	-0.37716139
6	1.17638396	1.47730133	1.16150948
1	0.35688960	1.20762124	1.85155736
1	1.95029109	1.98798127	1.75714365
16	2.49344358	-0.85326490	1.31927579
7	-0.18609710	1.25867553	-2.96410522
6	0.94250062	3.34054699	-2.17113870
1	0.69067153	4.39623684	-1.95081700
1	1.71461148	3.35875639	-2.95621970
6	-0.33532726	2.70009526	-2.71564008
1	-0.61836949	3.25738988	-3.62441616
1	-1.16091354	2.82995727	-2.00133080
16	-1.59756438	0.45774530	-3.53199896
8	-1.09304800	-0.79921626	-4.11565303
8	-2.44782430	1.37617526	-4.32159898
6	-2.45690953	0.11915183	-1.98381817
6	-3.77239440	0.55770861	-1.83142867
6	-4.45277094	0.25209141	-0.65043099
6	-3.83456325	-0.48049069	0.37395892
6	-2.50480446	-0.90174312	0.19246577
6	-1.81205799	-0.61136917	-0.98106354
1	-4.24536132	1.12867966	-2.62959744
1	-0.77887089	-0.93389137	-1.10847654
1	-2.00104441	-1.46397364	0.98088893
6	-4.58207071	-0.82994747	1.63594783
1	-5.48171095	0.59287411	-0.52318501
8	3.34958909	-1.49657139	0.26064802
8	3.09870843	-0.36340043	2.57729591
6	1.25492106	-2.09005520	1.78541591
6	0.73012166	-2.08132390	3.07782452
6	-0.24754301	-3.01983911	3.42216657
6	-0.69908950	-3.97145593	2.49662695
6	-0.14045332	-3.96500950	1.20532587
6	0.82895722	-3.03208015	0.84365592

1	1.10250954	-1.36134546	3.80593328
1	-0.65634750	-3.01918554	4.43436868
6	-1.75463000	-4.98286014	2.86820453
1	-0.46766394	-4.70666162	0.47405654
1	1.27064893	-3.04029288	-0.15265734
1	-5.43203613	-0.15540653	1.80023072
1	-4.97946771	-1.85536988	1.57909410
1	-3.92496792	-0.78560334	2.51478864
1	-1.41146843	-6.00766501	2.66595215
1	-2.01941272	-4.91477602	3.93081997
1	-2.67210136	-4.83150585	2.27934120
1	0.55593996	1.02755415	-3.63419334

Energy = -8139.840667 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 79

Atomic N.	X	Y	Z
8	4.29829132	0.40561975	-0.52952142
6	5.08573349	0.15697741	-1.68917619
1	5.15524661	1.04720742	-2.33563255
1	4.69246276	-0.67002183	-2.30929037
1	6.10309753	-0.11340000	-1.36273423
50	2.31202220	0.80483569	-0.46518189
7	1.81337839	-1.83136436	0.11165571
6	3.14441501	-2.47429103	0.09417855
1	3.05427703	-3.56870013	0.22999353
1	3.65321282	-2.27053237	-0.85339497
1	3.76247367	-2.05530942	0.89605262
7	1.58303806	-0.30022663	-2.24682913
6	0.99918149	-2.29762025	-1.03823302
1	0.98375441	-3.40556847	-1.06874943
1	-0.03106319	-1.94992090	-0.88383131
6	1.48288583	-1.74870188	-2.38210007
1	0.73751382	-2.03675814	-3.14418805
1	2.44145498	-2.20469353	-2.68238530
16	1.91906950	0.65425022	-3.52835880
7	0.11079449	-0.03029808	2.31433653
6	1.14500981	-2.18580823	1.39289984
1	0.86345704	-3.25843804	1.36080284
1	1.87713979	-2.07215204	2.20224592
6	-0.10562240	-1.36996634	1.75614624
1	-0.67150128	-1.94908439	2.49882619
1	-0.77282894	-1.25273696	0.88871407
16	0.56230201	0.10610719	3.94930044
8	1.39881877	1.31964795	4.01653734
8	1.03643800	-1.20485913	4.44871229
6	-1.00408157	0.44645511	4.77833211
6	-1.62973422	-0.56292568	5.50940290
6	-2.83473021	-0.28154912	6.15816142
6	-3.41442565	0.99352826	6.09098944
6	-2.75500681	1.99150451	5.35109298
6	-1.55398055	1.72887804	4.69670368
1	-1.16634632	-1.54637078	5.57788668
1	-1.03715109	2.50795086	4.13708069
1	-3.18832005	2.99167046	5.29304022
6	-4.69757326	1.30192931	6.82040455
1	-3.32868227	-1.06701787	6.73291009

8	2.33525457	1.92621164	-2.82326378
8	2.81623019	0.04400914	-4.53470309
6	0.36141632	1.01275435	-4.37283742
6	0.14759382	0.51333806	-5.65735168
6	-1.06568325	0.78152571	-6.29703123
6	-2.06189175	1.54567664	-5.67330267
6	-1.81637057	2.03656149	-4.37801313
6	-0.61486636	1.77516300	-3.72440531
1	0.93091216	-0.06507908	-6.14562741
1	-1.23677062	0.39311800	-7.30265694
6	-3.35530330	1.86266399	-6.38083244
1	-2.57871161	2.63662376	-3.87758465
1	-0.42628592	2.16774203	-2.72515194
1	-5.25234176	0.38637951	7.06200698
1	-4.49073703	1.82422017	7.76746237
1	-5.34913862	1.95680136	6.22604200
1	-3.32992963	2.88004994	-6.80136665
1	-3.54080825	1.16703657	-7.20914982
1	-4.21022775	1.81904547	-5.69226854
1	0.71323832	0.58791166	1.75323522

Energy = -8139.840693 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 80

Atomic N.	X	Y	Z
8	4.30311442	-0.42449622	0.54585898
6	5.49221417	0.28458244	0.88082991
1	5.61554417	1.21583695	0.29538964
1	6.35766901	-0.36163477	0.66219290
1	5.52206765	0.54925151	1.95206912
50	2.49804801	0.55639547	0.43864958
7	1.81792613	-1.71675292	-0.46339382
6	2.71335956	-2.15423869	-1.55671972
1	2.49062514	-3.19178131	-1.86489551
1	2.61270007	-1.48768768	-2.42051233
1	3.74388260	-2.08905508	-1.18865920
7	0.49903001	0.16190517	-2.41867563
6	0.38199640	-1.76335648	-0.83819308
1	0.02786526	-2.81291283	-0.82032876
1	-0.18036933	-1.22162566	-0.06238739
6	0.02054525	-1.21067019	-2.21913605
1	-1.07684768	-1.29957896	-2.32081630
1	0.47348699	-1.82302842	-3.00903954
16	0.47097527	0.78842273	-4.00442535
7	1.51033062	-0.61994765	2.07662583
6	2.05903275	-2.57232610	0.73615592
1	1.77288610	-3.61859768	0.51485203
1	3.13876860	-2.52442913	0.93041432
6	1.31226526	-2.06485599	1.97220888
1	1.72502265	-2.58926974	2.84888091
1	0.23678700	-2.30988487	1.91586728
16	2.07315700	0.02342449	3.47332218
8	2.75707338	1.27660287	2.98984768
8	2.80805835	-0.94178435	4.32296833
6	0.64303471	0.57423653	4.43826007
6	0.29192595	-0.11426768	5.59835364
6	-0.82536142	0.30483279	6.32697157

6	-1.59161123	1.40287764	5.91348469
6	-1.20712202	2.08374807	4.74378300
6	-0.09905684	1.67729837	4.00480418
1	0.90148462	-0.95434437	5.92929219
1	0.20514339	2.21850763	3.10879859
1	-1.78218521	2.95132764	4.41377224
6	-2.79839554	1.85298819	6.69869273
1	-1.09944394	-0.22844809	7.23915589
8	0.96195512	2.16943209	-3.87126511
8	1.14181080	-0.22536170	-4.83928159
6	-1.26163862	0.85928514	-4.51264184
6	-1.81812136	-0.20315631	-5.22650628
6	-3.16241728	-0.13740362	-5.60139240
6	-3.95471837	0.97265760	-5.27413860
6	-3.36266556	2.03170470	-4.56250697
6	-2.02405281	1.98410004	-4.17978461
1	-1.19611197	-1.05284934	-5.50585993
1	-3.59997201	-0.96066140	-6.16864762
6	-5.40649751	1.03900872	-5.67537303
1	-3.95812054	2.91281808	-4.31620251
1	-1.55929266	2.81854808	-3.65473512
1	-2.90659571	1.28174050	7.62923349
1	-2.72892972	2.91941996	6.95786227
1	-3.72148398	1.72419099	6.11344180
1	-5.63044577	1.97892723	-6.19963353
1	-5.67979084	0.20516701	-6.33369929
1	-6.06086534	1.00045382	-4.79137325
1	0.11232686	0.85471474	-1.77181550

Energy = -8139.843580 Hartree

Number of imaginary frequencies = 0.

Compound 11a isomer 81

Atomic N.	X	Y	Z
8	4.00682796	-0.63846090	-2.41404577
6	4.92041663	0.11898411	-3.20063210
1	5.59351860	0.75486461	-2.59191494
1	4.39233758	0.77484188	-3.91427979
1	5.55294406	-0.57731322	-3.77505899
50	3.08830946	0.24939504	-0.80569381
7	2.45771960	-2.18223674	-0.15191217
6	3.10927487	-3.07408546	-1.14058229
1	2.77900684	-4.11778075	-0.98885225
1	2.88260074	-2.74363455	-2.15809486
1	4.19719449	-3.01245394	-1.02283647
7	1.00674244	-0.16483612	-1.47426968
6	0.97880231	-2.25010226	-0.28161883
1	0.63880592	-3.30322468	-0.28667488
1	0.54144809	-1.74427780	0.58637880
6	0.48015665	-1.52802359	-1.53429519
1	-0.62402843	-1.54109011	-1.50119353
1	0.78539423	-2.04856334	-2.45646473
16	0.72550847	0.86538477	-2.71950069
7	2.09169084	-0.55593257	2.38319243
6	2.93767440	-2.58579225	1.19973007
1	2.88850026	-3.68836458	1.29113420
1	4.00355818	-2.31341318	1.25001044
6	2.20068472	-2.02173146	2.41567269

1	2.72668729	-2.38570219	3.31423464
1	1.18078720	-2.42917957	2.46591210
16	1.22962115	0.15060361	3.69212423
8	1.64154522	1.56664829	3.67638590
8	1.36132810	-0.66741903	4.91817528
6	-0.47179625	-0.00489164	3.11664532
6	-1.40596671	-0.63959758	3.93460902
6	-2.73439442	-0.71635439	3.50799268
6	-3.13386582	-0.17233299	2.27872177
6	-2.16570330	0.45610274	1.47368110
6	-0.83810152	0.54746672	1.88483691
1	-1.08813167	-1.06441774	4.88612965
1	-0.09355488	1.02757120	1.25012763
1	-2.45282235	0.87911748	0.50916086
6	-4.57042196	-0.24549373	1.82630078
1	-3.47143970	-1.21162694	4.14232697
8	1.86233487	1.84339603	-2.58117321
8	0.46997595	0.19002672	-4.01080034
6	-0.77977207	1.78381456	-2.30541539
6	-1.99212695	1.41340528	-2.88769702
6	-3.15473231	2.10835424	-2.54070841
6	-3.12019069	3.17222865	-1.62782408
6	-1.88059365	3.53267946	-1.06873064
6	-0.71386724	2.84618757	-1.39843784
1	-2.01421321	0.60652161	-3.61958091
1	-4.10389616	1.82518635	-2.99956083
6	-4.37677190	3.91461481	-1.24701343
1	-1.82923805	4.36817787	-0.36793824
1	0.24692930	3.13895427	-0.97543561
1	-5.15938728	-0.91582569	2.46463986
1	-5.04081057	0.74910257	1.85860110
1	-4.64244790	-0.60149515	0.78899549
1	-4.23491533	5.00209772	-1.32021848
1	-5.21946090	3.63407346	-1.89134868
1	-4.66200871	3.69853161	-0.20578377
1	2.99633352	-0.07267913	2.34986793

Energy = -8139.840684 Hartree

Number of imaginary frequencies = 0.

Compound I1a isomer 82

Atomic N.	X	Y	Z
8	4.34515774	-0.23971405	0.05524316
6	5.52306469	0.36205325	0.58367583
1	5.54031780	1.46079765	0.45049860
1	6.39543112	-0.05001509	0.05107236
1	5.64359588	0.14772963	1.65980302
50	2.49189563	0.53905514	0.49588516
7	1.84404577	-1.19969737	-1.24019250
6	2.65789840	-1.05889792	-2.46755959
1	2.46233717	-1.88600464	-3.17387440
1	2.44445817	-0.10246224	-2.95799153
1	3.71281893	-1.06558891	-2.16969768
7	0.22965512	1.20100293	-2.10379724
6	0.38522084	-1.21527483	-1.51504157
1	0.09713708	-2.20120902	-1.93026648
1	-0.13512773	-1.10847848	-0.55102336
6	-0.13275291	-0.16445617	-2.49981592

1	-1.22587102	-0.31041839	-2.57770982
1	0.29182703	-0.33015696	-3.49799589
16	0.03598422	2.43968397	-3.25960034
7	1.72279526	-1.29455617	1.54103573
6	2.24042789	-2.45295726	-0.53232157
1	1.99011266	-3.33225473	-1.15673536
1	3.32952142	-2.39716208	-0.40360463
6	1.58639685	-2.57419579	0.84622162
1	2.10313429	-3.38110970	1.39011004
1	0.52360407	-2.86180064	0.75906682
16	2.38067683	-1.24864655	3.03967470
8	2.96693051	0.13925454	3.08500383
8	3.22596870	-2.42270226	3.35727873
6	1.02310958	-1.25257523	4.23864782
6	0.80352543	-2.38406558	5.02364850
6	-0.25699106	-2.38574882	5.93377257
6	-1.09515195	-1.27058750	6.07416428
6	-0.84736847	-0.14318159	5.27093501
6	0.20363332	-0.12644295	4.35665277
1	1.46857943	-3.24150814	4.92703282
1	0.40144577	0.75602857	3.74803354
1	-1.48519148	0.73739902	5.37035284
6	-2.21495674	-1.26258185	7.08466350
1	-0.43005289	-3.26907762	6.55144625
8	0.40957078	3.67428554	-2.55090121
8	0.73503515	1.96392357	-4.46802316
6	-1.72691754	2.52946353	-3.64682747
6	-2.22752652	1.84949606	-4.75796458
6	-3.59449098	1.92214724	-5.03780094
6	-4.46432510	2.66323636	-4.22477049
6	-3.92831752	3.34465248	-3.11699874
6	-2.56827367	3.28397580	-2.82210171
1	-1.54785552	1.29648660	-5.40537552
1	-3.98972225	1.40046687	-5.91109826
6	-5.94003667	2.73513412	-4.52505993
1	-4.58676717	3.94164176	-2.48325559
1	-2.15138685	3.83338384	-1.97788889
1	-2.50372734	-2.28186763	7.37183114
1	-1.90964626	-0.73446734	8.00152724
1	-3.10340599	-0.74676781	6.69533296
1	-6.28852059	3.77727856	-4.55508712
1	-6.17721023	2.26584720	-5.48782110
1	-6.52473630	2.22298835	-3.74597607
1	-0.15898277	1.50921873	-1.20843220

Energy = -8139.843603 Hartree

Number of imaginary frequencies = 0.

Intermediate 1b (I1b)

Compound I1b isomer 1

Atomic N.	X	Y	Z
50	0.29443114	-0.34789876	-0.87369693
7	0.84214421	-0.68301334	2.46858151
6	1.97626522	-0.54987198	3.37967116
1	1.68577038	-0.70797163	4.44159678
1	2.43127504	0.44663206	3.29838712
1	2.74450122	-1.29028686	3.12076712

7	0.83968070	1.64209340	0.86190245
6	-0.17403892	0.33814531	2.70851054
1	-0.47206799	0.40583259	3.77932413
1	-1.07152104	0.06567588	2.13623950
6	0.28960297	1.71814978	2.23556017
1	-0.56715799	2.40205515	2.24420675
1	1.04186379	2.14560425	2.92246798
6	1.06574756	2.90483039	0.20716242
6	-0.02836383	3.66569509	-0.25626974
6	0.22329721	4.87875971	-0.91174112
6	1.51947109	5.35079505	-1.13439606
6	2.58779104	4.56709212	-0.68132473
6	2.38868999	3.35388954	-0.01489721
7	-0.56794922	-2.05567553	0.14601478
6	0.33318485	-2.05847663	2.50308151
1	-0.00444128	-2.33786857	3.52841607
1	1.18110740	-2.71434364	2.25326789
6	-0.82532458	-2.35522057	1.55389330
1	-1.02850678	-3.43715615	1.66505905
1	-1.73849346	-1.85504558	1.93751911
6	-1.51667094	-2.64944145	-0.74827061
6	-2.88337808	-2.26334089	-0.79030572
6	-3.75176511	-2.88125356	-1.70079533
6	-3.32082315	-3.87303340	-2.58562940
6	-1.96794390	-4.23081833	-2.55281480
6	-1.06574734	-3.64294407	-1.65941592
6	-1.45539549	3.20115322	-0.09473486
1	-0.62768785	5.46046400	-1.27427020
6	1.76503876	6.64080740	-1.87875875
1	3.61195000	4.90850961	-0.85011263
6	3.57820489	2.54034408	0.43846205
6	-3.42511185	-1.16261788	0.08771780
1	-4.79681986	-2.56076086	-1.72757854
6	-4.28036815	-4.54415164	-3.53837895
1	-1.60125241	-4.99653728	-3.24148321
6	0.37722780	-4.08794454	-1.66766964
1	-2.09079568	3.64550323	-0.87144104
1	-1.88118691	3.49327194	0.87866170
1	-1.53339190	2.10756033	-0.17575826
1	3.56894082	2.36893400	1.52686439
1	4.51134343	3.06397305	0.19705802
1	3.60133545	1.55252104	-0.05054087
1	2.00261556	6.44650586	-2.93651736
1	2.61338384	7.19441806	-1.45279778
1	0.88171350	7.29242270	-1.85363450
1	-4.30057025	-0.69243532	-0.37914665
1	-2.66507029	-0.38549868	0.25960428
1	-3.73930966	-1.53630098	1.07486890
1	0.73388996	-4.30705031	-0.65256235
1	1.04745312	-3.31270381	-2.07067951
1	0.49805691	-4.98478416	-2.28965938
1	-3.82293443	-4.70047252	-4.52551549
1	-5.19214414	-3.94713832	-3.67351638
1	-4.58598640	-5.53367957	-3.16305125
1	1.71386457	1.10239986	0.88925688
8	2.33366557	-0.52633638	-0.52456533
6	3.02002800	-1.68292825	-0.07847719
1	3.66269163	-2.08489285	-0.88295040

1 2.33845190 -2.48983248 0.24388988
 1 3.67753935 -1.43431194 0.77534483
 Energy = -7200.155530 Hartree
 Number of imaginary frequencies = 0.

Compound 11b isomer 2

Atomic N.	X	Y	Z
50	1.40852025	-1.48287568	-0.11780923
7	0.94522690	-0.81304707	2.21621989
6	2.19964346	-0.69961685	2.99318763
1	1.98355027	-0.62279398	4.07342462
1	2.76426662	0.18636767	2.68110736
1	2.80473508	-1.59181635	2.79408988
7	0.51468667	1.92649152	0.53822275
6	0.05771481	0.36440907	2.44418718
1	-0.15391218	0.41557769	3.52994111
1	-0.88863233	0.17152450	1.92328929
6	0.57677817	1.73070483	1.99429734
1	-0.08456020	2.47174333	2.46130550
1	1.58509506	1.93031666	2.40599951
6	0.64586662	3.26694417	0.06888253
6	-0.41063126	4.18710250	0.25831410
6	-0.27216333	5.49254327	-0.23128361
6	0.86562484	5.91306792	-0.92644035
6	1.88704121	4.97710368	-1.13046964
6	1.80088042	3.66827274	-0.64536542
7	-0.45568124	-2.38272851	0.31418240
6	0.23497015	-2.06473099	2.63326628
1	-0.13054427	-1.95362733	3.67108149
1	0.98841936	-2.86391414	2.60163007
6	-0.91467843	-2.42489696	1.69517929
1	-1.24678388	-3.44273312	1.97969924
1	-1.78568854	-1.76404906	1.88232941
6	-1.35074099	-2.84369975	-0.69001271
6	-2.52646189	-2.12137406	-1.02736266
6	-3.38043065	-2.61459632	-2.02125541
6	-3.11166411	-3.80136594	-2.71190446
6	-1.93677769	-4.48862526	-2.39115486
6	-1.05651552	-4.03697697	-1.39916636
6	-1.70105347	3.77759572	0.92524815
1	-1.09678261	6.19438692	-0.08244670
6	0.97365629	7.31425253	-1.47865098
1	2.78470986	5.27522050	-1.67819132
6	2.93226169	2.69888925	-0.89630231
6	-2.84415323	-0.79781696	-0.37756393
1	-4.27503728	-2.03967344	-2.27618816
6	-4.06718459	-4.32973657	-3.75474690
1	-1.69744021	-5.41360103	-2.92261293
6	0.19480922	-4.82960588	-1.10561483
1	-2.52895170	4.40904945	0.57729505
1	-1.66035896	3.87908391	2.02217689
1	-1.93971889	2.72832780	0.70153776
1	2.63001020	1.86791175	-1.55427488
1	3.30682773	2.24703843	0.03576497
1	3.77485739	3.20800465	-1.38073294
1	0.70743299	7.34259141	-2.54713660
1	1.99825304	7.70220097	-1.39068180

1	0.29999595	8.00437707	-0.95356856
1	-3.53153186	-0.21450097	-1.00411497
1	-1.92829427	-0.20822630	-0.22248435
1	-3.32596209	-0.92039185	0.60612750
1	0.44420663	-4.81749407	-0.03743520
1	1.07262920	-4.41328460	-1.62692165
1	0.08156245	-5.86824771	-1.44438304
1	-3.54533236	-4.93774788	-4.50615158
1	-4.58580668	-3.51188183	-4.27401953
1	-4.84110472	-4.96711952	-3.29785578
1	1.19839908	1.32373282	0.07432893
8	2.60797375	-2.92053037	0.78591902
6	3.96070207	-3.07767175	0.38455193
1	4.12863541	-4.09572762	-0.00913626
1	4.64219209	-2.93521772	1.24395342
1	4.27244452	-2.36288833	-0.40330053

Energy = -7200.167395 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 3

Atomic N.	X	Y	Z
50	0.98292514	-1.52520269	-0.15116078
7	-0.18437446	-0.67734446	1.84072916
6	0.65548389	-0.78716563	3.05560581
1	0.09148018	-0.47217075	3.95064225
1	1.54802436	-0.15936216	2.95560939
1	0.97607758	-1.82856777	3.18101744
7	0.11442710	2.85735454	0.66704497
6	-0.61685839	0.73246821	1.62172944
1	-1.27503553	1.04087615	2.45387498
1	-1.19834568	0.75211423	0.69176761
6	0.55168358	1.71602961	1.47809396
1	0.88142129	2.08182174	2.45809165
1	1.41692754	1.19803131	1.01523477
6	0.90791915	4.03739731	0.71753539
6	0.90409908	4.84163926	1.88034135
6	1.66787911	6.01631389	1.90044397
6	2.41757730	6.43864951	0.79888814
6	2.38227572	5.64476027	-0.35469176
6	1.64867787	4.45610736	-0.41528288
7	-0.80004110	-2.70853820	-0.07803981
6	-1.38099998	-1.57080448	1.96646175
1	-2.16407264	-1.04862914	2.54445106
1	-1.06648617	-2.46259484	2.52475799
6	-1.89243274	-2.01870887	0.59832838
1	-2.74212256	-2.70234570	0.76304752
1	-2.28882167	-1.14406096	0.04721529
6	-1.08351911	-3.83206053	-0.88945640
6	-2.09077260	-3.81195753	-1.89274690
6	-2.34333681	-4.96724086	-2.64405999
6	-1.62036173	-6.15039029	-2.46558430
6	-0.60667463	-6.14683298	-1.50097778
6	-0.32896671	-5.02457295	-0.71282223
6	0.05132514	4.48945229	3.07453847
1	1.65407198	6.63109213	2.80419635
6	3.21272844	7.72196971	0.83414464
1	2.95255749	5.95306527	-1.23489392

6	1.64755577	3.63585533	-1.68339750
6	-2.84642364	-2.54782649	-2.22757856
1	-3.11689310	-4.92676090	-3.41607146
6	-1.93222619	-7.38933258	-3.27014768
1	-0.01803114	-7.05442144	-1.34225596
6	0.76364799	-5.10771843	0.32391055
1	-0.18130497	5.38925106	3.65904643
1	0.55088831	3.78274987	3.75742003
1	-0.89073414	4.02186766	2.75413545
1	0.65865874	3.63415819	-2.17127209
1	1.91436006	2.58493486	-1.49640359
1	2.36442109	4.04474229	-2.40644057
1	2.74184726	8.50175070	0.21530610
1	4.23080858	7.57421738	0.44524650
1	3.29309966	8.11318927	1.85686961
1	-3.28252551	-2.61993329	-3.23251240
1	-2.18402884	-1.67091293	-2.19683712
1	-3.67282998	-2.34761587	-1.52763507
1	0.44094299	-4.66761504	1.27866132
1	1.66968309	-4.55881243	0.01789978
1	1.05698887	-6.15219563	0.49366310
1	-1.02970145	-7.98971898	-3.45028111
1	-2.37296857	-7.13359942	-4.24362616
1	-2.65387386	-8.03606655	-2.74542328
1	0.01196052	2.51873906	-0.29244319
8	0.11523365	0.11352012	-1.14837753
6	0.31129878	0.15860134	-2.55638664
1	1.37925522	0.09709946	-2.84693290
1	-0.08028901	1.11378973	-2.94460026
1	-0.22315962	-0.65252832	-3.08761082

Energy = -7200.169162 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 4

Atomic N.	X	Y	Z
50	0.03728920	-0.68605747	-0.71963219
7	0.13414835	-0.99129251	1.72840198
6	1.34673320	-1.75717036	2.09238978
1	1.37990114	-1.95661957	3.17798709
1	2.24206192	-1.20169623	1.79640027
1	1.33861017	-2.71310125	1.55499382
7	1.67381808	1.53319647	0.98502956
6	0.07488631	0.31094153	2.46139874
1	-0.10279669	0.10187787	3.53255364
1	-0.79220056	0.85744820	2.06464006
6	1.32256714	1.19105092	2.36848222
1	1.10360533	2.09097801	2.97912365
1	2.17712362	0.69890440	2.85506557
6	2.73962463	2.47128031	0.82995203
6	4.08102259	2.06158609	1.00390928
6	5.11053342	2.99872297	0.84574914
6	4.85958398	4.32872247	0.49595018
6	3.52652161	4.71005037	0.30276795
6	2.46558899	3.81249538	0.46540977
7	-1.76997825	-1.77198368	-0.27710535
6	-1.09115381	-1.79888016	2.04014712
1	-1.38466757	-1.62388724	3.09071101

1	-0.82363521	-2.85735286	1.92524866
6	-2.23875500	-1.49584312	1.07614707
1	-3.07865914	-2.15697682	1.34463184
1	-2.58468929	-0.45514925	1.22366697
6	-2.60494401	-2.48537135	-1.16341306
6	-3.96960326	-2.13286240	-1.36609708
6	-4.76261998	-2.89329588	-2.23493958
6	-4.26175045	-3.98902324	-2.94396889
6	-2.91059431	-4.30464468	-2.76621199
6	-2.08096405	-3.58664691	-1.89753669
6	4.42840136	0.62441690	1.30007507
1	6.14333647	2.66716382	0.98007756
6	5.98707370	5.31234836	0.29345370
1	3.30050249	5.74292142	0.02527452
6	1.04866439	4.28504001	0.24098252
6	-4.57260060	-0.90171183	-0.73117372
1	-5.80493437	-2.59584383	-2.38107641
6	-5.14769548	-4.80964645	-3.85023256
1	-2.48476668	-5.15146747	-3.31130531
6	-0.64221668	-4.01337891	-1.74827905
1	5.48377606	0.42748231	1.07176070
1	3.80676153	-0.05094806	0.69440464
1	4.27167589	0.36061497	2.35877285
1	0.38514140	4.02503563	1.07912943
1	0.60701574	3.83669735	-0.66245073
1	1.02372560	5.37475844	0.11461538
1	6.90039181	4.98599186	0.80842863
1	5.72035051	6.31071937	0.66785029
1	6.23194565	5.42195802	-0.77491547
1	-5.46353234	-0.58519197	-1.28931060
1	-3.85472310	-0.06957027	-0.72178771
1	-4.88380198	-1.06472527	0.31254246
1	-0.33205643	-4.00960893	-0.69268387
1	0.05003679	-3.33973947	-2.27988607
1	-0.49320113	-5.02169283	-2.15710262
1	-4.57992436	-5.23725357	-4.68820564
1	-5.96586157	-4.20452587	-4.26507694
1	-5.60830839	-5.65008395	-3.30612856
1	0.81608348	1.83574123	0.49759929
8	-0.84732469	1.18688904	-0.26812034
6	-1.52228202	1.84997270	-1.32826122
1	-0.84400077	2.12969584	-2.15880864
1	-1.97555377	2.77804252	-0.94140758
1	-2.33870661	1.24049888	-1.76060660

Energy = -7200.170796 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 5

Atomic N.	X	Y	Z
50	0.03365537	-0.70377840	-0.71830908
7	0.15686579	-0.98794566	1.73001786
6	1.37368954	-1.75032367	2.08733720
1	1.41816411	-1.94133831	3.17402884
1	2.26546099	-1.19651524	1.77770184
1	1.36058852	-2.71036372	1.55741278
7	1.69267198	1.53143018	0.95708500
6	0.10410415	0.31977400	2.45386111

1	-0.06513157	0.11827960	3.52781493
1	-0.76600555	0.86373354	2.06026136
6	1.35113930	1.19889366	2.34522283
1	1.13647851	2.10311835	2.95105335
1	2.20909985	0.71017064	2.82935367
6	2.75424013	2.47208596	0.78849425
6	4.09788206	2.06718125	0.95604053
6	5.12388119	3.00560666	0.78330785
6	4.86699079	4.33231442	0.42550238
6	3.53153679	4.70887771	0.23936738
6	2.47407192	3.80991906	0.41631436
7	-1.77230335	-1.77990932	-0.24777519
6	-1.06471400	-1.79372008	2.06062788
1	-1.34513868	-1.61368768	3.11392308
1	-0.79888277	-2.85277283	1.94718552
6	-2.22371897	-1.49432066	1.10941940
1	-3.06162284	-2.15212055	1.39223532
1	-2.56597318	-0.45212030	1.25525418
6	-2.62307236	-2.49054666	-1.12130757
6	-3.98691852	-2.12796709	-1.31018947
6	-4.79616066	-2.88674885	-2.16549909
6	-4.31218122	-3.99016347	-2.87426608
6	-2.96147416	-4.31552002	-2.71044228
6	-2.11615969	-3.59986201	-1.85522313
6	4.45078067	0.63292512	1.25976756
1	6.15845698	2.67763750	0.91274520
6	5.99042148	5.31730365	0.20767550
1	3.30081849	5.73907205	-0.04417371
6	1.05439581	4.27733691	0.19856700
6	-4.57118323	-0.88732314	-0.67636869
1	-5.83771189	-2.58174535	-2.30111450
6	-5.21459968	-4.80824889	-3.76640636
1	-2.54879433	-5.16866105	-3.25582504
6	-0.67923504	-4.03724349	-1.71926466
1	5.50562654	0.43748315	1.02782872
1	3.82809949	-0.04796887	0.66136608
1	4.29949846	0.37537466	2.32078395
1	0.39677736	4.01929039	1.04192468
1	0.60866148	3.82349597	-0.70009740
1	1.02561123	5.36637314	0.06719737
1	6.91187946	4.99025644	0.70743396
1	5.72910273	6.31461235	0.58881144
1	6.21823435	5.43000003	-0.86411884
1	-5.46456676	-0.56462677	-1.22701466
1	-3.84476726	-0.06260063	-0.67912184
1	-4.87311928	-1.04128866	0.37148082
1	-0.35874430	-4.03215326	-0.66678652
1	0.01270071	-3.37057754	-2.25999882
1	-0.54217375	-5.04803335	-2.12611451
1	-4.66241102	-5.23285528	-4.61629228
1	-6.04031300	-4.20190334	-4.16405845
1	-5.66476905	-5.65095300	-3.21706853
1	0.83083246	1.82786659	0.47306147
8	-0.83927049	1.17631980	-0.27426889
6	-1.51889009	1.83384820	-1.33491018
1	-0.84306896	2.11476193	-2.16704749
1	-1.97604691	2.76065028	-0.94957965
1	-2.33329612	1.21991394	-1.76482377

Energy = -7200.170810 Hartree
 Number of imaginary frequencies = 0.

Compound 11b isomer 6

Atomic N.	X	Y	Z
8	-0.03102861	-2.02003157	0.44059512
6	0.62549771	-2.75796712	1.45911504
1	0.01560744	-2.83791728	2.37970965
1	1.60341832	-2.32318794	1.75021823
1	0.81661450	-3.78498666	1.10221568
50	-0.00549216	0.10406461	0.53695135
7	-1.80715203	-0.26193862	-1.08436461
6	-2.21208481	1.02797709	-1.67954122
1	-3.11463790	0.90676220	-2.30452879
1	-1.39961398	1.42790316	-2.29662981
1	-2.42047623	1.74600973	-0.87852114
7	0.92301468	-0.95019874	-2.14907123
6	-1.51567818	-1.27634982	-2.13358483
1	-2.39489560	-1.37386546	-2.79787470
1	-1.37431984	-2.22964800	-1.60571287
6	-0.28064002	-0.99867078	-2.98667312
1	-0.22988564	-1.80399604	-3.74604831
1	-0.38328800	-0.05750539	-3.54445501
6	2.18263414	-0.84004319	-2.80490822
6	2.55940253	0.36837439	-3.43334291
6	3.81276512	0.45164013	-4.05374895
6	4.71757139	-0.61404150	-4.05468962
6	4.34017467	-1.78872515	-3.39285456
6	3.09317653	-1.92442710	-2.77419716
7	-1.84010233	0.48507426	1.60052667
6	-2.88071383	-0.79944062	-0.19452908
1	-2.52845428	-1.78795094	0.13001224
1	-3.81782604	-0.91629559	-0.77042754
6	-3.11362371	0.07732032	1.03338779
1	-3.74114264	0.95647470	0.76874566
1	-3.73044901	-0.52130628	1.73154293
6	-1.88241329	1.10484352	2.87963736
6	-2.16241286	0.34869153	4.04853746
6	-2.16710216	0.97891004	5.29998056
6	-1.90172723	2.34345541	5.44636595
6	-1.62002050	3.07872098	4.28903862
6	-1.61012651	2.49144317	3.01832224
6	1.67056429	1.58666090	-3.39337072
1	4.09730826	1.39374624	-4.52916424
6	6.05206475	-0.50692993	-4.75114787
1	5.03516204	-2.63155885	-3.36040647
6	2.74094731	-3.21439835	-2.07125817
6	-2.42034786	-1.13577295	3.97282015
1	-2.36902087	0.37609666	6.18986223
6	-1.93806025	3.00764364	6.80198226
1	-1.40684731	4.14767241	4.37515932
6	-1.31586429	3.35287348	1.81306449
1	2.26328954	2.49912353	-3.53781670
1	1.15461211	1.65739079	-2.42442907
1	0.90185948	1.57301906	-4.18339596
1	2.62871521	-3.07500576	-0.98435101
1	3.52763828	-3.96300376	-2.22722906

1	1.79434463	-3.64068082	-2.43777056
1	6.35532559	0.54137844	-4.87452831
1	6.01418185	-0.95859243	-5.75528471
1	6.84096438	-1.02824050	-4.19123416
1	-2.10493255	-1.63318940	4.89985423
1	-1.88395808	-1.58383295	3.12516575
1	-3.49092756	-1.35916668	3.83518381
1	-2.06294597	3.20322379	1.02042676
1	-0.33449135	3.12187531	1.37079829
1	-1.31525689	4.41525167	2.09101416
1	-1.77786188	2.27913925	7.60834689
1	-2.91205301	3.48952951	6.98362792
1	-1.16965141	3.78862434	6.88766426
1	0.90067188	-1.73204813	-1.48278239

Energy = -7200.172262 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 7

Atomic N.	X	Y	Z
8	0.65846309	-0.79516970	6.08381723
6	-0.32545785	0.03650815	6.69152616
1	-0.43557549	1.00971633	6.18705355
1	-0.02436194	0.21830300	7.73582582
1	-1.31244892	-0.45607097	6.70148940
50	1.31873477	-1.01672887	4.18800403
7	-0.64760944	-0.71009951	-0.73329841
6	-1.23620300	0.51489758	-1.24896987
1	-0.65652459	1.44029434	-1.05160356
1	-2.23455105	0.65160097	-0.80671743
1	-1.35701581	0.42792358	-2.33941718
7	2.84161765	-0.84211044	-2.38111356
6	0.51504300	-1.20821784	-1.45501498
1	0.21879082	-1.34374130	-2.51022580
1	0.75225164	-2.21085945	-1.05853865
6	1.80835005	-0.35063779	-1.45283793
1	1.56267518	0.68607263	-1.71220277
1	2.25875308	-0.32815637	-0.44903639
6	2.62244451	-0.76722302	-3.78081779
6	2.53067868	0.48889241	-4.42921653
6	2.35233781	0.52771962	-5.81770398
6	2.29298032	-0.62922851	-6.60133461
6	2.44256187	-1.85884302	-5.94955643
6	2.60104444	-1.95016192	-4.56310401
7	-0.14296253	-0.05383534	3.02344391
6	-0.70262266	-0.88446747	0.70924004
1	-0.43153097	-1.92835326	0.94282447
1	-1.75270043	-0.74788987	1.01786153
6	0.16883485	0.05302883	1.58882644
1	1.23430410	-0.20043541	1.45081863
1	0.04931591	1.09105499	1.23768487
6	-1.38657251	0.50815575	3.43797750
6	-2.42646827	-0.33141446	3.91384481
6	-3.64226393	0.23973408	4.30857238
6	-3.86917765	1.61964537	4.26360629
6	-2.82153661	2.43557740	3.82572549
6	-1.58869085	1.91291227	3.41536955
6	2.69965043	1.78491393	-3.67380204

1	2.28832356	1.50470030	-6.30425050
6	2.07068383	-0.55519913	-8.09271864
1	2.42678228	-2.78115203	-6.53587954
6	2.75465239	-3.30702402	-3.91747266
6	-2.25194251	-1.82687238	4.02322086
1	-4.43755629	-0.41933745	4.66539578
6	-5.20196723	2.20473097	4.66274989
1	-2.95729584	3.52028091	3.81761081
6	-0.48944867	2.86951754	3.02088159
1	3.06542331	2.57142728	-4.34706682
1	3.41679010	1.66683075	-2.84904934
1	1.75525509	2.14885325	-3.23773922
1	3.73202913	-3.42698484	-3.42012077
1	2.67860071	-4.10112178	-4.67061355
1	1.97852286	-3.49333952	-3.15758532
1	0.99941214	-0.62416959	-8.34109623
1	2.57875451	-1.37680341	-8.61623745
1	2.43984713	0.39368192	-8.50557291
1	-3.21894518	-2.31233572	4.20785314
1	-1.58590749	-2.09664882	4.85886206
1	-1.81419692	-2.25771030	3.11232837
1	-0.48435230	3.07442527	1.93861336
1	0.50031448	2.46927845	3.28057168
1	-0.62265274	3.83357687	3.52935646
1	-5.67655861	1.61610726	5.45966745
1	-5.89872133	2.21970149	3.80961244
1	-5.09552963	3.23945316	5.01555312
1	3.11512551	-1.78717313	-2.11587425

Energy = -7200.146803 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 8

Atomic N.	X	Y	Z
8	-1.16830905	-0.66149079	0.60789270
6	-1.61387545	-1.21350225	1.83912999
1	-2.61199493	-1.65947589	1.69332114
1	-1.70686465	-0.45302734	2.63784003
1	-0.94360391	-2.01025987	2.21863228
50	0.69786178	0.34395059	0.63010013
7	-0.02696592	1.29146439	-1.53039426
6	1.14097057	1.46548057	-2.42214060
1	0.84763445	1.94622351	-3.37197680
1	1.59890148	0.49379259	-2.63146818
1	1.88269468	2.09679716	-1.91818258
7	-0.01818843	-1.75050034	-1.74590715
6	-1.08804801	0.46289866	-2.18204460
1	-1.52518167	1.04563096	-3.01390943
1	-1.86792895	0.29680632	-1.42571976
6	-0.63398543	-0.88081940	-2.75525627
1	-1.53914079	-1.33832416	-3.20479414
1	0.06865726	-0.72576894	-3.58678981
6	0.29649716	-3.07480319	-2.17759462
6	1.43025029	-3.30969371	-2.98908477
6	1.72408807	-4.61759071	-3.39542077
6	0.94318842	-5.71105443	-3.00840956
6	-0.15443758	-5.46358891	-2.17607615
6	-0.49535287	-4.17188900	-1.75894369

7	-0.19499601	2.22452485	1.18198886
6	-0.59149652	2.63255515	-1.16442765
1	-1.31480330	2.94619987	-1.93837399
1	0.24190660	3.34707383	-1.15689562
6	-1.22156593	2.62956266	0.22878130
1	-1.56902131	3.65482942	0.43584831
1	-2.11554759	1.97727488	0.23223366
6	-0.06144633	2.92889084	2.39779983
6	-1.17584913	3.20870189	3.23797775
6	-0.98994109	3.93734334	4.42012232
6	0.26636553	4.38824290	4.83465381
6	1.35883157	4.08760070	4.01391350
6	1.22345649	3.37796678	2.81579624
6	2.36586638	-2.18986120	-3.36911480
1	2.60847211	-4.78531081	-4.01548032
6	1.26443270	-7.10835929	-3.48124680
1	-0.77333415	-6.30098172	-1.84373364
6	-1.68873331	-3.97210902	-0.85494294
6	-2.55549573	2.67571471	2.92954171
1	-1.86144457	4.13405426	5.05093371
6	0.44540874	5.13276647	6.13605435
1	2.35482970	4.43222135	4.30547444
6	2.45114807	3.12750525	1.97625195
1	3.33484359	-2.59035511	-3.69376917
1	2.53208137	-1.52334002	-2.51031644
1	1.97612607	-1.57502919	-4.19679249
1	-1.38627831	-3.66450059	0.15806173
1	-2.25827057	-4.90525770	-0.76048795
1	-2.37037524	-3.19463273	-1.23077169
1	0.68265952	-7.36732962	-4.38027319
1	1.02572479	-7.85727115	-2.71352951
1	2.32731604	-7.20857112	-3.73953470
1	-3.16757874	2.65802201	3.84085518
1	-2.50390743	1.65463106	2.52634657
1	-3.09530839	3.28390857	2.18695445
1	2.25018541	3.31168587	0.91040227
1	2.80303455	2.08540327	2.05248446
1	3.27817564	3.77451838	2.29786591
1	0.69005579	4.44432170	6.96102951
1	-0.46986768	5.66986548	6.42014245
1	1.26413235	5.86319670	6.07067793
1	-0.61665816	-1.74692876	-0.90530446

Energy = -7200.170797 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 9

Atomic N.	X	Y	Z
8	0.15982376	-1.08711453	1.21534090
6	0.54407591	-1.08642136	2.58127012
1	1.57349730	-0.70748365	2.74967769
1	0.50311706	-2.11207565	2.98938979
1	-0.14085876	-0.45506666	3.17401031
50	1.51223036	-0.48781773	-0.22254255
7	1.33565815	1.37189782	-2.25606063
6	2.58278813	1.22147611	-3.01955854
1	2.57345503	1.82643729	-3.94725386
1	2.73370452	0.17030932	-3.29271907

1	3.43202958	1.53273918	-2.39703612
7	0.21159848	-1.26530229	-1.73891954
6	0.17865283	0.84042829	-3.00274384
1	0.14566819	1.26994654	-4.02577426
1	-0.73336232	1.14405823	-2.47074881
6	0.19586053	-0.68515513	-3.07388943
1	-0.72339432	-0.99327153	-3.60545766
1	1.03374236	-1.01614396	-3.72525156
6	-0.20866667	-2.63332681	-1.68535146
6	0.61291849	-3.68321605	-2.16763542
6	0.15439127	-5.00743933	-2.10424082
6	-1.09937841	-5.33306773	-1.58167625
6	-1.90511028	-4.28549355	-1.11921976
6	-1.48654221	-2.95109068	-1.15890154
7	0.70796370	2.31020108	0.51582774
6	1.14997159	2.78111145	-1.86304051
1	0.79908357	3.38687702	-2.72344342
1	2.14066333	3.17680024	-1.58565857
6	0.19716509	2.99182220	-0.68946757
1	0.09485879	4.08153562	-0.52890322
1	-0.80355762	2.61093998	-0.92689697
6	0.12318707	2.64913556	1.77635915
6	-1.23567551	2.38046907	2.05100199
6	-1.74560587	2.71491499	3.31277825
6	-0.95681006	3.27997142	4.31891447
6	0.39652428	3.49839041	4.03636441
6	0.94854435	3.19836399	2.78753222
6	1.98023602	-3.41947742	-2.75202389
1	0.80478361	-5.80639220	-2.47085372
6	-1.56118891	-6.76777354	-1.48921315
1	-2.89441242	-4.51226138	-0.71261202
6	-2.39415229	-1.86830824	-0.63696546
6	-2.13143745	1.68682035	1.05572515
1	-2.79593884	2.49507578	3.51922188
6	-1.54270720	3.64837195	5.66035406
1	1.04551981	3.91754398	4.80915653
6	2.41970082	3.44715536	2.54356127
1	2.61811067	-4.30894210	-2.66437380
1	2.48299132	-2.58292501	-2.24443159
1	1.92315948	-3.16268013	-3.82214470
1	-1.96647680	-1.43687431	0.27985157
1	-3.39079064	-2.27264904	-0.41446013
1	-2.50033843	-1.04751371	-1.36094808
1	-2.63237403	-6.86002232	-1.71836784
1	-1.41239746	-7.16780283	-0.47358552
1	-1.00498842	-7.41345257	-2.18212331
1	-2.98486550	1.22796458	1.57095124
1	-1.58711099	0.88949234	0.53139304
1	-2.54240618	2.38103754	0.30518411
1	2.59363527	4.13547519	1.69998266
1	2.96921337	2.51544488	2.32867535
1	2.88346715	3.89711338	3.42988064
1	-0.82715451	3.46821750	6.47454718
1	-2.45311054	3.07125197	5.87027413
1	-1.81423074	4.71539469	5.69627995
1	1.71305214	2.48237616	0.57098881

Energy = -7200.163178 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 10

Atomic N.	X	Y	Z
8	0.90834565	0.08561077	1.16012445
6	2.29092209	0.08725364	1.48830181
1	2.82532070	0.96488795	1.07710136
1	2.81767845	-0.81844536	1.12725765
1	2.40029431	0.12097040	2.58526319
50	0.41404713	0.12418195	-0.90075620
7	-1.83505742	0.79019833	-0.13300131
6	-2.86362144	0.22001846	-1.03099026
1	-3.87483045	0.55535539	-0.74043342
1	-2.81978955	-0.87311203	-1.00212320
1	-2.66112985	0.54798179	-2.05769537
7	-1.12236244	-1.89648158	1.12143494
6	-2.08201796	0.40239611	1.29014220
1	-2.99604339	0.91730250	1.63957134
1	-1.22791530	0.77628671	1.87200485
6	-2.27052432	-1.09214449	1.55633199
1	-2.45582517	-1.18361706	2.64627402
1	-3.18387575	-1.45736571	1.06492111
6	-1.16826361	-3.28083939	1.46854677
6	-1.99582434	-4.17055260	0.74564903
6	-2.02088330	-5.52549627	1.10016566
6	-1.23592628	-6.03882831	2.13722299
6	-0.39611569	-5.14977388	2.81781797
6	-0.35071770	-3.78550292	2.50917853
7	0.47018262	2.27586514	-0.99028743
6	-1.82862097	2.28587541	-0.25169587
1	-2.57233596	2.70889075	0.44717446
1	-2.13319110	2.53409993	-1.27675824
6	-0.43700387	2.87444464	-0.01788744
1	-0.51043380	3.96404975	-0.16647607
1	-0.13492690	2.71035393	1.03400203
6	1.39489976	3.09656034	-1.67109125
6	2.22855939	4.02707046	-0.98963098
6	3.10682446	4.83878119	-1.72024598
6	3.22425864	4.75748611	-3.11008543
6	2.41832505	3.82192412	-3.76853541
6	1.51405086	3.00069723	-3.08719795
6	-2.80043695	-3.70214916	-0.44051903
1	-2.65926079	-6.20314122	0.52744589
6	-1.30026287	-7.49809951	2.51883408
1	0.24144166	-5.52556860	3.62218502
6	0.58127033	-2.87877041	3.27766264
6	2.25216069	4.11639066	0.51843276
1	3.74077129	5.54179545	-1.17265519
6	4.20791138	5.61443259	-3.86935924
1	2.48085992	3.73730373	-4.85696728
6	0.66128204	2.04256301	-3.88058057
1	-3.10071172	-4.55434768	-1.06365753
1	-2.20666551	-3.01023890	-1.05544047
1	-3.72308094	-3.17631662	-0.14525542
1	1.41178077	-2.51989194	2.65016255
1	1.01872931	-3.41306289	4.13043296
1	0.06828039	-1.98533636	3.66369355
1	-2.00043174	-7.66003377	3.35388215

1	-0.31895874	-7.87291414	2.84109749
1	-1.64459430	-8.11628167	1.67876041
1	3.18882680	4.57918524	0.85600901
1	2.17362380	3.11978595	0.97500297
1	1.42604192	4.71927252	0.92682055
1	-0.38254910	2.05575420	-3.53332247
1	1.00858047	1.00028306	-3.78773131
1	0.68273767	2.29885084	-4.94822657
1	5.13702488	5.06293925	-4.08578258
1	4.48420056	6.50980395	-3.29626602
1	3.79487962	5.94104819	-4.83457104
1	-0.25992341	-1.43963915	1.45631814

Energy = -7200.170773 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 11

Atomic N.	X	Y	Z
8	1.12856713	-0.64594224	-0.91769985
6	2.13705160	-0.55158507	-1.92690326
1	2.10820000	0.43390509	-2.42324235
1	2.03249705	-1.32307904	-2.71307113
1	3.12887928	-0.67891295	-1.46305110
50	-0.53033720	-1.83495768	-1.31134239
7	-2.35858716	-0.14927973	-0.95126598
6	-3.52331272	-0.90298702	-1.47515497
1	-4.46804814	-0.39633887	-1.21076390
1	-3.53987425	-1.91993229	-1.06566595
1	-3.44655625	-0.97127897	-2.56767570
7	-1.06659254	-2.02859891	0.74881422
6	-2.43507205	-0.03453389	0.53133778
1	-3.38523534	0.45147299	0.82489109
1	-1.59928910	0.59782765	0.85418608
6	-2.29032762	-1.39398154	1.20891812
1	-2.24450594	-1.20911667	2.29875035
1	-3.21323733	-1.99421632	1.05141485
6	-0.60500519	-3.15569453	1.49438830
6	-1.27264349	-4.40582683	1.47616269
6	-0.76186138	-5.47546709	2.22674446
6	0.39745366	-5.35393448	2.99620957
6	1.04991906	-4.11404110	3.00397385
6	0.57372663	-3.01920749	2.27521587
7	-0.00117548	2.01602080	-1.45116905
6	-2.36574883	1.18607600	-1.63205727
1	-3.39108712	1.59493269	-1.54060796
1	-2.17188008	0.99885482	-2.69861210
6	-1.40637381	2.26683934	-1.13868828
1	-1.71577258	3.18126879	-1.66607276
1	-1.58430123	2.47934980	-0.06470073
6	0.86655932	3.14201412	-1.32506734
6	1.75251106	3.26664752	-0.22721353
6	2.62151601	4.36256287	-0.17152208
6	2.63147024	5.35609834	-1.15813765
6	1.75207939	5.21306589	-2.23602997
6	0.87823380	4.12363306	-2.34361933
6	-2.51685689	-4.62471403	0.65036169
1	-1.28462182	-6.43527202	2.19642383
6	0.94448584	-6.52175643	3.78164391

1	1.95666297	-3.99114564	3.60244748
6	1.30100338	-1.69940077	2.34034652
6	1.76670066	2.24207331	0.88273897
1	3.30463748	4.44582286	0.67781503
6	3.54924250	6.55037387	-1.05111472
1	1.76063515	5.95838710	-3.03567839
6	0.00406327	3.98543580	-3.56541271
1	-2.67575076	-5.69471455	0.46322770
1	-2.44585186	-4.11294108	-0.32143609
1	-3.41883885	-4.24267115	1.15468146
1	1.59936320	-1.35109333	1.34136391
1	2.19272383	-1.78311559	2.97582996
1	0.65522188	-0.91197654	2.75800274
1	1.12609103	-6.24846274	4.83162350
1	1.90570878	-6.86459827	3.36847942
1	0.25117330	-7.37291789	3.76691902
1	2.47498997	2.53783928	1.66701790
1	2.04754174	1.23914649	0.52819017
1	0.77467902	2.13830552	1.34956035
1	-1.01355555	4.37630988	-3.39971004
1	-0.09671085	2.92813528	-3.84865651
1	0.42783476	4.54484947	-4.40976822
1	4.50991774	6.27932168	-0.59179509
1	3.10229125	7.34083337	-0.42714342
1	3.75214166	6.98860010	-2.03773101
1	0.36323780	1.18768900	-0.95989998

Energy = -7200.166837 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 12

Atomic N.	X	Y	Z
8	1.41646510	3.57672981	0.75025044
6	2.45265697	4.12863063	1.54595831
1	2.04183254	4.63640541	2.44017303
1	3.01379112	4.88028011	0.96448113
1	3.18221446	3.37334390	1.90219829
50	1.18185542	1.51904397	0.59303179
7	-1.01494725	1.71403410	1.82191101
6	-1.06835063	3.09203023	2.36834944
1	-2.08226337	3.31542772	2.74423730
1	-0.77113843	3.81495000	1.60248703
1	-0.35291831	3.17859512	3.19609968
7	-0.27100359	1.69597606	-0.95380510
6	-2.01010231	1.54858313	0.72540988
1	-2.99740318	1.92433368	1.05655116
1	-2.08692949	0.47739296	0.50589480
6	-1.55374486	2.25617871	-0.55066858
1	-2.31575476	2.06191374	-1.32680244
1	-1.55417213	3.35209597	-0.38741431
6	0.12045081	1.77439869	-2.31594723
6	0.13438592	2.99356607	-3.04558883
6	0.50376915	2.98321773	-4.39766598
6	0.89372342	1.81546370	-5.05993987
6	0.91830961	0.62891895	-4.31839222
6	0.53760228	0.58437328	-2.97275466
7	-0.23270833	-1.26609331	1.95796841
6	-1.24708618	0.77810626	2.96114285

1	-2.16362589	1.09178701	3.49713591
1	-0.40653568	0.92491270	3.65844465
6	-1.39824804	-0.70991455	2.65313656
1	-1.57510017	-1.20384371	3.62991636
1	-2.30433425	-0.88367085	2.05834601
6	-0.10821826	-2.68145106	1.87555783
6	-1.04124299	-3.45643457	1.14976346
6	-0.86236334	-4.84459673	1.07915650
6	0.22146101	-5.49337771	1.67734459
6	1.15723822	-4.70170432	2.35413813
6	1.01187919	-3.31615412	2.46847677
6	-0.15722805	4.31646794	-2.37901567
1	0.51374364	3.93238210	-4.94093701
6	1.26172633	1.83043793	-6.52428644
1	1.22882183	-0.29961080	-4.80519509
6	0.56694328	-0.73251874	-2.23785001
6	-2.18564803	-2.82527998	0.39551009
1	-1.58726857	-5.43175596	0.50963634
6	0.37606463	-6.99319622	1.60384255
1	2.02783259	-5.17619047	2.81380722
6	2.05621719	-2.51210840	3.20797740
1	0.24326211	5.14043351	-2.98452486
1	0.30148933	4.35943527	-1.37937033
1	-1.23714354	4.49896559	-2.25748349
1	1.41667877	-0.79861943	-1.53782002
1	0.65918485	-1.56904491	-2.94306716
1	-0.33795412	-0.86654764	-1.63013988
1	0.39865791	1.56655126	-7.15664755
1	2.05885034	1.10711503	-6.74633267
1	1.60474719	2.82539824	-6.83978148
1	-2.52683272	-3.49150165	-0.40720547
1	-1.87786501	-1.87189631	-0.05768221
1	-3.05644636	-2.62361591	1.04000214
1	1.62453743	-1.94063218	4.04584143
1	2.56855930	-1.78994039	2.55083243
1	2.82576639	-3.17382525	3.62413073
1	1.43083830	-7.28419195	1.50235173
1	-0.17754211	-7.41047822	0.75206081
1	-0.00838688	-7.47862051	2.51502502
1	0.61895019	-0.87106067	2.35773938

Energy = -7200.165741 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 13

Atomic N.	X	Y	Z
8	1.78280991	3.23096674	1.30724831
6	2.85806275	3.52940006	2.18252618
1	3.49108479	2.64945125	2.41624206
1	2.48869517	3.93370524	3.14498359
1	3.51153760	4.29431625	1.72880666
50	1.32550450	1.26401486	0.82125017
7	-0.85956491	1.50607586	2.06529607
6	-0.76915472	2.77581186	2.82682085
1	-1.75865412	3.04934082	3.23343269
1	-0.37904583	3.57374862	2.18758258
1	-0.06403637	2.64731663	3.65796604
7	-0.07052107	1.84784687	-0.67720694

6	-1.84619932	1.63266250	0.95602133
1	-2.79090895	2.06068337	1.34326046
1	-2.03930721	0.62622252	0.56705019
6	-1.28956012	2.47854943	-0.18939515
1	-2.05400884	2.49907614	-0.98689059
1	-1.17004910	3.52707368	0.14824280
6	0.35203220	2.09752362	-2.00916465
6	0.51599409	3.40807477	-2.53363003
6	0.90676202	3.57190048	-3.86949793
6	1.17533626	2.48804295	-4.71088843
6	1.05335393	1.20353072	-4.16958408
6	0.64541129	0.98820020	-2.84845457
7	-0.40428260	-1.52784858	1.72963377
6	-1.21702069	0.43232467	3.03827862
1	-2.10635745	0.75574065	3.61298328
1	-0.38156017	0.37314836	3.75439372
6	-1.52018089	-0.96235493	2.49540802
1	-1.77403267	-1.58143507	3.37949482
1	-2.42434160	-0.93925601	1.87322738
6	-0.43005454	-2.91882209	1.42907576
6	-1.42176052	-3.46535700	0.58319421
6	-1.39116059	-4.83728686	0.29874916
6	-0.39917380	-5.68567125	0.79836076
6	0.59828096	-5.11549190	1.59868505
6	0.59956172	-3.75655491	1.92612589
6	0.36146429	4.63194507	-1.66319961
1	1.03349379	4.58827533	-4.25302764
6	1.56873886	2.69530355	-6.15389157
1	1.26700023	0.33547561	-4.79917531
6	0.51405242	-0.42385880	-2.33472577
6	-2.47144956	-2.60318654	-0.07368157
1	-2.15986990	-5.24645060	-0.36175172
6	-0.40459295	-7.16415107	0.49365100
1	1.40043966	-5.74807300	1.98694887
6	1.70447092	-3.19576034	2.79142043
1	0.86132863	5.49199179	-2.12835003
1	0.80425963	4.46283729	-0.66975590
1	-0.69358657	4.91251708	-1.51349336
1	1.33935269	-0.69743467	-1.65613418
1	0.52263041	-1.14198472	-3.16530032
1	-0.41001282	-0.54897808	-1.75459363
1	0.68767077	2.67558106	-6.81553704
1	2.25289776	1.90861296	-6.50125641
1	2.06205560	3.66647813	-6.29825194
1	-2.86116424	-3.09585552	-0.97368824
1	-2.05110746	-1.63111965	-0.36937556
1	-3.33223771	-2.40841665	0.58619112
1	1.31481543	-2.71525379	3.70367417
1	2.30889826	-2.44261546	2.25916855
1	2.38691063	-3.99443354	3.10711930
1	0.61483794	-7.54937735	0.35249118
1	-0.98179567	-7.38255046	-0.41477901
1	-0.85768613	-7.73906184	1.31697320
1	0.47469397	-1.29512630	2.19270293

Energy = -7200.165744 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 14

Atomic N.	X	Y	Z
8	-0.08711343	-0.37117962	-1.42979174
6	0.70798385	-0.85331706	-2.50418221
1	1.56408494	-0.18850903	-2.73468566
1	0.08456675	-0.92028494	-3.41154056
1	1.11777120	-1.86316907	-2.31122980
50	0.83595668	-0.26783400	0.47568562
7	-1.46678117	-0.11119630	1.35048315
6	-1.49776987	0.76845998	2.53983533
1	-2.50886791	0.80222522	2.98250920
1	-1.18690199	1.78061824	2.26332296
1	-0.79469532	0.38163018	3.28733422
7	-0.99617828	2.18087843	-0.60068710
6	-2.43375397	0.35219599	0.30833986
1	-3.46009598	0.18753785	0.68522210
1	-2.27928986	-0.28690938	-0.57226955
6	-2.32900876	1.82260032	-0.10092378
1	-3.11751175	1.97762137	-0.86589152
1	-2.59440506	2.47664524	0.74225052
6	-0.86749275	3.50316879	-1.12510166
6	-0.76685457	4.60982697	-0.25096443
6	-0.63577896	5.89750710	-0.78639452
6	-0.57931268	6.12884817	-2.16437027
6	-0.64391588	5.01787461	-3.01310193
6	-0.79165070	3.71514261	-2.52325656
7	0.34087771	-2.31035212	0.94953527
6	-1.79603627	-1.51902969	1.75023301
1	-2.89270168	-1.65269455	1.74092264
1	-1.43690607	-1.65967037	2.77805822
6	-1.09543590	-2.54711597	0.86143572
1	-1.35410665	-3.54662971	1.24707533
1	-1.49543781	-2.48363972	-0.16843529
6	1.21332866	-3.40856122	1.10751725
6	1.13326726	-4.56405804	0.27890477
6	2.00269289	-5.63961938	0.49938932
6	2.98255099	-5.62115155	1.49657748
6	3.07035466	-4.47131731	2.28786553
6	2.21419656	-3.37702286	2.11900504
6	-0.73017336	4.42392078	1.24491607
1	-0.55093652	6.74274821	-0.09846067
6	-0.46545519	7.52844543	-2.71881016
1	-0.58499704	5.16663662	-4.09435479
6	-0.84817327	2.55718060	-3.49141780
6	0.17940791	-4.63702417	-0.89054672
1	1.92379745	-6.51287470	-0.15441383
6	3.93407156	-6.77851723	1.68400486
1	3.82190080	-4.42705319	3.08089321
6	2.36005427	-2.19181170	3.04014948
1	-0.32527151	5.31849595	1.73526001
1	-0.09726214	3.56363352	1.50708808
1	-1.72943799	4.24416684	1.67399317
1	0.05358728	1.92850896	-3.42872757
1	-0.92446486	2.92351804	-4.52294062
1	-1.70730848	1.89688823	-3.30110257
1	-1.45704043	7.93914817	-2.96752030
1	0.13428501	7.54855584	-3.63918741
1	-0.00233290	8.20990752	-1.99242545

1	0.51903463	-5.39357182	-1.61007423
1	0.11432483	-3.66994571	-1.40857055
1	-0.84572609	-4.90799288	-0.59327148
1	1.37957076	-1.83037750	3.38429201
1	2.85230728	-1.33780775	2.54621621
1	2.96776246	-2.45553304	3.91605384
1	4.79972174	-6.70025464	1.00654072
1	3.44465454	-7.73990959	1.47423502
1	4.32580450	-6.81129293	2.71004395
1	-0.70133413	1.46269296	-1.28053842

Energy = -7200.170765 Hartree
Number of imaginary frequencies = 0.

Compound 11b isomer 15

Atomic N.	X	Y	Z
8	1.41584803	0.10594494	-0.14793748
6	2.47299157	0.94057317	-0.62114616
1	2.08103042	1.82588018	-1.15424014
1	3.10574686	0.37019729	-1.32127400
1	3.12667770	1.31398379	0.19041047
50	1.07998148	0.06739286	1.91180744
7	-1.40725360	0.28133294	2.05452920
6	-1.81830197	1.49515847	2.78501487
1	-2.90657025	1.50163146	2.97477549
1	-1.54041723	2.38416978	2.20884816
1	-1.29111200	1.52616766	3.74707955
7	-0.92262827	1.92948121	-0.47904223
6	-2.12725162	0.12968808	0.75810322
1	-3.15892842	-0.21477386	0.96619647
1	-1.61627378	-0.66888117	0.20191410
6	-2.23078204	1.37610362	-0.11731006
1	-2.81950205	1.06698905	-1.00585737
1	-2.83268357	2.14985666	0.38512809
6	-0.95029438	2.89919947	-1.53047774
6	-1.26035547	4.24469692	-1.23325161
6	-1.26877585	5.19011050	-2.26704105
6	-0.96572132	4.84726207	-3.58880280
6	-0.64770622	3.51122835	-3.86123153
6	-0.64572910	2.53008464	-2.86275854
7	0.32569547	-1.92256686	1.86556800
6	-1.64294194	-0.92389996	2.89883763
1	-2.72829325	-1.05611026	3.06784836
1	-1.16501988	-0.72670054	3.87112300
6	-1.03687106	-2.18664401	2.28902043
1	-1.08722088	-2.97322308	3.06864956
1	-1.68383019	-2.55201579	1.46174977
6	1.10870520	-3.05508819	1.49916425
6	1.00716300	-3.62362331	0.20403614
6	1.78499491	-4.74114526	-0.12195743
6	2.67782611	-5.31697603	0.78954598
6	2.77368625	-4.74340557	2.06127666
6	2.00888506	-3.62857963	2.43059401
6	-1.53352282	4.68121070	0.18398220
1	-1.49870543	6.23060937	-2.02369205
6	-1.00106917	5.87894661	-4.69074167
1	-0.40398692	3.21771629	-4.88553335
6	-0.32992856	1.09638304	-3.22093865

6	0.09791283	-3.01680512	-0.83462820
1	1.69730199	-5.16714203	-1.12517162
6	3.53273272	-6.49896500	0.39936692
1	3.45980883	-5.17810564	2.79310307
6	2.15753894	-3.05393491	3.81953068
1	-1.44879046	5.77147865	0.27871701
1	-0.82146425	4.20760995	0.87486799
1	-2.54654491	4.40327851	0.51777573
1	0.58939559	0.73325694	-2.73755823
1	-0.20016368	0.99316065	-4.30560914
1	-1.13596075	0.41321936	-2.91263488
1	-1.97526952	5.87721012	-5.20517212
1	-0.23250213	5.68145139	-5.45063772
1	-0.84147064	6.89143372	-4.29600917
1	0.26100820	-3.48609823	-1.81365042
1	0.29133408	-1.93730166	-0.92042788
1	-0.96569898	-3.14907767	-0.57906856
1	1.18303053	-2.86651617	4.29114802
1	2.68728323	-2.08787641	3.80666575
1	2.73111610	-3.73646359	4.46051939
1	4.43350886	-6.17394235	-0.14531345
1	2.98768195	-7.18922061	-0.25954505
1	3.86816649	-7.05934304	1.28249449
1	-0.25750987	1.17032757	-0.68073182

Energy = -7200.166823 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 16

Atomic N.	X	Y	Z
8	0.77568316	-0.03091868	-1.66785888
6	1.68928640	0.62629699	-2.53882846
1	2.35668871	1.33885158	-2.01305156
1	1.16495409	1.19086888	-3.33206113
1	2.33096770	-0.12390778	-3.03122185
50	0.05879693	1.03136384	0.00076236
7	-1.16897578	-0.98732216	0.56485599
6	-1.88769206	-0.66649676	1.82434918
1	-2.63915064	-1.44220702	2.04977538
1	-2.38304658	0.30625368	1.73038508
1	-1.16469360	-0.61959749	2.64781344
7	-1.92729896	1.39112948	-0.67460799
6	-2.13000986	-1.05034841	-0.57978866
1	-2.86043913	-1.86068992	-0.39821996
1	-1.54144772	-1.29192144	-1.47341228
6	-2.85442694	0.27741730	-0.80236843
1	-3.31996314	0.21920327	-1.80388724
1	-3.70034775	0.37205895	-0.08789851
6	-2.35082176	2.65157508	-1.18049800
6	-2.62665933	3.72174841	-0.29080686
6	-3.01085432	4.96731558	-0.80138747
6	-3.14658796	5.19683983	-2.17544360
6	-2.86642147	4.13679239	-3.04316920
6	-2.46944017	2.87647489	-2.57740676
7	1.86447896	-2.42526991	-0.20324014
6	-0.49262280	-2.31149129	0.75655612
1	-1.29570897	-3.06037401	0.89885408
1	0.06885381	-2.25660774	1.70032372

6	0.45880539	-2.79144166	-0.35797052
1	0.34872688	-3.87938493	-0.43234042
1	0.15493308	-2.37748071	-1.32682372
6	2.62629006	-2.68781932	0.94783057
6	2.55740125	-3.91134693	1.66689142
6	3.35260248	-4.07754917	2.81088078
6	4.25394814	-3.11049846	3.25897016
6	4.37198700	-1.94780621	2.48803353
6	3.58977042	-1.72017130	1.35454866
6	-2.51615008	3.53682761	1.20385843
1	-3.21798694	5.78122684	-0.10148818
6	-3.59948863	6.53800766	-2.70069255
1	-2.94011119	4.29724373	-4.12237873
6	-2.13760928	1.79300207	-3.57436852
6	1.74037674	-5.09725059	1.20538242
1	3.27878614	-5.02513271	3.35125756
6	5.07297716	-3.31106787	4.51086329
1	5.09934434	-1.18439713	2.77646783
6	3.79772772	-0.45888149	0.55480693
1	-2.91766037	4.41246824	1.73066564
1	-1.47241531	3.40161876	1.52808694
1	-3.06896571	2.64793464	1.54020473
1	-1.37884996	1.10618917	-3.17401672
1	-1.76624263	2.22989658	-4.51111117
1	-3.02327763	1.18913835	-3.83183095
1	-3.23704251	6.71041159	-3.72325815
1	-3.24122596	7.36012797	-2.06588447
1	-4.69897220	6.60325074	-2.72809091
1	2.04953683	-5.99456714	1.75699599
1	1.89068102	-5.29554014	0.13386225
1	0.65677706	-4.97813957	1.36791473
1	2.89769292	0.17947121	0.53604513
1	4.06080771	-0.67366361	-0.49388393
1	4.61166707	0.13792638	0.98479591
1	6.09955064	-2.93821437	4.38488843
1	5.12834372	-4.37338584	4.78506450
1	4.63704408	-2.77293703	5.36803732
1	2.00711975	-1.49510290	-0.60073258

Energy = -7200.164918 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 17

Atomic N.	X	Y	Z
8	1.18585246	3.41900051	1.49478777
6	2.41305554	3.98032979	1.93098090
1	3.30115790	3.40347836	1.60206460
1	2.45252648	4.04326111	3.03581559
1	2.52035274	5.00485134	1.53493289
50	1.13415723	1.54143285	0.60802638
7	-0.15184696	0.67808393	2.60300533
6	-0.07590435	1.73611118	3.63994993
1	-0.78114944	1.51817639	4.46115409
1	-0.28613889	2.71501373	3.19832024
1	0.94387463	1.77101559	4.04408208
7	-0.90932761	1.74717199	0.04499493
6	-1.53812708	0.57165715	2.06742451
1	-2.25902606	0.51230139	2.90551885

8	1.20939945	0.57217053	-1.14357824
6	1.38826678	1.84215561	-1.74955551
1	0.44209070	2.19265611	-2.19933784
1	2.14130000	1.77589554	-2.55484654
1	1.72872874	2.62660813	-1.04273552
50	1.58647961	0.31521388	0.86666640
7	-0.00705584	-0.78204528	2.82597561
6	-0.00261249	-0.14355964	4.14577294
1	-0.53204439	-0.75457533	4.90354029
1	-0.48089819	0.84348174	4.10932253
1	1.03543778	-0.00109715	4.47362729
7	-1.23063218	1.39781509	1.36845980
6	-1.35918184	-0.93118356	2.26612202
1	-1.99074633	-1.58012271	2.90976286
1	-1.25130268	-1.42493683	1.29140668
6	-2.08157828	0.40435086	2.05974541
1	-2.96991380	0.21362188	1.44561028
1	-2.45516230	0.80202175	3.02095157
6	-1.91560079	2.40509353	0.61166028
6	-1.96100475	3.73713093	1.07905622
6	-2.60599064	4.71093925	0.30697553
6	-3.21881473	4.40001192	-0.91133608
6	-3.13960997	3.07751803	-1.36403742
6	-2.48728203	2.07466289	-0.63738748
7	1.49832724	-1.78993954	0.55613511
6	0.72648092	-2.06220885	2.89262231
1	0.20496848	-2.77834636	3.56156441
1	1.70587985	-1.83606800	3.34330879
6	0.94511577	-2.71703540	1.53163600
1	1.63039402	-3.56978491	1.70314651
1	-0.00620963	-3.17483202	1.18734210
6	1.97731175	-2.40249611	-0.64039765
6	1.09058168	-2.95283854	-1.59895717
6	1.60529378	-3.57175154	-2.74487604
6	2.97890866	-3.65923883	-2.98979361
6	3.84443110	-3.10515328	-2.04074747
6	3.37269995	-2.48140171	-0.87936192
6	-1.30869869	4.12724365	2.38625372
1	-2.63307963	5.73985624	0.67396697
6	-3.95012534	5.45238165	-1.70916622
1	-3.57365028	2.81790456	-2.33271901
6	-2.33564371	0.69421270	-1.22457148
6	-0.40337701	-2.85100710	-1.42757122
1	0.90480685	-3.98182105	-3.47770847
6	3.50916832	-4.29602394	-4.25215612
1	4.92387985	-3.16359196	-2.20460895
6	4.36672089	-1.90327348	0.09896198
1	-1.49525486	5.18540755	2.60734270
1	-0.21465925	3.99085082	2.36152976
1	-1.69525754	3.54186326	3.23568334
1	-1.28840973	0.36180402	-1.15013189
1	-2.62650693	0.69529639	-2.28265663
1	-2.96161842	-0.05659540	-0.71684221
1	-5.02963892	5.43658486	-1.49032458
1	-3.83578045	5.28717952	-2.78936467
1	-3.58278825	6.46046738	-1.47502051
1	-0.90917021	-2.89258879	-2.40124733
1	-0.66423524	-1.90386526	-0.93733038

1	-0.80841729	-3.67214999	-0.81365526
1	4.10181364	-2.14085376	1.13830303
1	4.41348313	-0.80354989	0.02982686
1	5.37656225	-2.28302810	-0.10644276
1	3.58941540	-3.55755991	-5.06590790
1	2.84792763	-5.09913591	-4.60569080
1	4.51117959	-4.71934059	-4.09689146
1	-0.64510120	1.86060043	2.06467706

Energy = -7200.160682 Hartree
Number of imaginary frequencies = 0.

Compound 11b isomer 19

Atomic N.	X	Y	Z
8	1.06714749	0.63954381	-0.69284613
6	1.49835868	1.86431303	-1.28620672
1	0.67779837	2.60365730	-1.32759117
1	1.84034900	1.67314880	-2.31694417
1	2.33564020	2.33981234	-0.73993433
50	1.81657774	0.19193331	1.20413455
7	-0.23166038	-0.55791565	2.42392883
6	-0.52897424	0.30039622	3.58634595
1	-1.34112796	-0.12427686	4.20310496
1	-0.81282451	1.30088857	3.24291224
1	0.37465319	0.38828395	4.20294176
7	-1.50724297	1.49597736	0.54756653
6	-1.42827029	-0.78083376	1.56334359
1	-2.09222199	-1.51110953	2.06547892
1	-1.06957298	-1.24322814	0.63290640
6	-2.27088270	0.44802248	1.23114117
1	-3.11570913	0.07178264	0.61765900
1	-2.72646970	0.86063258	2.14528083
6	-2.30364306	2.52537527	-0.04694209
6	-2.75930901	3.60175609	0.74563906
6	-3.52850021	4.61158268	0.15289784
6	-3.84993062	4.59683598	-1.20820381
6	-3.37600618	3.52952937	-1.98073365
6	-2.62076040	2.48954322	-1.42616992
7	1.69444025	-1.90940038	0.88617372
6	0.30143377	-1.87093932	2.88524186
1	-0.48317151	-2.41942050	3.43983145
1	1.12502746	-1.65029181	3.58208544
6	0.83487906	-2.71752770	1.73102647
1	1.37902108	-3.56983213	2.18549019
1	-0.01386499	-3.17367095	1.17614030
6	2.46308426	-2.60470817	-0.09127018
6	1.89185311	-2.98938687	-1.33080732
6	2.67324148	-3.67798126	-2.26650846
6	4.01570503	-3.99319523	-2.02592590
6	4.56959927	-3.60223915	-0.80279677
6	3.82107317	-2.91737644	0.16399874
6	-2.38819076	3.70016644	2.20387305
1	-3.86622541	5.44572642	0.77324459
6	-4.69791968	5.68486211	-1.82223428
1	-3.61012220	3.49644530	-3.04791457
6	-2.16612203	1.34388851	-2.30040797
6	0.46589088	-2.63176337	-1.66616387
1	2.21958651	-3.96604092	-3.21876903

6	4.84634590	-4.70369878	-3.06778589
1	5.61479393	-3.84124774	-0.58885643
6	4.47700712	-2.52007798	1.46524973
1	-2.55492543	4.71771506	2.58020036
1	-1.33104634	3.43564493	2.34894352
1	-2.98438556	3.01882832	2.83257325
1	-1.07027397	1.27693144	-2.37286184
1	-2.56190642	1.45875261	-3.31735155
1	-2.51386025	0.37411224	-1.91279917
1	-5.75615889	5.38270343	-1.87229132
1	-4.37729541	5.91353043	-2.84799752
1	-4.64915238	6.61039054	-1.23291754
1	0.24496145	-2.86503673	-2.71597867
1	0.29723363	-1.55788228	-1.49718820
1	-0.25614094	-3.18746390	-1.04655566
1	3.84691926	-2.76316248	2.33176922
1	4.66506889	-1.43534326	1.51240112
1	5.44383525	-3.02758011	1.58112974
1	5.25351770	-3.99168776	-3.80332570
1	4.24913248	-5.43886929	-3.62495161
1	5.69813615	-5.22676535	-2.61235720
1	-0.85844330	1.07724104	-0.13306574

Energy = -7200.166813 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 20

Atomic N.	X	Y	Z
8	3.59648095	1.25674291	-0.93593672
6	4.91284980	1.07768034	-0.43949256
1	5.60720092	0.88451068	-1.27528789
1	5.00328057	0.22941516	0.26892885
1	5.26759338	1.98502008	0.08684569
50	2.00340060	0.20062247	-0.12369463
7	1.05500334	2.37310373	0.74540294
6	2.12209358	3.39041637	0.58189515
1	1.71522229	4.40250017	0.75332281
1	2.56706685	3.31564987	-0.41506585
1	2.91854455	3.19680210	1.31175861
7	0.66455048	0.83794186	-1.65180333
6	-0.06498934	2.63528449	-0.20159671
1	-0.36401216	3.69950844	-0.14156852
1	-0.90973215	2.00572837	0.10095199
6	0.31534843	2.25191196	-1.63200442
1	-0.56817056	2.43575967	-2.26944603
1	1.10722755	2.93365929	-2.00056001
6	0.54462637	0.11162741	-2.86534499
6	1.14359579	0.53793199	-4.08162018
6	0.95420020	-0.21927250	-5.24548107
6	0.21723711	-1.40753612	-5.25577469
6	-0.32997515	-1.83952018	-4.04271394
6	-0.18681813	-1.10729333	-2.85875454
7	-0.39412573	0.13776458	2.30136466
6	0.62621963	2.40891727	2.17463228
1	0.39543457	3.45618812	2.44974930
1	1.50531561	2.11176201	2.76891902
6	-0.57663694	1.56429830	2.58894010
1	-0.72073315	1.75539927	3.67154777

1	-1.48547396	1.93055546	2.09396754
6	-1.28905105	-0.79207443	2.90131173
6	-2.66473642	-0.79638030	2.57610865
6	-3.50160829	-1.74684611	3.17596567
6	-3.02382857	-2.71211838	4.06692955
6	-1.65087928	-2.71760775	4.34103131
6	-0.77921502	-1.77838008	3.78211142
6	2.05102569	1.74336352	-4.13424960
1	1.42822342	0.12182659	-6.17021939
6	0.00750573	-2.18753008	-6.53156456
1	-0.90261333	-2.77058731	-4.01598160
6	-0.81985205	-1.62039258	-1.58944006
6	-3.24383747	0.14918516	1.55272051
1	-4.56197976	-1.74382932	2.91097999
6	-3.95374977	-3.70786118	4.71687035
1	-1.24234583	-3.47384471	5.01596942
6	0.69469345	-1.83567862	4.11117943
1	2.67834797	1.70545412	-5.03475181
1	2.70601898	1.77756185	-3.25025388
1	1.49100263	2.69172031	-4.16928803
1	-0.07467094	-2.04860037	-0.89814680
1	-1.55069004	-2.40943145	-1.81053725
1	-1.31406080	-0.80932468	-1.03810325
1	-0.91362464	-1.87092275	-7.04703806
1	-0.08471186	-3.26444083	-6.33371152
1	0.83995938	-2.03820579	-7.23317610
1	-4.17687557	-0.25770551	1.14223921
1	-2.54188580	0.30391721	0.72061141
1	-3.48186437	1.13770283	1.97755118
1	1.05755206	-0.89601072	4.55876521
1	1.31333185	-2.03210109	3.21980114
1	0.89628164	-2.64030704	4.82894599
1	-3.46690064	-4.68350528	4.85239309
1	-4.86102828	-3.85832530	4.11643465
1	-4.27352694	-3.36297945	5.71316236
1	0.56776865	-0.12882073	2.51329903

Energy = -7200.165737 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 21

Atomic N.	X	Y	Z
8	2.17101205	2.48395004	1.56803109
6	3.51733790	2.83031071	1.28410625
1	3.57820639	3.82968683	0.81254814
1	4.01976943	2.11510669	0.60150085
1	4.10902275	2.86442338	2.21604800
50	1.31934403	0.79942617	0.65220076
7	-0.52481333	2.41645358	0.22769934
6	-0.01956672	3.65138988	-0.40839875
1	-0.79561558	4.43788965	-0.41124849
1	0.29062275	3.45205121	-1.44030174
1	0.85335117	3.99139083	0.16135452
7	-0.66661376	0.18764171	-1.95108564
6	-1.71801628	1.88577399	-0.48016534
1	-2.49845673	2.67107936	-0.49812648
1	-2.10899835	1.05448892	0.12426109
6	-1.49988831	1.39806945	-1.91091076

1	-2.50416311	1.22695269	-2.34839028
1	-1.03003129	2.17635205	-2.52561171
6	-0.42012893	-0.38005078	-3.23813153
6	0.48107641	0.24436661	-4.12908411
6	0.72237276	-0.34620970	-5.37613239
6	0.11928859	-1.54665449	-5.76429171
6	-0.74304235	-2.16658773	-4.85231434
6	-1.02894149	-1.60468956	-3.60362231
7	-0.14822087	0.43415025	2.15947270
6	-0.87476532	2.71634906	1.65073918
1	-1.74734085	3.39603596	1.68461918
1	0.00028467	3.23117531	2.06978589
6	-1.14479219	1.45033934	2.46224406
1	-1.13860574	1.75521280	3.52515445
1	-2.17483963	1.07577066	2.27269668
6	0.00009946	-0.62355191	3.09822474
6	-0.35782156	-1.94660908	2.73327752
6	-0.19257238	-2.99303177	3.64821774
6	0.31481871	-2.77733162	4.93445202
6	0.68041119	-1.47205483	5.27920936
6	0.54069575	-0.39640938	4.39228861
6	1.22817140	1.49649391	-3.74327730
1	1.42810841	0.14007174	-6.05432233
6	0.37982698	-2.14923723	-7.12364414
1	-1.21500698	-3.11493277	-5.12108205
6	-1.96639503	-2.31984057	-2.65806316
6	-0.91059489	-2.24206514	1.35974098
1	-0.47481698	-4.00571530	3.34769304
6	0.44882728	-3.91284370	5.92070610
1	1.11096375	-1.28298845	6.26660363
6	1.01651379	0.97308903	4.81245660
1	2.15348430	1.58719343	-4.32656713
1	1.48987148	1.47921586	-2.67530805
1	0.63938244	2.40961121	-3.93089297
1	-1.44724844	-2.69102103	-1.75908804
1	-2.41640829	-3.19057732	-3.15070557
1	-2.78814544	-1.67158463	-2.31573175
1	-0.40710127	-1.86644028	-7.84081022
1	0.39941906	-3.24691857	-7.07985587
1	1.33772141	-1.80521110	-7.53616578
1	-1.32541825	-3.25820813	1.31848764
1	-0.12920724	-2.16746078	0.58590352
1	-1.70050612	-1.52698149	1.08778828
1	0.20393754	1.57286414	5.25466702
1	1.41236299	1.53779269	3.95562656
1	1.80148274	0.88818510	5.57587168
1	0.68731066	-4.85874838	5.41490223
1	-0.48882099	-4.06907884	6.47790779
1	1.23669144	-3.71026156	6.65902544
1	-1.08488501	-0.51705809	-1.34218273

Energy = -7200.168587 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 22

Atomic N.	X	Y	Z
8	3.24926305	2.19349946	-0.12937359
6	4.64372617	1.98013600	0.01654873

1	5.19127005	2.51227189	-0.78031661
1	4.93274339	0.91102975	-0.04015415
1	5.00725346	2.36783363	0.98803688
50	1.92432374	0.59407391	-0.11807816
7	0.97831707	1.44215480	2.06371513
6	1.91035683	2.49127558	2.54441288
1	1.45970973	3.04733156	3.38519064
1	2.17099543	3.16980087	1.72634827
1	2.83955937	2.01760651	2.88612543
7	0.28087777	1.81738190	-0.69879717
6	-0.31432892	2.04843333	1.63770036
1	-0.68348380	2.73335851	2.42523038
1	-1.03451694	1.23331385	1.50215603
6	-0.17301194	2.77544722	0.30017256
1	-1.17049832	3.16568679	0.02910698
1	0.47941222	3.66190748	0.42731287
6	-0.00077056	2.06052937	-2.06849031
6	0.32533374	3.28170454	-2.71765319
6	-0.01464251	3.45776908	-4.06596285
6	-0.64117569	2.45972471	-4.81810883
6	-0.91678745	1.24553976	-4.17925411
6	-0.61658218	1.02960194	-2.82982518
7	0.02980716	-1.48326096	1.81166042
6	0.81796735	0.45338658	3.17016600
1	0.55582974	0.99799000	4.09777027
1	1.81285429	0.00890684	3.33435838
6	-0.21410102	-0.65911552	3.00020948
1	-0.17291938	-1.25404115	3.93492969
1	-1.22558860	-0.23463126	2.95695492
6	-0.66431283	-2.72064210	1.69581189
6	-2.07012369	-2.75998253	1.55925467
6	-2.70561142	-4.00278336	1.43036991
6	-1.99885117	-5.20776925	1.40103718
6	-0.60351467	-5.14360704	1.50267410
6	0.07374515	-3.93032897	1.65184825
6	1.10657576	4.36542600	-2.01439085
1	0.24978777	4.40241636	-4.54955814
6	-1.01883536	2.68718947	-6.26227670
1	-1.39675832	0.44129365	-4.74352117
6	-0.95934544	-0.29643554	-2.19786393
6	-2.89937397	-1.50126923	1.48992221
1	-3.79322564	-4.01951115	1.32382258
6	-2.70602719	-6.52982094	1.22348178
1	-0.02120416	-6.06803798	1.47253140
6	1.58131497	-3.92207700	1.75758325
1	1.55916725	5.04328915	-2.75031103
1	1.90765246	3.93090395	-1.39709626
1	0.47438715	4.98024152	-1.35364047
1	-0.06699113	-0.92637043	-2.04496109
1	-1.65322590	-0.86204793	-2.83367620
1	-1.40660919	-0.15713454	-1.20459987
1	-2.06598882	3.01778158	-6.35483161
1	-0.91631588	1.76725942	-6.85484962
1	-0.39045470	3.46236223	-6.72202757
1	-3.85245563	-1.69962386	0.98304871
1	-2.37118081	-0.71499697	0.93155440
1	-3.14129143	-1.09856130	2.48673617
1	1.93030165	-3.45076878	2.69082367

1	2.05425912	-3.37974011	0.92207585
1	1.97242472	-4.94678288	1.74080434
1	-2.62389848	-6.88977476	0.18581457
1	-3.77495248	-6.44589074	1.45986646
1	-2.27286724	-7.30666909	1.86954279
1	1.03260625	-1.64418379	1.71290820

Energy = -7200.165700 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 23

Atomic N.	X	Y	Z
8	2.27381253	1.23000516	2.58184707
6	3.50718773	1.92063154	2.45912484
1	3.40241954	2.97735846	2.77094322
1	3.90788550	1.92270633	1.42505205
1	4.27233762	1.45612917	3.10606959
50	1.36845419	0.41818191	0.87204544
7	-0.63017146	1.53539195	1.84832203
6	-0.35515217	2.95479465	2.15582305
1	-1.16672169	3.38890270	2.76717735
1	-0.25487307	3.53492400	1.23160972
1	0.59228568	3.00329411	2.70557995
7	-1.06916981	1.27105611	-1.22986021
6	-1.90526599	1.37381616	1.10367161
1	-2.72462758	1.81707968	1.70237246
1	-2.10301227	0.29428153	1.03364303
6	-1.95673515	1.98022548	-0.29696907
1	-3.01598975	1.94648390	-0.62277037
1	-1.67955040	3.04192800	-0.27725668
6	-1.05599212	1.73572226	-2.58041228
6	-0.39697179	2.94145543	-2.90980612
6	-0.38037540	3.36372200	-4.24502368
6	-0.97391481	2.62161763	-5.27132955
6	-1.58971325	1.41257679	-4.92805590
6	-1.64828898	0.96014742	-3.60538682
7	0.27450651	-1.10663882	1.89035304
6	-0.69479639	0.76867602	3.13106658
1	-1.58558527	1.08196342	3.70802986
1	0.21100029	1.04398484	3.68787866
6	-0.70227957	-0.74254195	2.90564787
1	-0.49381593	-1.20446433	3.88849340
1	-1.72146801	-1.09231372	2.62977953
6	0.68583875	-2.46719315	1.84930788
6	0.34925405	-3.27273154	0.73149211
6	0.77176863	-4.60618847	0.67816131
6	1.52050478	-5.18626319	1.70831357
6	1.86143237	-4.37932728	2.79869322
6	1.46795264	-3.03764253	2.88918526
6	0.33292520	3.74935158	-1.86607603
1	0.13912530	4.29348251	-4.49036093
6	-0.96182734	3.11339568	-6.69851231
1	-2.04621399	0.80281739	-5.71170199
6	-2.32455190	-0.35507288	-3.29361703
6	-0.45782946	-2.70379089	-0.41060641
1	0.50220678	-5.21045390	-0.19230986
6	1.93314667	-6.63763761	1.65095170
1	2.47448536	-4.79959112	3.60095607

6	1.92723891	-2.21188378	4.06633915
1	1.10976748	4.36841654	-2.33285192
1	0.81024845	3.08914118	-1.12739844
1	-0.33879359	4.43329375	-1.32141824
1	-1.60873694	-1.11900199	-2.94794099
1	-2.81339717	-0.75628109	-4.18997579
1	-3.09509886	-0.25344944	-2.51352028
1	-1.86230892	3.70761832	-6.92132431
1	-0.93860422	2.27765358	-7.41099144
1	-0.09157997	3.75470805	-6.89317779
1	-0.79826795	-3.50372962	-1.08182367
1	0.13506811	-1.99358530	-1.00977070
1	-1.33665223	-2.15569236	-0.04094192
1	1.18714445	-2.21408411	4.88353211
1	2.09424191	-1.16390481	3.77728291
1	2.85943214	-2.61970648	4.47973680
1	2.11305120	-6.96396127	0.61726001
1	1.14957612	-7.29108146	2.06701981
1	2.84841978	-6.81641645	2.23168214
1	-1.30438529	0.27769434	-1.21325368

Energy = -7200.168613 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 24

Atomic N.	X	Y	Z
8	4.04542612	-0.59333636	-0.48134010
6	4.88528468	0.10710846	-1.38152280
1	4.42181311	1.02718931	-1.78105079
1	5.15946331	-0.53668595	-2.24019998
1	5.82409267	0.39626234	-0.87676600
50	2.13641497	-0.15764198	0.16039988
7	1.27759483	-1.07825170	-2.00939612
6	2.07208429	-2.26693387	-2.39312315
1	1.92894624	-2.50350190	-3.46246090
1	1.76681287	-3.13368698	-1.79636991
1	3.12976106	-2.06629936	-2.18457579
7	-1.03491807	-1.81810028	0.15771913
6	-0.18262040	-1.34991201	-2.15467238
1	-0.35191076	-1.70541765	-3.19011722
1	-0.71431268	-0.39736653	-2.03552630
6	-0.80444823	-2.36124184	-1.18949745
1	-1.77983018	-2.62831956	-1.61521206
1	-0.22201413	-3.30243528	-1.16886186
6	-1.99547196	-2.49408616	0.96622681
6	-1.58887311	-3.20359075	2.12195047
6	-2.55567550	-3.81900660	2.92394955
6	-3.92023215	-3.76635055	2.61485861
6	-4.30259476	-3.04041394	1.48243770
6	-3.37234550	-2.39271651	0.65940972
7	1.69635340	1.60030154	-0.97436311
6	1.65914280	0.07080685	-2.88870663
1	1.24632326	-0.08575017	-3.90307583
1	2.75441028	0.05879761	-2.96233725
6	1.20911094	1.42180229	-2.33725805
1	1.62831145	2.19302684	-3.01430267
1	0.10865739	1.51802910	-2.42650569
6	1.32543659	2.80397925	-0.30358840

6	-0.02189525	3.12027645	0.01727527
6	-0.31323828	4.32278836	0.67768932
6	0.68152020	5.22565488	1.05973377
6	2.00816696	4.89219184	0.76303351
6	2.34482133	3.71051187	0.09420531
6	-0.13020501	-3.28823915	2.50621405
1	-2.22901443	-4.36160751	3.81463911
6	-4.94106604	-4.47688933	3.47059837
1	-5.36463544	-2.94837351	1.24072041
6	-3.86145253	-1.55145965	-0.49442489
6	-1.15883975	2.17502866	-0.28280926
1	-1.35597166	4.54543955	0.91923303
6	0.34521510	6.49595519	1.80305775
1	2.80920889	5.57759641	1.05192549
6	3.79476605	3.42501960	-0.20940513
1	0.00177406	-3.94713660	3.37347180
1	0.28748651	-2.30467952	2.77608285
1	0.49276390	-3.68416501	1.68885450
1	-3.22088264	-0.66893248	-0.63255979
1	-4.89037441	-1.21457843	-0.31277991
1	-3.86938346	-2.10354014	-1.44849469
1	-5.02930376	-5.53761690	3.18630499
1	-5.93662526	-4.02560450	3.36295816
1	-4.66457378	-4.44833223	4.53363571
1	-2.00339489	2.36531291	0.39242800
1	-0.85469308	1.12544539	-0.15727312
1	-1.53677554	2.28731452	-1.31233206
1	3.94642587	3.22259143	-1.27851247
1	4.16551026	2.54040807	0.33036490
1	4.42260851	4.27891681	0.07742124
1	0.54094512	6.38920020	2.88185261
1	-0.71393017	6.76047942	1.68452445
1	0.95169657	7.34127056	1.44781176
1	-0.14684677	-1.73650483	0.65843350

Energy = -7200.163868 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 25

Atomic N.	X	Y	Z
8	3.49561244	0.73244298	-0.90021062
6	4.03448107	1.27057748	-2.09266197
1	3.29231736	1.82268807	-2.69803572
1	4.45815278	0.46700817	-2.72670363
1	4.85778979	1.96870996	-1.85743727
50	1.58793766	0.83111198	-0.12741329
7	0.93291384	-0.95462240	-1.75844060
6	1.98870860	-1.97999488	-1.88228071
1	1.78615930	-2.66523041	-2.72487583
1	2.05573519	-2.55219541	-0.95064099
1	2.94756760	-1.47162707	-2.03519975
7	-0.01646775	-2.17839036	0.88020507
6	-0.40696793	-1.55287102	-1.50767554
1	-0.77843227	-2.00371978	-2.44831257
1	-1.08986644	-0.72778942	-1.25744958
6	-0.49413408	-2.63447989	-0.43126872
1	-1.55665055	-2.94843089	-0.40041857
1	0.07699685	-3.51983477	-0.74282622

6	-0.35446328	-2.96857171	2.01604367
6	0.20226468	-4.25550385	2.19267028
6	-0.14068564	-4.99454650	3.33251883
6	-0.99506771	-4.49465254	4.31982952
6	-1.50006073	-3.20031611	4.14690108
6	-1.20238279	-2.43292738	3.01649342
7	0.51867190	1.89326295	-1.66599379
6	0.88767477	-0.12387717	-2.99826430
1	0.49206298	-0.72714864	-3.83729968
1	1.92552752	0.14678504	-3.23105105
6	0.06128693	1.14959796	-2.83230738
1	0.19556713	1.73691219	-3.76278454
1	-1.01698748	0.89248732	-2.79920176
6	-0.13948095	3.12134792	-1.37304838
6	-1.51270755	3.18993228	-1.01388242
6	-2.10118625	4.43259448	-0.73783018
6	-1.37830907	5.62647141	-0.78062475
6	-0.01717599	5.54622211	-1.09813549
6	0.60840708	4.33080013	-1.39412189
6	1.20917126	-4.81966883	1.22138996
1	0.30148526	-5.98581795	3.46109633
6	-1.36704145	-5.32247886	5.52618158
1	-2.15283792	-2.77336640	4.91236653
6	-1.77412451	-1.04037208	2.88335558
6	-2.35310235	1.94902197	-0.84688678
1	-3.15778083	4.45940429	-0.45731333
6	-2.03442739	6.95562630	-0.49463515
1	0.57926286	6.46203957	-1.12766087
6	2.07440735	4.32844717	-1.74985161
1	1.80036222	-5.61135452	1.69927658
1	1.89737796	-4.03375974	0.87720095
1	0.73666108	-5.26175690	0.32958730
1	-0.98841160	-0.26697901	2.87155146
1	-2.43680626	-0.81538680	3.72807045
1	-2.36327673	-0.92049076	1.95994162
1	-2.31896271	-5.85354178	5.36629353
1	-1.49075318	-4.69634891	6.42052023
1	-0.60216322	-6.08064691	5.74198242
1	-3.21767520	2.15291735	-0.20181148
1	-1.76180552	1.14322486	-0.38593290
1	-2.74261393	1.56530649	-1.80343783
1	2.24876920	3.83332228	-2.71485942
1	2.68354926	3.78871782	-1.00884497
1	2.45625530	5.35608026	-1.81017138
1	-1.44241782	7.55166222	0.21504825
1	-3.03911612	6.82174816	-0.07227159
1	-2.13630476	7.55582096	-1.41238477
1	-0.31248923	-1.21359252	1.03393461

Energy = -7200.162828 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 26

Atomic N.	X	Y	Z
8	3.10125401	-1.99249968	-1.27429731
6	4.37958121	-1.67576973	-1.80039882
1	4.42229438	-1.87135335	-2.88946584
1	5.15067434	-2.30165504	-1.31900034

1	4.66834454	-0.61652188	-1.64448230
50	1.83890535	-0.49609902	-0.57952424
7	0.24890270	-1.01332239	-2.47205610
6	0.97584578	-1.91907234	-3.39482071
1	0.27960938	-2.34883025	-4.13634519
1	1.47837376	-2.71090537	-2.83105545
1	1.75192825	-1.34895198	-3.92119785
7	0.46491341	-1.89380285	0.25571460
6	-0.84587164	-1.74630448	-1.77639505
1	-1.45245384	-2.30283224	-2.51664175
1	-1.47851859	-1.00245367	-1.27830366
6	-0.29307272	-2.68498094	-0.70409207
1	-1.15626998	-3.16339310	-0.20703018
1	0.27530381	-3.50464191	-1.18659888
6	0.65177171	-2.39657127	1.57027449
6	1.17721674	-3.68960876	1.83483180
6	1.30148186	-4.12508373	3.16176447
6	0.95594409	-3.32040557	4.25077975
6	0.48059341	-2.03267053	3.97804488
6	0.31748104	-1.56060574	2.67139566
7	-0.54377291	1.78492235	-1.43663504
6	-0.24924323	0.13581171	-3.28344725
1	-0.79862108	-0.26008934	-4.15941307
1	0.64405934	0.64842423	-3.67530095
6	-1.16374760	1.15443046	-2.60705704
1	-1.42227910	1.89512523	-3.39058091
1	-2.11017700	0.68064715	-2.31557079
6	-1.15976796	2.94969137	-0.89763416
6	-2.44205175	2.88896626	-0.30634280
6	-2.99847853	4.05739548	0.23099183
6	-2.32150448	5.28031243	0.22978897
6	-1.03499191	5.30840328	-0.32208567
6	-0.44577187	4.17381404	-0.88757006
6	1.68494309	-4.57962286	0.72604175
1	1.71276098	-5.12169889	3.34524769
6	1.08154159	-3.82185871	5.66951877
1	0.21024659	-1.37522392	4.80894592
6	-0.22265790	-0.17022874	2.44712294
6	-3.19810266	1.58944645	-0.17905381
1	-3.98775496	3.99578530	0.69153196
6	-2.95461882	6.52812050	0.79622784
1	-0.47085647	6.24440679	-0.31861848
6	0.94779275	4.26263953	-1.46562989
1	2.35964657	-5.34374907	1.13446036
1	2.23357238	-3.99209321	-0.02585518
1	0.87156756	-5.11061640	0.20561984
1	0.56129639	0.53197657	2.11754186
1	-0.65444966	0.23270093	3.37276929
1	-0.98595681	-0.16572821	1.65740513
1	0.10304066	-4.12414027	6.07597759
1	1.48201227	-3.04592442	6.33762323
1	1.74445489	-4.69590174	5.72580458
1	-3.92814376	1.65107761	0.63824146
1	-2.51210742	0.75723243	0.03487397
1	-3.75801192	1.33499294	-1.09345154
1	0.97726860	3.96646527	-2.52688945
1	1.66373043	3.61933173	-0.92763653
1	1.32467752	5.29079351	-1.40139363

1	-2.21231423	7.16156323	1.30137266
1	-3.74403303	6.28268068	1.51922005
1	-3.41445847	7.13751464	0.00192129
1	0.43702891	1.98053953	-1.63918262

Energy = -7200.165728 Hartree
Number of imaginary frequencies = 0.

Compound 11b isomer 27

Atomic N.	X	Y	Z
8	3.34874547	0.33329329	-1.69785977
6	4.64004329	-0.08038935	-1.28520904
1	5.32887573	0.78283850	-1.23229499
1	5.06626300	-0.80349349	-2.00539856
1	4.64824058	-0.56775454	-0.28858091
50	1.74556868	0.19152922	-0.35151182
7	0.59873490	-0.48526961	-2.45466078
6	1.36047809	-1.53020242	-3.17248324
1	0.96257914	-1.67205785	-4.19340481
1	1.30438313	-2.48211880	-2.63226289
1	2.40888982	-1.21278362	-3.21596120
7	-0.85147437	-1.79600879	-0.05355136
6	-0.83725384	-0.84659348	-2.33991005
1	-1.24032203	-1.03270340	-3.35409969
1	-1.36357864	0.03221013	-1.94081127
6	-1.16293543	-2.05612870	-1.46592779
1	-2.23623058	-2.28545232	-1.62069432
1	-0.60995797	-2.94315790	-1.79936930
6	-1.15816640	-2.82221098	0.88798387
6	-0.39702421	-4.01187131	0.92420900
6	-0.71208521	-4.99055282	1.87563097
6	-1.73797087	-4.82233584	2.81081845
6	-2.45012646	-3.61719234	2.78556711
6	-2.18440917	-2.61964016	1.84224418
7	0.66506483	1.92101598	-1.01320335
6	0.74021493	0.80925271	-3.18967715
1	0.23221437	0.74025557	-4.17026491
1	1.81798635	0.94410966	-3.35143742
6	0.19446232	1.99177434	-2.38910632
1	0.55380871	2.90904787	-2.89553353
1	-0.91237651	2.02618356	-2.46820564
6	0.43359407	3.05545988	-0.19209865
6	-0.87838448	3.42960664	0.20681520
6	-1.06898848	4.55705643	1.01535127
6	-0.00059555	5.33883773	1.46496199
6	1.28816705	4.95678610	1.07816609
6	1.52607050	3.84145360	0.26536439
6	0.78288053	-4.22083801	0.00786881
1	-0.11259589	-5.90410231	1.89983683
6	-2.07224473	-5.90428526	3.80900555
1	-3.24209541	-3.44740883	3.51923623
6	-2.97788782	-1.33341049	1.86602417
6	-2.07845105	2.60343711	-0.18225040
1	-2.08714619	4.82146516	1.31460123
6	-0.22483659	6.53054456	2.36465140
1	2.14230252	5.55464458	1.40793565
6	2.94838133	3.50798213	-0.11874677
1	1.48564533	-4.94121467	0.44588904

1	1.31613673	-3.27382827	-0.15995440
1	0.48623846	-4.61938463	-0.97628050
1	-2.34868459	-0.46216635	2.11331880
1	-3.76818344	-1.38408994	2.62508423
1	-3.46220324	-1.12405998	0.89903682
1	-2.90191767	-6.53374629	3.44974516
1	-2.38163255	-5.47940032	4.77386476
1	-1.21277085	-6.56497192	3.98501223
1	-2.90154786	2.75285188	0.52903052
1	-1.81548005	1.53517799	-0.19994003
1	-2.46047185	2.85959964	-1.18350932
1	3.01295161	3.09024722	-1.13141470
1	3.38587342	2.75367326	0.55696736
1	3.58395436	4.40136003	-0.05066755
1	-0.13245019	6.25125825	3.42650519
1	-1.22762151	6.95658848	2.22461020
1	0.51378333	7.32134892	2.17274060
1	-1.31243089	-0.93006539	0.22820513

Energy = -7200.167989 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 28

Atomic N.	X	Y	Z
8	2.69993381	-1.65792925	-2.30125929
6	3.96827406	-1.29851258	-2.82425849
1	3.90199915	-1.06148993	-3.90390864
1	4.67432819	-2.13906580	-2.71045689
1	4.41729520	-0.41839005	-2.32086285
50	1.71899421	-0.41898630	-0.95331184
7	-0.05825256	0.00390950	-2.69662056
6	0.46958288	-0.53778118	-3.97268240
1	-0.32941684	-0.57007646	-4.73413251
1	0.89426625	-1.53381616	-3.81442693
1	1.27926640	0.11059508	-4.33118873
7	0.22165171	-1.87648158	-0.54116452
6	-1.19198564	-0.82906424	-2.20597496
1	-1.91706305	-0.99390011	-3.02615203
1	-1.68320575	-0.27728223	-1.39620630
6	-0.69858942	-2.15849849	-1.63452424
1	-1.58222272	-2.70477488	-1.25825747
1	-0.27853581	-2.77939386	-2.45040670
6	0.41649815	-2.85583809	0.46780515
6	0.76371699	-4.20266739	0.17892959
6	0.90550823	-5.11879507	1.23070008
6	0.74924323	-4.75285270	2.57041633
6	0.45096766	-3.41319418	2.84427226
6	0.27783613	-2.46657969	1.82872582
7	-0.38642660	2.23685316	-0.59122218
6	-0.44764185	1.42275940	-2.94700690
1	-1.10481801	1.45865920	-3.83730987
1	0.47897546	1.95513258	-3.21587284
6	-1.16499706	2.18182233	-1.83304918
1	-1.37068947	3.19236094	-2.24030152
1	-2.14605066	1.73002803	-1.63699185
6	-0.79358425	3.15337780	0.41873999
6	-2.03391392	3.00722864	1.08088200
6	-2.38029134	3.92182906	2.08435413

6	-1.53267091	4.96146477	2.47775434
6	-0.29057378	5.06119521	1.83951217
6	0.09169102	4.18494401	0.81944000
6	1.06753845	-4.65622579	-1.22871044
1	1.17796156	-6.14991922	0.98857246
6	0.88752577	-5.76511330	3.68233660
1	0.33218116	-3.09312644	3.88307998
6	-0.06382433	-1.04333066	2.19295748
6	-2.96405914	1.85671302	0.78424726
1	-3.33909403	3.79375374	2.59317222
6	-1.94315501	5.94643319	3.54548464
1	0.40414695	5.84961836	2.13964931
6	1.44724480	4.33850750	0.16909789
1	1.64755033	-5.58847273	-1.20810451
1	1.64867769	-3.89264137	-1.76793526
1	0.15544652	-4.85515994	-1.81421841
1	0.79623507	-0.36456468	2.06644776
1	-0.38135754	-0.97617883	3.24188969
1	-0.85896117	-0.64965979	1.54570985
1	-0.09779776	-6.09212052	4.05149789
1	1.43150588	-5.34818873	4.54199536
1	1.42377464	-6.66093597	3.34095720
1	-3.62853640	1.67361188	1.63838907
1	-2.39699692	0.93551503	0.58711065
1	-3.60716475	2.04729387	-0.09005289
1	1.37118385	4.48803458	-0.92030381
1	2.09018034	3.45781312	0.33301682
1	1.97505595	5.20633124	0.58329799
1	-1.08252964	6.26739127	4.14842176
1	-2.69275217	5.51369712	4.22164134
1	-2.38591083	6.85274140	3.10235150
1	0.59683164	2.39139312	-0.81598153

Energy = -7200.165733 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 29

Atomic N.	X	Y	Z
8	0.77337858	-0.94632771	-1.12336473
6	0.66182574	-1.95865576	-2.10898261
1	1.66324845	-2.30123779	-2.42927271
1	0.11941802	-1.63133202	-3.02003874
1	0.12076204	-2.83424184	-1.70559571
50	0.10910474	0.97955513	-1.53620975
7	-1.09314513	2.95135435	-0.07987955
6	-2.09147033	3.71395709	-0.83341442
1	-2.39200926	4.63838015	-0.30124989
1	-2.98773932	3.10733495	-1.01043749
1	-1.67573257	3.98861779	-1.81219154
7	-1.74195309	0.10175789	0.22162630
6	-1.63630848	2.38958101	1.16356074
1	-2.22690803	3.14262947	1.72462049
1	-0.79048711	2.10309066	1.80320275
6	-2.50932583	1.15669753	0.92032588
1	-2.89199888	0.79916395	1.89358038
1	-3.38489494	1.41123423	0.31190377
6	-2.46428866	-1.10064418	-0.10627837
6	-3.47367830	-1.09247632	-1.09146984

6	-4.14180978	-2.29065673	-1.38084043
6	-3.82957793	-3.49434187	-0.74375414
6	-2.79434080	-3.48308979	0.19871935
6	-2.10634533	-2.31216551	0.53039812
7	1.44244859	1.64432930	0.01889193
6	0.13144098	3.74652929	0.11491581
1	-0.05465837	4.62803207	0.76345871
1	0.41552852	4.12272984	-0.88086195
6	1.28666189	2.92728914	0.69027894
1	2.19613183	3.55124763	0.58665369
1	1.14328215	2.81478084	1.78626676
6	2.65343460	0.96547917	0.34353090
6	2.86128811	0.40211938	1.62799898
6	4.07405805	-0.23438220	1.92510547
6	5.10456693	-0.34478713	0.98880575
6	4.88998587	0.21179743	-0.27717899
6	3.69548723	0.85732399	-0.61449226
6	-3.82678363	0.14573434	-1.88023238
1	-4.91738872	-2.27898713	-2.15061896
6	-4.58169771	-4.76467139	-1.05813841
1	-2.50602322	-4.41546132	0.68988039
6	-0.96855739	-2.36189545	1.52226200
6	1.78788416	0.43785421	2.68668496
1	4.20678839	-0.67066976	2.91918359
6	6.38974843	-1.06694065	1.31560287
1	5.68134274	0.14701630	-1.02900674
6	3.54426651	1.42992792	-2.00207744
1	-4.25106471	-0.13391619	-2.85320430
1	-2.94150368	0.77167384	-2.06532771
1	-4.58033938	0.76664591	-1.36850722
1	-0.01882967	-2.06601485	1.04597841
1	-0.84644305	-3.37993599	1.91373666
1	-1.13657211	-1.69868944	2.38651430
1	-5.36475466	-4.95764143	-0.30792471
1	-3.91307451	-5.63658451	-1.06034701
1	-5.07284893	-4.70615626	-2.03852785
1	1.88927241	-0.41337853	3.37311711
1	0.79108427	0.39851549	2.22545345
1	1.82993055	1.35547628	3.29588624
1	3.07262873	2.42231909	-1.98630358
1	2.91314110	0.78516214	-2.63655776
1	4.52159961	1.51097826	-2.49662111
1	6.36530727	-2.10710375	0.95321326
1	6.56598879	-1.10099945	2.39925976
1	7.25479214	-0.58061451	0.84275320
1	-0.94327394	-0.16231660	0.80553738

Energy = -7200.167082 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 30

Atomic N.	X	Y	Z
8	1.11480771	-1.23305516	-0.00287602
6	1.38038570	-2.60158944	0.25238422
1	0.88143760	-3.28968614	-0.46105224
1	1.03840422	-2.88045446	1.26597080
1	2.46617721	-2.80373610	0.19721417
50	0.03309907	-0.68651280	-1.69169482

7	-1.79515111	1.26037157	-2.26004685
6	-2.85942538	0.81913144	-3.16413405
1	-3.44672896	1.67267892	-3.55742370
1	-3.54374042	0.13386044	-2.64958668
1	-2.41606767	0.27565111	-4.00935474
7	-1.71995231	-0.18638711	0.29579181
6	-2.31725334	1.83111317	-1.01178918
1	-3.14464592	2.54464521	-1.20495504
1	-1.50712060	2.40006027	-0.53585914
6	-2.80821975	0.76009695	-0.03544485
1	-3.19630879	1.26097115	0.87007128
1	-3.64313435	0.19394244	-0.46439059
6	-2.06767069	-1.27340205	1.17493792
6	-2.92294380	-2.30860866	0.74215658
6	-3.22429057	-3.34909333	1.63177200
6	-2.69249947	-3.40740743	2.92287476
6	-1.81255167	-2.39055082	3.31133115
6	-1.48983153	-1.32544607	2.46471885
7	0.96051247	1.24917610	-1.51507765
6	-0.84514902	2.13996855	-2.96255954
1	-1.32395455	3.09296540	-3.27047129
1	-0.55226912	1.60541336	-3.88033155
6	0.40558127	2.44332718	-2.13748227
1	1.13164558	2.91346779	-2.82957338
1	0.16883581	3.23463070	-1.39443494
6	2.25769714	1.43887567	-0.95465116
6	2.45017746	2.22634158	0.20880285
6	3.74143103	2.41697538	0.71911281
6	4.86834843	1.84780648	0.12167643
6	4.66908514	1.07035487	-1.02470964
6	3.39777181	0.85637126	-1.56810526
6	-3.48527451	-2.36331520	-0.65815173
1	-3.88075901	-4.15200215	1.28730094
6	-3.05636837	-4.52621826	3.86839527
1	-1.35575809	-2.42666719	4.30311551
6	-0.50129396	-0.27668540	2.91645577
6	1.28690703	2.84473914	0.94290603
1	3.86341859	3.01937226	1.62377592
6	6.24757969	2.03449719	0.70728020
1	5.53329738	0.61764412	-1.51854507
6	3.26989475	0.00455486	-2.80670002
1	-3.70623719	-3.40183276	-0.93664759
1	-2.77393127	-1.96057634	-1.39407647
1	-4.42738571	-1.79875811	-0.75267674
1	0.39048420	-0.27260148	2.26709702
1	-0.17022848	-0.47997695	3.94215658
1	-0.93315568	0.73748854	2.90797601
1	-3.90610352	-4.24242298	4.50938792
1	-2.21831330	-4.77844862	4.53229389
1	-3.34744845	-5.43341189	3.32202811
1	1.51921661	2.96588572	2.00942461
1	0.39254949	2.21291909	0.84909442
1	1.02581795	3.84104146	0.55020370
1	2.56219722	0.43531610	-3.52858317
1	2.90363784	-1.00688681	-2.56290344
1	4.24538047	-0.11558043	-3.29693524
1	6.52733423	1.18215658	1.34692423
1	6.30125671	2.94059500	1.32593259

1 7.01064159 2.11140116 -0.08023099
 1 -0.95384480 0.33550593 0.73089070
 Energy = -7200.167093 Hartree
 Number of imaginary frequencies = 0.

Compound 11b isomer 31

Atomic N.	X	Y	Z
8	0.96021116	-1.02934397	0.83611636
6	2.32627231	-1.41339478	0.83110745
1	2.96985942	-0.54950802	1.07293490
1	2.66745577	-1.81766537	-0.14434322
1	2.50542811	-2.19610845	1.58973355
50	-0.19418671	-1.34512354	-0.84362217
7	-1.81032375	0.35630500	-2.31141294
6	-2.46470167	-0.50331305	-3.30821051
1	-3.24386240	0.04259498	-3.87534805
1	-2.93364074	-1.36319728	-2.81511141
1	-1.71269649	-0.88702130	-4.01024774
7	-1.94806764	-0.91373127	0.30986036
6	-2.75871810	0.78708691	-1.26563848
1	-3.67237350	1.21948643	-1.72443683
1	-2.26894775	1.56840032	-0.66831771
6	-3.13356052	-0.35734481	-0.32603019
1	-3.80761989	0.06396397	0.44227713
1	-3.74871368	-1.10227895	-0.87617644
6	-2.21131354	-1.64088466	1.51506556
6	-2.81677667	-2.92192760	1.49334846
6	-3.06628203	-3.59138906	2.70111155
6	-2.74134865	-3.03258164	3.93883862
6	-2.15241666	-1.76186742	3.94622032
6	-1.88129556	-1.06072696	2.76677742
7	1.03448154	1.18879015	-1.89222265
6	-1.15623110	1.49848184	-2.97712803
1	-1.90193204	2.26974663	-3.25861882
1	-0.72235245	1.12509335	-3.91907729
6	-0.04791940	2.15635646	-2.15958664
1	0.31926044	3.03082052	-2.72877404
1	-0.44020558	2.53746511	-1.20872078
6	2.29479514	1.69514739	-1.44476919
6	2.41989321	2.36855637	-0.20981894
6	3.68641475	2.82071674	0.18439385
6	4.83513846	2.60929160	-0.58339148
6	4.69201430	1.90334360	-1.78346357
6	3.44784360	1.44724976	-2.22883000
6	-3.20284635	-3.59909020	0.19999865
1	-3.52373130	-4.58396563	2.66638282
6	-2.99308520	-3.77862625	5.22740878
1	-1.89361480	-1.29860479	4.90222724
6	-1.23532088	0.29807213	2.83738513
6	1.24952778	2.55358092	0.72296365
1	3.77474571	3.33266403	1.14577918
6	6.18126073	3.12799918	-0.13914663
1	5.57411583	1.70105909	-2.39589791
6	3.35651907	0.68198685	-3.52951304
1	-3.23368647	-4.68937054	0.32674390
1	-2.49279067	-3.36535912	-0.60710590
1	-4.20055392	-3.28211385	-0.14434420

1	-0.21688117	0.24471293	2.42580402
1	-1.18615811	0.65007987	3.87656669
1	-1.78685918	1.03857896	2.24018003
1	-3.45521078	-3.12795926	5.98406850
1	-2.05267284	-4.15629171	5.65871702
1	-3.65487887	-4.64028580	5.06774933
1	1.60593518	2.73685337	1.74459982
1	0.62107400	1.65246776	0.74188340
1	0.61938605	3.41244901	0.44154659
1	2.68331729	1.16829901	-4.25481440
1	2.99378015	-0.34887355	-3.38139131
1	4.34413518	0.61096153	-4.00137163
1	6.98820414	2.43124073	-0.40521641
1	6.20920046	3.28576162	0.94726545
1	6.41365654	4.09268274	-0.61763131
1	1.18985073	0.64960201	-2.74532590

Energy = -7200.163172 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 32

Atomic N.	X	Y	Z
8	0.62838054	0.00851820	1.33510371
6	1.89998472	0.13886456	1.95566199
1	1.78486315	0.00266437	3.04407081
1	2.35218745	1.13618051	1.79512490
1	2.62946776	-0.61543481	1.59931548
50	0.54595860	0.33524112	-0.75813227
7	-1.89003832	0.53944510	-0.41944340
6	-2.60978518	-0.00120681	-1.59389381
1	-3.70054699	0.13509146	-1.48873436
1	-2.38515461	-1.06573638	-1.71197331
1	-2.27018304	0.52645076	-2.49329908
7	-0.97956913	-2.19639801	0.56892048
6	-2.34003824	-0.12219282	0.84397603
1	-3.38001715	0.19074336	1.05170419
1	-1.69443877	0.25921044	1.64750045
6	-2.31368697	-1.65181967	0.84702343
1	-2.69117380	-1.95855372	1.84408112
1	-3.03407498	-2.04996003	0.11783704
6	-0.84784353	-3.61285102	0.69270876
6	-1.33881501	-4.46591005	-0.32275764
6	-1.19188252	-5.85181456	-0.18470202
6	-0.55353438	-6.42696236	0.91883872
6	-0.04062975	-5.56535504	1.89483517
6	-0.17869042	-4.17513990	1.80669845
7	0.24757192	2.45648128	-0.52772010
6	-2.11761617	2.01915694	-0.32030162
1	-3.04553975	2.20741474	0.24890666
1	-2.25292674	2.39826937	-1.34163969
6	-0.92086546	2.74389146	0.29625957
1	-1.15073418	3.82181979	0.29366762
1	-0.80618527	2.44002215	1.35419507
6	1.13496228	3.50201737	-0.86149612
6	1.64861951	4.40204938	0.11395278
6	2.50275210	5.44093331	-0.27980194
6	2.90317076	5.62214334	-1.60618233
6	2.41253910	4.71692549	-2.55398710

6	1.54424893	3.67404154	-2.21483902
6	-1.95744804	-3.90957274	-1.58029331
1	-1.56912609	-6.49870929	-0.98093938
6	-0.43386225	-7.92536671	1.05906464
1	0.47878635	-5.98568583	2.75980785
6	0.40269508	-3.29912722	2.89115113
6	1.35949451	4.22677813	1.58650042
1	2.88801497	6.11572630	0.48982314
6	3.85759464	6.72473124	-1.99790116
1	2.70091963	4.83433080	-3.60228883
6	1.03790752	2.76496280	-3.30657707
1	-1.97331124	-4.67018838	-2.37142829
1	-1.38185543	-3.04342920	-1.93803570
1	-2.99769544	-3.57785538	-1.42933134
1	1.26934106	-2.72361171	2.53053208
1	0.74148089	-3.91052899	3.73700829
1	-0.32611391	-2.56785771	3.27111276
1	-1.28488201	-8.34063244	1.62225666
1	0.48112538	-8.20655082	1.59811095
1	-0.42014229	-8.41941900	0.07799762
1	2.12047075	4.74289976	2.18651372
1	1.36024070	3.16394012	1.86596682
1	0.38017667	4.63329583	1.88390765
1	-0.03996357	2.57316941	-3.19824931
1	1.53345480	1.78016841	-3.29249677
1	1.22150526	3.20770725	-4.29465476
1	4.89277885	6.35343673	-2.06710773
1	3.85051616	7.54027745	-1.26211093
1	3.60080253	7.14821608	-2.97945385
1	-0.29364197	-1.68934575	1.14963606

Energy = -7200.170833 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 33

Atomic N.	X	Y	Z
8	2.02977862	-0.28335124	0.05536304
6	3.25793589	-0.82124661	0.53018620
1	3.61123401	-0.24255090	1.40088268
1	4.06673420	-0.80474778	-0.22656130
1	3.14134840	-1.87495135	0.85123074
50	1.87664351	0.22381519	-1.96768942
7	-0.40620839	-0.76148156	-1.99671018
6	-0.63111675	-1.64321466	-3.16331588
1	-1.67393616	-2.00591631	-3.18778971
1	0.04538939	-2.50430389	-3.12639829
1	-0.42562461	-1.08288878	-4.08370286
7	0.28508286	-3.14611836	0.88670351
6	-0.68173234	-1.47858719	-0.71854907
1	-1.76320669	-1.70133658	-0.66280516
1	-0.42955260	-0.79032043	0.09687929
6	0.13851268	-2.76785366	-0.52485765
1	-0.30260268	-3.59930501	-1.08769399
1	1.15583833	-2.61307701	-0.91185453
6	-0.86908954	-3.31130672	1.69721881
6	-1.83621590	-4.30226208	1.40456754
6	-2.94359055	-4.44578694	2.25113675
6	-3.11832586	-3.66680827	3.39857973

6	-2.12051324	-2.73256243	3.70232107
6	-1.00688543	-2.53871760	2.87977841
7	0.59023974	1.89669316	-1.68250187
6	-1.28594508	0.44529474	-2.09956685
1	-2.31904742	0.16828433	-1.82119986
1	-1.27507560	0.76415115	-3.15114844
6	-0.76416520	1.59539289	-1.24402978
1	-1.42720782	2.46343096	-1.40992103
1	-0.86141305	1.33616989	-0.17003940
6	1.11882507	3.19617838	-1.45738402
6	1.20418776	3.77263821	-0.16314459
6	1.72010590	5.06779861	-0.01787227
6	2.18532874	5.81357913	-1.10500758
6	2.11782573	5.22439206	-2.37300663
6	1.59446403	3.94173677	-2.56943440
6	-1.66976682	-5.25780724	0.24811347
1	-3.68001165	-5.21804850	2.01354396
6	-4.33606289	-3.82338751	4.27714554
1	-2.21133211	-2.12750131	4.60804603
6	0.04789545	-1.53056858	3.27377642
6	0.80306082	2.99805751	1.06870354
1	1.77940087	5.49533321	0.98685236
6	2.77547968	7.19060348	-0.91591416
1	2.46925411	5.78641802	-3.24255146
6	1.52750800	3.37506648	-3.96664647
1	-2.26023113	-6.16742834	0.41893656
1	-0.61568133	-5.54544562	0.12360348
1	-2.00880148	-4.82970853	-0.70981052
1	1.01248989	-2.01471839	3.50147944
1	-0.26083623	-0.98652464	4.17495000
1	0.24437921	-0.78718588	2.48475728
1	-5.10313923	-3.07016143	4.03591335
1	-4.08406255	-3.69878322	5.33959763
1	-4.79671920	-4.81233248	4.14917752
1	1.26515739	3.43767824	1.96252585
1	1.11718955	1.94616681	0.98917288
1	-0.28709847	3.00645197	1.22957917
1	0.54464139	2.92672498	-4.16860816
1	2.27058877	2.57617518	-4.12404937
1	1.72413362	4.15834310	-4.71070211
1	3.87455340	7.14781383	-0.85134899
1	2.41099575	7.65916720	0.00817124
1	2.52673922	7.85275977	-1.75724997
1	0.92225605	-2.47801821	1.32017246

Energy = -7200.168588 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 34

Atomic N.	X	Y	Z
8	1.58962702	-0.37883174	-0.07529127
6	2.70577994	0.00300150	-0.86411952
1	2.92559787	1.07610339	-0.72591213
1	2.55728247	-0.16719486	-1.95049833
1	3.60037403	-0.57067665	-0.56274029
50	-0.04261310	-1.25780945	-0.97921908
7	-2.73912040	-0.64678970	-0.89029283
6	-3.39167174	-1.71966530	-1.65443086

1	-4.49598318	-1.65064890	-1.60378306
1	-3.08713713	-2.69887968	-1.26601539
1	-3.07432510	-1.66394050	-2.70439174
7	-0.79587260	-1.79471136	0.95422662
6	-2.99637005	-0.77812361	0.55711440
1	-4.08351651	-0.89271256	0.74975347
1	-2.65474042	0.14554620	1.04430822
6	-2.22737171	-1.94622974	1.17169587
1	-2.44403585	-1.94041632	2.25566866
1	-2.64763395	-2.90443955	0.79585197
6	0.02185255	-2.54327043	1.86060326
6	0.13650381	-3.95273906	1.76773820
6	0.94010292	-4.64507093	2.68631888
6	1.63492182	-3.98891698	3.70448052
6	1.50522850	-2.59701993	3.79055755
6	0.71923572	-1.86612665	2.89374414
7	-0.86411963	1.54216125	-1.70668957
6	-3.14923986	0.67057254	-1.41258861
1	-4.15879257	0.94281086	-1.04306115
1	-3.23216822	0.57944175	-2.50787411
6	-2.18056360	1.80567943	-1.09251471
1	-2.62412588	2.74641407	-1.46888422
1	-2.06179760	1.92079331	-0.00799029
6	0.05443156	2.63152063	-1.82595790
6	0.57366052	3.28392125	-0.68596504
6	1.48755027	4.33039389	-0.86797709
6	1.92592326	4.73744463	-2.13151462
6	1.42896137	4.04799216	-3.24333666
6	0.50194626	3.00919781	-3.11527384
6	-0.58308038	-4.74070841	0.69921214
1	1.02675019	-5.73118837	2.59404883
6	2.51509727	-4.74710795	4.66923996
1	2.03336324	-2.05935906	4.58275019
6	0.62646530	-0.36898621	3.03019259
6	0.22799922	2.84353889	0.71432125
1	1.89057970	4.82307470	0.02029535
6	2.89463406	5.88377388	-2.29247275
1	1.76934465	4.32618155	-4.24374347
6	0.00692974	2.29544348	-4.35271871
1	-0.06720079	-5.68996965	0.50300666
1	-0.64493687	-4.17963194	-0.24503697
1	-1.61489873	-4.98566337	0.99889508
1	1.13163845	0.11155255	2.17970315
1	1.09765815	-0.03526707	3.96445723
1	-0.41857381	-0.02714158	3.02026156
1	2.33842442	-4.43025762	5.70750594
1	3.58149814	-4.57247910	4.45655258
1	2.33682093	-5.82890171	4.60737380
1	0.98866161	3.19938172	1.42082042
1	0.19352687	1.74712340	0.77952933
1	-0.74076260	3.24357563	1.05387061
1	-1.08853713	2.35778825	-4.46162560
1	0.27907297	1.22673848	-4.35393037
1	0.44774040	2.74091222	-5.25289860
1	3.56221836	5.72799895	-3.15103595
1	3.51454183	6.01184142	-1.39495320
1	2.36249672	6.83346800	-2.46151191
1	-1.02525273	1.15548814	-2.63784857

Energy = -7200.163230 Hartree
 Number of imaginary frequencies = 0.

Compound 11b isomer 35

Atomic N.	X	Y	Z
8	1.53021321	-0.54110106	0.24007699
6	2.83900421	-0.20050705	-0.18970648
1	3.09555659	0.82472486	0.12994280
1	2.96750952	-0.24626915	-1.29104442
1	3.57753693	-0.89182329	0.25390556
50	0.11785209	-1.10846381	-1.15210820
7	-2.45158770	-0.21250158	-1.64313621
6	-2.98048536	-1.11707231	-2.67403189
1	-4.05772578	-0.94196491	-2.86274554
1	-2.84805129	-2.16059688	-2.36430101
1	-2.42412300	-0.97050593	-3.60923830
7	-1.14955781	-1.77984294	0.44083619
6	-3.07684655	-0.46688578	-0.33049289
1	-4.18316828	-0.46939710	-0.42119901
1	-2.78721342	0.35041698	0.34417807
6	-2.59725963	-1.77892267	0.28709115
1	-3.07854442	-1.86386800	1.27882399
1	-2.99402734	-2.63334034	-0.30318429
6	-0.65975432	-2.73044744	1.39340821
6	-0.64588946	-4.12013906	1.11738889
6	-0.16680268	-5.01491717	2.08677185
6	0.29529509	-4.58165502	3.33088964
6	0.26948010	-3.20582200	3.59323152
6	-0.19451623	-2.27832372	2.65526820
7	-0.26482746	1.83127920	-1.63227610
6	-2.60335705	1.19012446	-2.07290634
1	-3.65155617	1.52977645	-1.94564311
1	-2.39238973	1.22646393	-3.15417280
6	-1.67551586	2.17308627	-1.36403445
1	-1.92316585	3.19016004	-1.72153472
1	-1.85332839	2.16459414	-0.28175472
6	0.73303073	2.81037076	-1.33033583
6	0.96022863	3.24325483	-0.00530600
6	1.96864311	4.18722546	0.23013568
6	2.77569597	4.69867817	-0.79035087
6	2.55854913	4.22334069	-2.08858239
6	1.55363570	3.29516114	-2.37750442
6	-1.13024776	-4.67531922	-0.20081067
1	-0.15116131	-6.08305171	1.85334220
6	0.81179275	-5.55733251	4.36136421
1	0.62351647	-2.83958201	4.56077222
6	-0.18618478	-0.80976486	2.98983853
6	0.19982440	2.67169199	1.16481067
1	2.14346884	4.50887892	1.25977453
6	3.83857451	5.73171449	-0.50475919
1	3.18767834	4.58572846	-2.90522935
6	1.37283467	2.81055551	-3.79814560
1	-0.65882023	-5.64466010	-0.41039069
1	-0.90451654	-3.99427683	-1.03473184
1	-2.22046945	-4.83620945	-0.19937288
1	0.55969645	-0.29310678	2.36832723
1	0.05816058	-0.65568492	4.04947319

1	-1.15974477	-0.34323673	2.78102459
1	0.23619749	-5.49354941	5.29735355
1	1.86237621	-5.35085893	4.61631578
1	0.75033044	-6.59143828	3.99740305
1	0.76307085	2.82706873	2.09377216
1	0.04842918	1.59068238	1.04023117
1	-0.78412229	3.14881121	1.30001256
1	0.35966295	3.01215774	-4.18356881
1	1.55358893	1.72691316	-3.89434966
1	2.08032469	3.31544905	-4.46720064
1	4.70597166	5.60939251	-1.16786217
1	4.18924820	5.66712661	0.53402986
1	3.45273100	6.75220325	-0.65765069
1	-0.18474870	1.58540755	-2.62013204

Energy = -7200.163153 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 36

Atomic N.	X	Y	Z
8	1.77704163	0.29954958	1.18942277
6	2.30883054	0.62958502	-0.08203889
1	2.87750918	1.57594441	-0.03775398
1	1.53535341	0.74932173	-0.86040252
1	3.00096695	-0.16687332	-0.40820014
50	-0.10679685	0.45511452	1.96346433
7	-2.80648839	-0.19457080	1.39472761
6	-3.54535269	0.18348609	2.60496209
1	-4.64147507	0.09353815	2.46697475
1	-3.31577223	1.22041793	2.87942608
1	-3.23569551	-0.45894398	3.44018308
7	-0.87623456	1.90024071	0.55702536
6	-3.06669133	0.74189208	0.28804130
1	-4.15669370	0.92815490	0.18161769
1	-2.70927280	0.27965102	-0.64204029
6	-2.32808248	2.06914245	0.46978850
1	-2.58931655	2.70835582	-0.38832542
1	-2.73563106	2.60116674	1.35505503
6	-0.12431196	2.94980290	-0.04303722
6	0.66663161	3.83457862	0.73592671
6	1.38397780	4.86234523	0.10874123
6	1.35766831	5.05783988	-1.27472366
6	0.58152754	4.17746640	-2.03530725
6	-0.14909396	3.13520433	-1.45408115
7	-0.72335467	-2.23515976	0.72865509
6	-3.09055461	-1.59521476	1.04163675
1	-4.09656012	-1.69633919	0.58298857
1	-3.11896225	-2.16849169	1.98284416
6	-2.06473465	-2.23892316	0.11132404
1	-2.40789807	-3.26783571	-0.10568235
1	-2.02893433	-1.70925995	-0.84844457
6	0.27529409	-3.10065478	0.18474283
6	0.71814093	-2.97209378	-1.14963927
6	1.71476489	-3.83885778	-1.61813248
6	2.30683038	-4.81157148	-0.80850047
6	1.88257049	-4.89141580	0.52312720
6	0.88204095	-4.05955007	1.03264723
6	0.76280135	3.70694492	2.23671440

1	1.97860357	5.53752231	0.72992788
6	2.16776227	6.15221496	-1.92708485
1	0.55600429	4.29098421	-3.12264978
6	-0.90738489	2.19187327	-2.35461012
6	0.19774216	-1.89377678	-2.06673384
1	2.05532804	-3.72423283	-2.65023511
6	3.36282460	-5.74552168	-1.34791866
1	2.34439231	-5.62327975	1.19033995
6	0.48028702	-4.17907592	2.48458951
1	1.10739095	4.64960420	2.68304418
1	1.48586517	2.92773502	2.52970158
1	-0.20468599	3.44340005	2.68826666
1	-0.85478374	1.16419058	-1.96832427
1	-0.49157083	2.21036614	-3.37062365
1	-1.97594822	2.44941176	-2.43730891
1	1.67473819	6.53233898	-2.83247443
1	3.16257548	5.78554940	-2.22691668
1	2.32506766	6.99638839	-1.24173439
1	0.92485752	-1.68858787	-2.86283492
1	0.02589797	-0.95886210	-1.51588453
1	-0.74835728	-2.17645675	-2.55538734
1	-0.59110219	-4.41090656	2.60602974
1	0.68548958	-3.25292710	3.04661728
1	1.04276982	-4.98464997	2.97206057
1	4.13776089	-5.95119907	-0.59648902
1	3.85127568	-5.32479248	-2.23696780
1	2.92686025	-6.71436100	-1.63932477
1	-0.83370250	-2.45693685	1.71919858

Energy = -7200.159773 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 37

Atomic N.	X	Y	Z
8	2.16917782	-0.01284410	-0.37428513
6	1.70097709	-0.71842345	-1.50480237
1	0.64593375	-1.03998649	-1.41701627
1	2.29587045	-1.63433027	-1.67372771
1	1.79197384	-0.08626181	-2.40748082
50	1.35276626	0.35041673	1.47381758
7	-0.95245018	0.88075246	2.87203567
6	-0.75040813	1.95510266	3.84618929
1	-1.57202178	1.99940483	4.58882298
1	-0.68470640	2.92619540	3.34049896
1	0.19818575	1.79186259	4.37546912
7	-0.70810453	1.67910301	0.00996549
6	-2.09956607	1.13187513	1.99311611
1	-2.98352991	1.47825092	2.56817148
1	-2.38159614	0.18105155	1.51878650
6	-1.79331568	2.15425415	0.89882164
1	-2.72301409	2.34760459	0.33183904
1	-1.48589248	3.11387542	1.33351471
6	-0.39931457	2.56588388	-1.08400955
6	0.34481676	3.74286926	-0.85955129
6	0.64466225	4.56907908	-1.95072949
6	0.23906741	4.26554100	-3.25346967
6	-0.49250304	3.08909225	-3.45115142
6	-0.82666861	2.23913840	-2.39162593

7	0.15363886	-1.46420882	1.57887153
6	-0.98397150	-0.43123795	3.53806772
1	-1.88156104	-0.54013983	4.18320386
1	-0.10002754	-0.46561765	4.19490402
6	-0.92255574	-1.60170394	2.55837862
1	-0.78175878	-2.51285407	3.17075250
1	-1.91839896	-1.72834753	2.08528819
6	0.46345475	-2.67539867	0.89795519
6	-0.47468164	-3.29598051	0.02919731
6	-0.15316495	-4.50417914	-0.60338142
6	1.07954682	-5.13506568	-0.42101444
6	2.00137293	-4.51349092	0.42826473
6	1.72255430	-3.30911427	1.08471591
6	0.84367505	4.13084956	0.51023562
1	1.23484277	5.47112119	-1.77167932
6	0.56212289	5.18437260	-4.40664896
1	-0.81749032	2.82246325	-4.45970147
6	-1.63140148	0.98952152	-2.66552985
6	-1.80566237	-2.65753258	-0.28370689
1	-0.88934342	-4.95492468	-1.27486043
6	1.42055835	-6.41998884	-1.13676413
1	2.97343564	-4.98536609	0.59534473
6	2.78040138	-2.71665178	1.98249724
1	1.73664513	4.76350370	0.42708284
1	1.10674928	3.24907468	1.11269568
1	0.09027050	4.70755571	1.07191765
1	-1.04607760	0.07193364	-2.49259393
1	-1.95832717	0.96901344	-3.71238988
1	-2.53471149	0.92914361	-2.03825507
1	-0.27044008	5.87741732	-4.60651808
1	0.74388300	4.61920498	-5.33095596
1	1.45162685	5.79265983	-4.19546150
1	-2.15690309	-2.96457632	-1.27803343
1	-1.72399730	-1.56059285	-0.26471635
1	-2.58832603	-2.93768304	0.43955853
1	2.34732487	-2.30208792	2.90387208
1	3.31964997	-1.89811648	1.47742712
1	3.52573002	-3.47577647	2.25540922
1	2.05984824	-6.23042050	-2.01365320
1	0.51627348	-6.93185664	-1.49239239
1	1.96958725	-7.11127523	-0.48144291
1	-0.99473160	0.77684618	-0.37913957

Energy = -7200.161480 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 38

Atomic N.	X	Y	Z
8	2.18593480	-0.27225355	-0.06154404
6	1.85572570	-0.48438884	-1.41854692
1	0.77416726	-0.64268913	-1.58899320
1	2.37152700	-1.37819906	-1.81424439
1	2.17464131	0.38408258	-2.02425460
50	1.09343658	-0.38515105	1.67256602
7	-1.34613829	0.06654334	2.85462229
6	-1.19665452	0.71796790	4.15736707
1	-2.12853763	0.66520905	4.75515045
1	-0.92233386	1.77247440	4.03151189

1	-0.38764231	0.22930496	4.71714559
7	-0.48657550	1.68118179	0.50117207
6	-2.27373548	0.78445503	1.97400387
1	-3.19865099	1.07936261	2.51214567
1	-2.57874948	0.10131384	1.16847810
6	-1.64916278	2.03190673	1.34914986
1	-2.42832602	2.55816881	0.76682096
1	-1.31063652	2.73133912	2.12410408
6	0.12344214	2.80062572	-0.17199233
6	0.95233000	3.69429089	0.53753962
6	1.54644551	4.75724165	-0.15599681
6	1.35273136	4.95939541	-1.52525562
6	0.53055259	4.05574440	-2.20792274
6	-0.09386978	2.98691602	-1.55682837
7	-0.31901059	-1.89300623	0.98422690
6	-1.65732538	-1.36270694	3.01616235
1	-2.66333031	-1.51385132	3.46205671
1	-0.91782023	-1.76099706	3.72927688
6	-1.56231795	-2.14813955	1.70932503
1	-1.64509330	-3.21750986	1.98265204
1	-2.46462670	-1.94057553	1.09747731
6	-0.04240505	-2.85405629	-0.02905548
6	-0.87683627	-2.98357913	-1.17270274
6	-0.59712454	-3.95859087	-2.13889132
6	0.49481571	-4.82316821	-2.02987725
6	1.31601748	-4.68417325	-0.90618574
6	1.07341175	-3.72720719	0.08655690
6	1.23578878	3.53255682	2.01034384
1	2.20008894	5.43636731	0.39678599
6	1.99338982	6.12297499	-2.24227654
1	0.36562853	4.18495284	-3.28031094
6	-0.98216056	2.05214416	-2.34506559
6	-2.04043591	-2.05307632	-1.41205104
1	-1.24913394	-4.02952788	-3.01407689
6	0.80073175	-5.84327045	-3.10010834
1	2.17557042	-5.34978525	-0.78968584
6	2.01562032	-3.65526316	1.26259340
1	2.19978432	3.99022377	2.26686440
1	1.27368473	2.47322233	2.30375865
1	0.46896478	4.02474952	2.63116852
1	-0.55435168	1.03956250	-2.42342912
1	-1.11407448	2.42493728	-3.36823236
1	-1.98462312	1.95424785	-1.89948440
1	1.29201047	6.96742142	-2.33343161
1	2.30239636	5.84618864	-3.25959741
1	2.87738366	6.48686762	-1.70208971
1	-2.23891655	-1.95117041	-2.48749204
1	-1.83080374	-1.05542778	-0.99857921
1	-2.97027299	-2.41076923	-0.94127684
1	1.47749748	-3.48881146	2.20657800
1	2.73607713	-2.82860626	1.14663996
1	2.59753385	-4.58271138	1.34924191
1	1.54420124	-5.45819046	-3.81623960
1	-0.09938007	-6.10712915	-3.67173440
1	1.21528769	-6.76518953	-2.66849949
1	-0.80576291	1.01523049	-0.20753346

Energy = -7200.161486 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 39

Atomic N.	X	Y	Z
8	-0.56678880	-0.99200070	-0.56161438
6	-0.52306296	-2.32400786	-1.06085024
1	0.16157922	-2.43238546	-1.92300801
1	-1.53012078	-2.61314761	-1.40374695
1	-0.20903811	-3.06014238	-0.29430045
50	1.26283234	-0.22456863	0.17642961
7	0.24067770	1.97807347	0.11418849
6	1.32084637	2.93450731	0.46476797
1	0.99793003	3.97169923	0.27116120
1	2.21597903	2.71279588	-0.12521979
1	1.56214910	2.82836374	1.52949294
7	1.88744831	0.63330336	-1.68752472
6	-0.08155648	2.06636425	-1.34234253
1	-0.47376739	3.07425633	-1.57249253
1	-0.86285228	1.32035578	-1.53865351
6	1.13907367	1.76593133	-2.21618616
1	0.75624294	1.59914008	-3.23947811
1	1.78171629	2.66935885	-2.28593827
6	2.90271635	0.08046174	-2.51331339
6	4.26232893	0.12233660	-2.09911618
6	5.25424431	-0.44967601	-2.90324628
6	4.96045825	-1.06269834	-4.12702227
6	3.62281113	-1.09375558	-4.52873848
6	2.59355103	-0.54631896	-3.75056541
7	-1.84017413	0.09773005	1.74651949
6	-0.94482454	2.31749194	0.96065872
1	-1.31796792	3.30382392	0.62229797
1	-0.57334259	2.43399077	1.98673746
6	-2.11074188	1.32769110	0.98588478
1	-2.95955819	1.85800288	1.43998654
1	-2.42141185	1.07451445	-0.04151015
6	-2.79963562	-0.31967869	2.70533183
6	-3.48539821	-1.55050778	2.54565435
6	-4.40630348	-1.95788226	3.51659669
6	-4.68859490	-1.18503692	4.64879667
6	-3.98268663	0.01152752	4.80517772
6	-3.03765289	0.45168999	3.86959860
6	4.66663686	0.79522726	-0.80909398
1	6.29358344	-0.40172014	-2.56701445
6	6.04773969	-1.69335036	-4.96356296
1	3.36096631	-1.57885166	-5.47326598
6	1.17079180	-0.67771548	-4.23769660
6	-3.22715345	-2.43201072	1.34867127
1	-4.92754500	-2.90808142	3.37394053
6	-5.72347735	-1.62321122	5.65687769
1	-4.14908675	0.61628320	5.70052542
6	-2.23348804	1.69299908	4.16802167
1	5.75983386	0.87582620	-0.74495719
1	4.32253942	0.24029152	0.07789205
1	4.24112219	1.80622695	-0.73281887
1	0.46450784	-0.70481466	-3.39716372
1	1.05058241	-1.59497297	-4.83011252
1	0.87816391	0.16322021	-4.88772653
1	5.72154509	-1.83446625	-6.00263122

1	6.33179048	-2.68199817	-4.56921259
1	6.95755008	-1.07618237	-4.97123078
1	-3.93881500	-3.26690771	1.32514745
1	-2.21316219	-2.86170978	1.36865583
1	-3.31726775	-1.87891358	0.40171404
1	-2.54204526	2.56393704	3.56853864
1	-1.16714483	1.51631797	3.96048795
1	-2.34028277	1.97372768	5.22380595
1	-5.53814163	-1.17258607	6.64145729
1	-5.73114580	-2.71558008	5.77642931
1	-6.73698630	-1.32358388	5.34524204
1	-1.58871667	-0.63900401	1.07466701

Energy = -7200.166797 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 40

Atomic N.	X	Y	Z
8	0.80049264	0.76745171	1.85026980
6	1.37106324	-0.52893646	1.89631792
1	2.44597507	-0.47752988	2.14711102
1	1.28401400	-1.07781773	0.94262293
1	0.86830830	-1.12370640	2.67947630
50	0.27514248	1.97559228	0.28919006
7	-1.20144388	1.96867287	-2.13344289
6	-1.16770913	3.36012936	-2.59821708
1	-1.60902671	3.47095289	-3.60897088
1	-0.13280251	3.72225646	-2.63178370
1	-1.72087978	3.99627953	-1.89429138
7	1.46282796	1.01166306	-1.23400364
6	-0.33792974	1.10345240	-2.95510875
1	-0.51747977	1.28563476	-4.03619150
1	-0.59739954	0.05805901	-2.73993299
6	1.14527568	1.29736800	-2.63466159
1	1.71366919	0.62951702	-3.30100163
1	1.45580112	2.32245717	-2.92717929
6	2.73523640	0.40633722	-1.03048212
6	3.78505086	1.09213892	-0.36544719
6	5.02723786	0.46573271	-0.19449031
6	5.28317053	-0.82847771	-0.65497734
6	4.24096190	-1.49999589	-1.30261494
6	2.98385739	-0.91651141	-1.49416410
7	-2.38669969	0.55231887	0.21848006
6	-2.59135178	1.48932000	-2.05954723
1	-2.99160294	1.26422998	-3.07036481
1	-3.20063070	2.31727914	-1.66134711
6	-2.79565426	0.26425261	-1.17098678
1	-3.86353040	-0.01818833	-1.22859341
1	-2.22229886	-0.58907104	-1.55323652
6	-2.83604996	-0.32566127	1.25265429
6	-2.48339128	-1.69250769	1.26696233
6	-2.93936402	-2.49781246	2.31943120
6	-3.70995315	-1.99569294	3.37122975
6	-4.01059573	-0.62851132	3.35824332
6	-3.59169275	0.21193519	2.32342481
6	3.60948925	2.49203433	0.17053138
1	5.82398761	1.01698096	0.31206138
6	6.62021934	-1.49187874	-0.42756745

1	4.40246768	-2.52199437	-1.65661602
6	1.89650105	-1.73576184	-2.14417025
6	-1.58146314	-2.29932724	0.22150415
1	-2.65305629	-3.55248977	2.32396054
6	-4.20378297	-2.89222331	4.48060617
1	-4.58853204	-0.19842625	4.17989591
6	-3.93021190	1.68389761	2.37462762
1	4.58541851	2.97349514	0.31990445
1	3.09814718	2.48867900	1.14744480
1	3.01448753	3.11927257	-0.50916518
1	0.92398558	-1.52659016	-1.67659473
1	2.11211433	-2.80811228	-2.04883058
1	1.78809173	-1.52147228	-3.21993005
1	6.88721489	-2.15577107	-1.26156989
1	6.60881014	-2.10642658	0.48684727
1	7.42064749	-0.74853632	-0.31100012
1	-1.09631291	-3.20143984	0.61569466
1	-0.79363591	-1.59345553	-0.07525783
1	-2.12929739	-2.59540629	-0.68735942
1	-4.51297304	2.01138074	1.49741107
1	-3.02641343	2.31328809	2.42693713
1	-4.53176133	1.90726403	3.26412792
1	-4.18216672	-2.37773155	5.45136573
1	-3.59261647	-3.80102668	4.56117106
1	-5.24390653	-3.20931775	4.30389700
1	-2.69605034	1.49848479	0.44569667

Energy = -7200.159767 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 41

Atomic N.	X	Y	Z
8	0.06822209	-1.37137420	-0.50267013
6	0.11621213	-2.71995928	-0.05755899
1	0.98767981	-2.92364760	0.59579903
1	0.19390806	-3.38544980	-0.93358337
1	-0.79161049	-3.01662605	0.50161226
50	-0.21947942	0.11617720	0.97961099
7	-0.82373307	1.58847915	-0.90482660
6	-0.36778200	2.97010470	-0.63544448
1	-0.68494371	3.65677087	-1.43996753
1	0.72265323	2.99222420	-0.54588307
1	-0.80067867	3.30932928	0.31337419
7	1.99444151	0.52261025	-1.36172138
6	-0.28760645	1.08488095	-2.20684333
1	-0.77450921	1.64575075	-3.02588978
1	-0.58397291	0.02936340	-2.28355389
6	1.22422691	1.20871735	-2.40599137
1	1.42818417	0.79526961	-3.41513477
1	1.52124182	2.26660440	-2.44796504
6	3.40816706	0.48345101	-1.56109197
6	4.19657156	1.62876932	-1.30436893
6	5.58196265	1.56628742	-1.50128522
6	6.22199657	0.39768970	-1.92573351
6	5.42980925	-0.73596385	-2.14019575
6	4.04044724	-0.71516312	-1.97238811
7	-2.36642852	-0.04731088	0.88724218
6	-2.32301274	1.54359911	-0.92863418

1	-2.67829594	1.79640789	-1.94374075
1	-2.68399676	2.31130791	-0.23183546
6	-2.86415468	0.19206406	-0.46242403
1	-3.96443686	0.25723280	-0.47018078
1	-2.58133435	-0.59336499	-1.18904659
6	-3.24477117	-0.55756541	1.86720042
6	-4.07636384	-1.68735070	1.62645390
6	-4.95363410	-2.13054728	2.62527069
6	-5.03312328	-1.52072943	3.88000685
6	-4.19327497	-0.42656109	4.11577369
6	-3.31242041	0.06466393	3.14648139
6	3.58398396	2.89375804	-0.75830887
1	6.17990763	2.45670882	-1.29068991
6	7.71349821	0.36275297	-2.15689403
1	5.90462692	-1.66833874	-2.45627535
6	3.24216203	-1.97447533	-2.21387820
6	-3.98908894	-2.47940261	0.34272816
1	-5.57798926	-3.00401193	2.41705775
6	-5.95756256	-2.04371425	4.95328171
1	-4.23504733	0.07802536	5.08502755
6	-2.46657051	1.26902986	3.47608585
1	4.35597590	3.53755474	-0.31758232
1	2.84240633	2.65441260	0.01771221
1	3.07295810	3.48653997	-1.53445237
1	2.83285242	-2.38407234	-1.27741908
1	3.87547406	-2.74905645	-2.66442403
1	2.38666771	-1.80297264	-2.88398512
1	7.95660543	0.55703015	-3.21373829
1	8.13684738	-0.61842539	-1.90148956
1	8.22899155	1.12535292	-1.55750443
1	-4.39802849	-3.48747274	0.49103726
1	-2.94713717	-2.57413282	0.00634908
1	-4.55004194	-2.01945097	-0.48583141
1	-2.45180000	1.98672064	2.64236789
1	-1.41617456	0.99891518	3.67457541
1	-2.84735684	1.77543810	4.37305593
1	-5.42831969	-2.71942442	5.64436515
1	-6.79449426	-2.60843944	4.52051288
1	-6.37402235	-1.22542948	5.55786087
1	1.59451578	-0.41956136	-1.23041126

Energy = -7200.170791 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 42

Atomic N.	X	Y	Z
8	3.24053288	2.04970090	-0.82357362
6	4.63942143	1.81712382	-0.80172297
1	5.09980127	2.20438428	-1.72695655
1	4.90477702	0.74326552	-0.72415828
1	5.11691436	2.33637983	0.05184807
50	1.90346488	0.51214090	-0.42155513
7	1.22163923	1.71048197	1.69406849
6	2.21602312	2.79140309	1.90197361
1	1.87089238	3.48208436	2.69131695
1	2.39131053	3.32966411	0.96543245
1	3.17157677	2.34695558	2.20844706
7	0.22084756	1.68214561	-0.99960034

6	-0.10243729	2.28472087	1.32377818
1	-0.37062425	3.09257470	2.03161783
1	-0.84449690	1.48118844	1.39551720
6	-0.10351533	2.79493953	-0.11752615
1	-1.11983518	3.17016572	-0.33441370
1	0.57130933	3.66971039	-0.20174969
6	-0.21080055	1.72195736	-2.35118251
6	0.05918417	2.81791735	-3.21496673
6	-0.42810660	2.79613297	-4.52856772
6	-1.15223633	1.71579902	-5.04239083
6	-1.37290685	0.62416341	-4.19570912
6	-0.92488912	0.60783350	-2.86986847
7	0.21387163	-1.19020628	2.00424751
6	1.17372368	0.90704568	2.95103304
1	1.02487292	1.59445649	3.80605803
1	2.17475966	0.46268088	3.07257470
6	0.11436930	-0.18636578	3.06894759
1	0.25134793	-0.63194310	4.07494017
1	-0.88974213	0.25733710	3.06950485
6	-0.50059715	-2.41126528	2.15898246
6	-1.91375471	-2.43253496	2.19043697
6	-2.57182514	-3.66271640	2.32092278
6	-1.88469809	-4.87783597	2.39409698
6	-0.48744151	-4.83749808	2.31668960
6	0.21481518	-3.63375016	2.20581051
6	0.93151863	3.97042067	-2.77882220
1	-0.20469272	3.64589537	-5.17989494
6	-1.68931472	1.73464476	-6.45347708
1	-1.92665501	-0.24049320	-4.57146476
6	-1.21546598	-0.59299724	-2.00463353
6	-2.73280296	-1.17665003	2.02080492
1	-3.66468860	-3.66612738	2.33724429
6	-2.62035213	-6.18563653	2.55886750
1	0.07811729	-5.77210091	2.34832499
6	1.72364730	-3.65208863	2.12185895
1	1.30874440	4.51163413	-3.65670155
1	1.79006337	3.60993494	-2.19188182
1	0.38720885	4.69985707	-2.15760851
1	-0.31910959	-1.21505591	-1.84322763
1	-1.97693077	-1.23255815	-2.47015896
1	-1.55662880	-0.28795122	-1.00625721
1	-2.69536355	2.18272992	-6.49208751
1	-1.76878052	0.71977282	-6.86691195
1	-1.04523902	2.32626999	-7.11900532
1	-3.74103334	-1.42433072	1.66476112
1	-2.26704137	-0.50095027	1.28899171
1	-2.85118919	-0.61852564	2.96353107
1	2.19199420	-3.06284135	2.92711625
1	2.09275260	-3.24721122	1.16493817
1	2.09982522	-4.67908811	2.20558094
1	-2.11182257	-7.00243139	2.02836863
1	-3.64801502	-6.11696063	2.17732264
1	-2.68355194	-6.47635861	3.61965914
1	1.19725782	-1.39103987	1.82045944

Energy = -7200.165743 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 43

Atomic N.	X	Y	Z
8	2.95160923	1.14630850	1.81612614
6	4.22739978	1.53359638	1.33077758
1	4.37431162	2.62609342	1.42962092
1	4.38711900	1.27724867	0.26366943
1	5.02499697	1.03558967	1.91005201
50	1.56942313	0.26640962	0.50536548
7	0.05364223	1.92913482	1.57095640
6	0.63158077	3.28883123	1.52248379
1	0.06044089	3.98176599	2.16627530
1	0.62791519	3.67073451	0.49536530
1	1.66950555	3.22672207	1.87043859
7	-1.08633762	1.23937036	-1.25179030
6	-1.36071382	1.92032758	1.11729949
1	-1.93939147	2.62470994	1.74585697
1	-1.75631523	0.91292218	1.31186419
6	-1.60755330	2.27477680	-0.34756660
1	-2.70087392	2.41721892	-0.46402607
1	-1.14739830	3.23764858	-0.60339849
6	-1.28539084	1.44953969	-2.65034425
6	-0.51432929	2.41133609	-3.34082514
6	-0.71417986	2.58160064	-4.71661925
6	-1.63614901	1.81695844	-5.43863789
6	-2.36360584	0.84531327	-4.74157301
6	-2.21159381	0.65220388	-3.36435838
7	0.48013084	-0.79831474	2.00091199
6	0.13592059	1.42091249	2.97543892
1	-0.54115443	2.00813549	3.62449915
1	1.17429864	1.58841194	3.29178725
6	-0.18095675	-0.07048134	3.07344434
1	0.14845344	-0.39297851	4.07854309
1	-1.28037841	-0.23901770	3.05948631
6	0.63922084	-2.20095892	2.17212723
6	-0.06666222	-3.09896126	1.33109473
6	0.10216633	-4.47990246	1.48507052
6	0.95423577	-5.01673737	2.45680984
6	1.65100480	-4.12324425	3.27674143
6	1.51916739	-2.73391012	3.15172994
6	0.55446983	3.21282862	-2.64070207
1	-0.10636662	3.32183008	-5.24303395
6	-1.84886461	2.03908182	-6.91654811
1	-3.07817945	0.22038251	-5.28301953
6	-3.02236694	-0.41369003	-2.66379612
6	-1.00331178	-2.57955724	0.26694043
1	-0.45518271	-5.15609358	0.83098812
6	1.14631234	-6.50897763	2.58598478
1	2.33844592	-4.51725780	4.03053288
6	2.34859064	-1.83171929	4.03303513
1	1.30794921	3.55950504	-3.35957296
1	1.05679364	2.60436727	-1.87455434
1	0.14795162	4.10944010	-2.14434279
1	-2.39248055	-1.23896708	-2.29279029
1	-3.75360546	-0.85360318	-3.35311517
1	-3.57873392	-0.01492830	-1.80114646
1	-2.67838395	2.74122688	-7.09680993
1	-2.09890385	1.10164401	-7.43187818
1	-0.95326271	2.46303140	-7.39033024

1	-1.61684889	-3.39402834	-0.14116033
1	-0.44913099	-2.12565284	-0.57076142
1	-1.66976262	-1.80267904	0.66889608
1	1.80708555	-1.53998684	4.94800810
1	2.62638755	-0.90684528	3.50656311
1	3.26393673	-2.34637456	4.35464227
1	1.94033221	-6.86729133	1.91129358
1	0.22891439	-7.05537347	2.32629737
1	1.43542404	-6.78936609	3.60793981
1	-1.48676752	0.33973974	-0.98225667

Energy = -7200.168585 Hartree
Number of imaginary frequencies = 0.

Compound 11b isomer 44

Atomic N.	X	Y	Z
8	0.96126614	0.69936116	-3.41907134
6	1.61539007	-0.08979333	-4.40012015
1	1.45047893	-1.17821929	-4.27146662
1	2.70925986	0.08114350	-4.38407264
1	1.25054567	0.18245867	-5.40538688
50	0.09319183	-0.17692388	-1.75520238
7	1.79508621	1.04319740	-0.36166412
6	2.89027494	1.51717018	-1.23749123
1	3.61609676	2.11422584	-0.65686029
1	2.47070043	2.11616821	-2.05243573
1	3.40415291	0.66527755	-1.69581528
7	-0.89471904	1.61235949	-1.16795014
6	1.02191289	2.21002088	0.16713762
1	1.72569240	3.00905464	0.46553000
1	0.47960518	1.86542881	1.05812873
6	0.00086534	2.71613065	-0.84963086
1	-0.55893485	3.54359183	-0.37937038
1	0.52680992	3.15198302	-1.72225703
6	-2.23360972	1.88983713	-1.54820001
6	-2.56009007	2.77676870	-2.60868397
6	-3.90577852	3.02127099	-2.91256193
6	-4.95341894	2.40026626	-2.22490049
6	-4.61728552	1.49864725	-1.20913512
6	-3.28832346	1.23726768	-0.85587408
7	3.43783605	-1.88586585	1.50869760
6	2.32079721	0.24075000	0.77462943
1	1.45606888	-0.07007731	1.37926118
1	2.95869860	0.88763522	1.40965768
6	3.10724730	-1.01816026	0.37003175
1	2.52410630	-1.58519492	-0.36956846
1	4.05848071	-0.75104010	-0.11096401
6	2.39232118	-2.44383816	2.29572704
6	1.50027363	-3.39012605	1.73759371
6	0.50201358	-3.94216080	2.55067990
6	0.37244478	-3.62104440	3.90556554
6	1.30021646	-2.72602487	4.45082002
6	2.29923229	-2.12975606	3.67448268
6	-1.48711841	3.40465569	-3.46540997
1	-4.13810821	3.70188646	-3.73649603
6	-6.39484013	2.70458132	-2.55622676
1	-5.41471371	0.99048265	-0.66029504
6	-2.99611321	0.26976992	0.26458523

6	1.63860935	-3.86750985	0.31348430
1	-0.17978049	-4.67284613	2.10816137
6	-0.73185426	-4.21211028	4.74805022
1	1.24222754	-2.47484762	5.51289510
6	3.27347222	-1.17208667	4.32032189
1	-1.91459336	3.75054516	-4.41586232
1	-0.68316998	2.68457624	-3.68106846
1	-1.02234731	4.27865504	-2.98145678
1	-2.58535444	-0.68331743	-0.10763793
1	-3.91273996	0.03627865	0.82227128
1	-2.24740324	0.67772366	0.95807938
1	-6.76647861	3.56159364	-1.97165843
1	-7.04766299	1.84978827	-2.33208254
1	-6.51630857	2.95946470	-3.61827249
1	1.19632079	-4.86617924	0.20321890
1	2.69603757	-3.91838821	0.01674928
1	1.12276849	-3.20759784	-0.40425972
1	3.26014982	-0.17845091	3.84377769
1	4.31297866	-1.53883697	4.27682736
1	3.02779162	-1.03225771	5.38024941
1	-0.41683513	-4.33834842	5.79294212
1	-1.04745696	-5.19163139	4.36395167
1	-1.62062313	-3.56117273	4.75149019
1	4.12423971	-1.42620977	2.10441137

Energy = -7200.168585 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 45

Atomic N.	X	Y	Z
8	0.89024562	0.07893558	-1.37599022
6	1.69983115	-0.79391456	-2.14834812
1	2.55650169	-1.21628943	-1.58331029
1	2.11616958	-0.25670255	-3.01908240
1	1.10203965	-1.64272087	-2.52419395
50	1.41323045	0.48968630	0.57672875
7	-0.01707034	0.33443842	2.93648797
6	0.87491242	0.89730318	3.96036640
1	0.36160455	1.01442959	4.93479411
1	1.24217813	1.88019097	3.64185665
1	1.74410517	0.23899415	4.08973837
7	-0.02379009	2.08012684	0.60290563
6	-1.13313075	1.25086776	2.63114153
1	-1.64322157	1.56642201	3.56517825
1	-1.85635521	0.70517615	2.00970780
6	-0.66906122	2.47616291	1.84625408
1	-1.57007429	3.07764165	1.62535482
1	-0.04222559	3.12024149	2.50068136
6	0.03535791	3.11534493	-0.38488132
6	0.92234632	4.21307862	-0.25936800
6	0.93701342	5.20928313	-1.24794529
6	0.09448479	5.16169406	-2.36010383
6	-0.78203971	4.07426914	-2.46838396
6	-0.82717277	3.05701663	-1.50998952
7	0.09911329	-2.13078926	1.24126963
6	-0.48675759	-1.00055521	3.35169691
1	-1.28562281	-0.91650384	4.11656349
1	0.36067227	-1.50912744	3.83973592

6	-0.98716257	-1.87932071	2.20852358
1	-1.36795782	-2.82066820	2.64724527
1	-1.83124495	-1.40449069	1.69361338
6	-0.07990157	-3.18333978	0.28962595
6	-1.10148425	-3.12728898	-0.68376638
6	-1.21236159	-4.17869232	-1.60360715
6	-0.33635394	-5.26793715	-1.61254397
6	0.69307957	-5.28004401	-0.66433578
6	0.83505266	-4.26418536	0.28554913
6	1.86627715	4.34462770	0.91202150
1	1.63656576	6.04308808	-1.14285476
6	0.12489177	6.24049633	-3.41645027
1	-1.45393165	4.01310190	-3.32885774
6	-1.78248896	1.90596733	-1.68642636
6	-2.02780061	-1.94341228	-0.80416462
1	-2.00013527	-4.12205894	-2.35882918
6	-0.49699759	-6.39475327	-2.60397579
1	1.40868586	-6.10585793	-0.65933859
6	1.97260805	-4.32659986	1.27942087
1	2.73892171	4.95349893	0.64069690
1	2.22413209	3.36297335	1.25611915
1	1.38250630	4.83381340	1.77292327
1	-1.21742668	0.98253786	-1.87970049
1	-2.46454777	2.09446576	-2.52636925
1	-2.38002653	1.73542274	-0.77913727
1	-0.85295275	6.73720706	-3.50983717
1	0.36919805	5.82489445	-4.40577759
1	0.87204362	7.00945390	-3.17961834
1	-2.46212334	-1.90416567	-1.81122467
1	-1.48293924	-1.00427762	-0.63607677
1	-2.86708965	-1.99228397	-0.09193562
1	1.61704846	-4.32442244	2.32311660
1	2.67077825	-3.48043170	1.16639138
1	2.55463546	-5.24535297	1.13722860
1	0.47686437	-6.79168353	-2.92234316
1	-1.04151125	-6.06452515	-3.49867412
1	-1.06236946	-7.23257968	-2.16582073
1	0.95223386	-2.31787695	1.77032543

Energy = -7200.163159 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 46

Atomic N.	X	Y	Z
8	2.77510307	0.10510208	2.36941013
6	3.98798463	0.83996496	2.32270476
1	3.98579362	1.65678904	3.06948913
1	4.18332724	1.30162025	1.33345579
1	4.84410679	0.18075186	2.55112966
50	1.52456552	0.06427094	0.68525933
7	-0.20068103	0.56375358	2.40853448
6	0.18839100	1.72469790	3.23667460
1	-0.47194089	1.81800023	4.11763119
1	0.13466573	2.64903617	2.65060088
1	1.22467959	1.57469848	3.56196195
7	-1.23186327	1.63046290	-0.33551479
6	-1.60058486	0.68091655	1.92605176
1	-2.27031903	0.78537878	2.80165900

8	3.34013514	-0.30305817	-1.52450838
6	3.70777430	-0.58884982	-2.86056380
1	2.89783917	-0.39625290	-3.58796801
1	4.00987586	-1.64966938	-2.96341726
1	4.57501708	0.02772652	-3.15778213
50	1.57660988	0.42858188	-0.74838701
7	0.62700364	-1.88009396	-0.98248320
6	1.62026229	-2.90742308	-0.60948744
1	1.27281661	-3.91983594	-0.88319724
1	1.80799454	-2.86234739	0.46866994
1	2.56094265	-2.68187368	-1.12477592
7	0.04252739	-1.27455498	1.95939213
6	-0.67667485	-2.08239055	-0.29356235
1	-1.19484580	-2.94544359	-0.75494074
1	-1.29303918	-1.19438067	-0.49648613
6	-0.63399155	-2.34240592	1.21209499
1	-1.68864380	-2.46801182	1.52928291
1	-0.13819770	-3.30184586	1.41391934
6	-0.13746342	-1.24750606	3.37243199
6	0.42786248	-2.25100881	4.19129438
6	0.24387422	-2.18077172	5.57845254
6	-0.45757834	-1.13662041	6.18862705
6	-0.97099835	-0.12936209	5.36274197
6	-0.83016496	-0.16712458	3.97201471
7	0.31930547	0.55210884	-2.49292067
6	0.42038411	-1.89110413	-2.46113517
1	-0.11590428	-2.81297662	-2.75611128
1	1.41900675	-1.91597014	-2.91574243
6	-0.33168089	-0.66195048	-2.96699840
1	-0.32160941	-0.71881128	-4.07399462
1	-1.40003612	-0.73357595	-2.67812113
6	-0.25036069	1.79630913	-2.88610284
6	-1.55004897	2.20746411	-2.48224994
6	-2.05317182	3.44612046	-2.90379467
6	-1.31166954	4.32000058	-3.70246136
6	-0.01827081	3.92516160	-4.06242612
6	0.51984082	2.69270812	-3.67601888
6	1.28208328	-3.35192731	3.61365704
1	0.69158722	-2.95902546	6.20174484
6	-0.66165401	-1.09881952	7.68390327
1	-1.50474495	0.71166647	5.81231535
6	-1.40227445	0.94955272	3.12962160
6	-2.38883278	1.37764324	-1.54314131
1	-3.05241323	3.74376519	-2.57390251
6	-1.88484468	5.63656614	-4.16812306
1	0.59296934	4.59379249	-4.67439870
6	1.91422085	2.32954948	-4.12273494
1	1.93097521	-3.77991235	4.38852777
1	1.91824397	-2.96361248	2.80485547
1	0.68441567	-4.17943526	3.19878518
1	-0.61860514	1.50881217	2.59226672
1	-1.93844114	1.66944929	3.76016744
1	-2.11324103	0.57743619	2.37456403
1	-1.63244707	-1.53778367	7.96430241
1	-0.64899892	-0.06843856	8.06520321
1	0.11787660	-1.66776144	8.20835088
1	-3.13733537	2.00331548	-1.03970484
1	-1.75587108	0.91065242	-0.77328632

1	-2.93180007	0.56872082	-2.05769184
1	1.92623926	1.36098646	-4.64089261
1	2.61363954	2.23892341	-3.27769986
1	2.31081726	3.09482719	-4.80284484
1	-1.12227466	6.42797778	-4.17225247
1	-2.71350483	5.96187498	-3.52470990
1	-2.27668916	5.55891152	-5.19487179
1	-0.21381755	-0.36866863	1.56470491

Energy = -7200.162832 Hartree
Number of imaginary frequencies = 0.

Compound 11b isomer 48

Atomic N.	X	Y	Z
8	1.63448837	-3.76231230	-0.31948749
6	2.57733289	-4.31839612	-1.21990929
1	2.07933963	-4.96826937	-1.96523653
1	3.30444559	-4.94156735	-0.67012758
1	3.15421915	-3.55590481	-1.78235870
50	1.27374894	-1.72105934	-0.30579944
7	-1.06132875	-2.19729282	-1.11845386
6	-1.17457674	-3.66886723	-1.26157390
1	-2.22907038	-3.95395089	-1.42411139
1	-0.77215991	-4.17154286	-0.37784317
1	-0.57624128	-3.99527960	-2.12066700
7	0.09296433	-1.69951618	1.45240175
6	-1.89686214	-1.71104240	0.01187260
1	-2.93262207	-2.08908334	-0.09148455
1	-1.90516401	-0.61559654	-0.03895195
6	-1.29992609	-2.11526742	1.36121147
1	-1.90741741	-1.62970652	2.14398966
1	-1.42588090	-3.20696706	1.52178961
6	0.56109915	-1.22275008	2.70779573
6	1.46498383	-1.99205575	3.48330431
6	1.92863482	-1.48743665	4.70686632
6	1.52564594	-0.24391611	5.20119935
6	0.64172193	0.51219428	4.42180497
6	0.15803757	0.05198259	3.19236477
7	-0.56559178	0.71624694	-2.02645312
6	-1.43941076	-1.59412125	-2.43201113
1	-2.36191424	-2.08671048	-2.79413745
1	-0.63812526	-1.86224100	-3.13930561
6	-1.69975949	-0.08981611	-2.49160869
1	-1.95314676	0.12471027	-3.54900430
1	-2.59743861	0.15466227	-1.90736102
6	-0.51933775	2.09118525	-2.38819619
6	-1.50709420	2.99891768	-1.94198231
6	-1.40491611	4.34815704	-2.30686240
6	-0.34633717	4.83996771	-3.07541553
6	0.64365396	3.93212837	-3.47016125
6	0.57601210	2.57357699	-3.14778766
6	1.93832587	-3.34866715	3.02050047
1	2.62075527	-2.09620074	5.29500347
6	2.00883099	0.26097107	6.53973265
1	0.33259565	1.50106322	4.77168658
6	-0.74129016	0.94214671	2.37160571
6	-2.62979298	2.57038915	-1.02891077
1	-2.17148257	5.04072710	-1.95002922

6	-0.27497860	6.29408090	-3.47242841
1	1.49571010	4.28925532	-4.05389913
6	1.67536920	1.64099504	-3.60032474
1	2.24282809	-3.96254727	3.87913213
1	2.80651682	-3.27108484	2.34750360
1	1.16631055	-3.87672002	2.44861726
1	-0.44214146	0.92753663	1.31326240
1	-0.70246013	1.97650804	2.73717645
1	-1.79537923	0.62180630	2.41092897
1	1.27925167	0.04007504	7.33522903
1	2.15498935	1.35028459	6.52853368
1	2.95876128	-0.20996494	6.82632221
1	-3.03310799	3.43691559	-0.48925825
1	-2.27737567	1.83886592	-0.28757791
1	-3.46852548	2.11082287	-1.57593525
1	1.29020312	0.81569555	-4.22123013
1	2.21126786	1.18425368	-2.75184721
1	2.41691406	2.18438431	-4.19875964
1	0.76094279	6.66076020	-3.47211410
1	-0.86093769	6.92386925	-2.78960785
1	-0.67444821	6.45057487	-4.48721839
1	0.31034112	0.26014382	-2.28440263

Energy = -7200.163012 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 49

Atomic N.	X	Y	Z
8	3.50051837	0.25045051	-1.25114810
6	3.94574498	0.37691841	-2.58942824
1	3.21056148	0.87561124	-3.24676556
1	4.17056280	-0.61727156	-3.02293818
1	4.87873005	0.96699663	-2.62235746
50	1.69589834	0.76081842	-0.40185726
7	0.66635025	-1.23426748	-1.48064531
6	1.60469270	-2.38563074	-1.44752755
1	1.32014166	-3.13092542	-2.21051624
1	1.56276440	-2.86378453	-0.46322410
1	2.62182101	-2.02071307	-1.63592517
7	0.03883576	-2.32722936	1.37113526
6	-0.67548132	-1.63533862	-0.96142159
1	-0.87951203	-2.67148118	-1.28591842
1	-1.42423595	-0.98540487	-1.43627027
6	-0.87423354	-1.50994806	0.55139876
1	-0.80681927	-0.44258545	0.83662626
1	-1.90587129	-1.81861355	0.76380608
6	-0.46127148	-2.80041010	2.62000274
6	-1.45334347	-3.80736901	2.64655602
6	-1.91091265	-4.27781395	3.88402671
6	-1.40247444	-3.80413495	5.09779700
6	-0.38931541	-2.83917262	5.04680231
6	0.08663565	-2.32575826	3.83572750
7	0.64509524	1.58618174	-2.07987910
6	0.56337408	-0.72878676	-2.88347461
1	-0.01775497	-1.44292797	-3.49627963
1	1.58727241	-0.69988514	-3.27899108
6	-0.05248940	0.66534702	-2.96923978
1	0.03722402	0.98690407	-4.02614357

1	-1.14239558	0.60486162	-2.77348752
6	0.16627119	2.92812348	-2.03162548
6	-1.13550464	3.26182136	-1.57040932
6	-1.54545911	4.60268087	-1.55156741
6	-0.70681652	5.64491404	-1.95247553
6	0.58366068	5.30916401	-2.37838894
6	1.03122513	3.98479472	-2.42565608
6	-1.97721189	-4.42789953	1.37412519
1	-2.67356730	-5.06073758	3.89382051
6	-1.93403450	-4.30722447	6.41824759
1	0.04105195	-2.46494268	5.97904180
6	1.18400585	-1.28690061	3.83813557
6	-2.08603930	2.21692123	-1.04030008
1	-2.55029089	4.83630573	-1.18893086
6	-1.15683888	7.08463984	-1.89039724
1	1.26488648	6.10330021	-2.69556235
6	2.42845740	3.69741478	-2.91603126
1	-2.38725457	-5.42605782	1.57535893
1	-1.17510996	-4.52048490	0.62768062
1	-2.78368174	-3.83594453	0.91211852
1	2.11723050	-1.66537077	3.38859072
1	1.42289171	-0.98281415	4.86470569
1	0.90421810	-0.38033798	3.27895691
1	-2.72015727	-3.64203632	6.80968382
1	-1.14215781	-4.35558825	7.17836160
1	-2.37393238	-5.30858474	6.31701663
1	-2.78996745	2.66462793	-0.32648832
1	-1.53731793	1.41405961	-0.52661410
1	-2.68516688	1.74885862	-1.83804142
1	2.41994693	2.97065090	-3.73983897
1	3.06523982	3.26678329	-2.12831672
1	2.90954344	4.61947128	-3.26791710
1	-0.75688741	7.58798140	-0.99583782
1	-2.25157904	7.16061585	-1.84985758
1	-0.80590195	7.65282565	-2.76358509
1	0.89613584	-1.79566755	1.53155767

Energy = -7200.163607 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 50

Atomic N.	X	Y	Z
8	3.55715547	-0.30834584	-0.88604795
6	4.18330807	-0.29926274	-2.15472854
1	3.56262635	0.16031126	-2.94578019
1	4.43079201	-1.33050218	-2.47488533
1	5.13240060	0.26435224	-2.10768304
50	1.71973915	0.41247400	-0.29297868
7	0.69244131	-1.63437028	-1.31238606
6	1.51246635	-2.83363215	-1.04707258
1	1.16375200	-3.69776274	-1.64063523
1	1.46985684	-3.07927434	0.01947120
1	2.55398025	-2.60248898	-1.29814142
7	-0.46686584	-1.71430690	1.51828084
6	-0.73902906	-1.84345464	-0.96236564
1	-1.20241295	-2.49533235	-1.72822187
1	-1.23730251	-0.86539693	-1.03191443
6	-1.03650134	-2.47388627	0.39794178

1	-2.14045961	-2.54827045	0.46439452
1	-0.65877332	-3.50520342	0.42484888
6	-0.93912183	-2.02302794	2.82669079
6	-0.61978007	-3.25739034	3.43612715
6	-1.08746486	-3.51798376	4.73089028
6	-1.83842326	-2.58842615	5.45658101
6	-2.10555972	-1.35455687	4.85114301
6	-1.67715832	-1.05701592	3.55372285
7	0.87770225	1.11493428	-2.14733784
6	0.80671444	-1.25344450	-2.75150217
1	0.28579661	-2.00208955	-3.37811883
1	1.87552942	-1.28443645	-2.99889969
6	0.26369205	0.14381488	-3.04304724
1	0.50638774	0.36261203	-4.10228215
1	-0.84406962	0.13129748	-2.99126436
6	0.49157328	2.47737736	-2.29437607
6	-0.83406200	2.93047937	-2.05180276
6	-1.14907800	4.28675890	-2.21373546
6	-0.19472809	5.23463529	-2.59092868
6	1.11627252	4.78713801	-2.78911284
6	1.47332696	3.44109886	-2.65225452
6	0.26985354	-4.26644353	2.75379709
1	-0.82823556	-4.47329393	5.19439967
6	-2.35008125	-2.90470375	6.84115782
1	-2.67130654	-0.59901206	5.40197487
6	-1.99150467	0.29266935	2.95089691
6	-1.91044790	2.00165485	-1.54905222
1	-2.17373069	4.61256349	-2.01411053
6	-0.56349089	6.68520328	-2.78739143
1	1.88931159	5.50718669	-3.07036997
6	2.90353400	3.03317050	-2.90484402
1	0.71427667	-4.94642896	3.49187884
1	1.08403342	-3.76105057	2.21409381
1	-0.27505014	-4.88958807	2.02656498
1	-1.08037711	0.87641593	2.73930098
1	-2.60360719	0.88744295	3.64001698
1	-2.54930568	0.20481907	2.00474472
1	-3.38556940	-3.27932223	6.80707116
1	-2.34867674	-2.01323330	7.48345536
1	-1.73864057	-3.67743270	7.32632406
1	-2.70736507	2.56848432	-1.05024395
1	-1.49278007	1.28492764	-0.82566015
1	-2.38113827	1.41779270	-2.35619324
1	2.96184926	2.22917249	-3.65111439
1	3.39611174	2.65159359	-1.99750179
1	3.48851253	3.88901785	-3.26653665
1	0.23783178	7.35376691	-2.44292147
1	-1.48226062	6.94165693	-2.24275087
1	-0.73854451	6.91048009	-3.85154590
1	-0.57792493	-0.71493178	1.34197058

Energy = -7200.162838 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 51

Atomic N.	X	Y	Z
8	2.17180962	-3.20087997	-0.66456025
6	3.37772457	-3.50361245	-1.34681332

1	3.17609037	-4.03872583	-2.29508257
1	4.00906717	-4.15893830	-0.72236523
1	3.97831359	-2.60555224	-1.59678475
50	1.52003744	-1.23752702	-0.48232472
7	-0.44100866	-1.79010431	-1.97414709
6	-0.15557211	-3.12086301	-2.56410372
1	-1.05496627	-3.51693294	-3.06753897
1	0.19073653	-3.81194981	-1.78948191
1	0.65210486	-3.02197316	-3.30060376
7	-0.03566347	-1.76904283	0.87049079
6	-1.56686208	-1.88132879	-1.00246970
1	-2.41367503	-2.42677984	-1.46180947
1	-1.88302484	-0.85932576	-0.76375154
6	-1.12456142	-2.55004397	0.29947123
1	-1.99295736	-2.55034145	0.98252961
1	-0.88466775	-3.61450391	0.10694480
6	0.20138219	-1.83046558	2.26855483
6	0.37312252	-3.05518396	2.96817711
6	0.57333547	-3.03416518	4.35525310
6	0.64209178	-1.84388872	5.08530567
6	0.51520069	-0.64308401	4.37798749
6	0.29299492	-0.61286143	2.99688647
7	-0.25847289	1.29089962	-1.92890908
6	-0.72506997	-0.85784758	-3.10472723
1	-1.49394054	-1.31510315	-3.75700452
1	0.20123197	-0.80070698	-3.69886264
6	-1.20435981	0.55348867	-2.77330040
1	-1.36759798	1.05351989	-3.74930888
1	-2.18727885	0.51526969	-2.28579134
6	-0.42181683	2.69914538	-1.80327677
6	-1.56607860	3.25006495	-1.18395725
6	-1.67197989	4.64315164	-1.06906454
6	-0.67292181	5.51142972	-1.51654873
6	0.46884953	4.94273224	-2.09489195
6	0.61178281	3.56119411	-2.24913016
6	0.43035605	-4.37768215	2.24216091
1	0.70967650	-3.98663661	4.87521407
6	0.83224423	-1.85322491	6.58323187
1	0.57467152	0.30515976	4.91914902
6	0.14431121	0.71626167	2.29936751
6	-2.64769715	2.38072893	-0.59126041
1	-2.56143016	5.05666646	-0.58696289
6	-0.79645639	7.00649791	-1.34639811
1	1.27326314	5.59453896	-2.44509399
6	1.86586668	3.00369998	-2.88189936
1	0.91283681	-5.13494754	2.87436161
1	1.00209163	-4.28476705	1.30618608
1	-0.56997538	-4.76082215	1.98369522
1	1.04064112	0.97988026	1.71322364
1	-0.01779191	1.52158242	3.02791885
1	-0.69010418	0.69716325	1.58556735
1	-0.13420921	-1.79514254	7.10952189
1	1.43522005	-0.99746398	6.91782431
1	1.33005735	-2.77413009	6.91682234
1	-3.20604631	2.93512647	0.17392747
1	-2.21629225	1.48591027	-0.11981963
1	-3.37882490	2.04281022	-1.34327561
1	1.64657487	2.39913518	-3.77709871

1	2.43327457	2.36249233	-2.18708630
1	2.53390934	3.81720507	-3.19040353
1	-0.19198394	7.36254414	-0.49734512
1	-1.83685214	7.30230230	-1.15778884
1	-0.44514175	7.54260489	-2.23956014
1	0.69441070	1.08334284	-2.22917011

Energy = -7200.165706 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 52

Atomic N.	X	Y	Z
8	1.62009542	-0.37338654	-0.57721606
6	2.55174754	-1.35960332	-0.16331848
1	3.53617431	-1.16983215	-0.62677058
1	2.25292782	-2.39317911	-0.43407506
1	2.68323399	-1.33164174	0.93323622
50	-0.09521661	-0.91750421	-1.58279549
7	-2.71845011	-0.26410586	-1.05814966
6	-3.73213365	-1.30725803	-1.24228291
1	-4.76110390	-0.90128626	-1.17709558
1	-3.62894225	-2.09682548	-0.48713406
1	-3.59939084	-1.76837471	-2.22975061
7	-1.32632500	-1.49659063	1.15847868
6	-2.76331550	0.34905125	0.27806036
1	-3.73805832	0.85126759	0.45672295
1	-1.97813416	1.11599078	0.30674083
6	-2.51233207	-0.64939973	1.41302670
1	-2.34448964	-0.07623926	2.33279672
1	-3.40963234	-1.26755503	1.59847578
6	-0.65501917	-2.01456532	2.31530124
6	0.16286018	-1.16292132	3.08995905
6	0.81290255	-1.69306305	4.21127922
6	0.70756992	-3.04160164	4.57035745
6	-0.08097366	-3.87224565	3.76652307
6	-0.76664083	-3.38303143	2.64871497
7	-0.38611961	1.13286395	-2.07982843
6	-2.82777731	0.73005329	-2.14496507
1	-3.80164651	1.26043638	-2.09455307
1	-2.80444764	0.16234585	-3.08872447
6	-1.69856951	1.75646262	-2.15483461
1	-1.81147834	2.33400898	-3.09285826
1	-1.86390523	2.49256365	-1.33995056
6	0.70436251	2.00983433	-2.35968722
6	1.09039090	3.02730686	-1.45326709
6	2.14637663	3.88653703	-1.78401920
6	2.85208890	3.76997288	-2.98455114
6	2.46818724	2.75486144	-3.86812984
6	1.41609755	1.87817152	-3.57945632
6	0.39610299	0.27219450	2.69073729
1	1.44524235	-1.02980570	4.80651358
6	1.45764825	-3.59262279	5.75911909
1	-0.17368537	-4.93161901	4.01831111
6	-1.60478433	-4.32303713	1.81187028
6	0.40880088	3.18147460	-0.11796650
1	2.43585307	4.66019248	-1.06747612
6	4.01222216	4.68240940	-3.30364672
1	3.00050454	2.64296931	-4.81665108

6	1.05930775	0.80435239	-4.57902330
1	1.23288838	0.69586458	3.26033979
1	-0.47988291	0.91409705	2.87510532
1	0.63658357	0.33454201	1.61792422
1	-2.65135659	-3.98871020	1.73139185
1	-1.61546572	-5.32602205	2.25607321
1	-1.21182857	-4.42851479	0.78690274
1	2.45764725	-3.94924146	5.46549201
1	0.92722830	-4.44312475	6.20866688
1	1.59897846	-2.82708539	6.53387794
1	1.07866058	3.66351625	0.60628342
1	0.11806567	2.19799444	0.27399766
1	-0.50062492	3.80102477	-0.18441552
1	-0.02730405	0.71949298	-4.71665879
1	1.41335525	-0.18823473	-4.25386906
1	1.52586901	1.01135237	-5.55146010
1	4.97261139	4.21040616	-3.04168398
1	3.94649274	5.62490591	-2.74343827
1	4.05157088	4.92224558	-4.37565345
1	-1.61161426	-2.28253473	0.57307702

Energy = -7200.160670 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 53

Atomic N.	X	Y	Z
8	1.28500896	-0.57152222	-0.88369419
6	2.04196255	-1.69442663	-1.30181726
1	1.49486252	-2.36187481	-1.99937773
1	2.33901277	-2.30762554	-0.43139814
1	2.96628454	-1.37084634	-1.81534895
50	-0.58668781	-0.21634155	-1.71496774
7	-2.95019463	0.77932384	-0.77680262
6	-4.12938761	0.11761514	-1.33931223
1	-5.05968140	0.68035713	-1.12477660
1	-4.23420148	-0.89555195	-0.93292960
1	-4.01216837	0.02999755	-2.42784081
7	-1.21396674	-0.99935797	0.78993652
6	-2.94602757	0.76863477	0.69170852
1	-3.93411625	1.06005653	1.10375837
1	-2.22156299	1.52052716	1.03283947
6	-2.55360546	-0.59290229	1.26929957
1	-2.58501730	-0.52934311	2.37221489
1	-3.27633388	-1.36375157	0.97762233
6	-0.74390625	-2.28860997	1.22835754
6	-1.34260936	-3.47575816	0.75720834
6	-0.84116453	-4.70617634	1.20464213
6	0.24143160	-4.79827454	2.08337546
6	0.84369508	-3.60561226	2.50175193
6	0.37348353	-2.35408499	2.09325942
7	-0.32333910	1.84058500	-1.13343063
6	-2.77664839	2.12078151	-1.36002691
1	-3.60593409	2.80023078	-1.07211037
1	-2.82141994	1.98895074	-2.45292751
6	-1.44066060	2.76317791	-0.98655969
1	-1.32356693	3.64797374	-1.64274795
1	-1.51103667	3.17948106	0.04116294
6	0.95558725	2.46436803	-1.04422350

6	1.44232444	2.97531747	0.18608135
6	2.69364337	3.60384004	0.23678751
6	3.49834759	3.75074628	-0.89564876
6	3.01527728	3.23400533	-2.10287737
6	1.77132437	2.60022457	-2.19775910
6	-2.46871330	-3.47185793	-0.24872574
1	-1.30414209	-5.62178650	0.82847143
6	0.74798871	-6.13572399	2.56558293
1	1.71270740	-3.64645199	3.16265534
6	1.08622215	-1.09916128	2.53854375
6	0.66056935	2.82196321	1.46654022
1	3.05495152	3.97470013	1.20019983
6	4.82983001	4.45942219	-0.82543466
1	3.62540261	3.32825270	-3.00531590
6	1.32738313	2.06598426	-3.53699349
1	-2.47170318	-4.41114565	-0.81673068
1	-2.36543720	-2.64420004	-0.96572871
1	-3.45744274	-3.38406045	0.23082804
1	1.49973166	-0.55467396	1.67280994
1	1.91830640	-1.34922757	3.20795038
1	0.42118862	-0.41221977	3.08713276
1	0.33037442	-6.38451946	3.55402808
1	1.84214276	-6.13737766	2.66634390
1	0.46472133	-6.94262187	1.87665401
1	1.33469678	2.78860458	2.33287340
1	0.06813099	1.89652452	1.44768998
1	-0.04139447	3.65575333	1.63096910
1	0.26694573	2.27893381	-3.73108680
1	1.45063545	0.97140115	-3.59427050
1	1.92884138	2.50076778	-4.34664713
1	4.72995494	5.52468919	-1.08920474
1	5.55670140	4.01933710	-1.52226535
1	5.25434846	4.41272893	0.18684750
1	-0.53195072	-0.29816908	1.09285453

Energy = -7200.167095 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 54

Atomic N.	X	Y	Z
8	1.18392763	-0.51792875	-0.60293946
6	2.37669683	-0.38988729	-1.38079872
1	2.42436300	0.59479529	-1.87819907
1	2.46051670	-1.16142052	-2.16955448
1	3.25555795	-0.48886551	-0.72262381
50	-0.27908681	-1.84084011	-1.28823145
7	-2.20208955	-0.29154651	-1.04904889
6	-3.32161906	-1.13879477	-1.52869588
1	-4.29398219	-0.67647924	-1.28576438
1	-3.26659548	-2.13262006	-1.06951474
1	-3.24417171	-1.25118740	-2.61759033
7	-1.08921746	-2.22202068	0.63808869
6	-2.27935016	-0.09614480	0.42544947
1	-3.21665269	0.42764155	0.69261355
1	-1.42853232	0.53532376	0.71170891
6	-2.17642513	-1.42306195	1.17428277
1	-2.01941425	-1.17575945	2.24115022
1	-3.15403602	-1.95377406	1.13818540

6	-0.59728955	-3.27557305	1.46209681
6	-0.97533914	-4.61945329	1.21987919
6	-0.45857969	-5.64161318	2.02651716
6	0.42120215	-5.37761561	3.08190973
6	0.78995469	-4.04695946	3.30876655
6	0.30316086	-2.99503841	2.52244831
7	0.00568952	2.01423358	-1.50154551
6	-2.27162230	0.99884640	-1.80977888
1	-3.32853577	1.32798474	-1.80003374
1	-1.99910759	0.76930213	-2.85060762
6	-1.43494971	2.17917636	-1.32213025
1	-1.76221219	3.03149984	-1.93598117
1	-1.71889475	2.44407310	-0.28291462
6	0.77869030	3.20868344	-1.38462015
6	1.53678694	3.48371286	-0.22021685
6	2.32200432	4.64136343	-0.17387339
6	2.36682098	5.55372342	-1.23536503
6	1.61049729	5.26520490	-2.37547048
6	0.82589973	4.10877367	-2.47456227
6	-1.93082928	-4.96759947	0.10273606
1	-0.75791706	-6.67382166	1.82601945
6	0.93866567	-6.48993288	3.96229490
1	1.49225633	-3.81798483	4.11493381
6	0.76465515	-1.58397653	2.78919366
6	1.49899199	2.55718766	0.97285242
1	2.90806839	4.84097757	0.72707764
6	3.19200913	6.81488652	-1.14226466
1	1.64852282	5.94699419	-3.22911058
6	0.08571147	3.81489040	-3.75574509
1	-2.21547645	-6.02672232	0.15529461
1	-1.48728683	-4.78974356	-0.88943179
1	-2.84834840	-4.36356511	0.15271978
1	0.98414049	-1.05951026	1.84788711
1	1.66254426	-1.58420183	3.42106963
1	-0.00421660	-0.99646521	3.31748653
1	0.28064518	-6.64632521	4.83202388
1	1.94055042	-6.26021019	4.35027982
1	0.99087866	-7.44229127	3.41730483
1	2.11975673	2.95553719	1.78536927
1	1.85532635	1.54383168	0.73583737
1	0.47445884	2.44397619	1.36099400
1	-0.96911913	4.13299448	-3.71193836
1	0.08989545	2.73555686	-3.96347771
1	0.54546963	4.34585093	-4.59958261
1	4.14360693	6.63530358	-0.62269562
1	2.65917343	7.59869452	-0.58057749
1	3.41624877	7.21996346	-2.13819353
1	0.37755227	1.24795076	-0.92139293

Energy = -7200.166634 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 55

Atomic N.	X	Y	Z
8	1.10069050	-1.17723598	-0.40800173
6	2.05283097	-2.12242706	0.04899611
1	1.60373635	-2.96495059	0.61452318
1	2.78834739	-1.63846091	0.71722232

1	2.60890345	-2.55878036	-0.80150099
50	-0.92966854	-1.56032181	-0.17926640
7	-3.12288387	-0.02683018	0.36585263
6	-4.10460869	-0.68780328	1.22912900
1	-5.07054690	-0.14487665	1.24570929
1	-3.72842511	-0.76013048	2.25667688
1	-4.27917944	-1.70916953	0.86496145
7	-0.50662105	0.39340846	1.63608623
6	-2.69837652	1.27662274	0.89271894
1	-3.56551506	1.88218061	1.22797242
1	-2.21663644	1.83044458	0.07556010
6	-1.70890154	1.14866951	2.05283802
1	-1.44605050	2.16306502	2.40413565
1	-2.16817677	0.63044656	2.90261967
6	0.48538849	0.16318809	2.65495309
6	0.22900322	-0.71421960	3.72910187
6	1.22983480	-0.91145435	4.69104054
6	2.47695550	-0.28649525	4.61228385
6	2.72037109	0.54576914	3.51301080
6	1.75112521	0.78334504	2.53402894
7	-1.25259716	-0.16526222	-1.78784139
6	-3.60446391	0.02498164	-1.02533045
1	-4.50146873	0.67180489	-1.12157506
1	-3.90808365	-1.00199342	-1.28409375
6	-2.53229150	0.49415043	-2.00872451
1	-2.92461817	0.28606402	-3.02358114
1	-2.45028307	1.60095901	-1.95756685
6	-0.30482141	0.05075773	-2.83078937
6	0.29790471	1.31940720	-3.02795019
6	1.20803423	1.50636216	-4.07683715
6	1.55503624	0.47497917	-4.95282805
6	0.96487089	-0.77632434	-4.74362345
6	0.05001264	-1.00551219	-3.70993066
6	-1.06267443	-1.48607177	3.85451598
1	1.02753678	-1.59846670	5.51645081
6	3.52790413	-0.49895922	5.67463117
1	3.69749713	1.02308421	3.40758880
6	2.07852866	1.65581952	1.34542257
6	0.01696362	2.47652461	-2.10255790
1	1.67214587	2.48918532	-4.19887118
6	2.51453999	0.70547505	-6.09573633
1	1.22162138	-1.60494794	-5.40922545
6	-0.53645623	-2.38633604	-3.55033242
1	-0.89940018	-2.40548741	4.43150598
1	-1.45829867	-1.77178789	2.86880765
1	-1.84358428	-0.91226240	4.38003670
1	2.01503410	1.08019429	0.40648867
1	3.09832095	2.05057674	1.43026093
1	1.39995516	2.52041226	1.26087307
1	3.54247168	0.33769215	6.39089219
1	4.53320868	-0.56731879	5.23628625
1	3.33902032	-1.41767378	6.24561442
1	0.87216617	3.16467216	-2.06892465
1	-0.18182710	2.11506778	-1.08388006
1	-0.86149916	3.06249454	-2.41856068
1	-1.61225701	-2.35055893	-3.32921841
1	-0.05648972	-2.93359014	-2.72164576
1	-0.38256239	-2.98074853	-4.46099902

1	3.12871869	-0.18478791	-6.29039257
1	3.18874469	1.54761328	-5.88772377
1	1.97642827	0.93944027	-7.02846215
1	-0.05458475	0.89638747	0.86717531

Energy = -7200.167058 Hartree
Number of imaginary frequencies = 0.

Compound 11b isomer 56

Atomic N.	X	Y	Z
8	1.08315460	-0.88098516	-0.29421227
6	1.88477682	-1.65677947	-1.18866793
1	1.42262963	-1.71691268	-2.18974072
1	2.04155479	-2.69362146	-0.83558441
1	2.87628240	-1.18618575	-1.29193897
50	0.05560995	-1.89862418	1.21203565
7	-2.15195404	-0.82536783	0.83919967
6	-2.97974511	-1.49816349	1.87036706
1	-3.94485814	-0.97803327	1.99802679
1	-2.44794463	-1.51698057	2.82875554
1	-3.17202664	-2.53191784	1.55630634
7	-0.00663274	-0.23611602	2.53196013
6	-1.89023574	0.59244386	1.21245956
1	-2.84247092	1.15230378	1.27647911
1	-1.27761103	1.02855514	0.41301464
6	-1.12094776	0.69423418	2.52766062
1	-0.78168212	1.74352045	2.61843118
1	-1.81443976	0.53612146	3.38370079
6	1.02521765	-0.00012912	3.48664320
6	1.07083875	-0.73067097	4.69974314
6	2.10569126	-0.49342777	5.61356678
6	3.10603802	0.45386249	5.36867112
6	3.04678155	1.17270780	4.16955865
6	2.03344542	0.96317235	3.22548438
7	-1.11939106	-0.49729748	-2.19245798
6	-2.88236582	-0.95679264	-0.46367679
1	-3.94073351	-0.69314842	-0.27417076
1	-2.84395143	-2.02012344	-0.74316158
6	-2.41895659	-0.11165553	-1.64763955
1	-3.17955261	-0.27228642	-2.42619776
1	-2.48498979	0.96662692	-1.39502470
6	-0.81624558	0.02771095	-3.48511452
6	0.07668700	1.11512421	-3.64670239
6	0.38534427	1.55954647	-4.93750753
6	-0.17807573	0.97771360	-6.07990701
6	-1.05822625	-0.09375689	-5.89949266
6	-1.38123495	-0.58490836	-4.62780827
6	0.01170188	-1.75681547	5.02752135
1	2.12569773	-1.06207753	6.54714972
6	4.23232580	0.66888039	6.35109942
1	3.82006028	1.91491970	3.95350283
6	2.03433461	1.74711306	1.93680044
6	0.68593194	1.80940868	-2.45076192
1	1.08063616	2.39543835	-5.05096374
6	0.14236298	1.50307599	-7.45882227
1	-1.49084578	-0.58383792	-6.77564491
6	-2.28240651	-1.78754006	-4.49679134
1	0.14322588	-2.13307066	6.05054479

1	0.05102171	-2.62041127	4.34553944
1	-1.00045983	-1.33412809	4.94716428
1	1.80130661	1.09589184	1.08195785
1	3.01023044	2.22324152	1.77435877
1	1.27845752	2.54953723	1.94816518
1	3.91657050	0.44333794	7.37890735
1	4.59773585	1.70451816	6.32246188
1	5.08847864	0.01457461	6.12146240
1	1.32797653	2.63767889	-2.77628879
1	1.28949628	1.13295902	-1.82771727
1	-0.09124321	2.22945799	-1.79283152
1	-3.32954998	-1.50610037	-4.29660040
1	-1.95389901	-2.42497801	-3.66381604
1	-2.28073328	-2.37628161	-5.42349283
1	1.19332628	1.81471347	-7.53611912
1	-0.47532222	2.38194375	-7.70345024
1	-0.04781521	0.74416833	-8.22970137
1	-0.35838276	-0.33537682	-1.51669252

Energy = -7200.166669 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 57

Atomic N.	X	Y	Z
8	1.79173159	-0.32610929	0.27194373
6	3.07256669	0.27669188	0.41785452
1	3.02059694	1.36102257	0.64402718
1	3.68664880	0.16011633	-0.49440874
1	3.61335856	-0.20737277	1.24864584
50	0.23893285	0.83398115	-0.54689605
7	-1.17871601	-1.11081766	-0.22144726
6	-2.52210549	-0.69782036	-0.70169402
1	-3.18706868	-1.57339242	-0.79344913
1	-2.43142101	-0.20377184	-1.67541512
1	-2.95802858	0.00783574	0.01598552
7	0.12482286	-0.08695710	-2.46257097
6	-0.55381604	-2.06780382	-1.18652432
1	-1.17766874	-2.97863665	-1.25228321
1	0.42798980	-2.33454459	-0.77622958
6	-0.36518950	-1.45233546	-2.57323162
1	0.33044158	-2.11508119	-3.12082831
1	-1.32055941	-1.49362050	-3.13940466
6	0.67513713	0.50353153	-3.63394650
6	0.00102249	1.57272273	-4.27813038
6	0.56717840	2.16754424	-5.41203828
6	1.78479328	1.73359838	-5.94863087
6	2.44377784	0.68351829	-5.30158506
6	1.91956972	0.06512418	-4.15914473
7	0.41375317	-1.10981581	2.82963504
6	-1.35848157	-1.75834713	1.11871440
1	-1.96147688	-2.67180379	0.95140843
1	-1.96721398	-1.07687623	1.73027925
6	-0.08547830	-2.12628674	1.90689351
1	-0.29187560	-3.06260899	2.43802824
1	0.74533915	-2.33044691	1.22096943
6	-0.36572383	-0.49390487	3.82314367
6	-1.30149908	-1.19648436	4.62934177
6	-2.04051627	-0.49093226	5.59094495

6	-1.86997743	0.87326679	5.83270408
6	-0.88157384	1.53006177	5.09009731
6	-0.13294876	0.88307398	4.10541841
6	-1.32461276	2.07861243	-3.76122995
1	0.03458718	2.99110382	-5.89502902
6	2.35713996	2.36503910	-7.19498775
1	3.40964711	0.34308175	-5.68512689
6	2.71021200	-1.02939907	-3.48471398
6	-1.47563129	-2.69773768	4.57857391
1	-2.75838928	-1.05139239	6.19585746
6	-2.70487193	1.60666921	6.85411221
1	-0.68213588	2.58796847	5.27999253
6	0.93889113	1.64807159	3.37088785
1	-1.77054760	2.78601402	-4.47271886
1	-1.22132639	2.59736621	-2.79526411
1	-2.03445029	1.25420171	-3.60237635
1	2.51219495	-1.05198844	-2.40395244
1	3.78670249	-0.88545661	-3.64818045
1	2.45602443	-2.02442553	-3.88549123
1	1.97955789	1.86668375	-8.10216709
1	3.45300698	2.29013320	-7.21466102
1	2.08380978	3.42651373	-7.26944142
1	-2.04466456	-3.03229530	5.45564756
1	-0.50501392	-3.21525829	4.59314106
1	-2.02146280	-3.05025179	3.68832377
1	0.73610162	1.72094180	2.28853247
1	1.93000558	1.17820100	3.48046191
1	1.01303285	2.67179508	3.75821039
1	-2.11022616	2.35391853	7.39864239
1	-3.13605107	0.91346278	7.58923062
1	-3.54201758	2.14370656	6.37947108
1	1.02416569	-0.47159844	2.31607889

Energy = -7200.164930 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 58

Atomic N.	X	Y	Z
8	0.81491068	3.58342951	2.10686587
6	1.45888584	4.84780332	2.17954660
1	2.45055780	4.86521037	1.68531152
1	1.61043249	5.13888061	3.23367519
1	0.84039800	5.62978946	1.70105972
50	1.72171618	1.99691863	1.10887139
7	-0.45628817	1.80284214	0.00293947
6	-0.90172620	3.08205806	-0.59098992
1	-1.93981146	3.00369037	-0.95870983
1	-0.24784135	3.36681535	-1.42303312
1	-0.83880542	3.85628249	0.18293071
7	0.43850069	-0.34307296	-3.05298257
6	-0.51512530	0.68079021	-0.97013806
1	-1.55898574	0.54660300	-1.31078300
1	-0.21912562	-0.22580175	-0.42506624
6	0.41015461	0.84314890	-2.18822536
1	0.11344719	1.71044989	-2.78802398
1	1.44043267	1.03042439	-1.84470925
6	-0.74513015	-0.75708347	-3.72220663
6	-1.28202696	-2.04663511	-3.47754306

6	-2.41634220	-2.46499469	-4.18000306
6	-3.05449979	-1.64565261	-5.11875960
6	-2.48837252	-0.39277423	-5.37197627
6	-1.33986092	0.06241440	-4.71109577
7	0.70270434	0.44538773	2.13402071
6	-1.29803195	1.50278927	1.20250837
1	-2.33759913	1.29968461	0.88606435
1	-1.27721395	2.41490038	1.81494501
6	-0.74468606	0.33677576	2.02085188
1	-1.25628973	0.37143023	3.00112976
1	-1.04170941	-0.63328484	1.56692505
6	1.33834255	-0.36121589	3.11966867
6	2.13863727	-1.46261582	2.72401263
6	2.77804026	-2.24177011	3.69565609
6	2.65153201	-1.97031801	5.06283482
6	1.86113147	-0.88018240	5.44114754
6	1.20929538	-0.06927370	4.50263900
6	-0.63696842	-2.98034645	-2.47998102
1	-2.81672816	-3.46201028	-3.97956319
6	-4.30787360	-2.09877258	-5.82766170
1	-2.93481572	0.24933502	-6.13574042
6	-0.72852698	1.37856831	-5.12656663
6	2.30660318	-1.80973821	1.26385334
1	3.38757436	-3.09052713	3.37399616
6	3.37712113	-2.80306391	6.09253543
1	1.75827900	-0.63883703	6.50273875
6	0.40700403	1.11741201	4.97811792
1	-1.19585251	-3.92232583	-2.42060891
1	-0.60557404	-2.55162185	-1.46550280
1	0.39934374	-3.23774517	-2.75593792
1	-1.05265878	2.21789570	-4.48954094
1	-1.02461422	1.62659733	-6.15422343
1	0.36893376	1.33485183	-5.08011480
1	-4.28503360	-3.17758390	-6.03525043
1	-4.44133986	-1.56963203	-6.78087039
1	-5.20381984	-1.90461656	-5.21661886
1	2.81979470	-2.77420228	1.15327908
1	2.89898902	-1.05073005	0.72912846
1	1.33517640	-1.87061911	0.75220731
1	-0.65808768	0.86424642	5.10788749
1	0.45938194	1.94808629	4.25957374
1	0.77419058	1.46493678	5.95299315
1	4.38077955	-2.39648580	6.29577342
1	3.50908435	-3.83864120	5.74998667
1	2.83441026	-2.82324813	7.04741946
1	0.85558002	-1.12502569	-2.55066757

Energy = -7200.168737 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 59

Atomic N.	X	Y	Z
8	1.62328820	1.14340251	0.92624990
6	2.21933338	-0.13351387	0.82854300
1	1.49643385	-0.94099200	0.60604824
1	2.71830872	-0.40915085	1.77542769
1	2.98621738	-0.13142846	0.03179876
50	-0.33315388	1.76556089	0.93055778

7	-2.84866923	1.35493340	-0.09543291
6	-3.48386039	2.61875900	-0.47416959
1	-4.57424133	2.50131181	-0.63468782
1	-3.03654538	3.01416477	-1.39428976
1	-3.31962185	3.36005241	0.31962900
7	-0.43208918	0.60526290	-1.66800811
6	-2.85733751	0.37618164	-1.18790410
1	-3.85014066	0.32732505	-1.68178815
1	-2.66644370	-0.61774552	-0.75853097
6	-1.79401925	0.66551267	-2.24729390
1	-1.91398530	-0.06258907	-3.07102565
1	-1.93761016	1.66142833	-2.68518329
6	0.63401820	0.81112439	-2.61658016
6	0.92631872	2.10681969	-3.09216089
6	1.98254967	2.26951611	-3.99783377
6	2.76340381	1.19670609	-4.43845192
6	2.45149619	-0.07838509	-3.95493636
6	1.39854040	-0.29253929	-3.05877124
7	-1.16867960	-0.04615968	1.80460821
6	-3.40500226	0.84768125	1.16901825
1	-4.46630973	0.54078636	1.05430619
1	-3.38092576	1.69131804	1.87732318
6	-2.60465430	-0.31548949	1.75224269
1	-3.00846007	-0.49229309	2.76760338
1	-2.84585055	-1.23898088	1.18598306
6	-0.45365112	-0.93283064	2.65847923
6	-0.34785676	-2.31910169	2.36352261
6	0.33886820	-3.17226051	3.23748431
6	0.94403218	-2.70885123	4.40800950
6	0.84144089	-1.34188242	4.68831525
6	0.16281518	-0.45323040	3.84638797
6	0.14912493	3.32158039	-2.64905628
1	2.20949487	3.27730538	-4.35416116
6	3.92718928	1.41211414	-5.37506530
1	3.04065994	-0.93661480	-4.28687489
6	1.09883767	-1.69616221	-2.58527251
6	-0.91106532	-2.90132548	1.09048881
1	0.41491017	-4.23263183	2.98084486
6	1.70924589	-3.63756224	5.31994179
1	1.29984230	-0.94954035	5.60011496
6	0.10549152	1.00371214	4.23396073
1	0.76644792	4.22450370	-2.73936740
1	-0.17680357	3.23647853	-1.60199937
1	-0.74944823	3.48103871	-3.26773476
1	1.30718552	-1.82555965	-1.51086125
1	1.72345245	-2.42052644	-3.12227385
1	0.04801577	-1.97903251	-2.75508688
1	3.74845217	2.26019641	-6.04979811
1	4.12063207	0.52010410	-5.98612134
1	4.84891548	1.63025308	-4.81293209
1	-0.34323790	-3.79164851	0.78837773
1	-0.86655607	-2.16440967	0.27483980
1	-1.96463972	-3.20647899	1.19533442
1	-0.88399492	1.43981504	4.03635037
1	0.84329324	1.59654412	3.66817376
1	0.33798756	1.12956243	5.29999830
1	2.79427397	-3.56388956	5.14405791
1	1.41987021	-4.68478281	5.15911350

1 1.53693412 -3.39328661 6.37787933
 1 -0.31246833 -0.32017964 -1.24736072
 Energy = -7200.161555 Hartree
 Number of imaginary frequencies = 0.

Compound 11b isomer 60

Atomic N.	X	Y	Z
8	0.83086329	1.41337155	0.95277085
6	1.45573784	2.07763670	2.04627028
1	1.33913454	3.17841020	2.01013747
1	2.53702812	1.85990841	2.04636717
1	1.04382263	1.74019095	3.01758317
50	-0.49523579	2.55019991	-0.21097602
7	-2.25150059	0.83581541	-0.24385760
6	-3.38247327	1.46460859	-0.96970568
1	-4.18644854	0.73113059	-1.15316080
1	-3.03192540	1.85994231	-1.93004179
1	-3.78253378	2.29465181	-0.37421554
7	-0.17691173	1.48045469	-2.00780984
6	-1.64437893	-0.24575315	-1.08299171
1	-2.42976219	-0.97542751	-1.35559265
1	-0.90840020	-0.75768582	-0.45341589
6	-0.97558313	0.31175133	-2.33662851
1	-0.35679508	-0.50441160	-2.75548977
1	-1.73865999	0.52921303	-3.11696873
6	0.79443612	1.88781316	-2.96777981
6	0.53193795	2.96078473	-3.85457233
6	1.51336224	3.35739698	-4.77231942
6	2.75508223	2.71736858	-4.84986973
6	3.00388356	1.66164210	-3.96549197
6	2.05355530	1.23665207	-3.02857125
7	-0.72190033	-1.01114396	1.86324248
6	-2.76766328	0.29079782	1.05046058
1	-3.36127227	-0.61270435	0.82587093
1	-3.45904010	1.04621903	1.45488214
6	-1.74363170	0.00152794	2.15700865
1	-1.24656196	0.95074741	2.41914683
1	-2.32024265	-0.29958003	3.04234205
6	-0.49216014	-2.08200224	2.75812952
6	-1.53368568	-2.96707980	3.13684419
6	-1.25201411	-4.02005693	4.01779526
6	0.03118107	-4.26477738	4.51317239
6	1.05961737	-3.42583645	4.06907840
6	0.82768369	-2.34767806	3.21010315
6	-0.79215568	3.68722347	-3.82257539
1	1.29741290	4.18831698	-5.44923125
6	3.78607500	3.13665130	-5.87036405
1	3.97431460	1.15866877	-3.99432131
6	2.38578332	0.11335105	-2.07819595
6	-2.91854194	-2.88248124	2.53900756
1	-2.06805310	-4.69150706	4.29782745
6	0.29954561	-5.38791818	5.48533567
1	2.08291203	-3.60855865	4.40728535
6	1.98786495	-1.48862237	2.77003327
1	-0.87291071	4.37921803	-4.67115360
1	-0.91569764	4.27465106	-2.89925005
1	-1.63894101	2.98743571	-3.86813598

1	2.03372927	0.34139739	-1.06168362
1	3.46857923	-0.06698800	-2.05556428
1	1.90453874	-0.83106824	-2.38066150
1	3.68740598	2.55043176	-6.79796995
1	4.80708420	2.98113935	-5.49543904
1	3.67631897	4.19577996	-6.14025477
1	-3.45466278	-3.82713371	2.69752977
1	-2.86233187	-2.70114901	1.45511161
1	-3.54032936	-2.08335125	2.97103415
1	1.88436180	-0.44908635	3.11503856
1	2.09237061	-1.44957557	1.67416363
1	2.92802929	-1.88168977	3.17660470
1	1.27899985	-5.85210985	5.30346484
1	-0.46813278	-6.17051699	5.41388528
1	0.30119060	-5.02497382	6.52572570
1	0.13669483	-0.52163278	1.59100671

Energy = -7200.167003 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 61

Atomic N.	X	Y	Z
8	0.88217836	1.53979528	-0.15588105
6	1.45393555	2.43245898	0.78563192
1	0.70307523	3.02607436	1.34733560
1	2.12104066	3.14932123	0.27377950
1	2.05754696	1.87948910	1.52708562
50	-1.16223917	1.43888419	-0.38396474
7	-3.02159089	-0.68174618	-0.38280190
6	-4.32147933	-0.07543579	-0.69677779
1	-5.11443386	-0.83834806	-0.82661723
1	-4.24876505	0.50825951	-1.62292375
1	-4.61270166	0.61128221	0.10925704
7	-0.84008756	0.24619846	-2.12337036
6	-2.51407012	-1.48114880	-1.51324471
1	-3.32030708	-2.12343148	-1.92613921
1	-1.71715570	-2.13601772	-1.13620427
6	-1.92092283	-0.60183590	-2.61660628
1	-1.55094905	-1.27037057	-3.40963701
1	-2.73260317	-0.01101437	-3.09336303
6	0.28066573	0.37763095	-2.99331704
6	0.55366967	1.60143923	-3.65569273
6	1.64967834	1.69388980	-4.52191393
6	2.50469142	0.61317336	-4.76100608
6	2.23080888	-0.58697043	-4.09860903
6	1.14714332	-0.72303349	-3.22222690
7	-1.20863779	-0.33117161	1.98684877
6	-3.09745292	-1.46047126	0.86580768
1	-3.54730866	-2.45829000	0.68597928
1	-3.78224338	-0.92920410	1.54707104
6	-1.75554483	-1.64181977	1.57172850
1	-1.91469668	-2.30498664	2.44195329
1	-1.03549188	-2.14368298	0.91242431
6	-0.20715134	-0.32860910	3.01258861
6	1.07294460	-0.88254151	2.78782357
6	2.01413787	-0.83834576	3.82453738
6	1.74611761	-0.24439616	5.06211004
6	0.48549475	0.33328603	5.24535051

6	-0.49533284	0.29757024	4.24836565
6	-0.31312703	2.81946430	-3.45053222
1	1.83653845	2.64354655	-5.03068708
6	3.70088183	0.75030079	-5.67225446
1	2.89085053	-1.44517506	-4.25258392
6	0.94705856	-2.03408441	-2.50487133
6	1.47610261	-1.44593872	1.44867863
1	3.00446320	-1.26164349	3.63969377
6	2.77837686	-0.23527292	6.16341242
1	0.25235495	0.82440926	6.19318525
6	-1.83891297	0.94273935	4.50371625
1	-0.16506458	3.54220315	-4.26436305
1	-0.06073699	3.33571301	-2.50950326
1	-1.38010395	2.55997193	-3.40254889
1	0.64453034	-1.85823765	-1.46351528
1	1.87295158	-2.62410899	-2.51054139
1	0.16334296	-2.65442162	-2.97024857
1	3.50805372	1.46819787	-6.48169235
1	3.97321402	-0.21276747	-6.12544990
1	4.58246997	1.11269726	-5.11952692
1	2.56720320	-1.55010350	1.39575583
1	1.16151021	-0.77145802	0.63765812
1	1.04736429	-2.44330338	1.26303809
1	-2.67172192	0.22675957	4.40839696
1	-2.03940587	1.77743680	3.81141013
1	-1.87854614	1.35268660	5.52032134
1	2.64347493	0.62516091	6.83265018
1	3.79756217	-0.19634241	5.75540140
1	2.70865741	-1.14492458	6.78087022
1	-1.99130550	0.24061362	2.30874877

Energy = -7200.163061 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 62

Atomic N.	X	Y	Z
8	0.83840948	-1.21637110	-0.17411403
6	2.12331850	-1.73229543	0.14518833
1	2.27560255	-1.85172504	1.23490084
1	2.94683684	-1.09569135	-0.23518182
1	2.23458438	-2.72952898	-0.31260012
50	0.32359654	0.66028724	0.66683423
7	-1.99240604	0.05819151	0.05880456
6	-2.74396153	1.27361716	-0.32559110
1	-3.79969984	1.03531003	-0.54476536
1	-2.28410207	1.73440281	-1.20532800
1	-2.70559953	1.99217405	0.50196422
7	-0.27128425	0.04505678	-2.45832659
6	-2.04052414	-0.97387320	-1.02220300
1	-3.07453816	-1.35925489	-1.09261547
1	-1.38356938	-1.79544996	-0.70381873
6	-1.63241598	-0.50269481	-2.41915278
1	-1.74690148	-1.38555384	-3.08110414
1	-2.34289184	0.24796989	-2.79462908
6	0.22778739	0.37120098	-3.75601725
6	-0.19859776	1.55158026	-4.40740280
6	0.30776715	1.85539806	-5.67736490
6	1.24239225	1.03838886	-6.32148808

6	1.67929679	-0.10682276	-5.64631188
6	1.18857583	-0.45842691	-4.38344533
7	-0.45201238	-0.23368205	2.46704534
6	-2.56096667	-0.51327435	1.32423005
1	-3.39220472	-1.19639357	1.07355405
1	-2.96291257	0.32375535	1.90984492
6	-1.49402693	-1.20992621	2.16955475
1	-1.98183187	-1.55954070	3.09389627
1	-1.12436433	-2.10727636	1.63799132
6	0.05717964	-0.14780393	3.78040236
6	0.48461937	-1.29769182	4.50269633
6	0.95404830	-1.15962726	5.81546675
6	1.04655195	0.08033222	6.45366445
6	0.65836643	1.20843983	5.72254812
6	0.16740723	1.12190891	4.41526467
6	-1.13586207	2.52141592	-3.73306841
1	-0.02418752	2.77538870	-6.16539394
6	1.75173817	1.37224760	-7.70291755
1	2.42208776	-0.75517176	-6.11809418
6	1.70531830	-1.70473047	-3.70437092
6	0.52682992	-2.66540587	3.86239295
1	1.28582422	-2.05709203	6.34528341
6	1.52912376	0.19732741	7.87950666
1	0.72427351	2.19504395	6.18935169
6	-0.25286469	2.38779314	3.71143315
1	-1.08922702	3.50454761	-4.21883320
1	-0.86480042	2.64034718	-2.67391255
1	-2.18669489	2.19085102	-3.77205280
1	2.32949134	-1.46434692	-2.82973882
1	2.32067143	-2.29172061	-4.39780547
1	0.89094323	-2.35032693	-3.34339430
1	1.14126973	0.88487479	-8.47985256
1	2.78715487	1.03256160	-7.84227706
1	1.71694266	2.45385124	-7.89179830
1	1.22269375	-3.31735687	4.40663640
1	0.85649173	-2.60213757	2.81586069
1	-0.45288436	-3.16830447	3.85704942
1	-1.20581404	2.25069529	3.17890373
1	0.48354649	2.70970423	2.95667899
1	-0.36416242	3.21115702	4.42955954
1	2.16411993	-0.65518714	8.15736552
1	0.68515840	0.22062168	8.58780753
1	2.10741220	1.11897444	8.03477781
1	0.35387686	-0.60073167	-1.95148853

Energy = -7200.170817 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 63

Atomic N.	X	Y	Z
8	2.96796769	2.46458091	0.63830251
6	4.26338311	2.38506389	1.20999188
1	4.99240702	2.90442744	0.56438329
1	4.62151772	1.34399744	1.34273489
1	4.29121188	2.87167963	2.20426688
50	1.80864792	0.75755680	0.39972443
7	0.18247535	1.67182406	2.10325233
6	0.85017946	2.83515535	2.73674801

1	0.12705856	3.40720882	3.34430389
1	1.30474563	3.47314399	1.97266665
1	1.65826515	2.47594664	3.38671692
7	0.34847797	1.78227661	-0.76386807
6	-0.95277624	2.12328639	1.25052305
1	-1.59125945	2.82599232	1.81990618
1	-1.54099785	1.23735329	0.98403416
6	-0.45483036	2.76248135	-0.04583791
1	-1.34387888	3.03736063	-0.64155295
1	0.06522219	3.71306510	0.18576073
6	0.49460390	1.90539381	-2.17055216
6	0.93152123	3.10264947	-2.79887255
6	1.01985246	3.15468151	-4.19677583
6	0.72223377	2.05624412	-5.00867862
6	0.33591122	0.86972347	-4.37524273
6	0.21190648	0.77468420	-2.98481495
7	-0.43110197	-1.34463633	1.87486512
6	-0.24738898	0.75765453	3.20182283
1	-0.82340392	1.34227875	3.94495003
1	0.67425680	0.42513910	3.70611698
6	-1.09450332	-0.45974335	2.83835202
1	-1.30932719	-0.97446192	3.79659977
1	-2.06734573	-0.14099743	2.44200321
6	-0.96464726	-2.65000311	1.68165969
6	-2.24946372	-2.83855037	1.12344490
6	-2.72174060	-4.14384461	0.93125822
6	-1.95892511	-5.27204303	1.24585196
6	-0.67236072	-5.06248325	1.75689909
6	-0.16467362	-3.78004383	1.98442769
6	1.38536092	4.29671069	-1.99415786
1	1.36366575	4.08304815	-4.66160602
6	0.80060125	2.14969266	-6.51371820
1	0.10646995	-0.01031668	-4.98223807
6	-0.23100564	-0.52872815	-2.36828912
6	-3.09770180	-1.67649452	0.66871481
1	-3.71409433	-4.27624044	0.49272780
6	-2.50290766	-6.66645534	1.04987566
1	-0.04245350	-5.92400982	1.99217664
6	1.23317218	-3.61465953	2.53462305
1	2.00385428	4.95799651	-2.61551850
1	1.97725118	3.97796604	-1.12259271
1	0.54154517	4.89913508	-1.62085387
1	0.60222322	-1.06191652	-1.88062974
1	-0.64523299	-1.19918528	-3.13280070
1	-0.98290034	-0.36015609	-1.58571405
1	-0.18309277	2.38456473	-6.95141189
1	1.13523343	1.20225468	-6.95898602
1	1.49496761	2.94052001	-6.82928560
1	-3.82437293	-2.00634473	-0.08478298
1	-2.47465622	-0.88789806	0.22269470
1	-3.67098038	-1.22335591	1.49355458
1	1.24393577	-3.04363395	3.47734669
1	1.89955290	-3.09140932	1.82894278
1	1.68296807	-4.59399228	2.73923427
1	-1.71746553	-7.36225144	0.72369444
1	-3.30555833	-6.68054294	0.30038450
1	-2.92201079	-7.06618245	1.98706706
1	0.56041097	-1.41215748	2.10617678

Energy = -7200.165719 Hartree
 Number of imaginary frequencies = 0.

Compound 11b isomer 64

Atomic N.	X	Y	Z
8	1.62605677	1.25898117	2.99249960
6	2.89082590	1.88334420	3.14654997
1	2.77640302	2.96070517	3.37281412
1	3.53182149	1.80441157	2.24502413
1	3.44503081	1.42362225	3.98391307
50	1.11389640	0.39866692	1.14854043
7	-0.99575625	1.66480236	1.56117323
6	-0.71787253	3.08315764	1.86986003
1	-1.61515620	3.57681856	2.28270435
1	-0.40002805	3.61664585	0.96697308
1	0.09570965	3.11522278	2.60424486
7	-0.66998981	1.25285954	-1.51061938
6	-2.05490888	1.51752572	0.52909216
1	-2.97265879	2.02451651	0.88380233
1	-2.28547396	0.44444311	0.45495443
6	-1.72320428	2.04897180	-0.86436274
1	-2.66753814	2.04098559	-1.44519217
1	-1.40311198	3.09762524	-0.82116439
6	-0.27585154	1.64367926	-2.82627002
6	0.50968704	2.80212542	-3.01908978
6	0.90627863	3.14579961	-4.31779366
6	0.57141539	2.37011229	-5.43207634
6	-0.17804040	1.20803055	-5.21441536
6	-0.61263972	0.83482511	-3.93825946
7	-0.28624374	-1.01358376	1.93018440
6	-1.40889411	0.97060902	2.81820549
1	-2.38742351	1.36172202	3.15505710
1	-0.64217511	1.22521137	3.56190544
6	-1.45787123	-0.54716214	2.65652468
1	-1.52574869	-0.96646638	3.67732345
1	-2.39824950	-0.85861809	2.15080431
6	0.04413541	-2.39077075	2.05690445
6	-0.04741052	-3.24524873	0.92758782
6	0.29416459	-4.59705648	1.04409444
6	0.72361098	-5.14942753	2.25681507
6	0.82621125	-4.29623839	3.35952376
6	0.50443629	-2.93394951	3.28566665
6	0.97787593	3.63898741	-1.85495847
1	1.52189518	4.03842040	-4.45459576
6	0.99465862	2.77545255	-6.82324217
1	-0.43953777	0.57236349	-6.06405365
6	-1.41636281	-0.43304427	-3.76271914
6	-0.50673057	-2.70774352	-0.40638366
1	0.21555176	-5.23867145	0.16215852
6	1.05472875	-6.61843330	2.36891750
1	1.19023004	-4.69651958	4.30991882
6	0.70381298	-2.06280426	4.50216647
1	1.88191496	4.20015608	-2.12405702
1	1.20829259	3.00363895	-0.98741166
1	0.22286373	4.37813037	-1.53992808
1	-0.86191366	-1.20271343	-3.20085476
1	-1.66567599	-0.86669573	-4.73901377

1	-2.36238766	-0.25654980	-3.22739709
1	0.19276834	3.32906433	-7.33707763
1	1.23230620	1.89943395	-7.44235471
1	1.87814232	3.42732779	-6.79793972
1	-0.70909462	-3.52886358	-1.10719063
1	0.25673865	-2.05752834	-0.86380719
1	-1.41906210	-2.10332415	-0.29777902
1	-0.21489689	-1.98306048	5.10647484
1	0.99978721	-1.04252431	4.21732867
1	1.47804145	-2.48828182	5.15468411
1	1.62493911	-6.97052831	1.49740959
1	0.14043168	-7.23040974	2.42532107
1	1.64585516	-6.82583070	3.27094862
1	-0.95860925	0.27365259	-1.51806361

Energy = -7200.168789 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 65

Atomic N.	X	Y	Z
8	3.74476095	1.03105954	-0.54225334
6	5.01096423	0.59385141	-0.07642715
1	5.72076346	0.53096417	-0.91916059
1	4.98059785	-0.40406754	0.40612303
1	5.43129605	1.30367052	0.66228534
50	2.01522227	-0.00406031	-0.04168318
7	1.26135600	1.98609565	1.31640692
6	2.43373983	2.88866390	1.42254050
1	2.12640503	3.86890278	1.82738455
1	2.91136701	3.00579475	0.44496188
1	3.17364317	2.43924996	2.09714018
7	0.81970355	1.12951649	-1.39047146
6	0.21510000	2.59052019	0.44462378
1	0.02400099	3.63469049	0.75890816
1	-0.70149342	2.00258159	0.56981693
6	0.61528003	2.52585570	-1.02952510
1	-0.21648775	2.95375758	-1.61763762
1	1.48739348	3.18610046	-1.20625239
6	0.67939053	0.73893023	-2.74784437
6	1.37158821	1.38041306	-3.80997851
6	1.15478227	0.95755834	-5.12862152
6	0.29956604	-0.10190128	-5.44553915
6	-0.34177438	-0.75434583	-4.38654958
6	-0.17463714	-0.35522335	-3.05597970
7	-0.47683309	-0.38359367	2.25749569
6	0.77892215	1.72399331	2.70432131
1	0.64667138	2.69315788	3.22293977
1	1.59669498	1.19691337	3.22174608
6	-0.52139518	0.94323254	2.88133636
1	-0.69018454	0.88293216	3.97549724
1	-1.36582107	1.51622996	2.47660839
6	-1.48900205	-1.32315786	2.60222823
6	-2.84198331	-1.09682449	2.26121735
6	-3.79904578	-2.06199109	2.60196790
6	-3.46396681	-3.25728632	3.24446527
6	-2.11237623	-3.48077869	3.53341474
6	-1.12384455	-2.53977468	3.23067766
6	2.40147926	2.45262186	-3.54720938

1	1.70101986	1.45989287	-5.93200407
6	0.06530891	-0.51879060	-6.87779057
1	-1.00887347	-1.59370329	-4.60105738
6	-0.91288095	-1.08877983	-1.96418835
6	-3.27325292	0.12232670	1.48377475
1	-4.84076382	-1.87800707	2.32704629
6	-4.52015946	-4.26786743	3.62113052
1	-1.81498107	-4.41556267	4.01515022
6	0.32023591	-2.83733087	3.56248764
1	3.06247430	2.56297738	-4.41716119
1	3.01485183	2.19785193	-2.66946014
1	1.94590340	3.43827284	-3.35951172
1	-0.24559072	-1.74456347	-1.38013624
1	-1.70387054	-1.72175222	-2.38758134
1	-1.35432941	-0.38665565	-1.24422788
1	-0.83584798	-0.03848728	-7.29206458
1	-0.07888360	-1.60504562	-6.96238557
1	0.91040673	-0.23457632	-7.51979481
1	-4.22321062	-0.06977602	0.96871131
1	-2.52106464	0.39073907	0.72798805
1	-3.42771246	1.00209169	2.12912024
1	0.75976259	-2.07518208	4.22646126
1	0.95302900	-2.88797399	2.66091209
1	0.40495494	-3.80488442	4.07232460
1	-4.14707276	-5.29633862	3.51927544
1	-5.41462874	-4.16423182	2.99227818
1	-4.83865786	-4.13978966	4.66798718
1	0.44199014	-0.79910635	2.41374184

Energy = -7200.165738 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 66

Atomic N.	X	Y	Z
8	2.60697821	1.29737936	2.19935777
6	4.01364618	1.34429412	2.01973582
1	4.35760529	2.38352568	1.85694921
1	4.36596628	0.74389470	1.15641967
1	4.52796851	0.95927004	2.91808240
50	1.42527229	0.21631593	0.84409937
7	0.08080631	2.31011764	0.90927582
6	0.92368571	3.49665315	0.65111415
1	0.37266375	4.42708623	0.87805640
1	1.24495674	3.51838723	-0.39631632
1	1.81217504	3.42464028	1.28955426
7	-0.46665046	0.88625035	-1.81320393
6	-1.15453331	2.32742275	0.08464997
1	-1.70819014	3.26314703	0.29441951
1	-1.78458012	1.49445713	0.42880382
6	-0.96560066	2.21389350	-1.42661164
1	-1.94620750	2.44171210	-1.89107711
1	-0.27034294	2.97858937	-1.79564882
6	-0.27778671	0.65235940	-3.20931973
6	0.81614298	1.23753492	-3.88605365
6	0.99114940	0.97337094	-5.25006321
6	0.13264336	0.13160565	-5.96498187
6	-0.92305921	-0.46577163	-5.26712216
6	-1.14842936	-0.21681679	-3.90876985

7	-0.18749815	-0.15699205	2.19281070
6	-0.28164278	2.28381618	2.36028054
1	-0.95562750	3.13045802	2.59150785
1	0.66303053	2.41535916	2.90495605
6	-0.91708270	0.95837292	2.77679384
1	-0.91083786	0.94440082	3.88246113
1	-1.99186661	0.93249092	2.49142133
6	-0.37318041	-1.43364328	2.79066180
6	-1.02190674	-2.46511180	2.06543633
6	-1.18561112	-3.72977843	2.64358686
6	-0.73152758	-4.01648652	3.93545371
6	-0.07809887	-2.99737053	4.63667895
6	0.11539593	-1.72060759	4.09397078
6	1.82620259	2.08968785	-3.15903073
1	1.84564319	1.42344225	-5.76175691
6	0.33105858	-0.11407772	-7.44112628
1	-1.59930044	-1.14235706	-5.79551625
6	-2.30345592	-0.89222258	-3.20584719
6	-1.53419171	-2.21666811	0.66707585
1	-1.68863801	-4.51166858	2.06818651
6	-0.95204310	-5.37431088	4.55806918
1	0.31609331	-3.20616570	5.63525971
6	0.88522179	-0.69126933	4.88543004
1	2.78408743	2.09186173	-3.69481127
1	1.99663815	1.70772667	-2.14194500
1	1.50324277	3.14044561	-3.07399446
1	-1.96284767	-1.62072251	-2.45168016
1	-2.92145036	-1.44216861	-3.92628181
1	-2.95749578	-0.17134597	-2.69078898
1	-0.21686441	0.62757797	-8.04396117
1	-0.03391316	-1.10727001	-7.73566113
1	1.39097818	-0.04096082	-7.72022751
1	-2.18482589	-3.03896441	0.34021547
1	-0.70733068	-2.13567915	-0.05727258
1	-2.10058605	-1.27558708	0.61360007
1	1.46836207	-0.03414818	4.22367919
1	1.56866520	-1.18302558	5.59059398
1	0.21773249	-0.04834119	5.48262390
1	-0.14173586	-5.63192447	5.25411689
1	-1.01167882	-6.16157541	3.79419700
1	-1.89317572	-5.40201386	5.13040256
1	-1.09421791	0.17749821	-1.43091868

Energy = -7200.168595 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 67

Atomic N.	X	Y	Z
8	3.56610969	-0.94939040	-2.42911544
6	3.26042466	-0.87221035	-3.80933969
1	2.48541337	-0.11946414	-4.04258893
1	2.90599389	-1.85187746	-4.18570445
1	4.16526893	-0.60919219	-4.38601088
50	2.81244335	0.13222435	-0.84402023
7	0.79545447	-1.33680514	-0.91951503
6	1.17113997	-2.74302881	-1.18708701
1	0.28088567	-3.34545364	-1.43960533
1	1.65901341	-3.17879295	-0.30851501

1	1.89091250	-2.76170302	-2.01389822
7	-0.31662588	-1.38434386	2.76067126
6	-0.09352634	-1.22812425	0.26732599
1	-0.97913201	-1.87448574	0.11734999
1	-0.44957513	-0.19019200	0.31348208
6	0.57479408	-1.57481764	1.60941250
1	0.93449152	-2.60955180	1.60809185
1	1.45788044	-0.93431850	1.75982745
6	-1.49689166	-2.16744659	2.87722113
6	-1.41815674	-3.56946843	3.05607810
6	-2.60201698	-4.30465757	3.19874422
6	-3.86433408	-3.70324250	3.20664929
6	-3.91673823	-2.30949643	3.08776764
6	-2.76483046	-1.53446872	2.92000886
7	1.32770742	1.34422778	-1.81306218
6	0.11998101	-0.76662683	-2.12409921
1	-0.88658912	-1.21168151	-2.23351833
1	0.72309992	-1.06792635	-2.99051407
6	0.02136049	0.75723830	-2.08401933
1	-0.36400513	1.07361767	-3.07422435
1	-0.75750164	1.06469388	-1.35649939
6	1.38439571	2.76522608	-1.71104307
6	0.75268483	3.48196814	-0.65961721
6	0.84227960	4.88059604	-0.61673595
6	1.55625798	5.61092068	-1.56945669
6	2.19934264	4.89463001	-2.58571222
6	2.12789751	3.50020755	-2.67327417
6	-0.09295900	-4.28242828	3.17472209
1	-2.52582057	-5.38586282	3.34069777
6	-5.12371940	-4.52545778	3.33566525
1	-4.88600979	-1.80550141	3.11923676
6	-2.88753749	-0.03303556	2.80272730
6	0.02658847	2.77602857	0.45854976
1	0.35124387	5.41131011	0.20359072
6	1.66655521	7.11432538	-1.48647862
1	2.76931306	5.43841639	-3.34380680
6	2.83454242	2.79637661	-3.80488380
1	-0.21196578	-5.21128612	3.74766796
1	0.64952938	-3.65098037	3.68302061
1	0.32825393	-4.56356358	2.19556730
1	-2.37183356	0.49481980	3.62239609
1	-3.94139770	0.26904326	2.84019237
1	-2.46855386	0.34790958	1.85746602
1	-5.52907233	-4.79221527	2.34651062
1	-5.90972730	-3.97544499	3.87109315
1	-4.93514338	-5.46418007	3.87415535
1	-0.01682205	3.41273430	1.35189014
1	0.54235281	1.84110517	0.72471725
1	-1.01074620	2.51726137	0.19081381
1	2.14780996	2.14358812	-4.36078304
1	3.65198018	2.15337117	-3.44526611
1	3.26502035	3.52652104	-4.50280827
1	2.63695330	7.41914828	-1.06360968
1	0.88034188	7.53873778	-0.84806708
1	1.58847116	7.57749116	-2.48037022
1	-0.53295726	-0.39501551	2.86993931

Energy = -7200.163954 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 68

Atomic N.	X	Y	Z
8	3.16066170	-0.29014915	-2.06145647
6	3.37756397	-0.00750251	-3.42932106
1	2.54433521	0.54790354	-3.89955417
1	3.52374674	-0.94345294	-4.00451896
1	4.29267138	0.59912394	-3.55697159
50	1.63737346	0.27364013	-0.77174697
7	0.35850198	-1.68452214	-1.75021217
6	1.25910138	-2.84112062	-1.93974766
1	0.79678208	-3.59871571	-2.59837769
1	1.49114174	-3.30225866	-0.97374268
1	2.19854202	-2.47940288	-2.37453621
7	-0.27077661	-1.63081943	1.28846126
6	-0.90155371	-2.08474009	-1.07333031
1	-1.40919781	-2.85189953	-1.69091606
1	-1.55915189	-1.20359898	-1.05879823
6	-0.77830487	-2.63677721	0.34626233
1	-1.78609632	-3.00297194	0.62912486
1	-0.11995083	-3.51428267	0.36926805
6	-0.18629483	-2.00864853	2.66111659
6	0.80451625	-2.91957907	3.09179225
6	0.87437056	-3.25470732	4.44987092
6	0.01444731	-2.69917922	5.40285302
6	-0.92943455	-1.76456992	4.96125731
6	-1.04954767	-1.41401443	3.61248920
7	0.20716854	1.16270351	-2.12485221
6	0.04228062	-1.08667250	-3.08098618
1	-0.61979853	-1.76690917	-3.65049250
1	0.99450436	-1.00998055	-3.62030615
6	-0.59371176	0.29943481	-2.98110729
1	-0.64783298	0.69420727	-4.01585523
1	-1.64815308	0.20493451	-2.65066195
6	-0.24285214	2.49756811	-1.93332206
6	-1.48123096	2.80725292	-1.30876194
6	-1.86905190	4.14531892	-1.14730572
6	-1.06614194	5.20964852	-1.56110103
6	0.16891349	4.89758214	-2.14278754
6	0.59023446	3.57849456	-2.33695721
6	1.82480128	-3.48195344	2.13379400
1	1.64911578	-3.95436829	4.77359022
6	0.09577600	-3.09889410	6.85626463
1	-1.59894064	-1.29568324	5.68665491
6	-2.08090604	-0.39234639	3.19152600
6	-2.37254523	1.73189430	-0.74043475
1	-2.82400474	4.35716140	-0.65824128
6	-1.50245215	6.64385023	-1.38261986
1	0.82529710	5.70887533	-2.46903300
6	1.92197080	3.32542019	-2.99934123
1	2.72863739	-3.79256903	2.67353348
1	2.10905768	-2.72870032	1.38498878
1	1.45264257	-4.36843884	1.59428100
1	-1.61683147	0.52635913	2.79546210
1	-2.69895591	-0.09583744	4.04795727
1	-2.75798416	-0.77942091	2.41361871
1	-0.58389699	-3.93757104	7.07627752

1	-0.18720942	-2.26866412	7.51764576
1	1.11033393	-3.42204126	7.12611110
1	-2.99479583	2.13414497	0.06997836
1	-1.76408723	0.90796198	-0.33835617
1	-3.05340893	1.29993529	-1.49153245
1	1.81329006	2.66550958	-3.87074715
1	2.64128499	2.83456524	-2.32562989
1	2.37129055	4.27101536	-3.33016444
1	-0.75012273	7.22708000	-0.83095569
1	-2.45017087	6.70631908	-0.83167337
1	-1.64588023	7.14221476	-2.35384830
1	-0.83908040	-0.78715615	1.20612523

Energy = -7200.162748 Hartree
Number of imaginary frequencies = 0.

Compound 11b isomer 69

Atomic N.	X	Y	Z
8	3.90742425	0.02429759	0.27336834
6	4.94821887	0.96270162	0.05547028
1	4.58679315	2.00775750	-0.02792126
1	5.50488755	0.73218868	-0.87358550
1	5.66728888	0.92841449	0.89198482
50	1.91598694	0.59497645	0.12359028
7	1.68528214	-0.88260609	-1.91188895
6	3.06130953	-1.27877635	-2.29922393
1	3.02943135	-2.08397741	-3.05412026
1	3.62618749	-1.59652292	-1.41747659
1	3.57933283	-0.40985303	-2.72483210
7	1.21703840	-1.26136827	0.89852484
6	0.93773278	-2.05354364	-1.37340249
1	1.04297556	-2.91332037	-2.06284881
1	-0.11937079	-1.77106065	-1.30818626
6	1.41275140	-2.41701301	0.03356146
1	0.79492171	-3.26388937	0.38261449
1	2.45336851	-2.79471749	-0.01252122
6	1.07236632	-1.46051130	2.29644045
6	2.00412273	-2.20418578	3.07000269
6	1.77418878	-2.38351828	4.44075755
6	0.66965498	-1.82946168	5.09494635
6	-0.21616203	-1.06176445	4.33091717
6	-0.04144276	-0.87221831	2.95548895
7	-0.73778780	1.02767665	-1.97127818
6	1.04016044	-0.28941218	-3.11994878
1	1.15818782	-0.99277156	-3.96679628
1	1.62402151	0.61050300	-3.37208142
6	-0.44160987	0.07146051	-3.04336099
1	-0.70657571	0.47174989	-4.04279280
1	-1.04664953	-0.83493978	-2.91098197
6	-2.00477745	1.67616787	-1.97826982
6	-3.20068950	0.94515654	-1.79588367
6	-4.42214756	1.63207964	-1.78756172
6	-4.50362201	3.02051706	-1.92601327
6	-3.30396301	3.72960555	-2.06175305
6	-2.06275407	3.08746362	-2.09525764
6	3.28271656	-2.73622431	2.46868923
1	2.50564248	-2.95400439	5.02016027
6	0.43353517	-2.06277076	6.56796657

1	-1.08379463	-0.60597902	4.81571160
6	-1.04632915	-0.05008949	2.18778009
6	-3.19373992	-0.54259130	-1.54435615
1	-5.33913518	1.05616884	-1.63904979
6	-5.83543915	3.73108542	-1.93632930
1	-3.33225184	4.81854733	-2.14988571
6	-0.80015020	3.90531766	-2.24012746
1	4.01163720	-2.95220819	3.26110846
1	3.72304669	-2.00269319	1.77614202
1	3.12760127	-3.67175522	1.90744909
1	-0.65507056	0.94807572	1.92878813
1	-1.95875558	0.10058078	2.77973590
1	-1.30537398	-0.53119684	1.23515502
1	-0.20910343	-2.94216337	6.73570113
1	-0.06475483	-1.20271669	7.03656366
1	1.37747682	-2.24373219	7.10055433
1	-4.11409027	-0.84671210	-1.02948675
1	-2.33824257	-0.82967169	-0.91608101
1	-3.13611781	-1.12863248	-2.47578494
1	-0.21140588	3.60817374	-3.12331015
1	-0.13998082	3.81173784	-1.36191605
1	-1.04318976	4.96926776	-2.35061735
1	-5.77619600	4.70365041	-1.42830150
1	-6.61134267	3.13254716	-1.44045917
1	-6.17677248	3.92306482	-2.96606252
1	0.00349870	1.72763904	-1.92941838

Energy = -7200.165740 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 70

Atomic N.	X	Y	Z
8	3.34294878	0.08099391	-1.45477543
6	4.61314082	0.04050682	-0.82405475
1	4.56252383	0.18233310	0.27469577
1	5.26628579	0.83485859	-1.22680392
1	5.11525339	-0.92894105	-1.00545574
50	1.61434316	0.30937218	-0.28812046
7	0.83947304	-1.57084159	-1.72380248
6	1.81220716	-2.68380118	-1.72153319
1	1.56638684	-3.42235186	-2.50574201
1	1.81852190	-3.18576893	-0.74749924
1	2.80745951	-2.26212601	-1.90559702
7	-0.75500651	-1.67763455	0.95534638
6	-0.54514083	-2.05400814	-1.48755269
1	-0.79792979	-2.80039650	-2.26544686
1	-1.21620361	-1.19496744	-1.63259887
6	-0.82539012	-2.67620998	-0.12133726
1	-1.82524136	-3.15120321	-0.18390548
1	-0.11780965	-3.48652617	0.09564123
6	-1.03215755	-2.14023424	2.27785407
6	-0.08090307	-2.92189891	2.97057758
6	-0.36934892	-3.34558278	4.27419398
6	-1.55840526	-3.00314448	4.92571495
6	-2.47101697	-2.19775473	4.23424433
6	-2.23471203	-1.76684137	2.92457259
7	0.41427440	1.18822085	-1.81967623
6	0.91061510	-0.87217401	-3.04448760

1	0.53438698	-1.54179402	-3.84110520
1	1.97628869	-0.66961011	-3.21671752
6	0.14523331	0.45004433	-3.04436445
1	0.46372662	0.99393923	-3.95285605
1	-0.94447247	0.27192334	-3.17855999
6	0.13384568	2.58220344	-1.82876395
6	-0.90921911	3.09748756	-1.01789593
6	-1.17442737	4.47223854	-1.01039291
6	-0.43793910	5.37159792	-1.78889724
6	0.59294487	4.85450103	-2.58067629
6	0.89913390	3.48795822	-2.61175163
6	1.25571883	-3.25920054	2.35858007
1	0.37691535	-3.94252438	4.80448758
6	-1.85405590	-3.49295973	6.32268007
1	-3.40079160	-1.89915836	4.72485752
6	-3.25475572	-0.89640882	2.22726661
6	-1.74145362	2.17626049	-0.15866343
1	-1.98625222	4.84982112	-0.38281208
6	-0.71762741	6.85426622	-1.74277809
1	1.19677457	5.53931867	-3.18268025
6	2.06556317	3.01182529	-3.44324906
1	1.99449983	-3.47214233	3.14182813
1	1.62577158	-2.42249622	1.74838969
1	1.20676167	-4.15094029	1.71204889
1	-2.87685993	0.12336168	2.04622164
1	-4.15868668	-0.79884546	2.84108412
1	-3.55904607	-1.30930506	1.25279389
1	-2.47086920	-4.40546714	6.30126138
1	-2.40641074	-2.74160026	6.90363818
1	-0.93031400	-3.73502231	6.86509281
1	-2.62476549	2.70067722	0.23003672
1	-1.16712371	1.80286867	0.70485882
1	-2.07492382	1.29577605	-0.72673224
1	1.75053022	2.69602544	-4.45146910
1	2.56619568	2.15343591	-2.97173820
1	2.79654401	3.82057297	-3.57633458
1	-0.09146730	7.35350252	-0.98593620
1	-1.76585523	7.05633846	-1.48305547
1	-0.50458909	7.33374098	-2.70814557
1	-1.38309720	-0.90608862	0.72599770

Energy = -7200.168583 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 71

Atomic N.	X	Y	Z
8	2.26201653	-2.68259616	-1.74608413
6	3.36197559	-2.67670893	-2.64136228
1	3.84382029	-1.68268434	-2.73821137
1	3.05163199	-2.99199796	-3.65647482
1	4.13394641	-3.38479075	-2.29399355
50	1.50485925	-0.90510931	-0.98397877
7	-0.62645472	-1.30199685	-2.27841035
6	-0.34546783	-2.41620228	-3.21638017
1	-1.28382965	-2.77885594	-3.67159447
1	0.17161883	-3.22810258	-2.69584286
1	0.32220675	-2.05818748	-4.01045793
7	0.23368607	-1.91439042	0.39423125

6	-1.57014360	-1.74264694	-1.21293905
1	-2.44002756	-2.25158772	-1.67106103
1	-1.91428483	-0.84682169	-0.68327045
6	-0.87633591	-2.64973587	-0.19644591
1	-1.62007600	-2.90630587	0.57931941
1	-0.59729342	-3.60566158	-0.68227757
6	0.70318950	-2.28573029	1.68126615
6	1.07580597	-3.61715560	2.01189975
6	1.50167233	-3.91044738	3.31397773
6	1.60637096	-2.93157651	4.30745082
6	1.27875995	-1.61757177	3.95725616
6	0.82785311	-1.27856028	2.67616547
7	-0.66090705	1.68132191	-1.48804603
6	-1.15606035	-0.16578795	-3.08830425
1	-1.98586071	-0.53683191	-3.72039469
1	-0.34493388	0.13087448	-3.77268642
6	-1.67517557	1.06646970	-2.35089754
1	-2.02871442	1.76231269	-3.13836856
1	-2.56126416	0.80727060	-1.75695204
6	-0.90676514	2.99025694	-0.98603200
6	-1.97040740	3.24146646	-0.08960618
6	-2.15754541	4.54316047	0.39461472
6	-1.31427611	5.60211788	0.04666883
6	-0.24114455	5.32192808	-0.80789592
6	-0.02479538	4.04432829	-1.33226573
6	1.10528765	-4.70992204	0.97053775
1	1.79008650	-4.93943242	3.54695524
6	2.04432060	-3.28412013	5.70884337
1	1.36045232	-0.82789545	4.70904583
6	0.47184173	0.15528794	2.37202898
6	-2.86712216	2.13591951	0.41090367
1	-2.97954073	4.72299891	1.09216074
6	-1.55355282	6.99904724	0.56640319
1	0.44937396	6.12360408	-1.08150700
6	1.15273539	3.80002193	-2.24754004
1	1.73761296	-5.54029854	1.31188336
1	1.50650024	-4.33076050	0.01825306
1	0.10540775	-5.12622481	0.76768642
1	1.24061714	0.65249257	1.75698804
1	0.36992040	0.73542111	3.29869219
1	-0.46269470	0.21744892	1.79856973
1	1.19089527	-3.60986502	6.32523020
1	2.50239330	-2.42315591	6.21465064
1	2.77323567	-4.10680308	5.70564440
1	-3.33520666	2.42409960	1.36093054
1	-2.29382892	1.21219924	0.57586321
1	-3.68186272	1.90182131	-0.29304667
1	0.84165637	3.40727058	-3.22933652
1	1.86985895	3.07931154	-1.82073323
1	1.69971767	4.73394334	-2.42604051
1	-0.60766692	7.51664771	0.77833206
1	-2.15024815	6.98546994	1.48830306
1	-2.10005490	7.60996190	-0.16967461
1	0.24221496	1.66204736	-1.96264330

Energy = -7200.165744 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 72

Atomic N.	X	Y	Z
8	2.07168885	-0.70930852	0.20777692
6	2.09521936	0.41261884	1.06579174
1	2.99777403	1.02532278	0.88832181
1	2.11591468	0.08026682	2.12030098
1	1.22643733	1.08500634	0.93533387
50	0.85522660	-1.24122425	-1.35767456
7	-1.70905788	-1.23029691	-2.34679621
6	-2.06535882	-2.52932967	-2.92088984
1	-2.97470839	-2.46694542	-3.55152478
1	-2.24119444	-3.26586739	-2.12737564
1	-1.23168666	-2.89592430	-3.53502063
7	-1.22607680	-1.21193993	0.59438349
6	-2.69104522	-0.76664346	-1.36083889
1	-3.72982123	-0.90025538	-1.72845329
1	-2.54287915	0.31243927	-1.21168228
6	-2.55213401	-1.47209599	-0.01188507
1	-3.37092923	-1.12916938	0.64773412
1	-2.67247231	-2.55720670	-0.12300682
6	-1.03760385	-1.79866219	1.89765917
6	-0.79221002	-3.18179169	2.02854283
6	-0.59076651	-3.71220705	3.30933227
6	-0.61724148	-2.91976717	4.46089637
6	-0.85598183	-1.55019604	4.30409937
6	-1.07524525	-0.97647656	3.04696001
7	0.34396417	0.78215125	-1.97994924
6	-1.41584106	-0.25192738	-3.40634872
1	-2.32559488	0.00177749	-3.99092610
1	-0.70898719	-0.74355001	-4.09384398
6	-0.78294941	1.03338843	-2.87636988
1	-0.45742672	1.60868799	-3.76410418
1	-1.57222687	1.65687652	-2.40745473
6	1.16563806	1.92428847	-1.76317520
6	0.67006169	3.07459763	-1.09050816
6	1.49189300	4.19598628	-0.91926071
6	2.80941814	4.23135466	-1.38273152
6	3.29282062	3.09256176	-2.03523792
6	2.50694211	1.95085878	-2.23305730
6	-0.71981301	-4.10285962	0.83596735
1	-0.38536647	-4.78153762	3.40139040
6	-0.41516941	-3.52463974	5.82899077
1	-0.87575095	-0.90482933	5.18553640
6	-1.34153998	0.50758685	2.94302432
6	-0.71626615	3.10636812	-0.49538038
1	1.08867456	5.06361563	-0.38940700
6	3.69105738	5.43580375	-1.15559578
1	4.31854079	3.09142591	-2.41380624
6	3.11748891	0.77211543	-2.94987309
1	-0.09319897	-4.97468705	1.06365096
1	-0.29314325	-3.59814356	-0.04318791
1	-1.71460727	-4.48493670	0.55299420
1	-0.52213634	1.04244770	2.43609062
1	-1.44156162	0.94731186	3.94297071
1	-2.27026950	0.72758938	2.39331990
1	-1.37465579	-3.84150133	6.26771480
1	0.03913611	-2.80440546	6.52259642
1	0.23101868	-4.41153697	5.78234507

1	-0.75365850	3.79418762	0.36009565
1	-1.01373026	2.10441667	-0.15199759
1	-1.47819507	3.44180952	-1.21719545
1	2.40781403	0.30817342	-3.64953331
1	3.43235046	-0.00863451	-2.23770024
1	4.01118241	1.08008885	-3.50910995
1	4.29897214	5.31796726	-0.24429094
1	3.09638125	6.35169933	-1.03655969
1	4.38806221	5.58576602	-1.99203196
1	-1.11517576	-0.19805934	0.67996468

Energy = -7200.161481 Hartree
Number of imaginary frequencies = 0.

Compound 11b isomer 73

Atomic N.	X	Y	Z
8	1.79890292	-1.26677849	-1.05976332
6	3.11204966	-1.66360021	-1.45118107
1	3.46190210	-1.05803164	-2.30540521
1	3.16932479	-2.72705043	-1.75495207
1	3.82157051	-1.51844415	-0.61843988
50	0.33242010	-2.75328740	-1.06418021
7	-1.22407785	-1.29720108	-2.27954043
6	-2.01160099	-2.23283679	-3.11633592
1	-2.79781355	-1.69262322	-3.67142298
1	-2.48287483	-2.99707168	-2.48522091
1	-1.34817338	-2.73939265	-3.82953790
7	-0.96127060	-1.99915146	0.45850999
6	-2.08400477	-0.67695963	-1.22565238
1	-3.05500164	-0.37386096	-1.65758389
1	-1.54681438	0.20171460	-0.85096957
6	-2.27845841	-1.63601426	-0.05111028
1	-2.85210548	-1.09829024	0.72444913
1	-2.92027674	-2.49062922	-0.35863794
6	-0.85019846	-2.43788335	1.80727168
6	-1.54119029	-3.56944586	2.31178679
6	-1.37941162	-3.93812070	3.65507066
6	-0.54116286	-3.23348359	4.52292214
6	0.15251278	-2.13135529	4.00701548
6	0.01276216	-1.71860747	2.67772546
7	0.33452088	1.36084969	-1.50413668
6	-0.51076432	-0.31948868	-3.18038804
1	-1.03219362	-0.31010132	-4.15181471
1	0.50174257	-0.71638602	-3.35339216
6	-0.41760179	1.14288346	-2.74131711
1	0.04354677	1.67122280	-3.60054126
1	-1.43435213	1.55454843	-2.64595825
6	0.76109521	2.68376283	-1.21763156
6	-0.18254364	3.71065485	-0.97102432
6	0.27048697	5.00580970	-0.68565623
6	1.62868341	5.32356156	-0.60449463
6	2.54674137	4.28660943	-0.80789764
6	2.14385366	2.98399641	-1.11798280
6	-2.41027208	-4.42320859	1.42090519
1	-1.91300363	-4.81807724	4.02489970
6	-0.39778059	-3.63446639	5.97159242
1	0.81592644	-1.56269612	4.66418451
6	0.75682258	-0.50186402	2.18673261

6	-1.66573329	3.43427854	-0.92843798
1	-0.47214493	5.78402618	-0.49056645
6	2.09075466	6.73160480	-0.31622257
1	3.61690366	4.49688494	-0.73361892
6	3.18483553	1.91463258	-1.33577685
1	-2.56671251	-5.41338314	1.86857800
1	-1.94853610	-4.56175983	0.43097649
1	-3.40361159	-3.97743107	1.25381860
1	1.48309977	-0.75084223	1.39898327
1	1.28945833	-0.01684532	3.01547057
1	0.06912967	0.22611535	1.73317320
1	-1.00185580	-2.98623560	6.62629405
1	0.64476607	-3.55250759	6.31035085
1	-0.73047977	-4.66844124	6.13468744
1	-2.18037337	4.20686434	-0.34244004
1	-1.86805976	2.45801935	-0.46482854
1	-2.12719506	3.42722631	-1.92918986
1	3.07783004	1.43723852	-2.32231071
1	3.11195900	1.11103703	-0.58736597
1	4.19363363	2.34203176	-1.27490387
1	2.97811647	6.73903084	0.33219138
1	1.30274085	7.31745655	0.17606255
1	2.36268771	7.26090851	-1.24353282
1	1.06686956	0.65088480	-1.38228823

Energy = -7200.163125 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 74

Atomic N.	X	Y	Z
8	1.61035592	-1.33931385	-0.66991295
6	2.08527718	-0.98217714	0.61159209
1	3.15595301	-0.71062207	0.57379951
1	1.97900492	-1.83742943	1.30447830
1	1.55537313	-0.11661235	1.05206870
50	0.27869518	-0.45443532	-1.95728350
7	-2.06550535	0.96263733	-2.17642900
6	-2.91808819	0.42346801	-3.23775251
1	-3.72667122	1.12849184	-3.51647955
1	-3.37404817	-0.52294081	-2.92238647
1	-2.30567839	0.21687896	-4.12593800
7	-1.60864479	-0.84621413	0.14840897
6	-2.77349953	1.08199446	-0.89735827
1	-3.77855451	1.53390954	-1.03026752
1	-2.20116250	1.76350567	-0.25194492
6	-2.92809660	-0.25912328	-0.18041406
1	-3.53662840	-0.10067939	0.72939827
1	-3.47736933	-0.97581489	-0.80409676
6	-1.67141119	-2.08845664	0.87725879
6	-2.00385861	-3.28826847	0.21483695
6	-2.03243603	-4.47977936	0.95191241
6	-1.73711571	-4.52275926	2.31726175
6	-1.40407902	-3.31987271	2.95050996
6	-1.37394763	-2.10418456	2.25969675
7	0.62601547	1.59543841	-1.30949833
6	-1.40596623	2.20332804	-2.61411604
1	-2.13792916	3.02669455	-2.75558208
1	-0.96048730	1.98583555	-3.59807991

6	-0.30591352	2.66550749	-1.66031368
1	0.22156270	3.49322208	-2.17186661
1	-0.77424530	3.13422722	-0.77004475
6	1.84000219	2.06364285	-0.73184844
6	1.85410221	2.71663541	0.53087233
6	3.05970537	3.19455462	1.06047051
6	4.27732499	3.04668102	0.39162160
6	4.25679871	2.39499646	-0.84584000
6	3.07584231	1.90476783	-1.41603208
6	-2.31011279	-3.33462610	-1.26157887
1	-2.27568434	-5.40773033	0.42872120
6	-1.79111430	-5.81872600	3.08925676
1	-1.16190931	-3.32355581	4.01600960
6	-1.02000202	-0.83569418	3.00125392
6	0.60101294	2.86401335	1.35857297
1	3.04353271	3.68410628	2.03831279
6	5.57140662	3.53643346	0.99580337
1	5.19308572	2.26835370	-1.39606508
6	3.15516110	1.21724288	-2.75657265
1	-2.08774026	-4.32992086	-1.66719046
1	-1.71730151	-2.59832749	-1.82382395
1	-3.37487799	-3.13327538	-1.46513596
1	-0.05483223	-0.41754209	2.67249892
1	-0.93405650	-1.03476148	4.07652047
1	-1.78166458	-0.05056135	2.87268281
1	-2.74808256	-5.92183457	3.62476154
1	-0.99152172	-5.87117122	3.84093335
1	-1.69224804	-6.68525217	2.42222360
1	0.84774534	2.91229797	2.42774505
1	-0.07495162	2.01186039	1.19357724
1	0.03727627	3.77815221	1.11228928
1	2.31598075	1.49768310	-3.40889782
1	3.13016181	0.12051085	-2.64494081
1	4.09504649	1.46971670	-3.26564837
1	6.08909511	2.72833046	1.53700947
1	5.39697998	4.35118413	1.71160069
1	6.26190617	3.90141832	0.22250500
1	-1.09696781	-0.16605846	0.71687445

Energy = -7200.161479 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 75

Atomic N.	X	Y	Z
8	0.46020433	0.08203552	2.71759184
6	1.78820750	0.01589100	3.21350906
1	1.78580269	-0.31333670	4.26730358
1	2.27346190	1.00973967	3.17556499
1	2.43456499	-0.68778799	2.65107359
50	-0.08821466	-0.95114264	0.99560073
7	-0.88389179	1.21394985	0.20051481
6	-1.53512018	1.09673059	-1.12720169
1	-2.14970188	1.99075056	-1.33095722
1	-2.17499427	0.20678011	-1.14038075
1	-0.77062772	1.01697821	-1.90637626
7	-2.16625092	-0.94872620	1.38972650
6	-1.90768539	1.48112317	1.25819920
1	-2.44877295	2.41690118	1.02592524

8	0.55308721	-0.12249632	1.14306959
6	1.14627139	-0.93577123	2.14916737
1	1.52464431	-0.28920866	2.95793501
1	2.00157504	-1.53088102	1.77177311
1	0.42664291	-1.64289081	2.60295907
50	-0.22682971	-1.15446994	-0.53279733
7	-1.37461126	0.90111137	-1.13149224
6	-2.23404129	0.56014382	-2.29317931
1	-2.93707849	1.38257418	-2.50967734
1	-2.79496935	-0.35574881	-2.08109457
1	-1.59923012	0.39232909	-3.17180659
7	-2.20772671	-1.36235612	0.26380471
6	-2.20661892	1.09183981	0.09499259
1	-2.88508094	1.95284048	-0.04991990
1	-1.51229142	1.31241172	0.91643981
6	-3.01566059	-0.16225526	0.43620631
1	-3.38200484	-0.02520134	1.46986541
1	-3.92790813	-0.20361444	-0.19632201
6	-2.73615882	-2.57948388	0.77121023
6	-3.03349620	-3.65296368	-0.11131534
6	-3.52380390	-4.86056490	0.39958051
6	-3.75265527	-5.05380833	1.76632373
6	-3.45378179	-3.99402351	2.62721417
6	-2.94867004	-2.77222044	2.16388040
7	1.72710146	1.73360700	-0.67843939
6	-0.62351508	2.14516269	-1.48525827
1	-1.36176335	2.96861576	-1.54461323
1	-0.21514307	1.98836147	-2.49176421
6	0.52306657	2.57176522	-0.56714250
1	0.77242575	3.60665667	-0.84057216
1	0.18270446	2.60534836	0.48131556
6	2.97916281	2.38049931	-0.84821101
6	3.98410821	2.27182689	0.14673377
6	5.22023198	2.89568702	-0.05090282
6	5.50616805	3.63695843	-1.20340749
6	4.51139646	3.71900104	-2.18184979
6	3.26496605	3.09574569	-2.03679512
6	-2.84264580	-3.51638196	-1.60306720
1	-3.74509601	-5.67287276	-0.29793863
6	-4.32155676	-6.35113242	2.28862161
1	-3.59626786	-4.12524571	3.70364443
6	-2.59585325	-1.70611281	3.17277861
6	3.73873472	1.48997142	1.41368003
1	5.97946980	2.80795036	0.73050976
6	6.85636756	4.28363070	-1.40002379
1	4.71558377	4.26513747	-3.10628459
6	2.28654191	3.13650383	-3.18466200
1	-3.28565047	-4.37400729	-2.12644476
1	-1.77934078	-3.46849503	-1.88642624
1	-3.31191720	-2.59855105	-1.98554100
1	-1.78285828	-1.06548016	2.80572365
1	-2.28467555	-2.16354628	4.12182860
1	-3.45430171	-1.05266000	3.39949073
1	-5.42325387	-6.33676575	2.27600115
1	-4.01037801	-6.53566492	3.32602195
1	-4.00088323	-7.20573623	1.67704810
1	4.56477395	1.63537918	2.12125521
1	3.65789135	0.40920408	1.21722883

1	2.80475224	1.79145339	1.91120432
1	1.44239544	3.82231079	-3.01094543
1	1.86228505	2.13612474	-3.35957381
1	2.78758124	3.46711872	-4.10364536
1	7.59928887	3.55495714	-1.76180675
1	7.24350973	4.69881516	-0.45870367
1	6.80744158	5.09624260	-2.13720567
1	1.71754820	1.06332548	0.10132114

Energy = -7200.166754 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 77

Atomic N.	X	Y	Z
8	1.54227829	0.42217609	-0.91624624
6	2.96140595	0.48527300	-0.83109488
1	3.37220345	-0.08242236	0.02831939
1	3.31997881	1.52725106	-0.73839634
1	3.40358410	0.06024625	-1.74810079
50	0.44758864	0.29373150	0.87614181
7	-1.53681289	0.19693646	-0.52159229
6	-2.67452580	0.07648379	0.42540209
1	-3.63277803	0.23590416	-0.09765258
1	-2.56815414	0.81507478	1.22761326
1	-2.67056531	-0.92865019	0.86444644
7	-0.34557704	2.26859515	0.91182991
6	-1.50845989	1.56391919	-1.12851464
1	-2.43833890	1.72632993	-1.70479417
1	-0.65283751	1.58723742	-1.81461201
6	-1.33688476	2.66121632	-0.07783124
1	-1.05707003	3.58104104	-0.62441812
1	-2.31546903	2.88620254	0.39835335
6	0.17949704	3.29216904	1.74890400
6	-0.13197456	3.31150699	3.13295594
6	0.41623268	4.30395813	3.95401814
6	1.26328335	5.29880386	3.45193185
6	1.56844417	5.26623241	2.08776709
6	1.05032689	4.28656712	1.23053016
7	0.42858612	-2.03635962	-2.25201531
6	-1.72161565	-0.84556855	-1.58292563
1	-2.65161265	-0.58561123	-2.12472624
1	-1.90217108	-1.80208320	-1.07159042
6	-0.57764134	-1.03601788	-2.59894437
1	-1.03808894	-1.27002121	-3.56567596
1	-0.02328913	-0.09946262	-2.73304728
6	0.13518471	-3.36684762	-1.90910331
6	-0.84447382	-4.14850397	-2.57893405
6	-1.07138469	-5.46743989	-2.15769274
6	-0.34434621	-6.07579129	-1.13300698
6	0.67603003	-5.31946777	-0.54431380
6	0.93012329	-3.99592095	-0.90801750
6	-1.05182995	2.27683099	3.73606415
1	0.16628851	4.30290598	5.01831343
6	1.81246061	6.38110141	4.35013164
1	2.24835815	6.01690003	1.67533817
6	1.46134648	4.28544713	-0.22171508
6	-1.59473595	-3.66703930	-3.80037798
1	-1.83373894	-6.04784822	-2.68431276

6	-0.63719564	-7.48702121	-0.68479953
1	1.30108771	-5.77192104	0.22993526
6	2.06882659	-3.25582328	-0.25288766
1	-1.30689152	2.54449243	4.76987207
1	-0.59307021	1.27579076	3.75355238
1	-1.98504605	2.18622711	3.16192477
1	1.45702284	3.26651021	-0.63340778
1	2.46540304	4.71473174	-0.33958934
1	0.77948709	4.89195459	-0.84020611
1	1.10575908	7.22183765	4.43727240
1	2.75494572	6.78663707	3.95775782
1	1.99666901	6.00535174	5.36607639
1	-2.08714924	-4.51775047	-4.28906475
1	-0.91534131	-3.20830778	-4.53395267
1	-2.38046653	-2.92788991	-3.57450134
1	1.72411491	-2.37816502	0.32056225
1	2.80192717	-2.88969066	-0.99016613
1	2.60166033	-3.91275944	0.44573557
1	0.28521477	-8.02825477	-0.43058372
1	-1.15993818	-8.05406069	-1.46721987
1	-1.27721946	-7.50000794	0.21225822
1	1.14137487	-1.59686698	-1.66697635

Energy = -7200.164915 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 78

Atomic N.	X	Y	Z
8	0.44726557	0.64068310	-1.25162156
6	1.57896060	0.72360881	-2.10702044
1	2.47645508	1.11830896	-1.59051224
1	1.34899842	1.40478780	-2.94342255
1	1.85474232	-0.25431091	-2.54606306
50	0.55507487	-0.74970065	0.34541265
7	-1.89237244	-0.46419300	0.48201292
6	-2.33323656	-0.56729485	1.89083091
1	-3.43285485	-0.50277397	1.96872993
1	-1.87832249	0.23199725	2.48403437
1	-2.00350194	-1.53102257	2.29723921
7	-0.55440140	2.24997745	0.85579522
6	-2.34459155	0.82058124	-0.13541317
1	-3.44461167	0.78900345	-0.24322943
1	-1.89745537	0.86334534	-1.13850686
6	-1.99731292	2.09517671	0.63589192
1	-2.42203381	2.93178450	0.04395788
1	-2.52181030	2.11461520	1.60220732
6	-0.14623937	3.48638478	1.44252785
6	-0.31832807	3.70874173	2.82830149
6	0.09532538	4.92583344	3.38429970
6	0.69551769	5.92941581	2.61721826
6	0.88967229	5.67739240	1.25447429
6	0.47756632	4.48263931	0.65283031
7	-0.20688853	-2.36214891	-0.86290448
6	-2.43560615	-1.61910056	-0.30695576
1	-3.44373993	-1.36302257	-0.67918407
1	-2.52408776	-2.47126542	0.37939012
6	-1.50068094	-2.02657995	-1.44610155
1	-1.94803997	-2.90301781	-1.94267239

1	-1.45459121	-1.21622156	-2.19833164
6	0.47348378	-3.51646037	-1.30670548
6	0.66682626	-3.79866840	-2.68751432
6	1.32181130	-4.97710445	-3.07147904
6	1.82658148	-5.89180605	-2.14430278
6	1.65503056	-5.59178674	-0.78766293
6	0.99448947	-4.43832157	-0.35361048
6	-0.87703185	2.63612690	3.72891984
1	-0.03588923	5.08052427	4.45836654
6	1.10723604	7.24426295	3.23438287
1	1.37117629	6.43700936	0.63332733
6	0.72252923	4.26863077	-0.82216154
6	0.25117546	-2.82243406	-3.76306966
1	1.46267048	-5.16845404	-4.13898663
6	2.55666111	-7.13906155	-2.58199108
1	2.03388051	-6.28915088	-0.03529416
6	0.82658412	-4.20915894	1.12764480
1	-0.62938216	2.84536571	4.77754061
1	-0.45959973	1.65516341	3.45895862
1	-1.97475767	2.55946122	3.66486491
1	1.48954453	3.49919987	-1.00107368
1	1.07078614	5.19740848	-1.29139083
1	-0.18408889	3.93989654	-1.35153428
1	0.30339227	7.99272501	3.14805038
1	1.99410241	7.66092195	2.73758307
1	1.33401017	7.13108919	4.30325680
1	0.81202091	-3.01483790	-4.68717609
1	0.44171391	-1.78595140	-3.45147683
1	-0.81943072	-2.88796162	-4.01286732
1	-0.19251342	-3.86999867	1.36589901
1	1.51129384	-3.43401493	1.50962404
1	1.03336371	-5.13096800	1.68756480
1	3.64155837	-7.04965760	-2.41305380
1	2.40352047	-7.33590756	-3.65146857
1	2.21636266	-8.02230586	-2.02158448
1	-0.06798315	2.06260042	-0.03479480

Energy = -7200.170790 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 79

Atomic N.	X	Y	Z
8	1.46755223	-0.17972377	-1.09138967
6	2.87769840	-0.36901274	-1.12230707
1	3.12973305	-1.12553147	-1.88466124
1	3.29115346	-0.72222064	-0.15593335
1	3.41033519	0.56333302	-1.38661750
50	0.59273700	0.45743111	0.71292840
7	-1.53877824	0.32040731	-0.44411699
6	-2.55509771	0.71051284	0.56612482
1	-3.53357928	0.88097352	0.08575312
1	-2.23547409	1.62425859	1.07933338
1	-2.65512300	-0.09519431	1.30361951
7	0.13900938	2.46225588	0.16035658
6	-1.37034910	1.40722719	-1.45810260
1	-2.32767485	1.56077905	-1.99017414
1	-0.61526148	1.05788967	-2.17308043
6	-0.89543603	2.71758756	-0.83004774

1	-0.54492328	3.35743754	-1.66116016
1	-1.75771442	3.25830795	-0.38376509
6	0.92784486	3.57009165	0.57794015
6	0.80682974	4.07493852	1.89820688
6	1.61115126	5.14484173	2.30848902
6	2.53529935	5.75119007	1.44984078
6	2.65100184	5.24085116	0.15308834
6	1.87376635	4.16589973	-0.29757291
7	-0.18467361	-2.66746434	-1.49239838
6	-2.01538963	-0.94040689	-1.10030624
1	-2.95148515	-0.68612888	-1.63420660
1	-2.28176050	-1.64418750	-0.29864024
6	-1.04809530	-1.64266162	-2.07424463
1	-1.65162923	-2.06277946	-2.88698515
1	-0.36775069	-0.91437160	-2.53155325
6	-0.65014104	-3.74864280	-0.72527524
6	0.14202889	-4.18608180	0.37517719
6	-0.28307873	-5.26213721	1.15665004
6	-1.47677870	-5.94762285	0.90262288
6	-2.20867168	-5.54953329	-0.21738014
6	-1.81723689	-4.49092319	-1.05081342
6	-0.18174610	3.47657332	2.87034407
1	1.50548968	5.52051392	3.32972099
6	3.36427034	6.92900905	1.90288141
1	3.38416077	5.67977253	-0.52934789
6	2.08634982	3.63703536	-1.69512073
6	1.45596561	-3.51701125	0.69058620
1	0.34479528	-5.57120888	1.99647157
6	-1.94353398	-7.07203276	1.79493710
1	-3.11310576	-6.10271887	-0.48447524
6	-2.61432395	-4.26632921	-2.31619413
1	-0.25169389	4.09270900	3.77641920
1	0.10638197	2.45959352	3.17952809
1	-1.18459240	3.39911530	2.42641747
1	1.86429030	2.56205875	-1.74928251
1	3.12229223	3.80527723	-2.01879856
1	1.43615455	4.14347053	-2.42731726
1	2.82837367	7.87788899	1.74056482
1	4.31016753	6.98994436	1.34757795
1	3.59815517	6.86736960	2.97460578
1	1.95016855	-4.01942274	1.53136176
1	1.33093398	-2.45664486	0.96986905
1	2.14885238	-3.54320014	-0.16636165
1	-1.95779095	-4.18982742	-3.19552286
1	-3.23659123	-3.35697184	-2.29196408
1	-3.29282735	-5.11368210	-2.47940954
1	-2.66844927	-7.71619045	1.27888541
1	-2.43429317	-6.68726778	2.70350121
1	-1.10362411	-7.70031182	2.12430048
1	0.65573196	-2.21910108	-1.12357700

Energy = -7200.164924 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 80

Atomic N.	X	Y	Z
8	1.38628016	0.02177897	1.11345021
6	2.41891005	-0.90923972	1.39114760

1	2.86881290	-1.27959167	0.45297352
1	2.07567244	-1.79490344	1.96513080
1	3.21838449	-0.42661306	1.98180290
50	-0.53016884	-0.32247591	1.78445054
7	-3.05091011	-0.33654308	0.52551140
6	-4.03112816	-0.55859653	1.59604637
1	-5.07288529	-0.47571478	1.22798053
1	-3.88722673	0.17940981	2.39500680
1	-3.88249912	-1.55588619	2.03121387
7	-1.01625575	1.67414992	1.20968934
6	-3.10589831	1.04946386	0.02499441
1	-4.15901483	1.35888882	-0.14310778
1	-2.58319703	1.08317139	-0.94022660
6	-2.41183638	2.02980365	0.97369048
1	-2.48001239	3.03201056	0.52111556
1	-2.99174463	2.10127410	1.91857746
6	-0.10423916	2.76808009	1.24464801
6	0.52457376	3.15899191	2.45358279
6	1.40251145	4.25011773	2.45973073
6	1.69124221	4.98178690	1.30371861
6	1.07942657	4.57775458	0.11301249
6	0.19742615	3.49195218	0.06083972
7	-0.87922602	-2.11172745	-0.55510391
6	-3.22144117	-1.32837430	-0.55096998
1	-4.05803577	-1.04647478	-1.22248920
1	-3.50894857	-2.28287297	-0.08026911
6	-1.96785540	-1.56041287	-1.39148979
1	-2.23198034	-2.24992056	-2.21448438
1	-1.63204769	-0.62284366	-1.85331719
6	0.19596530	-2.78031520	-1.22701324
6	1.08579082	-2.07522297	-2.06749793
6	2.12561043	-2.78157676	-2.68647244
6	2.33331469	-4.14950280	-2.48406398
6	1.46342173	-4.81657603	-1.61483589
6	0.39849268	-4.16068986	-0.98864982
6	0.27892987	2.41936222	3.74570349
1	1.87285845	4.53804858	3.40380365
6	2.61311013	6.17700741	1.34275311
1	1.30899933	5.11128737	-0.81360482
6	-0.37846973	3.08087114	-1.27058572
6	0.99467086	-0.58186270	-2.25475417
1	2.81441163	-2.22709917	-3.32845718
6	3.45126029	-4.88268450	-3.18486001
1	1.61227236	-5.88111548	-1.41831100
6	-0.50648800	-4.93410076	-0.05622725
1	0.56768446	3.03689454	4.60702206
1	0.87590453	1.49372374	3.79650796
1	-0.77600591	2.13228612	3.85888557
1	-0.39888426	1.98590601	-1.35728015
1	0.22003045	3.49104225	-2.09459821
1	-1.41238289	3.43704344	-1.41122719
1	2.05084268	7.10982593	1.51034958
1	3.15871687	6.29284669	0.39585146
1	3.34906799	6.08952892	2.15367431
1	1.92540230	-0.19846307	-2.69168852
1	0.84506207	-0.08148666	-1.28577342
1	0.17615547	-0.29036181	-2.93157055
1	-1.56021800	-4.90838737	-0.37916936

1	-0.46759695	-4.54998898	0.97680176
1	-0.20463170	-5.98793275	-0.01822374
1	3.83658453	-5.70843858	-2.57127559
1	4.28677402	-4.20876924	-3.41742768
1	3.10611536	-5.31669586	-4.13680198
1	-1.29946037	-2.77084729	0.10216064

Energy = -7200.163059 Hartree
Number of imaginary frequencies = 0.

Compound 11b isomer 81

Atomic N.	X	Y	Z
8	0.33916231	0.38267153	-1.37555757
6	1.37630119	0.25632735	-2.33869903
1	1.09502481	0.81656764	-3.24611670
1	1.55106090	-0.79374848	-2.64164084
1	2.34370907	0.66183858	-1.98125498
50	0.57001401	-0.70897846	0.42701793
7	-1.83936249	-0.28547441	0.74708790
6	-2.13314065	-0.10966700	2.18667342
1	-3.21603945	0.02204855	2.35798355
1	-1.59417677	0.76047981	2.57409463
1	-1.79231484	-0.99883215	2.73063584
7	-0.39778211	2.38997525	0.48847704
6	-2.31646301	0.88603367	-0.05101332
1	-3.42218692	0.88528845	-0.04655454
1	-1.97213921	0.72677151	-1.08250249
6	-1.85897646	2.26205089	0.43615904
1	-2.31807768	2.99576229	-0.25782601
1	-2.28398727	2.47941775	1.42677093
6	0.09910105	3.69360750	0.79331614
6	0.06654351	4.17648437	2.12201379
6	0.56493222	5.45561622	2.39944784
6	1.11629543	6.27178666	1.40660973
6	1.17252560	5.76296555	0.10425502
6	0.67196029	4.49722992	-0.22222933
7	-0.36091042	-2.47140974	-0.38982336
6	-2.49554741	-1.53702545	0.24299172
1	-3.53050685	-1.30526231	-0.06620820
1	-2.53235210	-2.24678624	1.07963700
6	-1.70051285	-2.18555044	-0.89054612
1	-2.22290413	-3.11490401	-1.17023319
1	-1.71355586	-1.52656660	-1.77952781
6	0.23687097	-3.71591097	-0.68343404
6	0.27202518	-4.24762362	-2.00368727
6	0.85157131	-5.50212902	-2.23291941
6	1.43217185	-6.25923332	-1.21126346
6	1.41451939	-5.71707335	0.07813083
6	0.83319421	-4.47624103	0.36197673
6	-0.43180511	3.31510397	3.25489921
1	0.54136552	5.81232569	3.43239765
6	1.62083798	7.65849605	1.72552804
1	1.61348829	6.37164915	-0.68930536
6	0.76925111	4.00294334	-1.64615035
6	-0.23428150	-3.46049689	-3.18978348
1	0.87051346	-5.88550346	-3.25705747
6	2.08948179	-7.58883777	-1.49443055
1	1.85441354	-6.28672897	0.90137265

6	0.83155537	-3.98306605	1.78725368
1	-0.08046443	3.70415237	4.21920164
1	-0.06743320	2.28394293	3.13907379
1	-1.53224504	3.27509286	3.30381798
1	1.49308406	3.17898894	-1.74349206
1	1.09822046	4.81166794	-2.31083500
1	-0.19271171	3.62421475	-2.02230051
1	0.83183209	8.41255660	1.57482472
1	2.46457944	7.93732207	1.07956561
1	1.94919102	7.73443534	2.77106443
1	0.21341731	-3.84147893	-4.11707846
1	0.01930473	-2.39539745	-3.09470846
1	-1.32754633	-3.51779284	-3.30893876
1	-0.14566534	-3.55901651	2.06226703
1	1.57575541	-3.18679286	1.95376204
1	1.07027825	-4.80140654	2.47963120
1	3.15252750	-7.46258730	-1.75614171
1	1.60673357	-8.10467439	-2.33597227
1	2.04743540	-8.25070132	-0.61816270
1	-0.00716049	2.02108242	-0.39254392

Energy = -7200.170794 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 82

Atomic N.	X	Y	Z
8	0.49098647	0.69496067	-1.20672012
6	1.61978416	0.76110890	-2.06719714
1	1.44274700	1.53358874	-2.83425616
1	1.80774544	-0.19198633	-2.59750760
1	2.55152325	1.02956060	-1.53069794
50	0.51683712	-0.80183385	0.29417010
7	-1.91011962	-0.38367386	0.45616268
6	-2.35720942	-0.54912543	1.85694631
1	-3.45112263	-0.42484611	1.94232382
1	-1.85605417	0.18297885	2.49774981
1	-2.08522571	-1.55429440	2.20094514
7	-0.42373618	2.22297188	1.00118078
6	-2.28684618	0.96129194	-0.07840447
1	-3.38628071	0.99844066	-0.18970690
1	-1.83191420	1.04444934	-1.07542669
6	-1.87240556	2.16274104	0.77312076
1	-2.24851028	3.05732814	0.23558435
1	-2.39805949	2.14952881	1.73886762
6	0.05255927	3.39562383	1.66231504
6	-0.11457064	3.54507564	3.05822477
6	0.36685436	4.70058862	3.68691842
6	1.02981237	5.71049904	2.98282020
6	1.21710530	5.52874931	1.60775381
6	0.73890649	4.39857728	0.93503592
7	-0.33542858	-2.28599805	-1.01413326
6	-2.51820470	-1.45355254	-0.40196940
1	-3.51043136	-1.11795152	-0.75319320
1	-2.65441377	-2.34128263	0.22930826
6	-1.60858597	-1.84018673	-1.56859492
1	-2.10606870	-2.65570385	-2.11818124
1	-1.51591051	-0.98722677	-2.26748146
6	0.27194649	-3.45211278	-1.52713108

6	0.44261768	-3.66555388	-2.92436226
6	1.02369542	-4.85590963	-3.38022276
6	1.47743134	-5.85147596	-2.51031726
6	1.32812662	-5.62131236	-1.13853771
6	0.73905809	-4.45701220	-0.63324314
6	-0.74072799	2.45584202	3.89205387
1	0.23811939	4.79890575	4.76788680
6	1.51598636	6.95951882	3.67768448
1	1.74646267	6.29393276	1.03417258
6	0.97733244	4.25937302	-0.54993605
6	0.08155930	-2.60590890	-3.93902285
1	1.14825050	-4.99281116	-4.45814710
6	2.14068961	-7.10557450	-3.02743357
1	1.66637923	-6.38322576	-0.43083736
6	0.58957140	-4.30743786	0.86004148
1	-0.48908054	2.58860661	4.95212801
1	-0.37846612	1.46981219	3.56649683
1	-1.84052969	2.44647026	3.81926302
1	1.68676540	3.44834828	-0.77599793
1	1.39534734	5.18766608	-0.95933336
1	0.05208301	4.03231278	-1.10026871
1	0.78104002	7.77543600	3.58880897
1	2.45703176	7.32180766	3.24123742
1	1.68043605	6.78274509	4.74919341
1	0.62093103	-2.78181710	-4.87900698
1	0.34129187	-1.60284696	-3.57260372
1	-0.99300842	-2.58822460	-4.17917282
1	-0.40387445	-3.91569866	1.12469039
1	1.32577071	-3.60500319	1.28453438
1	0.73460799	-5.27340045	1.36195423
1	3.23157472	-6.97535474	-3.11408730
1	1.76511950	-7.37706079	-4.02361932
1	1.96854205	-7.95652595	-2.35355401
1	0.05415637	2.06308891	0.10073213

Energy = -7200.170806 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 83

Atomic N.	X	Y	Z
8	3.11914885	2.26743887	-0.72307636
6	4.52759171	2.15289192	-0.60237416
1	5.01580619	2.53262629	-1.51639611
1	4.87197572	1.10961781	-0.45201559
1	4.90471643	2.74984529	0.25061761
50	1.88494187	0.64464620	-0.32745779
7	0.96863550	1.87738361	1.67641414
6	1.85708397	3.04573204	1.89104738
1	1.40534710	3.74076647	2.62048837
1	2.05128796	3.55332590	0.94121290
1	2.82233087	2.69689389	2.27979942
7	0.15795947	1.64432172	-1.07110121
6	-0.36935031	2.32117016	1.19417888
1	-0.74925107	3.13476540	1.84174315
1	-1.04730483	1.46229153	1.25893063
6	-0.31397733	2.76426889	-0.26797882
1	-1.34012324	3.04314682	-0.56795204
1	0.29228054	3.68776678	-0.35268842

6	-0.18401281	1.58894428	-2.44741842
6	0.04843132	2.66760967	-3.34326003
6	-0.34915051	2.55000966	-4.68183089
6	-0.94435297	1.39074321	-5.18865471
6	-1.12539228	0.31914536	-4.30753456
6	-0.76466521	0.39577040	-2.95749987
7	0.17166424	-1.07808166	2.06931538
6	0.90131237	1.13096672	2.96712333
1	0.64274597	1.84218536	3.77526001
1	1.92400850	0.77593472	3.17297139
6	-0.07435916	-0.03871634	3.07473367
1	0.03220347	-0.42603355	4.10814076
1	-1.10827304	0.32104423	2.99217403
6	-0.45552701	-2.34388007	2.24445432
6	-1.86145688	-2.47654364	2.18355364
6	-2.43125915	-3.74724489	2.33955237
6	-1.66008554	-4.89783442	2.52714776
6	-0.26790364	-4.74972889	2.54052108
6	0.34628607	-3.50089589	2.40827448
6	0.79218986	3.90794850	-2.90969096
1	-0.15648534	3.38877961	-5.35676545
6	-1.38774735	1.30370218	-6.62940622
1	-1.57745021	-0.60563917	-4.67628058
6	-1.00355014	-0.79269467	-2.06004474
6	-2.75982221	-1.30032350	1.89005313
1	-3.51907740	-3.83744138	2.28377612
6	-2.30294395	-6.25050949	2.71613606
1	0.36370382	-5.63315824	2.66287508
6	1.85426152	-3.40217266	2.42630979
1	1.17990438	4.44152641	-3.78769990
1	1.63764948	3.64714532	-2.25492540
1	0.15049839	4.61425870	-2.35871711
1	-0.07082749	-1.33868139	-1.83936486
1	-1.69309970	-1.50446532	-2.53287008
1	-1.41027665	-0.48199436	-1.08845868
1	-2.43716581	1.61972443	-6.74477315
1	-1.31422494	0.27599463	-7.01135899
1	-0.78024341	1.95330934	-7.27474587
1	-3.71749382	-1.64486624	1.47924446
1	-2.29476679	-0.62561021	1.15688031
1	-2.98915880	-0.70830083	2.79073701
1	2.21754695	-2.73480997	3.22477723
1	2.25834993	-3.02077754	1.47389966
1	2.30107037	-4.38960686	2.59545192
1	-1.70953136	-7.04687664	2.24600520
1	-3.31296808	-6.27651644	2.28554528
1	-2.39531814	-6.50204525	3.78476165
1	1.17766376	-1.20819284	1.95823335

Energy = -7200.165749 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 84

Atomic N.	X	Y	Z
8	4.19064125	0.24349517	0.57741010
6	5.50148965	0.30665953	0.03307991
1	5.62402298	-0.29497092	-0.88939802
1	6.23751302	-0.06285342	0.76827598

1	5.77189862	1.34941709	-0.21732331
50	2.70290679	-0.84857675	-0.38671905
7	1.40224557	1.21274584	-0.12864493
6	2.11366914	2.39662332	-0.65760443
1	1.57243254	3.32517285	-0.40495996
1	2.21653357	2.32735070	-1.74644577
1	3.11577861	2.41777310	-0.21299119
7	-1.41567259	0.64065972	-2.67279609
6	0.02202207	1.09932793	-0.66837712
1	-0.55770416	1.99695224	-0.38221262
1	-0.43813422	0.23031369	-0.17880434
6	-0.05261057	0.89785604	-2.19161916
1	0.34906674	1.77000600	-2.71884690
1	0.57160437	0.03616738	-2.47889629
6	-2.41176842	1.64577823	-2.53885049
6	-2.29942768	2.87084365	-3.23882495
6	-3.31641269	3.82546436	-3.10765810
6	-4.46155442	3.60276685	-2.33719183
6	-4.58093094	2.36149183	-1.70085483
6	-3.58261044	1.38581966	-1.78235771
7	1.47984500	-1.15990443	1.31700564
6	1.37869978	1.28483108	1.36521885
1	0.75046838	2.13573634	1.68676130
1	2.41865848	1.46703362	1.66971743
6	0.89109739	-0.01702681	2.00005864
1	1.16724829	0.03303695	3.07014272
1	-0.21923890	-0.06607649	1.98382315
6	1.39177073	-2.42127827	1.97097503
6	0.52742132	-3.42333037	1.46168917
6	0.45712603	-4.66881491	2.09664609
6	1.21872117	-4.96379713	3.23354178
6	2.06924664	-3.96867515	3.72539652
6	2.17597180	-2.71033772	3.11778248
6	-1.15293222	3.14580114	-4.18146212
1	-3.21819122	4.76530923	-3.65722018
6	-5.52880178	4.66068364	-2.19384829
1	-5.47728774	2.14503043	-1.11420769
6	-3.77371709	0.06376933	-1.07611648
6	-0.32401794	-3.16098357	0.24224043
1	-0.21826600	-5.42871238	1.69438392
6	1.15193224	-6.32563836	3.88253005
1	2.68503364	-4.17984283	4.60401946
6	3.14435216	-1.69620669	3.67632123
1	-1.45477688	3.87714955	-4.94257941
1	-0.83170198	2.22526343	-4.68928301
1	-0.27155548	3.56438815	-3.66836501
1	-3.78984671	-0.78754665	-1.77708506
1	-4.72878988	0.05254323	-0.53675312
1	-2.97786276	-0.13638070	-0.34094463
1	-5.37491472	5.26182321	-1.28347160
1	-6.53032795	4.21449479	-2.12216105
1	-5.52261380	5.35278336	-3.04678592
1	-1.03403040	-3.98343855	0.08344515
1	0.28683349	-3.06353893	-0.66890229
1	-0.89204222	-2.22487245	0.34384015
1	2.65642378	-1.02182394	4.39917555
1	3.56733779	-1.06864389	2.87867796
1	3.96336156	-2.19774023	4.20891535

1	1.85395009	-7.02764436	3.40478520
1	0.14732064	-6.76240156	3.79578010
1	1.41416245	-6.27561805	4.94797229
1	-1.75106597	-0.24568717	-2.29904867

Energy = -7200.168737 Hartree
Number of imaginary frequencies = 0.

Compound 11b isomer 85

Atomic N.	X	Y	Z
8	3.55633771	-0.29839305	-0.76729029
6	4.36836445	0.46960784	-1.64132278
1	3.78550842	1.13355978	-2.31166329
1	4.97403065	-0.19402501	-2.28357588
1	5.06659436	1.11210095	-1.07162638
50	1.47526898	-0.03262450	-0.78605032
7	1.83069291	0.05135544	1.67646015
6	2.87952014	1.02956878	2.03450437
1	3.17310328	0.92089936	3.09414121
1	2.52397786	2.05221991	1.86551424
1	3.74565672	0.84742330	1.38733328
7	-0.78352648	1.62288518	1.01803970
6	0.61527583	0.22232331	2.51302020
1	0.90123063	0.12596907	3.57843070
1	-0.05710664	-0.61638304	2.28113781
6	-0.15024239	1.53268319	2.34173990
1	-0.89348391	1.58017459	3.16306242
1	0.51130867	2.39714217	2.48120122
6	-1.55450145	2.79602698	0.75481794
6	-0.90980871	4.02775644	0.50378388
6	-1.68899137	5.15861963	0.22784131
6	-3.08522695	5.10808861	0.16825571
6	-3.70167089	3.86995351	0.38404171
6	-2.96603334	2.71810983	0.68222145
7	0.98808100	-1.97635465	-0.05014427
6	2.37791817	-1.32887254	1.85833073
1	2.55113401	-1.52232427	2.93401490
1	3.34087646	-1.33874354	1.33014612
6	1.46814598	-2.39879316	1.25690579
1	2.06592491	-3.32814832	1.21545570
1	0.62359283	-2.62625153	1.94411850
6	0.48448737	-2.98884592	-0.91233163
6	-0.89394129	-3.01220048	-1.24385236
6	-1.38862849	-3.99774996	-2.10670004
6	-0.55957538	-4.97887446	-2.66105508
6	0.80021933	-4.94310064	-2.33385583
6	1.33940263	-3.97050433	-1.48219251
6	0.59419053	4.13632881	0.47226847
1	-1.18018144	6.10475231	0.02682615
6	-3.90170480	6.34722652	-0.10865215
1	-4.79048740	3.79636947	0.32569748
6	-3.68512214	1.40719745	0.90304819
6	-1.83921246	-1.98224505	-0.67359864
1	-2.45560597	-4.00282897	-2.34565855
6	-1.10572900	-6.01563271	-3.61354538
1	1.47314027	-5.68650837	-2.77046994
6	2.82633713	-3.95933452	-1.22224578
1	0.90499991	4.99634531	-0.13469211

1	1.04050299	3.22737158	0.04334617
1	1.02438201	4.28019764	1.47719928
1	-3.47027030	0.67584373	0.10652297
1	-4.77101092	1.56274211	0.91079462
1	-3.41129645	0.93666491	1.86027635
1	-4.24905153	6.81138192	0.82808534
1	-4.79406643	6.11544644	-0.70623796
1	-3.31333335	7.10103624	-0.64874720
1	-2.88319105	-2.26876768	-0.85892350
1	-1.67793487	-0.99165755	-1.12922857
1	-1.69237523	-1.86477981	0.40985890
1	3.08931551	-4.52706074	-0.31447682
1	3.19931025	-2.93346450	-1.08742778
1	3.36476435	-4.42664412	-2.05762900
1	-0.99780851	-5.68958419	-4.66047240
1	-2.17466522	-6.19774700	-3.43706988
1	-0.57362744	-6.97191894	-3.51500174
1	-1.36418446	0.79499126	0.87729522

Energy = -7200.168581 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 86

Atomic N.	X	Y	Z
8	2.80465803	1.37430177	0.14954297
6	3.19267488	2.73394375	0.16372658
1	3.07588459	3.22541387	-0.81918665
1	4.25843307	2.79780029	0.44201278
1	2.62253957	3.33576778	0.90223742
50	1.15091239	0.52829380	-0.74007567
7	-0.03882938	0.63216076	1.48425259
6	0.89586908	1.15584459	2.50824038
1	0.38949090	1.22522615	3.48682640
1	1.25766738	2.14695879	2.21777335
1	1.76465495	0.49337936	2.58615019
7	-0.16896213	2.21401588	-0.94891375
6	-1.11934156	1.62601384	1.21837217
1	-1.49771072	2.01611789	2.18284608
1	-1.94056962	1.10211844	0.71131227
6	-0.64802404	2.76551850	0.31345336
1	-1.51602184	3.42349450	0.13979071
1	0.09967276	3.38183023	0.85267555
6	-0.51077617	2.87930113	-2.15213331
6	-0.29232166	4.27455076	-2.33091909
6	-0.66745514	4.88980827	-3.53225736
6	-1.23999909	4.18167197	-4.59221915
6	-1.43192349	2.80804026	-4.41494786
6	-1.09178484	2.14956762	-3.22745380
7	-0.41999934	-2.63279428	0.39320372
6	-0.62786675	-0.64616762	1.98847386
1	-1.37341160	-0.38829597	2.76410321
1	0.17016709	-1.20990545	2.49149120
6	-1.26593944	-1.55113901	0.91106391
1	-2.18214317	-1.98729525	1.32653397
1	-1.58189519	-0.94370700	0.04897507
6	0.02498971	-3.64790466	1.28005678
6	-0.90582735	-4.51635720	1.90301417
6	-0.43626497	-5.52166904	2.75767908

6	0.92568969	-5.72888242	2.99652985
6	1.83175121	-4.90206023	2.32306115
6	1.41221110	-3.87022940	1.47636514
6	0.40348371	5.11220943	-1.28476907
1	-0.47753496	5.96053071	-3.64778557
6	-1.65547853	4.87484873	-5.86737433
1	-1.88093421	2.22406358	-5.22286237
6	-1.38103114	0.67326687	-3.11691566
6	-2.38423705	-4.44215372	1.60740549
1	-1.16713341	-6.18596846	3.22630948
6	1.40136918	-6.80300937	3.94451386
1	2.90447387	-5.05825759	2.46184926
6	2.44464562	-3.02477351	0.77119883
1	0.77776157	6.04254376	-1.73143074
1	1.25446496	4.57305336	-0.84651307
1	-0.25999009	5.39443977	-0.45252033
1	-0.47450503	0.05600706	-3.22991986
1	-2.08525924	0.35927469	-3.89863048
1	-1.81077821	0.42344111	-2.13571424
1	-2.70927312	5.19417586	-5.82442746
1	-1.55241391	4.21169038	-6.73737446
1	-1.05046800	5.77385780	-6.04902566
1	-2.85413505	-5.41937504	1.77940826
1	-2.56177858	-4.14825297	0.56308021
1	-2.91176068	-3.71703031	2.24895947
1	2.35220364	-1.95380503	1.01503712
1	2.37252637	-3.10061627	-0.32599671
1	3.45736121	-3.33893210	1.05257227
1	2.35971877	-7.23054536	3.61906969
1	0.67081298	-7.61968333	4.02278551
1	1.55233509	-6.40120150	4.95927222
1	0.34535532	-2.24453119	-0.16185893

Energy = -7200.161704 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 87

Atomic N.	X	Y	Z
8	3.48965463	2.43975366	0.38898099
6	3.34405884	3.81715770	0.10757486
1	2.82640820	4.00955037	-0.84952278
1	4.34384914	4.28036886	0.04546767
1	2.78105439	4.35756951	0.89827001
50	2.16767993	0.90767513	-0.02014415
7	1.21819950	1.09343965	2.30715780
6	2.01627175	2.11878783	3.02022813
1	1.60208798	2.29037595	4.02955508
1	2.01597147	3.05776859	2.46050510
1	3.05695196	1.78388224	3.09983349
7	0.34681756	2.03252905	-0.29771195
6	-0.16426715	1.57744819	2.05466222
1	-0.59559643	1.99751637	2.98433846
1	-0.76518617	0.71744916	1.73712562
6	-0.19855098	2.61254679	0.92558598
1	-1.25607288	2.88777704	0.77755103
1	0.31391599	3.53858760	1.25526504
6	-0.32433220	2.29194834	-1.51596751
6	-0.70070488	3.61158545	-1.90165065

6	-1.39725216	3.81629308	-3.09980307
6	-1.72770108	2.77123663	-3.96631530
6	-1.32550339	1.48459287	-3.59584655
6	-0.64484350	1.22251357	-2.40112382
7	0.54910610	-1.78353836	1.37953165
6	1.27150790	-0.15230677	3.12961448
1	1.04048087	0.10847751	4.18009343
1	2.32017933	-0.49041471	3.11051177
6	0.35059566	-1.31146966	2.75387449
1	0.55210830	-2.10686228	3.49930817
1	-0.69861782	-1.02070020	2.89907989
6	-0.00273957	-3.04526428	1.01807980
6	-1.40156744	-3.24331327	0.97904370
6	-1.89984824	-4.49574026	0.59533508
6	-1.06511200	-5.55267957	0.22168806
6	0.31585490	-5.32082595	0.22496233
6	0.86109195	-4.09527492	0.61855561
6	-0.30343454	4.82706240	-1.09656760
1	-1.66452202	4.84058802	-3.37463310
6	-2.50256773	3.01791695	-5.23831757
1	-1.56481065	0.64205776	-4.25046118
6	-0.28446091	-0.20652133	-2.08199581
6	-2.37118521	-2.12543177	1.27425755
1	-2.98346036	-4.63467744	0.56295879
6	-1.62891635	-6.89841352	-0.16551287
1	0.99421414	-6.12045014	-0.08293214
6	2.35962127	-3.90100727	0.60078752
1	-0.36664131	5.72845077	-1.72017967
1	0.72650485	4.73862566	-0.72459224
1	-0.94781732	4.99345073	-0.21932763
1	0.76763684	-0.43393443	-2.32587187
1	-0.90341176	-0.90006987	-2.66677212
1	-0.41231461	-0.43263529	-1.01383731
1	-3.58569219	2.89040525	-5.07975115
1	-2.20660413	2.31764003	-6.03183741
1	-2.34660511	4.04037821	-5.60940247
1	-3.34589784	-2.33445368	0.81515589
1	-2.00165036	-1.17003390	0.87425265
1	-2.54497930	-1.98969079	2.35386991
1	2.75387958	-3.62288954	1.59165722
1	2.67019274	-3.11257220	-0.10457223
1	2.86278982	-4.82636957	0.29453508
1	-1.06083140	-7.35020746	-0.99060671
1	-2.67881448	-6.81677450	-0.47714397
1	-1.59064034	-7.60438915	0.67933452
1	1.54446823	-1.76449482	1.15381173

Energy = -7200.161278 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 88

Atomic N.	X	Y	Z
8	3.67706496	-0.03762737	-0.61414219
6	4.40463454	-0.42043731	-1.76479408
1	3.78729297	-0.45514287	-2.68159695
1	4.85873535	-1.42186493	-1.62654747
1	5.23181596	0.28902462	-1.94785439
50	1.69524516	0.50657060	-0.38694157

7	1.17723126	-1.96345975	-0.39633380
6	2.19548578	-2.71134477	0.36881359
1	2.10597153	-3.79906555	0.19475326
1	2.08459400	-2.50691983	1.43889451
1	3.18677124	-2.35888135	0.06116953
7	-0.42639037	-0.84965246	1.98428849
6	-0.20236555	-2.34552611	0.00341041
1	-0.38069000	-3.39801942	-0.29293677
1	-0.89508512	-1.72752167	-0.58606226
6	-0.55507600	-2.22503122	1.48560493
1	-1.58934528	-2.61156022	1.58854058
1	0.07858785	-2.88955797	2.08753006
6	-0.90924377	-0.58923236	3.30084966
6	-0.20711840	-1.06931126	4.42929949
6	-0.69792913	-0.77997793	5.70878799
6	-1.84643711	-0.00832354	5.91262276
6	-2.50127036	0.49461091	4.78225897
6	-2.05944629	0.21547203	3.48480520
7	0.88587554	0.12681959	-2.35122846
6	1.36298857	-2.22110531	-1.85514273
1	1.07012551	-3.26185035	-2.09191636
1	2.43663335	-2.11533355	-2.05522575
6	0.58842977	-1.24478493	-2.73911047
1	0.90358712	-1.44760047	-3.78254083
1	-0.49302274	-1.48861632	-2.70773591
6	0.24984253	1.16938868	-3.08080203
6	-1.15933337	1.35485815	-3.08383451
6	-1.72508198	2.40330619	-3.82338515
6	-0.94809468	3.30599806	-4.55231420
6	0.44101175	3.13532509	-4.51954915
6	1.04804897	2.09590298	-3.80719357
6	1.09101137	-1.82304168	4.28415632
1	-0.14313140	-1.15022633	6.57463277
6	-2.36709477	0.26573129	7.30280743
1	-3.38834121	1.11977681	4.91095804
6	-2.80215592	0.78864594	2.29968924
6	-2.07492557	0.49102511	-2.25348580
1	-2.81146480	2.52749737	-3.80669153
6	-1.57460039	4.44733542	-5.31653249
1	1.07689247	3.82754809	-5.07802927
6	2.55022906	1.96131081	-3.84493023
1	1.67332998	-1.76795830	5.21280903
1	1.69390113	-1.39713839	3.46900026
1	0.93706346	-2.89183304	4.06325116
1	-2.18441792	1.49882223	1.72535730
1	-3.69370969	1.33402485	2.63288967
1	-3.13594031	0.00578349	1.60018362
1	-3.10495463	-0.49347620	7.60770924
1	-2.86361354	1.24396593	7.36017774
1	-1.55646647	0.24850802	8.04388970
1	-3.01471762	1.01735398	-2.04093902
1	-1.59595607	0.23637029	-1.29591772
1	-2.33638537	-0.45637834	-2.75168240
1	2.85149014	0.95771743	-4.17498630
1	3.01011965	2.11464226	-2.85671207
1	2.98429833	2.70006272	-4.53148219
1	-1.44265499	5.40272404	-4.78425064
1	-2.65286500	4.29224537	-5.45447602

1 -1.11647911 4.56489619 -6.30918655
 1 -0.88250433 -0.21546347 1.32734984
 Energy = -7200.162763 Hartree
 Number of imaginary frequencies = 0.

Compound 11b isomer 89

Atomic N.	X	Y	Z
8	3.16967791	-2.04623408	1.05224776
6	4.54617254	-2.05724684	0.71080872
1	4.79422988	-2.93461444	0.08241750
1	5.16055684	-2.11824308	1.62558811
1	4.86799497	-1.15294440	0.15552930
50	1.89784039	-0.59785604	0.27835653
7	0.69613023	-2.40228879	-1.01813589
6	1.54065591	-3.61812764	-0.92363516
1	0.98664361	-4.49852800	-1.29405909
1	1.86752751	-3.77268497	0.10923024
1	2.44130304	-3.47895533	-1.53516628
7	0.29135849	-1.17775732	1.55038566
6	-0.55886126	-2.57719572	-0.23437445
1	-1.02980706	-3.54488154	-0.49399777
1	-1.23756695	-1.76109876	-0.50810045
6	-0.29377459	-2.48151476	1.26837089
1	-1.26646051	-2.58251206	1.78262805
1	0.31644083	-3.34749737	1.59298639
6	0.15508018	-0.62468451	2.85051003
6	0.51824669	-1.32856708	4.03029776
6	0.32382178	-0.72514524	5.28027641
6	-0.18999992	0.56782840	5.41731969
6	-0.50202430	1.26712937	4.24610908
6	-0.34621051	0.69977292	2.97657685
7	-0.12200596	0.27174032	-2.32393320
6	0.44359142	-2.15192372	-2.46760350
1	0.06159851	-3.08382327	-2.92747092
1	1.42720887	-1.95415450	-2.92335187
6	-0.52671438	-1.03638143	-2.84947989
1	-0.57339441	-1.04348647	-3.95722124
1	-1.53965034	-1.27933113	-2.50301057
6	-0.75505755	1.43438420	-2.84641249
6	-2.13525866	1.66667621	-2.64852788
6	-2.70713577	2.83867430	-3.16147815
6	-1.95881284	3.80436378	-3.84048542
6	-0.58554078	3.57467678	-3.98746396
6	0.02705499	2.41225764	-3.51043590
6	1.18839078	-2.68008047	3.96873019
1	0.61508143	-1.28041677	6.17638026
6	-0.41258919	1.18248567	6.77843063
1	-0.89584376	2.28451534	4.31961047
6	-0.72238147	1.50167688	1.75567480
6	-2.99437542	0.72207936	-1.84454632
1	-3.77382312	3.00985566	-2.99573118
6	-2.60655551	5.04703632	-4.40167257
1	0.03123762	4.32087510	-4.49453425
6	1.51477399	2.22031361	-3.69442518
1	1.70179373	-2.89068488	4.91633795
1	1.92739643	-2.71254599	3.15362833
1	0.47102072	-3.49929914	3.79985484

1	0.16341384	1.87114228	1.21226170
1	-1.32237873	2.37756628	2.03576078
1	-1.28486727	0.88905300	1.03846859
1	-1.44524970	1.01995588	7.12717384
1	-0.24331663	2.26823022	6.76204497
1	0.25766353	0.74280132	7.52989649
1	-3.87786269	1.24584651	-1.45759058
1	-2.43516887	0.31516102	-0.98971107
1	-3.35934293	-0.12940505	-2.44126992
1	1.74935454	1.29743283	-4.24959182
1	2.05022814	2.16667058	-2.73199529
1	1.94278906	3.05922439	-4.25683535
1	-1.94411220	5.91948255	-4.31555015
1	-3.54580571	5.27767280	-3.88127958
1	-2.84482876	4.92438296	-5.47028031
1	0.89049938	0.36914633	-2.40453515

Energy = -7200.165742 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 90

Atomic N.	X	Y	Z
8	2.76273722	-1.18367626	-2.27622746
6	4.14281218	-1.38843830	-2.02646855
1	4.44400273	-1.13710601	-0.98870206
1	4.75907553	-0.76937745	-2.70428030
1	4.41737597	-2.44587829	-2.19864409
50	1.57831151	-0.26536021	-0.80790138
7	-0.02133176	-1.98560453	-1.63199255
6	0.60275815	-3.32563050	-1.67716481
1	-0.03490772	-4.03523411	-2.23446144
1	0.75924499	-3.70796368	-0.66204732
1	1.57753226	-3.22680213	-2.16896768
7	-0.69584900	-1.32064057	1.31465441
6	-1.34811342	-2.02957112	-0.96606023
1	-1.98666908	-2.76579301	-1.49135130
1	-1.81427687	-1.04345283	-1.10326644
6	-1.34752489	-2.37271206	0.52225561
1	-2.40514923	-2.52239335	0.81813795
1	-0.84088274	-3.32840184	0.70587366
6	-0.67403500	-1.48089831	2.73135165
6	0.14649222	-2.46353542	3.32897281
6	0.15861105	-2.58023134	4.72489790
6	-0.59258526	-1.74028701	5.55278991
6	-1.36328021	-0.74406718	4.94139474
6	-1.42235628	-0.60205301	3.55150320
7	0.23727800	0.76361906	-2.12666489
6	-0.17020801	-1.47245242	-3.02853183
1	-0.90809600	-2.08819371	-3.57692740
1	0.81612383	-1.59081282	-3.49657448
6	-0.57593421	0.00109492	-3.06313838
1	-0.42748674	0.34551629	-4.10540688
1	-1.66511669	0.10021494	-2.87257317
6	0.14133046	2.17836590	-2.19205078
6	-1.04725160	2.86099191	-1.81671842
6	-1.10721836	4.25799416	-1.89817342
6	-0.02140111	5.02473373	-2.33079913
6	1.14928206	4.34604914	-2.68591592

6	1.25276923	2.95091691	-2.62689800
6	1.05499082	-3.34027875	2.50344725
1	0.80199663	-3.33902483	5.17749206
6	-0.57963611	-1.90457967	7.05331561
1	-1.94229664	-0.05712292	5.56362276
6	-2.26353404	0.49709142	2.94417399
6	-2.24098378	2.11295906	-1.27868301
1	-2.03036150	4.76157773	-1.59769599
6	-0.09495309	6.53201364	-2.38134431
1	2.01206329	4.91973064	-3.03561665
6	2.54871926	2.29615750	-3.04341683
1	1.89427094	-3.70224004	3.11114301
1	1.46159685	-2.78094144	1.64836458
1	0.53731970	-4.22992710	2.10859089
1	-1.65007178	1.24432507	2.41369081
1	-2.81687481	1.03275117	3.72531889
1	-3.00161378	0.10837154	2.22470105
1	-1.43446706	-2.51018851	7.39407734
1	-0.64528132	-0.93424983	7.56457632
1	0.33493903	-2.40950070	7.39209168
1	-2.86122217	2.76780408	-0.65241047
1	-1.91138528	1.25431140	-0.67475734
1	-2.88702175	1.71729131	-2.07879238
1	2.38090376	1.33021944	-3.53636835
1	3.19899919	2.09318302	-2.17571130
1	3.11368502	2.95632272	-3.71548564
1	0.35016101	6.98339383	-1.48023108
1	-1.13456126	6.88075534	-2.44404208
1	0.45334111	6.93095472	-3.24646602
1	-1.12478542	-0.42408938	1.08249168

Energy = -7200.167989 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 91

Atomic N.	X	Y	Z
8	2.96615970	-2.40988570	-0.83141353
6	4.23586463	-2.30336855	-1.45410585
1	4.22549786	-2.76018419	-2.46280459
1	4.99455297	-2.83588913	-0.85510430
1	4.58122160	-1.25606169	-1.57046032
50	1.79995507	-0.72209858	-0.50506033
7	0.11962409	-1.61047020	-2.16919326
6	0.77597688	-2.74704679	-2.86041519
1	0.03666765	-3.31174751	-3.45520786
1	1.26763964	-3.39965239	-2.13245414
1	1.55364390	-2.35955531	-3.53094341
7	0.39646022	-1.79357283	0.68613504
6	-0.97589108	-2.10015802	-1.28595844
1	-1.62718080	-2.79598924	-1.84921128
1	-1.56404549	-1.22975682	-0.97295507
6	-0.41988378	-2.76643139	-0.02725961
1	-1.28163174	-3.07027941	0.59396721
1	0.10405989	-3.70262340	-0.30414142
6	0.59854735	-1.95080669	2.08242344
6	1.07292844	-3.15785920	2.66282397
6	1.21699958	-3.24333746	4.05443811
6	0.93916482	-2.16928206	4.90494512

6	0.51460565	-0.97224768	4.31729486
6	0.33539417	-0.84417304	2.93565594
7	-0.51966969	1.38722908	-1.82861227
6	-0.36343537	-0.67156892	-3.22391707
1	-0.96099858	-1.24220932	-3.96086452
1	0.53396456	-0.31314737	-3.75357445
6	-1.20985153	0.52415582	-2.79278508
1	-1.46696269	1.06444642	-3.72624444
1	-2.16304215	0.18172704	-2.36957856
6	-1.06153069	2.67645391	-1.56421756
6	-2.32390506	2.82639416	-0.94504399
6	-2.79926994	4.11629435	-0.67540486
6	-2.06079936	5.26602442	-0.97166121
6	-0.79731864	5.09338097	-1.54844933
6	-0.28763492	3.82748650	-1.85355235
6	1.50818363	-4.32622107	1.81140982
1	1.58917876	-4.17872913	4.48183427
6	1.07889668	-2.29859738	6.40285924
1	0.29908801	-0.11044850	4.95482608
6	-0.14500985	0.46881784	2.36972888
6	-3.14107136	1.63672846	-0.50502289
1	-3.77240067	4.21808387	-0.18811580
6	-2.60718448	6.64332543	-0.68259298
1	-0.18656901	5.97137060	-1.77288253
6	1.08678117	3.70275652	-2.46959719
1	2.15700640	-4.99560487	2.39182638
1	2.06303794	-3.97898761	0.92645751
1	0.65713446	-4.92877838	1.45515041
1	0.66330013	1.02445389	1.86541170
1	-0.53775003	1.11475113	3.16605736
1	-0.92362257	0.31100142	1.61149498
1	0.11316643	-2.54010920	6.87550694
1	1.43597401	-1.36315659	6.85612528
1	1.78228425	-3.09897928	6.67060544
1	-3.84360179	1.92827735	0.28610847
1	-2.49288585	0.84024787	-0.11176899
1	-3.73825856	1.20715371	-1.32540333
1	1.06383503	3.16677303	-3.43245003
1	1.79018207	3.16386429	-1.81326309
1	1.51449075	4.69536739	-2.65680177
1	-1.79960814	7.35573677	-0.46536405
1	-3.28697415	6.62897796	0.18040172
1	-3.17338931	7.03917806	-1.54037664
1	0.45990888	1.47855661	-2.09925459

Energy = -7200.165825 Hartree

Number of imaginary frequencies = 0.

Compound 11b isomer 92

Atomic N.	X	Y	Z
1	3.25598217	0.80995245	-1.36953512
8	4.21949739	0.79024475	-1.60233783
6	4.32451650	0.67714186	-3.01973377
1	3.90548003	-0.27217905	-3.39934477
1	5.39283881	0.70428575	-3.27322993
1	3.82654502	1.51047691	-3.54898073
50	1.67637499	0.43346032	1.35384570
7	0.85192966	2.69320375	1.68925098

6	1.77788324	3.48839371	2.52430843
1	1.35641815	4.48530094	2.73842573
1	2.73486604	3.61013757	2.00195454
1	1.96402853	2.96277426	3.46935562
7	1.46235770	1.16984460	-0.76127282
6	0.71954755	3.28745629	0.32529232
1	0.88752023	4.37746690	0.38040315
1	-0.30884476	3.11851847	-0.01471892
6	1.69633761	2.61037462	-0.64545943
1	1.68564249	3.12744337	-1.61063294
1	2.72294579	2.75283055	-0.25621533
6	0.65862757	0.60045732	-1.77574665
6	-0.15455485	1.28957665	-2.73491579
6	-0.88962167	0.54549574	-3.67527532
6	-0.87412453	-0.84455544	-3.75745190
6	-0.04745378	-1.50716087	-2.84744156
6	0.70383616	-0.82972112	-1.88671365
7	-0.37805989	0.13429363	1.90100091
6	-0.46886484	2.51699341	2.35920144
1	-1.05981186	3.44695576	2.26986664
1	-0.27177874	2.32664540	3.42349431
6	-1.21821509	1.31955921	1.77416753
1	-2.15118276	1.19497171	2.34986497
1	-1.52613885	1.54934325	0.73443821
6	-0.99563330	-1.11756922	2.14827439
6	-2.06296954	-1.60746277	1.34650045
6	-2.64870824	-2.84301473	1.65438063
6	-2.20807256	-3.63960039	2.71451452
6	-1.14617185	-3.15525007	3.48595181
6	-0.53877758	-1.92076462	3.23053021
6	-0.30152033	2.79555077	-2.89055593
1	-1.50747103	1.10270975	-4.38461496
6	-1.71288361	-1.59533719	-4.76186645
1	0.02485627	-2.59732372	-2.88307480
6	1.57455643	-1.66694933	-0.98365599
6	-2.55312656	-0.85925625	0.13014934
1	-3.46572090	-3.20113117	1.02205230
6	-2.82974442	-4.98591199	2.99834852
1	-0.78603623	-3.74869703	4.33069830
6	0.57483851	-1.45879473	4.13768860
1	-1.12378717	2.99958111	-3.58853461
1	0.59545964	3.26676169	-3.32060444
1	-0.54059245	3.32659946	-1.96132357
1	2.59408038	-1.26518425	-0.87811759
1	1.65796140	-2.68966666	-1.37502476
1	1.14326473	-1.78140756	0.03044192
1	-2.60358375	-2.04039601	-4.28989656
1	-1.14824134	-2.41896851	-5.22253515
1	-2.06241014	-0.93239102	-5.56483519
1	-3.11817320	-1.53264267	-0.52707689
1	-1.71631172	-0.44265427	-0.44729028
1	-3.22038251	-0.02241560	0.39011398
1	0.46830530	-0.39435708	4.39227568
1	1.56754827	-1.57050356	3.67098216
1	0.58468032	-2.04668116	5.06513201
1	-2.24816537	-5.80022093	2.53722700
1	-3.85150508	-5.04707311	2.60008172
1	-2.87008642	-5.18955988	4.07779965

Energy = -7200.146634 Hartree
 Number of imaginary frequencies = 0.

Intermediate 2a (I2a)

Compound I2a isomer 1

Atomic N.	X	Y	Z
8	-1.62435130	-1.42755766	2.25691749
8	-0.16746672	0.01005725	-0.68141312
6	-0.94040210	-0.96851797	-1.36949191
1	-1.50812936	-0.55929622	-2.22676334
1	-1.66892648	-1.45998426	-0.69874991
1	-0.27058712	-1.74781981	-1.77603092
8	0.52485012	-1.12890326	2.68596109
6	-0.48568355	-1.84680074	2.12270172
6	-0.16067639	-3.14254855	1.40651872
1	0.51140495	-2.93025143	0.55925470
1	-1.11203400	-3.48954148	0.98792281
6	0.45766255	-4.22987978	2.31095940
1	-0.08222006	-4.26030963	3.27102130
1	0.28364986	-5.20404620	1.83037201
6	1.96155960	-4.06262030	2.55030175
1	2.48275280	-4.13366189	1.57985281
1	2.32774414	-4.90373068	3.15898039
6	2.35450362	-2.74432616	3.22432547
1	1.94889491	-2.69142753	4.24781055
1	3.45140862	-2.70275394	3.32305794
6	1.92013842	-1.49261656	2.46967487
1	2.11048126	-1.56880171	1.38843419
1	2.46258574	-0.61608155	2.84522020
50	-0.73049482	1.99282194	-0.96432178
7	-0.47525758	2.82181740	1.48578055
6	-0.91412686	4.23077915	1.42177737
1	-0.75876686	4.74042892	2.39039522
1	-1.97549669	4.28175223	1.15417904
1	-0.34881484	4.76136303	0.64614200
6	-1.20251650	2.07746754	2.54603186
1	-1.04465539	2.58651338	3.51808375
1	-0.74923401	1.07980020	2.61951811
6	-2.70705618	1.92452218	2.34760077
1	-3.11252635	1.48674571	3.27529816
1	-3.20271564	2.89167621	2.19724283
6	0.98118051	2.73313463	1.77625481
1	1.20257798	1.66758340	1.92589928
1	1.21897536	3.27606722	2.71155243
6	1.84187891	3.25364449	0.62707326
1	1.81469534	4.35545606	0.56417230
1	2.88879175	2.97719526	0.84640499
1	-2.71395701	0.10575362	1.37738902
7	-2.99852154	1.07678475	1.16941659
16	-4.68664238	1.06256329	0.79871650
8	-5.42187324	0.18704217	1.73787038
8	-5.06847124	2.48288291	0.65038414
6	-4.68973950	0.27299439	-0.81795443
6	-4.46455863	1.04811443	-1.95896128
6	-4.50493625	0.43338960	-3.20825083
6	-4.76144245	-0.94358054	-3.33284690

6	-4.98939102	-1.69182090	-2.16824342
6	-4.95894128	-1.09250602	-0.90705630
1	-4.27279273	2.11574467	-1.86208856
1	-4.32784208	1.03146430	-4.10389434
6	-4.79113477	-1.59245984	-4.69351705
1	-5.19991971	-2.75962418	-2.24834547
1	-5.15368206	-1.66647288	-0.00168934
1	-5.53701294	-1.11334114	-5.34428150
1	-3.81720624	-1.49486739	-5.19565585
1	-5.03395769	-2.66008615	-4.62458815
7	1.35422475	2.61756055	-0.58640891
16	2.21037306	2.70994521	-1.97440775
8	1.23220268	2.22427295	-2.99942975
8	2.89402119	4.01095869	-2.16444125
6	3.51640149	1.45596074	-1.84620898
6	4.84164558	1.80793825	-2.09634518
6	5.83239872	0.82397648	-2.02396644
6	5.51303825	-0.50264248	-1.70362837
6	4.16619826	-0.82546609	-1.45498237
6	3.16439604	0.14167781	-1.52073419
1	5.08245768	2.83994895	-2.34968206
1	6.87113631	1.09348772	-2.22470075
6	6.58652292	-1.55877311	-1.60917484
1	3.90072495	-1.85800361	-1.21499145
1	2.11646293	-0.10394523	-1.32078518
1	7.50915471	-1.23750798	-2.10931623
1	6.83754325	-1.77464111	-0.55874554
1	6.25952232	-2.50407174	-2.06437715

Energy = -8524.649205 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 2

Atomic N.	X	Y	Z
8	-1.45946535	-2.49039748	2.72214438
8	1.08024657	-0.40145877	1.40760174
6	2.46163675	-0.39262992	1.74561979
1	2.90876886	0.61741979	1.73510242
1	3.05711668	-1.01223064	1.05044566
1	2.58234184	-0.80307487	2.76425367
8	0.42994290	-3.46479678	3.29918509
6	-0.45236011	-3.07674148	2.34591856
6	-0.18290340	-3.42642887	0.89692884
1	0.78197301	-2.99166428	0.59399453
1	-0.95759135	-2.91356497	0.31613946
6	-0.21454356	-4.94195223	0.60555103
1	-1.07264839	-5.40017359	1.12363216
1	-0.40068720	-5.07165568	-0.47125550
6	1.08020889	-5.67572607	0.97104369
1	1.90083460	-5.26826846	0.35576868
1	0.98591022	-6.73803311	0.69698027
6	1.47603234	-5.56842655	2.44750210
1	0.73091754	-6.06268753	3.09204971
1	2.42685573	-6.10320242	2.60472983
6	1.67104728	-4.13974179	2.94560978
1	2.22858567	-3.52651569	2.22107326
1	2.22640005	-4.13656640	3.89141803
50	0.20741709	0.78557703	-0.04769353

7	-0.56139522	2.27778203	1.83746012
6	-1.48589282	3.30646698	1.31692823
1	-1.81599330	3.99062500	2.11954796
1	-2.36214844	2.83154956	0.85985143
1	-0.97524033	3.89101226	0.54263552
6	-1.15265113	1.49315741	2.95540381
1	-1.24779760	2.14464567	3.84621963
1	-0.43440365	0.69291164	3.18849384
6	-2.52733321	0.88901191	2.68328755
1	-2.86649234	0.40061734	3.61022673
1	-3.25655175	1.67605306	2.44909574
6	0.70572385	2.88728377	2.33004184
1	1.27216805	2.07877572	2.81230229
1	0.48331005	3.65916377	3.09115971
6	1.55314905	3.48203028	1.20299785
1	1.13697508	4.44961509	0.86752177
1	2.55984962	3.68015276	1.60698042
1	-2.21026193	-1.01463287	1.89483851
7	-2.48659923	-0.07037939	1.55600195
16	-4.01230317	-0.19463864	0.77747148
8	-5.05138639	-0.72454360	1.68887657
8	-4.23107934	1.11212801	0.11638314
6	-3.65434382	-1.45263675	-0.46044409
6	-3.01127042	-1.09123073	-1.64696019
6	-2.76151983	-2.07368139	-2.60305624
6	-3.14468074	-3.40959090	-2.38941239
6	-3.79541249	-3.73803605	-1.19026380
6	-4.05411368	-2.76732763	-0.21999323
1	-2.71924707	-0.05548653	-1.81408250
1	-2.25868892	-1.79965643	-3.53215584
6	-2.85161498	-4.46322735	-3.42788964
1	-4.10981404	-4.76806429	-1.01352914
1	-4.56825247	-3.01382261	0.70820873
1	-3.15162656	-4.12868720	-4.43075808
1	-1.77312712	-4.68012079	-3.47137956
1	-3.37463990	-5.40202610	-3.20680378
7	1.59668850	2.51005148	0.11847046
16	2.93291509	2.33076548	-0.80554327
8	4.19039721	2.54162300	-0.04793029
8	2.67839365	1.02572799	-1.49566159
6	2.88671953	3.61876297	-2.07936134
6	1.91005828	3.56226550	-3.07828091
6	1.86554288	4.56415626	-4.04491565
6	2.78448792	5.62902742	-4.03156142
6	3.75205748	5.66087769	-3.01782209
6	3.81168132	4.66164263	-2.04207127
1	1.20174985	2.73355746	-3.10021447
1	1.10539904	4.52073146	-4.82748953
6	2.74126202	6.69287849	-5.10002509
1	4.47548485	6.47803015	-2.99132340
1	4.57190448	4.67539814	-1.26189586
1	3.18095490	6.32257853	-6.03920210
1	1.70849469	6.99387021	-5.32414137
1	3.30447782	7.58580290	-4.79998078

Energy = -8524.652794 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 3

Atomic N.	X	Y	Z
8	0.83960289	-1.16612145	0.15080389
8	2.12044523	-0.35002623	-2.26746974
6	3.15424740	-0.45920574	-3.23703592
1	2.87562187	0.01508488	-4.19559949
1	3.43255660	-1.50968454	-3.46253989
1	4.06171801	0.04377186	-2.85857758
8	2.16853657	0.14040791	1.30214438
6	1.99655402	-0.94692767	0.53530222
6	3.16767626	-1.84823058	0.22498111
1	3.95166950	-1.25328881	-0.26963414
1	2.80335037	-2.57235108	-0.51297921
6	3.74416825	-2.59052671	1.45189091
1	2.92065179	-2.99874112	2.05504543
1	4.31699267	-3.44867311	1.07015801
6	4.66563362	-1.73192560	2.32329028
1	5.54536937	-1.42818674	1.72873771
1	5.04883130	-2.34588343	3.15242356
6	3.99979348	-0.47673509	2.89638432
1	3.16741737	-0.74795527	3.56422696
1	4.73188386	0.07452506	3.50885543
6	3.48226769	0.49375207	1.84227918
1	4.18687093	0.61332293	1.00482206
1	3.29785764	1.48211667	2.27938007
50	0.55713287	-1.74076410	-2.41644681
7	-2.35984017	-2.29197718	-0.98555563
6	-3.01001211	-2.76291457	-2.21469864
1	-4.11420880	-2.65025547	-2.17394093
1	-2.63591402	-2.22071260	-3.09053417
1	-2.78061224	-3.82852872	-2.35048096
7	-1.06166728	-0.18766497	-2.56534127
6	-2.61292127	-0.86900089	-0.72128566
1	-3.66656587	-0.68732549	-0.40861937
1	-1.96773129	-0.55867897	0.11328257
6	-2.35668085	0.05616675	-1.91517059
1	-2.41439357	1.08968537	-1.52852973
1	-3.16683146	-0.05876030	-2.65211160
16	-0.94625100	0.24539456	-4.13738669
7	-1.01690130	-2.80554057	1.78907132
6	-2.83372331	-3.15430055	0.11549027
1	-3.94648085	-3.20345321	0.09817115
1	-2.45902429	-4.17107665	-0.07586044
6	-2.46419660	-2.74346673	1.53799822
1	-2.94492784	-3.46398226	2.21426943
1	-2.88342024	-1.74829117	1.76914864
16	-0.53788287	-2.58859967	3.39388080
8	0.93475876	-2.45205060	3.34782193
8	-1.18873887	-3.64608615	4.18965701
6	-1.22855005	-1.00958076	3.95639024
6	-2.24111520	-1.01275550	4.91617964
6	-2.77405485	0.20473552	5.34688969
6	-2.31272342	1.42296099	4.82751545
6	-1.29772827	1.39357597	3.85486887
6	-0.74961133	0.18889221	3.41690765
1	-2.59383346	-1.96134885	5.31929851
1	0.03996809	0.18307036	2.66442717
1	-0.93100333	2.33130104	3.43273149

6	-2.87320970	2.73608518	5.31300832
1	-3.56448438	0.20593538	6.09967477
8	0.22009540	-0.60835518	-4.60190008
8	-2.21691806	0.15668327	-4.89314768
6	-0.40201427	1.96823315	-4.22753116
6	-1.11494633	2.87130876	-5.01526698
6	-0.68597348	4.19982405	-5.07569740
6	0.44155520	4.62976843	-4.36161694
6	1.13263340	3.69356466	-3.57120962
6	0.72183859	2.36407963	-3.49563413
1	-1.98984992	2.53087400	-5.56771260
1	-1.23884230	4.91344492	-5.68946954
6	0.91932816	6.05761145	-4.45297548
1	2.00912292	4.01422931	-3.00409951
1	1.25680499	1.63213952	-2.88037836
1	-3.84843790	2.60153085	5.79799317
1	-2.19797554	3.19991814	6.04881756
1	-2.99149581	3.45077995	4.48715939
1	1.77971711	6.13798365	-5.13579450
1	0.13244757	6.72122153	-4.83386686
1	1.24677756	6.43415285	-3.47397726
1	-0.45020356	-2.19819856	1.17869774

Energy = -8524.640152 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 4

Atomic N.	X	Y	Z
8	1.75829770	-3.08221377	-1.32587777
8	2.43586322	-2.58027249	2.10677262
6	1.65800392	-2.98960185	3.22721599
1	1.62700606	-2.22702112	4.02250562
1	2.10645156	-3.90329713	3.65433995
1	0.61629093	-3.22239545	2.94058925
8	1.16696215	-4.87392713	-0.17399050
6	2.12613946	-4.05881099	-0.68927315
6	3.58754802	-4.40360233	-0.48039563
1	3.80097741	-4.37760742	0.60086533
1	4.14492943	-3.57656989	-0.93597182
6	4.02928697	-5.74740629	-1.09613867
1	3.60374939	-5.84695635	-2.10808063
1	5.12147648	-5.71327562	-1.22531664
6	3.67542717	-6.97486770	-0.25032778
1	4.19619719	-6.89665972	0.71959829
1	4.06919975	-7.87899390	-0.74041168
6	2.17652685	-7.15363200	0.01087610
1	1.63399510	-7.34642408	-0.92911672
1	2.02451581	-8.04200255	0.64553793
6	1.51641743	-5.97266024	0.71529969
1	2.13620005	-5.58775406	1.53948763
1	0.54516238	-6.26922735	1.13025758
50	2.32347679	-0.76747930	1.15939289
7	-1.63972182	-0.53990551	-1.20574863
6	-3.09951994	-0.42941047	-1.20784147
1	-3.45659966	-0.11877868	-0.21614370
1	-3.41491829	0.33221414	-1.93381609
1	-3.59983445	-1.38932097	-1.46340551
7	0.30774824	0.87928497	-3.44272504

6	-1.15183481	-0.95072761	-2.53520834
1	-1.19477489	-2.05479519	-2.64620533
1	-1.82136920	-0.52503227	-3.29608210
6	0.27456900	-0.47261278	-2.83670611
1	0.74641394	-1.16141913	-3.55092367
1	0.89342246	-0.49280310	-1.93051961
16	0.95726072	2.20767365	-2.59748411
7	0.11281880	-0.33291410	1.56754655
6	-1.20328145	-1.50412689	-0.17985356
1	-1.86238010	-2.39959325	-0.20262164
1	-0.19978644	-1.87153877	-0.43889101
6	-1.18326229	-0.95624755	1.25336694
1	-1.38507067	-1.78667644	1.95018608
1	-1.99932422	-0.22414033	1.37976780
16	0.28006511	0.41861432	2.99338901
8	1.81628526	0.47464527	3.08155809
8	-0.44696694	-0.16787674	4.14075573
6	-0.25232690	2.14035409	2.86770990
6	-1.14056599	2.64789252	3.81635875
6	-1.53052560	3.98652479	3.72946902
6	-1.04015653	4.81924458	2.71316420
6	-0.15314289	4.27420246	1.76807317
6	0.24254929	2.94043619	1.83371211
1	-1.50961219	1.99810901	4.60865507
1	0.91126429	2.52817200	1.07697475
1	0.22763777	4.90209695	0.96064025
6	-1.43690247	6.27238023	2.64089614
1	-2.22591457	4.38982120	4.46793774
8	1.41382662	1.75447566	-1.26519078
8	1.87357211	2.88601511	-3.54099342
6	-0.45899998	3.30253269	-2.35572699
6	-0.49674935	4.51722496	-3.04005503
6	-1.58304033	5.37250864	-2.83990268
6	-2.62691458	5.02763881	-1.96860298
6	-2.55821185	3.79458517	-1.29701609
6	-1.47981185	2.93003074	-1.47769133
1	0.31643750	4.78008789	-3.71533927
1	-1.61911606	6.32414715	-3.37341869
6	-3.78459372	5.96651739	-1.73643290
1	-3.36254330	3.50917467	-0.61604037
1	-1.43083480	1.96861618	-0.96245645
1	-2.34702277	6.47058306	3.22152760
1	-0.63830271	6.91441819	3.04414448
1	-1.60852635	6.58810059	1.60246921
1	-3.62611536	6.56604325	-0.82609889
1	-3.90830703	6.66637678	-2.57299851
1	-4.72566664	5.41649813	-1.60160109
1	0.74857667	0.90333707	-4.36239910

Energy = -8524.630090 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 5

Atomic N.	X	Y	Z
8	3.07372645	-2.74699434	-0.98412147
8	3.74772591	-1.13025940	-3.64495793
6	4.18631849	0.22503281	-3.62743511
1	3.56966177	0.87747249	-4.26755739

1	5.22166333	0.26243493	-4.00748004
1	4.18019213	0.64991992	-2.60684560
8	4.98404200	-1.75695019	-0.49404696
6	4.28965757	-2.72267953	-1.14342747
6	5.02968578	-3.72990892	-1.99811042
1	5.52439893	-3.19160800	-2.82290928
1	4.25001241	-4.35515480	-2.44872984
6	6.04038356	-4.60741719	-1.23037475
1	5.58784852	-4.94981499	-0.28561801
1	6.21878405	-5.51248274	-1.82993141
6	7.38606378	-3.92790441	-0.95787323
1	7.86197606	-3.68620674	-1.92388138
1	8.05637160	-4.64110664	-0.45357679
6	7.29146666	-2.64732049	-0.12258957
1	6.92344770	-2.86650933	0.89299346
1	8.30000044	-2.21945549	-0.00177740
6	6.40957683	-1.56267344	-0.73108066
1	6.58270770	-1.44934565	-1.81222040
1	6.60462494	-0.59549849	-0.25221396
50	1.80965169	-1.73624112	-3.37197212
7	-0.40343878	1.16279232	0.48335568
6	0.01876796	2.51458178	0.84424679
1	0.78555299	2.87349770	0.14534469
1	-0.83888126	3.19736330	0.77674361
1	0.43508924	2.57368447	1.87475090
7	-3.34412843	-0.98012016	1.51852092
6	-1.50486592	0.70035764	1.33420285
1	-1.14216755	0.26966389	2.29204516
1	-2.12404801	1.57235533	1.58975641
6	-2.37796086	-0.32733115	0.60483524
1	-1.75106517	-1.13700983	0.20574514
1	-2.88367469	0.15139731	-0.24521885
16	-4.85475118	-0.22054450	1.77550903
7	1.14045690	-0.09412541	-1.96830040
6	0.72371595	0.22535953	0.50238446
1	1.31485097	0.33604935	1.44181183
1	0.33250096	-0.80177214	0.49437637
6	1.68258954	0.36657859	-0.68235019
1	2.56103991	-0.26145199	-0.47022740
1	2.04833417	1.40142835	-0.77758408
16	0.58299880	0.98078747	-3.05909257
8	0.82327315	0.18725684	-4.35350460
8	1.15231322	2.34175816	-2.94867512
6	-1.21460616	1.15161823	-2.98641773
6	-1.77037732	2.37748336	-2.62118729
6	-3.15889627	2.50342527	-2.56667827
6	-4.00191455	1.42206693	-2.86783921
6	-3.41117930	0.20514054	-3.24915281
6	-2.02572068	0.06204295	-3.30901587
1	-1.11545284	3.21759411	-2.39513759
1	-1.58035802	-0.88395520	-3.61819886
1	-4.04848077	-0.64397733	-3.50227458
6	-5.49801147	1.55325013	-2.75246831
1	-3.59782833	3.46072979	-2.28006593
8	-5.10398848	0.81055409	0.74227580
8	-5.79758237	-1.33879930	1.99161539
6	-4.63300430	0.64245768	3.34451474
6	-4.46932785	-0.10147393	4.51680290

6	-4.33657191	0.56956135	5.72910460
6	-4.37086811	1.97497181	5.79081830
6	-4.54370228	2.69181162	4.59889463
6	-4.67719308	2.03465622	3.37254945
1	-4.45283872	-1.18995751	4.47471905
1	-4.20661327	-0.00565946	6.64767842
6	-4.23696743	2.68425655	7.11473222
1	-4.57728477	3.78225998	4.62768434
1	-4.81703398	2.58767099	2.44457772
1	-5.83271659	2.56699559	-3.01020821
1	-6.01611028	0.83804110	-3.40450222
1	-5.81422586	1.35258327	-1.71693439
1	-5.09564553	2.46451555	7.76688023
1	-3.33439933	2.35734847	7.65088582
1	-4.18281416	3.77209254	6.98333320
1	-3.58477618	-1.93119049	1.23007631

Energy = -8524.635549 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 6

Atomic N.	X	Y	Z
8	3.49508964	-2.39651688	-0.43605072
8	2.58850392	-2.32168871	2.65397249
6	1.40729590	-2.72760880	3.33835907
1	0.55027245	-2.84553246	2.65040265
1	1.11060013	-2.01659072	4.12675799
1	1.59813511	-3.70282864	3.81843798
8	2.17805689	-4.14730411	-0.15340827
6	3.37852012	-3.53439224	0.00310994
6	4.51442566	-4.27492064	0.67681562
1	4.21623329	-4.50247818	1.71330285
1	5.33622178	-3.55188641	0.73320098
6	4.97437285	-5.55364586	-0.05368816
1	5.04603787	-5.35364389	-1.13513280
1	5.99650350	-5.78175501	0.28346638
6	4.09045006	-6.77869887	0.20107178
1	4.11985829	-7.01777264	1.27818417
1	4.51892507	-7.64915158	-0.31954788
6	2.62882306	-6.60583230	-0.22384637
1	2.54945683	-6.47564609	-1.31547380
1	2.07088564	-7.52436874	0.02082540
6	1.90942475	-5.44437377	0.45358802
1	2.13417830	-5.39340158	1.52997863
1	0.82345755	-5.54651691	0.33821769
50	2.88331268	-0.47920485	1.81703399
7	0.61749448	0.27452743	-1.93672653
6	1.83695859	0.06062440	-2.72460549
1	1.73624973	-0.77826292	-3.44665188
1	2.09318336	0.96731489	-3.28788760
1	2.67202388	-0.16728156	-2.05161545
7	-0.41125982	3.03033914	-2.66430610
6	-0.54310590	0.52342560	-2.80231058
1	-0.65843426	-0.29140329	-3.55444567
1	-1.44581625	0.51084514	-2.17309935
6	-0.47831896	1.85527354	-3.55088774
1	-1.35784935	1.95676216	-4.20155545
1	0.39553153	1.88295936	-4.21894817

16	-1.77830891	4.01670838	-2.52450125
7	0.71739665	-0.01730571	1.22830916
6	0.35045527	-0.88030927	-1.05737480
1	-0.30352241	-1.61680198	-1.56889393
1	1.29711010	-1.40349767	-0.86096046
6	-0.29639834	-0.51118793	0.28136664
1	-0.79664802	-1.40570952	0.68963606
1	-1.07688031	0.25169701	0.11588243
16	0.23557065	0.68342571	2.60513842
8	1.55585085	0.65429540	3.39454322
8	-0.96025957	0.11768119	3.26744961
6	-0.11235894	2.43082519	2.31102644
6	-1.15697001	3.04509408	3.00129553
6	-1.40546797	4.40326651	2.78352211
6	-0.63219598	5.14969935	1.88222598
6	0.41785971	4.50161126	1.20562776
6	0.68351187	3.15102398	1.41433937
1	-1.76424565	2.46062158	3.69142389
1	1.48829988	2.64951718	0.87543706
1	1.01499234	5.06240865	0.48556086
6	-0.92949490	6.59959688	1.60733191
1	-2.22463330	4.88885364	3.31673139
8	-1.39099726	5.07454900	-1.57148338
8	-2.21319862	4.31747111	-3.90136376
6	-3.09292400	3.03733790	-1.75754188
6	-4.10231228	2.49468770	-2.55391467
6	-5.08962965	1.70736901	-1.95523122
6	-5.08122024	1.45574954	-0.57555082
6	-4.05401178	2.02068767	0.20168185
6	-3.06368067	2.81121911	-0.37757589
1	-4.11646701	2.70450792	-3.62283969
1	-5.88275970	1.28305577	-2.57363588
6	-6.15691658	0.61935451	0.07027144
1	-4.02726121	1.83583696	1.27739399
1	-2.27761565	3.25189214	0.23566688
1	-1.71313304	6.98320741	2.27237243
1	-0.03089092	7.21994028	1.73633246
1	-1.26264942	6.72341598	0.56621174
1	-6.85822072	1.25258671	0.63514413
1	-6.73712396	0.06409030	-0.67748447
1	-5.72836501	-0.09966703	0.78222769
1	-0.01998366	2.81183006	-1.74233592

Energy = -8524.636828 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 7

Atomic N.	X	Y	Z
8	0.88415974	-1.14492158	-0.03827853
8	1.97048987	-0.03054679	-2.42825753
6	2.93131765	0.00605547	-3.47541352
1	3.21809088	-1.00204453	-3.84050930
1	3.85170832	0.49261649	-3.10682738
1	2.56990888	0.57671729	-4.35009869
8	2.25225717	0.07923182	1.15667584
6	2.05849888	-0.92646641	0.29041064
6	3.23017455	-1.74805625	-0.19154721
1	3.96115211	-1.07686037	-0.66945706

1	2.83627642	-2.40243712	-0.97785960
6	3.91067072	-2.59508104	0.90760946
1	3.14261338	-3.09378197	1.51586259
1	4.47990857	-3.38705340	0.39867726
6	4.86533128	-1.80132407	1.80439705
1	5.69327388	-1.40569098	1.18984344
1	5.32168812	-2.48554512	2.53572012
6	4.20550039	-0.63798091	2.55175430
1	3.42887800	-1.00741110	3.23933160
1	4.96221419	-0.12905313	3.17089522
6	3.58974277	0.41960981	1.64446757
1	4.23122242	0.65154673	0.78029851
1	3.40824069	1.34916607	2.19663409
50	0.43948262	-1.45138154	-2.62507337
7	-2.34804834	-2.26729644	-1.07368330
6	-3.06627382	-2.62800152	-2.30223399
1	-4.16805461	-2.56534794	-2.17680526
1	-2.77229858	-1.97904173	-3.13499364
1	-2.81169149	-3.66235204	-2.57037596
7	-1.23250483	0.04647860	-2.49022960
6	-2.62997889	-0.89320332	-0.63666774
1	-3.66541398	-0.78985526	-0.23899664
1	-1.94024782	-0.64985191	0.18435495
6	-2.48665574	0.16637961	-1.73386011
1	-2.55073660	1.14833350	-1.23120220
1	-3.34168634	0.10068726	-2.42467386
16	-1.23933840	0.65640335	-4.00691569
7	-0.80030699	-3.01720104	1.53406929
6	-2.71428673	-3.26336619	-0.04681349
1	-3.82312478	-3.35788207	0.00225849
1	-2.31795503	-4.23647803	-0.37367840
6	-2.26279276	-2.99342575	1.38571851
1	-2.66823058	-3.80386225	2.00730825
1	-2.70203856	-2.04895547	1.75264581
16	-0.21951273	-2.94656323	3.11814424
8	1.24095128	-2.74584275	2.99096035
8	-0.77762292	-4.10568800	3.83926759
6	-0.92240867	-1.46249964	3.88647027
6	-1.86424821	-1.60389223	4.90602013
6	-2.40642160	-0.45900323	5.49519732
6	-2.02445488	0.82331790	5.07524084
6	-1.08024349	0.93388764	4.03920180
6	-0.52379390	-0.19693596	3.44334154
1	-2.15550614	-2.60198694	5.23121804
1	0.20966877	-0.09446272	2.64254560
1	-0.77643537	1.92365274	3.69268261
6	-2.59376544	2.05665353	5.73013691
1	-3.14150953	-0.56627978	6.29494516
8	-0.08361098	-0.09624731	-4.64137511
8	-2.55645577	0.60605718	-4.68248179
6	-0.75300279	2.39737793	-3.93572019
6	-1.54638320	3.35634103	-4.56404960
6	-1.16055666	4.69813261	-4.50154859
6	0.00275451	5.08607643	-3.82202566
6	0.77585324	4.09278401	-3.19349553
6	0.40952330	2.74932823	-3.24250512
1	-2.44863404	3.04835116	-5.09095539
1	-1.77604550	5.45540610	-4.99074019

6	0.43082742	6.53187173	-3.77846232
1	1.68218331	4.37931634	-2.65573035
1	1.00842947	1.97295589	-2.75357988
1	-3.52721674	1.83391503	6.26253188
1	-1.88457243	2.47145910	6.46326559
1	-2.79434836	2.84538338	4.99225159
1	1.27946622	6.70901831	-4.45730152
1	-0.38374344	7.20145051	-4.08277290
1	0.75915044	6.82190805	-2.77051216
1	-0.29945181	-2.32671182	0.95535390

Energy = -8524.640149 Hartree
Number of imaginary frequencies = 0.

Compound I2a isomer 8

Atomic N.	X	Y	Z
8	1.25906533	-3.11739098	-1.26695833
8	1.78615870	-0.92477798	2.25782128
6	2.05441067	-0.59118134	3.61716432
1	2.84551719	0.17376021	3.69706179
1	2.39784243	-1.49785261	4.14587233
1	1.16794746	-0.20324766	4.14985828
8	2.21934026	-4.06470033	0.48737902
6	2.22142998	-3.14280695	-0.51649719
6	3.41269336	-2.21363561	-0.65942055
1	3.49245837	-1.59996605	0.25435978
1	3.15461402	-1.53810785	-1.48341419
6	4.75338673	-2.92303838	-0.94386213
1	4.60024922	-3.71681210	-1.69318954
1	5.42907787	-2.18887420	-1.40797874
6	5.43602033	-3.49457982	0.30306338
1	5.66484541	-2.66283040	0.99101952
1	6.40358249	-3.93584843	0.01688304
6	4.60630352	-4.53952972	1.05566600
1	4.45559255	-5.43982521	0.43750767
1	5.16393461	-4.86574317	1.94888851
6	3.24317139	-4.04280812	1.52629603
1	3.28592546	-3.03172353	1.96025885
1	2.83361214	-4.72296847	2.28376854
50	0.60381330	0.19119359	0.98575506
7	-1.36432995	-1.45103231	1.47833532
6	-0.92219905	-2.86131465	1.45509613
1	-1.74135542	-3.53859139	1.76054975
1	-0.57004296	-3.14162837	0.45597644
1	-0.07777770	-2.97229054	2.14563882
7	-3.23824251	-1.02231828	-1.78641087
6	-2.48832891	-1.20993200	0.54425120
1	-3.37050146	-1.80522741	0.85155498
1	-2.76452614	-0.14938752	0.60362303
6	-2.15231198	-1.52296459	-0.92026395
1	-2.06906211	-2.60334162	-1.09170467
1	-1.17535212	-1.08762966	-1.18843365
16	-3.05507664	0.51130986	-2.50572471
7	-0.76664116	1.06744878	2.45246178
6	-1.75437186	-1.08532149	2.86713822
1	-2.68172852	-1.61592869	3.15707196
1	-0.94100299	-1.43293907	3.51884615
6	-1.92378424	0.42387905	3.05765526

1	-1.97717974	0.62705051	4.14016670
1	-2.86803744	0.77783899	2.60683329
16	-0.14091489	2.47002426	2.99783744
8	1.13778700	2.53633404	2.20033482
8	-0.07617651	2.57338406	4.47397056
6	-1.21609193	3.81148344	2.43406475
6	-1.49858265	4.86722080	3.30126327
6	-2.31695217	5.90869370	2.85749758
6	-2.86054092	5.90500823	1.56451985
6	-2.56790897	4.82137823	0.71808676
6	-1.74830965	3.77724170	1.14182069
1	-1.08610087	4.85980363	4.30935524
1	-1.54688899	2.93769594	0.47595237
1	-2.99478624	4.78529126	-0.28575027
6	-3.73212037	7.03818462	1.08379216
1	-2.54181942	6.73640703	3.53273929
8	-4.28994665	0.71349136	-3.28302645
8	-2.64445657	1.41707848	-1.41344735
6	-1.67985853	0.39235001	-3.66821443
6	-0.38706218	0.72242083	-3.25583857
6	0.66423275	0.59912607	-4.16567460
6	0.44306673	0.15416385	-5.47761214
6	-0.87164960	-0.15427238	-5.86774860
6	-1.93440363	-0.04074097	-4.97355944
1	-0.20860017	1.08346550	-2.24289010
1	1.67552479	0.85824646	-3.84786431
6	1.58935591	-0.00618863	-6.44337816
1	-1.06615852	-0.48000629	-6.89114232
1	-2.95644800	-0.25573027	-5.28498312
1	-4.06703151	7.66871985	1.91725167
1	-3.18357261	7.68054402	0.37763705
1	-4.61876670	6.66253189	0.55436990
1	1.27410544	0.18870587	-7.47694667
1	2.41836163	0.67021079	-6.19846442
1	1.98231053	-1.03436500	-6.40935552
1	-3.53873642	-1.68228689	-2.50456084

Energy = -8524.648506 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 9

Atomic N.	X	Y	Z
8	1.62499053	-4.87669429	-1.60735347
8	1.87396176	-2.22189948	1.20203137
6	1.84344728	-3.12466507	2.30645919
1	2.73335213	-2.99138024	2.94531970
1	1.84122193	-4.15813352	1.92202079
1	0.95661664	-2.99273489	2.95074145
8	3.45435771	-4.89343506	-0.35981145
6	2.66908237	-4.32013844	-1.31860318
6	3.14915749	-3.04844701	-1.99719362
1	3.25490865	-2.25536696	-1.23939740
1	2.33604455	-2.75308275	-2.67034144
6	4.46189092	-3.20432041	-2.79291794
1	4.43497616	-4.14593524	-3.36536135
1	4.50199842	-2.39380606	-3.53593733
6	5.72809138	-3.14247389	-1.93252726
1	5.77721308	-2.15068787	-1.45069790

1	6.61337562	-3.21364054	-2.58399837
6	5.81045171	-4.22006944	-0.84664060
1	5.88220143	-5.22420011	-1.29599324
1	6.73381510	-4.07286626	-0.26250537
6	4.64258903	-4.21581427	0.13571656
1	4.37219975	-3.19755647	0.45643949
1	4.89978316	-4.79553149	1.03138007
50	1.02166984	-0.36331966	1.11745542
7	-1.08205945	-1.44122082	0.00893817
6	-0.73679280	-2.33761026	-1.11516617
1	-1.63410308	-2.84211673	-1.51776344
1	-0.25118270	-1.77201694	-1.91800447
1	-0.03434878	-3.10012432	-0.76068236
7	-0.50425113	0.93188603	-1.75818281
6	-2.07817403	-0.41019665	-0.36795069
1	-3.08320553	-0.87169942	-0.44592482
1	-2.12492569	0.32532608	0.45016045
6	-1.83217995	0.31075251	-1.69646154
1	-2.65040011	1.04297759	-1.82299457
1	-1.89234389	-0.39749530	-2.53235476
16	0.09450258	1.39840302	-3.28306133
7	-0.59102535	-0.63243889	2.61518538
6	-1.60004553	-2.25858715	1.13990942
1	-2.55370758	-2.74416346	0.85530234
1	-0.85549037	-3.04560410	1.31813869
6	-1.78715579	-1.44511099	2.42253846
1	-1.93019584	-2.15376162	3.25499220
1	-2.69631425	-0.81896075	2.36240962
16	-0.01675523	-0.30779714	4.11209215
8	1.38244259	0.14866310	3.81311141
8	-0.25737331	-1.40418763	5.07865311
6	-0.91183002	1.13457032	4.74256570
6	-1.90213599	0.96116761	5.70973198
6	-2.60650984	2.07653081	6.17064569
6	-2.32922563	3.36241111	5.68501249
6	-1.32240597	3.50696094	4.71398420
6	-0.61398978	2.40459916	4.24010384
1	-2.10051545	-0.03517134	6.10322488
1	0.17893790	2.52343678	3.50143808
1	-1.08568623	4.50139972	4.33025879
6	-3.06537753	4.56791049	6.21401413
1	-3.38046512	1.94414779	6.92903484
8	1.39317307	2.03025815	-2.99629780
8	-0.04407295	0.20795293	-4.14269665
6	-1.01585410	2.67109285	-3.92466182
6	-2.08038540	2.30826979	-4.75212022
6	-2.94029981	3.30206746	-5.22455316
6	-2.74902433	4.65016910	-4.88567765
6	-1.66562964	4.98447003	-4.05421623
6	-0.79717703	4.00674253	-3.57252659
1	-2.21439079	1.26532009	-5.03689381
1	-3.77088135	3.02470695	-5.87592803
6	-3.66060406	5.72265624	-5.42565653
1	-1.49477791	6.02933733	-3.78864311
1	0.05777305	4.27102363	-2.95031711
1	-4.01529892	4.28345437	6.68456740
1	-2.46324880	5.09053390	6.97357380
1	-3.27696000	5.29202515	5.41533606

1	-3.19231941	6.23687004	-6.27920861
1	-4.61282777	5.30307318	-5.77384792
1	-3.87391691	6.48679869	-4.66594366
1	-0.34638470	1.68649747	-1.08547153

Energy = -8524.642525 Hartree
Number of imaginary frequencies = 0.

Compound I2a isomer 10

Atomic N.	X	Y	Z
8	-0.38295160	-0.95151655	-1.29337711
8	1.23136025	0.41736124	1.61291282
6	2.34766599	-0.42855528	1.89527801
1	2.32444198	-0.86336234	2.91244731
1	3.28590535	0.14987403	1.80961192
1	2.38661317	-1.27570755	1.19109423
8	1.80674936	-0.98335915	-1.56586435
6	0.63011968	-0.30777710	-1.53525203
6	0.61322652	1.17575204	-1.83194670
1	1.22291497	1.69361365	-1.07508388
1	-0.42390865	1.49305291	-1.67552372
6	1.07760803	1.55176789	-3.25465403
1	0.62113678	0.86487218	-3.98593688
1	0.67753350	2.55104016	-3.48193932
6	2.59877835	1.58220087	-3.43478640
1	3.01605683	2.35552634	-2.76712463
1	2.83583099	1.90026310	-4.46195052
6	3.30074009	0.25214345	-3.14247963
1	2.99190721	-0.52268536	-3.86307349
1	4.38760323	0.38128898	-3.27260006
6	3.07303029	-0.28132864	-1.73225805
1	3.14652758	0.51338951	-0.97454058
1	3.81292763	-1.05282755	-1.48698972
50	-0.20368926	0.56123646	3.10462923
7	-2.81014889	0.08950870	2.26582703
6	-3.46092767	-0.64398415	3.36448008
1	-4.54315936	-0.78731531	3.17786446
1	-2.98746297	-1.62279844	3.50579331
1	-3.33757363	-0.07593425	4.29512912
7	-1.09467161	-2.13634835	1.28118397
6	-2.99856494	-0.59026537	0.96859313
1	-4.07513294	-0.58882186	0.69381435
1	-2.46195411	-0.02047744	0.19788496
6	-2.52057283	-2.04172610	0.92721542
1	-2.71549541	-2.42421699	-0.08880289
1	-3.08671375	-2.66032611	1.63454698
16	-0.55360008	-3.65598348	1.82038580
7	-1.03026441	2.31793547	1.99666796
6	-3.31931544	1.47823001	2.19728811
1	-4.33498213	1.50408822	1.75140801
1	-3.39483269	1.85254560	3.22813129
6	-2.37496239	2.40815519	1.43267185
1	-2.77042359	3.43237377	1.52163523
1	-2.35468045	2.15488938	0.35863809
16	-0.36191927	3.64014946	2.69075521
8	0.60435914	3.03338613	3.67278649
8	-1.35848923	4.63627232	3.15237605
6	0.65968011	4.47423348	1.44856363

6	0.34510327	5.77265559	1.05047648
6	1.15311539	6.40763697	0.10279574
6	2.27353310	5.76449291	-0.44152351
6	2.56200796	4.45332891	-0.02094789
6	1.76405471	3.80097969	0.91729616
1	-0.51522059	6.27525890	1.49108558
1	1.97629541	2.77752878	1.23705458
1	3.43408404	3.94014232	-0.43294007
6	3.16834164	6.46893474	-1.43095283
1	0.91130003	7.42470186	-0.21173539
8	0.89864094	-3.50287068	2.01613549
8	-1.45632305	-4.04821740	2.92221306
6	-0.81630532	-4.81948306	0.46076561
6	-1.84109097	-5.76215174	0.54889941
6	-2.03480038	-6.65406769	-0.50847400
6	-1.22097695	-6.61308251	-1.65011517
6	-0.20090197	-5.64761116	-1.71172794
6	0.01011865	-4.75197995	-0.66537182
1	-2.46266283	-5.79792126	1.44288379
1	-2.83194088	-7.39691223	-0.44306574
6	-1.41507274	-7.59784699	-2.77573870
1	0.43947870	-5.59838732	-2.59430387
1	0.80664451	-4.00986138	-0.72013643
1	2.64773081	7.30230096	-1.92020036
1	4.05636919	6.88363769	-0.92882000
1	3.52857064	5.78127751	-2.20864720
1	-0.70970274	-8.43848124	-2.68388497
1	-2.42946928	-8.01696987	-2.77196325
1	-1.23587801	-7.12988908	-3.75313675
1	-0.50136303	-1.81697645	0.49864997

Energy = -8524.650404 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 11

Atomic N.	X	Y	Z
8	-0.35673969	-1.30359574	-0.95170019
8	1.35355793	1.02193569	1.17356265
6	2.68365008	0.51896559	1.31230470
1	2.97741111	0.33425872	2.36280573
1	3.40411776	1.24648025	0.89523984
1	2.79867339	-0.43906339	0.77922552
8	1.65798770	-0.90396615	-1.75846033
6	0.37067844	-0.52475894	-1.55406675
6	-0.11242532	0.80110803	-2.10022836
1	0.46841348	1.60990301	-1.62987063
1	-1.14443066	0.90388665	-1.74635281
6	-0.06162130	0.91923080	-3.63797074
1	-0.44764888	-0.00771799	-4.09267678
1	-0.75773205	1.71820119	-3.93346741
6	1.32516094	1.24750395	-4.20047239
1	1.63712036	2.23248805	-3.81269391
1	1.25661607	1.35377521	-5.29429698
6	2.40980031	0.22069585	-3.85924139
1	2.18967618	-0.75388050	-4.32480359
1	3.37067681	0.55651783	-4.28211307
6	2.62251613	0.00465443	-2.36479619
1	2.62339894	0.95365275	-1.80748676

1	3.57972642	-0.49775248	-2.17989627
50	0.26156309	1.21597216	2.92740516
7	-2.23674109	0.01823905	2.84846849
6	-2.44778610	-0.57119936	4.18156339
1	-3.46987084	-0.98338748	4.29052970
1	-1.71715730	-1.36691138	4.36929311
1	-2.29953849	0.20522314	4.94259766
7	-0.22964666	-1.95843868	1.89878247
6	-2.48901951	-0.96150702	1.77257038
1	-3.56183364	-1.25043068	1.76913211
1	-2.27559731	-0.48066115	0.80829577
6	-1.67235256	-2.25012260	1.87106484
1	-1.94531125	-2.88031434	1.00808010
1	-1.92285790	-2.80250223	2.78512106
16	0.76899173	-3.16803836	2.55701353
7	-1.19175948	2.45149836	1.76385712
6	-3.09495323	1.21167869	2.66881432
1	-4.14926903	0.91544468	2.49114214
1	-3.05995037	1.78573163	3.60570483
6	-2.59831935	2.12366217	1.54512763
1	-3.21978326	3.03313019	1.55411390
1	-2.72981803	1.64425937	0.55963138
16	-0.75904750	4.00995837	2.00942591
8	0.50646955	3.86905089	2.81201152
8	-1.86454490	4.86009277	2.51304659
6	-0.25447188	4.71426854	0.41809515
6	-0.96317121	5.78664917	-0.12128278
6	-0.54933894	6.33045512	-1.34089116
6	0.56707143	5.82201479	-2.01918442
6	1.25892071	4.73745332	-1.44949043
6	0.85708708	4.17686378	-0.23840708
1	-1.81780340	6.19128678	0.41980277
1	1.38331316	3.32558333	0.20107045
1	2.13370053	4.33280461	-1.96398451
6	1.03766340	6.43950038	-3.31267997
1	-1.10049343	7.17102037	-1.76689631
8	2.14400377	-2.66249499	2.40095942
8	0.19937029	-3.49710279	3.88006791
6	0.58503432	-4.62978305	1.50791233
6	-0.12652393	-5.73186771	1.98243141
6	-0.26407341	-6.85458982	1.16258192
6	0.29674376	-6.88716438	-0.12237289
6	1.00331868	-5.75853607	-0.57418641
6	1.15427622	-4.63120716	0.23036446
1	-0.55016344	-5.70630338	2.98576061
1	-0.81584584	-7.72149415	1.53062073
6	0.16902739	-8.11125479	-0.99386437
1	1.44338833	-5.76452958	-1.57307211
1	1.70730665	-3.76263285	-0.12720509
1	0.24167122	7.02469765	-3.79093597
1	1.88648413	7.11837770	-3.13582381
1	1.37924941	5.67407279	-4.02340069
1	1.09563897	-8.70562701	-0.96984482
1	-0.64934953	-8.76021962	-0.65688968
1	-0.01308250	-7.83878433	-2.04245513
1	0.11059733	-1.70440768	0.95786343

Energy = -8524.650398 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 12

Atomic N.	X	Y	Z
8	3.09620915	0.22137505	1.05930577
8	3.97306618	-0.87379615	-1.79850762
6	4.21676358	-2.27388733	-1.87330049
1	3.62047530	-2.75807220	-2.66436235
1	3.99503295	-2.78968734	-0.92061972
1	5.28333789	-2.43113880	-2.10644841
8	4.21061683	0.98042757	2.79131575
6	4.17287317	0.63745098	1.48190420
6	5.42171506	0.74480947	0.63731391
1	5.78955624	1.78446521	0.65109796
1	5.11560752	0.49266693	-0.38682466
6	6.54789026	-0.21743671	1.07789583
1	6.11685852	-1.21130491	1.27832616
1	7.22152073	-0.34732753	0.21839675
6	7.36450894	0.26431596	2.28058915
1	7.87269924	1.20608995	2.00988460
1	8.16174689	-0.46475763	2.49267340
6	6.54388373	0.49889028	3.55283808
1	6.10745383	-0.44415099	3.92043733
1	7.20989514	0.86400724	4.35145656
6	5.42215689	1.51965332	3.39905077
1	5.75134106	2.40517715	2.83320022
1	5.06840280	1.85619445	4.38107823
50	2.16332357	0.01312609	-1.45945845
7	-0.34416039	-0.78106043	2.18757957
6	0.55361311	-0.59568628	3.32825751
1	0.30567469	-1.27358722	4.17418966
1	1.59218453	-0.77493423	3.02654774
1	0.49025945	0.44181923	3.68029490
7	0.99890955	-1.68998690	-0.51765528
6	-0.24456765	-2.14005157	1.64031845
1	-0.25021911	-2.89212466	2.46255107
1	-1.13501827	-2.33806334	1.02715877
6	1.00374278	-2.38303459	0.77755852
1	1.11827650	-3.46918131	0.62158855
1	1.90164046	-2.04848158	1.31616342
16	0.51609857	-2.49935582	-1.84703626
7	-1.77974303	1.03838163	0.51875319
6	-1.72555666	-0.41976029	2.52953164
1	-2.26425040	-1.24405751	3.04576374
1	-1.69244106	0.43387727	3.22106113
6	-2.50799105	0.00842772	1.28242561
1	-3.49118746	0.39615116	1.57953063
1	-2.67913596	-0.84375120	0.60715405
16	-2.11048634	2.66764259	0.87063814
8	-0.83934727	3.38273166	0.63393224
8	-2.84538163	2.79965610	2.15065901
6	-3.26635981	3.11913253	-0.44379582
6	-4.60499467	3.35279216	-0.13403675
6	-5.48448422	3.71916349	-1.15690408
6	-5.04086306	3.85967204	-2.47943020
6	-3.68300620	3.62094110	-2.75935490
6	-2.79332780	3.25457696	-1.75214393
1	-4.94246548	3.25618253	0.89727981

1	-1.73940306	3.08217428	-1.97025804
1	-3.31866023	3.72735328	-3.78289743
6	-5.98576310	4.28624741	-3.57484393
1	-6.53384272	3.90365355	-0.91955104
8	1.04825296	-1.57598525	-2.93731915
8	0.88518413	-3.93250102	-1.87836832
6	-1.28579676	-2.44235565	-2.02488494
6	-2.01731509	-3.62735347	-1.94295532
6	-3.40729203	-3.57852231	-2.07837311
6	-4.07287403	-2.36473270	-2.30199709
6	-3.30816852	-1.18689771	-2.38132216
6	-1.92272876	-1.21708444	-2.24178195
1	-1.49553970	-4.57069564	-1.78691692
1	-3.98315399	-4.50356024	-2.01384727
6	-5.57024918	-2.31898728	-2.47597996
1	-3.80573049	-0.22942624	-2.54736690
1	-1.34344781	-0.29578607	-2.29633034
1	-7.03267859	4.12560235	-3.28724786
1	-5.86418089	5.35730549	-3.79956993
1	-5.79328356	3.73750970	-4.50695986
1	-5.83658983	-2.18201305	-3.53544758
1	-6.04297680	-3.24748984	-2.13138992
1	-6.01093159	-1.47836957	-1.92220985
1	-0.76517796	0.89679317	0.64199576

Energy = -8524.639804 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 13

Atomic N.	X	Y	Z
8	1.64108142	0.25694205	0.82862353
8	3.26541715	2.26806024	2.03695090
6	3.68408796	3.61359754	2.23468123
1	3.21382016	4.28810517	1.50082154
1	4.77968195	3.66576741	2.11326769
1	3.45372781	3.99441325	3.25053796
8	3.49860612	-0.64751952	1.57069917
6	2.80584304	-0.10813949	0.57398906
6	3.39942332	0.05681395	-0.79838830
1	4.20744397	0.80389642	-0.70454287
1	2.61849172	0.52622928	-1.40728737
6	3.92372814	-1.23393535	-1.46052340
1	3.18000057	-2.03624126	-1.33815506
1	4.00593681	-1.03589493	-2.53963903
6	5.28666419	-1.70169301	-0.94085076
1	6.03647369	-0.91619258	-1.13899235
1	5.60416776	-2.58550944	-1.51495132
6	5.30506835	-2.04213989	0.55237720
1	4.63008411	-2.88474088	0.77001035
1	6.31826803	-2.36853414	0.83789794
6	4.94082004	-0.88112578	1.46634939
1	5.41857525	0.06474170	1.17142220
1	5.21691152	-1.09702804	2.50452949
50	1.53713526	1.53918223	2.90812101
7	-1.26497386	0.27421340	3.25957069
6	-1.28556506	-0.67220902	4.37520456
1	-2.29611522	-0.78394651	4.82216244
1	-0.92984084	-1.65613814	4.04704541

1	-0.59997470	-0.31388480	5.15541837
7	-0.52468478	-1.79466011	1.30379839
6	-2.14257672	-0.11852500	2.15392234
1	-3.21642827	-0.04216516	2.44076219
1	-1.97921862	0.58979193	1.32889062
6	-1.93507320	-1.54034117	1.62772099
1	-2.59093650	-1.64659564	0.74420888
1	-2.25512006	-2.29041230	2.36328345
16	-0.13279682	-3.18815819	0.45337969
7	-0.13617331	2.69115005	1.99463462
6	-1.58241367	1.62596655	3.73848148
1	-2.61959671	1.67998812	4.13780827
1	-0.90708740	1.83203034	4.58526751
6	-1.43701288	2.73509599	2.69184504
1	-1.58008701	3.69717645	3.21151292
1	-2.26084170	2.65548288	1.95970300
16	-0.05766284	3.76740508	0.72954871
8	1.28397261	3.63963480	0.12100859
8	-0.56240004	5.10355372	1.13448914
6	-1.25681355	3.13415359	-0.48727388
6	-2.41805713	3.85480334	-0.76116590
6	-3.32322963	3.36184567	-1.70727041
6	-3.08140928	2.15868682	-2.38329922
6	-1.90084979	1.45170872	-2.08885531
6	-0.99031887	1.93090158	-1.14889669
1	-2.59505516	4.79554701	-0.24033336
1	-0.07428701	1.38405007	-0.92028399
1	-1.69599764	0.51002686	-2.60311103
6	-4.04963854	1.63521841	-3.41567783
1	-4.23328443	3.92540777	-1.92232016
8	1.31845548	-3.09084887	0.18609495
8	-0.72001917	-4.31882765	1.19533771
6	-0.98501644	-3.11154162	-1.14365854
6	-2.21313185	-3.75711259	-1.30138981
6	-2.86726459	-3.68565938	-2.53365607
6	-2.31168642	-2.98106880	-3.61196573
6	-1.06810001	-2.35155784	-3.42822488
6	-0.40490503	-2.40832156	-2.20336695
1	-2.63021301	-4.32914572	-0.47323244
1	-3.82333801	-4.19647029	-2.66134989
6	-3.03391747	-2.88631010	-4.93213630
1	-0.60982075	-1.81474092	-4.26120918
1	0.56634985	-1.93180536	-2.07152333
1	-4.99123846	2.19878178	-3.40398615
1	-3.62555561	1.71270185	-4.42867122
1	-4.28200667	0.57430677	-3.24279410
1	-2.33112510	-2.89901016	-5.77588660
1	-3.74584995	-3.71158455	-5.06046247
1	-3.60358554	-1.94583104	-4.99799189
1	0.02205904	-0.99181200	0.97194517

Energy = -8524.627412 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 14

Atomic N.	X	Y	Z
8	3.01204442	0.97297476	0.86644332
8	1.69060010	3.03242865	-0.91769374

6	2.87100297	3.06185616	-1.69824430
1	2.85389875	3.92602733	-2.38440376
1	2.99398779	2.15642824	-2.33228664
1	3.77416435	3.15066217	-1.06419576
8	4.93922783	0.52140447	1.78852604
6	4.07454484	0.35499543	0.77099673
6	4.43577355	-0.53187428	-0.39882154
1	5.35036238	-0.13325306	-0.87164055
1	3.61881755	-0.42382355	-1.12288798
6	4.62418235	-2.02533012	-0.05128525
1	3.78018008	-2.34941714	0.57360687
1	4.53869797	-2.58689217	-0.99333876
6	5.96413168	-2.36316220	0.60597989
1	6.78496991	-2.13155050	-0.09574785
1	6.00901139	-3.44833342	0.78492836
6	6.22271179	-1.62496188	1.92261446
1	5.46808630	-1.89150288	2.67959117
1	7.19888110	-1.93559151	2.32943836
6	6.25689720	-0.10808434	1.78678961
1	6.80674641	0.20920349	0.88622162
1	6.73635682	0.35075070	2.65944281
50	0.89918866	1.04147514	-0.48402513
7	-0.19630159	2.72277291	1.16902993
6	0.89011438	3.13202911	2.09230145
1	0.49773369	3.79193855	2.88762174
1	1.35272272	2.25008898	2.54640768
1	1.65419924	3.65598107	1.50819090
7	0.04824256	0.00360629	1.41951523
6	-1.24541854	1.97171369	1.89623949
1	-1.67415421	2.59757914	2.70282848
1	-2.04485122	1.73570131	1.17989068
6	-0.70218120	0.66787733	2.47803920
1	-1.56758221	0.06746800	2.81473564
1	-0.08331111	0.86003659	3.37116379
16	0.57696817	-1.50734942	1.72898201
7	-0.94125000	3.04657582	-1.71018615
6	-0.75424196	3.95592115	0.55217155
1	-1.30384021	4.53264384	1.32091876
1	0.10609510	4.55398008	0.22543137
6	-1.67613886	3.74460892	-0.64563847
1	-2.02520668	4.73700502	-0.97503051
1	-2.56848075	3.15791001	-0.37738054
16	-1.61428573	3.07344532	-3.27223373
8	-0.49269985	2.75403000	-4.17614383
8	-2.43521157	4.29056255	-3.46253201
6	-2.74770235	1.66841899	-3.23158581
6	-4.12252619	1.89508356	-3.18752657
6	-4.99000806	0.79915555	-3.17348501
6	-4.49963253	-0.51374465	-3.20755875
6	-3.10711782	-0.70918751	-3.25450576
6	-2.22807246	0.37089883	-3.26824646
1	-4.49897905	2.91738920	-3.17757537
1	-1.14987045	0.21634422	-3.31203090
1	-2.70676074	-1.72455559	-3.28405277
6	-5.43877519	-1.69368350	-3.21909056
1	-6.06750663	0.96988784	-3.14053731
8	1.40746858	-1.88415528	0.54714029
8	1.16051678	-1.66422710	3.08746140

6	-0.89959348	-2.56936134	1.69459242
6	-1.26325428	-3.29472592	2.82736606
6	-2.39641999	-4.11407715	2.78090793
6	-3.16902015	-4.21760395	1.61687374
6	-2.77969404	-3.47198880	0.48858130
6	-1.65615693	-2.64993762	0.52110349
1	-0.65423084	-3.21575593	3.72752197
1	-2.68220914	-4.68411542	3.66713877
6	-4.38827026	-5.10491237	1.56447005
1	-3.36766239	-3.54237953	-0.42934533
1	-1.35935655	-2.07417258	-0.35649434
1	-6.46344410	-1.39363218	-2.96619880
1	-5.46290345	-2.16460396	-4.21377088
1	-5.11919101	-2.46644556	-2.50563923
1	-4.28054643	-5.88188378	0.79293761
1	-4.56084292	-5.60453981	2.52606540
1	-5.29061380	-4.52706985	1.31488241
1	0.07698948	3.30902541	-1.74372961

Energy = -8524.634503 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 15

Atomic N.	X	Y	Z
8	4.25693893	1.55681384	2.83032561
8	2.37317654	1.97927278	-0.51374201
6	2.53619054	3.39087787	-0.64185425
1	3.03507336	3.64176937	-1.59380333
1	3.16454144	3.75463944	0.18809592
1	1.57996830	3.94224753	-0.61961045
8	5.44626293	2.26468639	1.10183892
6	4.76484267	1.28021165	1.75856112
6	4.70472873	-0.10728352	1.14290256
1	4.19474760	-0.04505015	0.16793987
1	4.06411960	-0.69441588	1.81105511
6	6.07596958	-0.79711291	0.98593344
1	6.67514283	-0.63517761	1.89689587
1	5.90079325	-1.88150485	0.92215043
6	6.86318045	-0.35551530	-0.25213988
1	6.28197931	-0.62228301	-1.15173490
1	7.80148819	-0.92956189	-0.30927498
6	7.18226905	1.14217917	-0.30050663
1	7.86156992	1.42474466	0.52047860
1	7.71621501	1.36667543	-1.23857397
6	5.95671391	2.04968403	-0.24339836
1	5.14063650	1.68680813	-0.88775065
1	6.22080103	3.06338810	-0.57062244
50	0.72636436	0.88586391	-1.04454234
7	-0.13198970	1.08075420	1.41234804
6	0.90437491	0.72982452	2.40705441
1	0.54530311	0.89881171	3.43868149
1	1.19951314	-0.31932814	2.29591468
1	1.78869190	1.35366086	2.23604597
7	-0.46787703	-1.85033557	0.79409695
6	-1.38935271	0.31942526	1.60354360
1	-1.94278407	0.72367579	2.47499581
1	-2.02021862	0.48641297	0.71663980
6	-1.23582823	-1.18392054	1.85188749

1	-2.25408049	-1.59884813	1.96374132
1	-0.70250892	-1.36245349	2.79406947
16	0.16828472	-3.39735855	1.11397324
7	-0.82043350	2.46642321	-0.88748187
6	-0.40591703	2.54162831	1.49177925
1	-0.85079612	2.79414656	2.47389066
1	0.56835394	3.04262482	1.41879698
6	-1.31147222	3.03725614	0.36207575
1	-1.26263674	4.13865566	0.34753625
1	-2.36410776	2.75592824	0.54945976
16	-0.91444161	3.29536453	-2.29468525
8	0.05273838	2.54163122	-3.16182314
8	-0.77917103	4.75967492	-2.11761244
6	-2.56385361	3.01441602	-2.98725750
6	-3.52632269	4.02092129	-2.90257497
6	-4.80489271	3.78527103	-3.41449820
6	-5.13205655	2.56191668	-4.01692472
6	-4.14020253	1.56808175	-4.09215118
6	-2.86158060	1.78514752	-3.58231251
1	-3.26415941	4.97917098	-2.45543652
1	-2.08969622	1.01925158	-3.66004798
1	-4.37317632	0.61216035	-4.56553768
6	-6.50169662	2.32698823	-4.60332434
1	-5.55932491	4.57175414	-3.35145061
8	0.81544654	-3.80159170	-0.14533010
8	0.90319086	-3.26668000	2.38606258
6	-1.23230319	-4.50186600	1.40147007
6	-1.69102658	-4.71366828	2.70349049
6	-2.78514049	-5.55654487	2.90750758
6	-3.42296538	-6.19321598	1.83155828
6	-2.93576972	-5.96313901	0.53332813
6	-1.84495858	-5.12445588	0.30975237
1	-1.17975927	-4.24149816	3.54170193
1	-3.14452612	-5.72931607	3.92346829
6	-4.57969201	-7.13177464	2.06352100
1	-3.41303175	-6.45738788	-0.31479406
1	-1.45189282	-4.96877123	-0.69482107
1	-7.24797080	3.00072818	-4.16289407
1	-6.49661393	2.50499951	-5.69006770
1	-6.83333984	1.29149097	-4.44673946
1	-4.22652552	-8.17264311	2.13055178
1	-5.10253214	-6.90145736	3.00062726
1	-5.30427967	-7.08719003	1.23967629
1	-0.90670580	-1.84670972	-0.13010484

Energy = -8524.642538 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 16

Atomic N.	X	Y	Z
8	3.05512558	1.07135854	0.73648562
8	1.57413670	3.25183346	-0.79745033
6	2.75200864	3.41640348	-1.56715370
1	3.63905366	3.55178130	-0.92034811
1	2.66423363	4.30354819	-2.21777598
1	2.95637552	2.55054025	-2.23482830
8	5.08522519	0.82011964	1.50559724
6	4.09887872	0.41834245	0.67807792

6	4.30580283	-0.77173021	-0.22663372
1	5.16620618	-0.57650134	-0.88958910
1	3.40571680	-0.84503463	-0.84728754
6	4.51085421	-2.10411023	0.53082600
1	3.76773583	-2.17801872	1.33845285
1	4.26926536	-2.91299390	-0.17296394
6	5.92713181	-2.31361820	1.07170096
1	6.63961930	-2.33757373	0.22818412
1	5.98369878	-3.30290199	1.55119619
6	6.38398989	-1.24510789	2.06951413
1	5.75369650	-1.25683829	2.97320057
1	7.41114239	-1.46856975	2.40133942
6	6.39329920	0.17040574	1.50649890
1	6.81296266	0.20180294	0.48851957
1	6.98727340	0.83852849	2.14148646
50	0.87960550	1.19438960	-0.58701017
7	-0.20485311	2.61957191	1.31520375
6	0.91088058	2.99565518	2.21670169
1	0.53406454	3.56979263	3.08307958
1	1.42729425	2.09907532	2.57341842
1	1.62568358	3.59552920	1.64348163
7	0.07655344	-0.11679000	1.17572546
6	-1.17315835	1.74980597	2.02133119
1	-1.54663712	2.25589285	2.93276721
1	-2.02395370	1.57830892	1.34732342
6	-0.55837676	0.39940853	2.38232630
1	-1.37719704	-0.25536931	2.73345576
1	0.15099351	0.49661190	3.22220717
16	0.57832299	-1.66661420	1.21718017
7	-1.08551843	3.19559136	-1.48567408
6	-0.85639259	3.87370141	0.85252800
1	-1.40358479	4.33635315	1.69648620
1	-0.04621950	4.55272608	0.55693367
6	-1.81594517	3.72665482	-0.32527179
1	-2.24444795	4.72033563	-0.53392758
1	-2.65479830	3.05419138	-0.08806516
16	-1.83967290	3.31753374	-3.01013672
8	-0.73640555	3.25275029	-3.98720164
8	-2.81138512	4.43382989	-3.00945246
6	-2.78710036	1.78398009	-3.10733342
6	-4.17145267	1.81666907	-2.93412118
6	-4.89373746	0.62530544	-3.02774654
6	-4.25127316	-0.59291941	-3.29845678
6	-2.85631408	-0.59255416	-3.46884584
6	-2.11909550	0.58716892	-3.37697407
1	-4.66775014	2.76760151	-2.74336416
1	-1.03830089	0.58432533	-3.51718615
1	-2.33857389	-1.53077660	-3.67644306
6	-5.04494647	-1.86786822	-3.43806875
1	-5.97702998	0.64453725	-2.89478410
8	1.23817729	-1.91306546	-0.09741020
8	1.33334435	-2.01504458	2.45350504
6	-0.93499281	-2.67532368	1.25588087
6	-1.13153846	-3.59781753	2.28197806
6	-2.29453789	-4.37458890	2.28991374
6	-3.26333950	-4.24000386	1.28627591
6	-3.04207263	-3.29625002	0.26658211
6	-1.88816354	-2.51577657	0.24522605

1	-0.37548568	-3.69654824	3.06029872
1	-2.45109427	-5.09676812	3.09364822
6	-4.50798145	-5.09283201	1.28488595
1	-3.78950397	-3.17074902	-0.51995360
1	-1.72535341	-1.78233720	-0.54563811
1	-5.90237526	-1.88416046	-2.75170239
1	-5.44405168	-1.96768134	-4.45952968
1	-4.42314202	-2.75130467	-3.24246174
1	-4.45651932	-5.86197432	0.49876926
1	-4.64247390	-5.60679527	2.24518694
1	-5.40601431	-4.49030727	1.08772652
1	-0.09559172	3.54325742	-1.54031689

Energy = -8524.634715 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 17

Atomic N.	X	Y	Z
8	2.68388455	-2.80297863	1.67971446
8	2.71438904	-0.29344009	-1.18684479
6	3.11848528	-0.09794107	-2.53761149
1	3.53826270	0.91214641	-2.68331900
1	2.29170617	-0.21254440	-3.26114164
1	3.89981173	-0.83545417	-2.79562463
8	3.35590798	-0.73777775	2.06371363
6	3.55999856	-1.95765053	1.52142100
6	4.84055994	-2.24089254	0.76582432
1	4.88330158	-1.55863592	-0.09932116
1	4.73273952	-3.26044425	0.37738828
6	6.12630802	-2.12542421	1.61142879
1	5.97160946	-2.61694974	2.58552177
1	6.91425521	-2.69857549	1.10012474
6	6.61743255	-0.68861409	1.81415110
1	6.85802115	-0.25526882	0.82815268
1	7.55986732	-0.70599702	2.38332973
6	5.61580868	0.22810011	2.52340045
1	5.43110190	-0.11448318	3.55451824
1	6.04819187	1.23860930	2.60512979
6	4.27554798	0.36939233	1.81207259
1	4.37786315	0.49761450	0.72350259
1	3.72201356	1.23042042	2.20585737
50	0.85312452	0.13567484	-0.40175713
7	0.06694114	-2.39250602	-0.99777886
6	1.10035315	-2.94888475	-1.89545636
1	0.79109610	-3.93544795	-2.29031843
1	1.28228795	-2.26951159	-2.73381732
1	2.03780881	-3.05611768	-1.33895782
7	-0.40226696	0.06120100	-2.23517862
6	-1.19566193	-2.15928891	-1.73966519
1	-1.55665298	-3.10664621	-2.18797585
1	-1.94799341	-1.81744956	-1.01531592
6	-1.05479139	-1.09584916	-2.83176682
1	-2.07084621	-0.85423400	-3.19162332
1	-0.49336487	-1.48558692	-3.69792140
16	-0.29469705	1.48031850	-3.02854334
7	-0.12833370	-1.92201936	2.10708763
6	-0.15076752	-3.37127475	0.10250261
1	-0.68266959	-4.25366661	-0.30536198

1	0.83958766	-3.71300157	0.43217237
6	-0.92283062	-2.88475538	1.32769966
1	-1.18153791	-3.77525502	1.92438480
1	-1.87275842	-2.40694846	1.04175528
16	-0.75772922	-1.50456379	3.63248524
8	0.39086482	-1.00009650	4.40828320
8	-1.62268171	-2.58795977	4.15418221
6	-1.84289147	-0.11482870	3.23775821
6	-3.22688837	-0.28284174	3.29436142
6	-4.05455374	0.80807740	3.01910043
6	-3.51616300	2.06318281	2.69635763
6	-2.11832759	2.19996271	2.64372914
6	-1.27794259	1.12079964	2.91308474
1	-3.63890505	-1.25433950	3.56537696
1	-0.19496805	1.23063833	2.87742263
1	-1.68162763	3.16697739	2.38720608
6	-4.41587019	3.24803463	2.44707176
1	-5.13800368	0.68266863	3.06483085
8	0.57198144	2.28083249	-2.09545421
8	0.09106962	1.35645861	-4.45376239
6	-1.94722376	2.22522316	-3.01343645
6	-2.53876125	2.60848459	-4.21611422
6	-3.81083919	3.18801150	-4.19561999
6	-4.49766138	3.38762250	-2.99053049
6	-3.87807672	2.98544374	-1.79289699
6	-2.61078805	2.40763704	-1.79578098
1	-1.99980864	2.45177621	-5.14973305
1	-4.27651290	3.48945125	-5.13570039
6	-5.86248900	4.02924028	-2.96825833
1	-4.39959214	3.12744901	-0.84409260
1	-2.13974346	2.09778418	-0.86180019
1	-4.65263341	3.76312934	3.39114898
1	-3.93780415	3.98354259	1.78650093
1	-5.36965399	2.94038051	1.99724840
1	-5.81396813	5.03914372	-2.53302173
1	-6.27915914	4.12032840	-3.97921532
1	-6.56703616	3.44854942	-2.35598669
1	0.86129320	-2.20816166	2.22970241

Energy = -8524.648517 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 18

Atomic N.	X	Y	Z
8	4.15375834	0.25797532	0.56996468
8	3.02219323	-1.82003715	-1.49906553
6	4.21178580	-1.48652456	-2.20210149
1	4.20438394	-1.95354152	-3.20337203
1	5.10049893	-1.86427124	-1.66386621
1	4.35293291	-0.39882367	-2.34464720
8	5.89301097	0.29869920	1.90853283
6	4.88933269	-0.38805367	1.30893393
6	4.73349270	-1.86979937	1.57234219
1	5.66936829	-2.38369841	1.29174836
1	3.95307028	-2.21489403	0.88269766
6	4.36420260	-2.21677398	3.03159860
1	3.58013400	-1.52847108	3.37876394
1	3.91103221	-3.21863162	3.02998231

6	5.55132813	-2.20887999	3.99816427
1	6.27877509	-2.97917621	3.68583173
1	5.20078947	-2.50315079	4.99942573
6	6.27507978	-0.86202144	4.09429843
1	5.60360810	-0.08387471	4.49145284
1	7.11163037	-0.94791271	4.80716324
6	6.85698336	-0.36612196	2.77488669
1	7.34999089	-1.17984145	2.21851086
1	7.59964214	0.42111623	2.95316458
50	1.84296378	-0.30847333	-0.71529755
7	0.03029561	-1.80971719	-1.86598012
6	0.31948205	-2.03229420	-3.29451226
1	-0.36670988	-2.77799187	-3.73799573
1	0.23887416	-1.09007309	-3.84858846
1	1.35067607	-2.39616478	-3.37494097
7	-0.97865050	0.93388247	-2.55283970
6	-1.35433839	-1.34502702	-1.62287156
1	-2.06060928	-2.19282249	-1.73501888
1	-1.41572845	-1.01249952	-0.57629552
6	-1.87105928	-0.23225400	-2.53644832
1	-2.88877670	0.01548819	-2.18122718
1	-1.96100573	-0.58235034	-3.57244425
16	-1.38210849	2.21786073	-3.59365447
7	0.96833372	-1.69930288	0.80030525
6	0.28789131	-3.06308151	-1.11009638
1	-0.41392465	-3.85766314	-1.43204539
1	1.31244875	-3.36807972	-1.36264859
6	0.17405525	-2.86961703	0.40045423
1	0.53802317	-3.78609316	0.89263689
1	-0.88689239	-2.75606680	0.69067626
16	0.65709830	-1.10539359	2.30466777
8	1.63665675	-0.00939092	2.51534006
8	0.53649389	-2.21014975	3.28699613
6	-0.98228737	-0.32192161	2.22275512
6	-2.12361190	-1.03813305	2.58959456
6	-3.38074223	-0.44134000	2.45187545
6	-3.51522674	0.86681634	1.96461569
6	-2.34896564	1.57184361	1.61703465
6	-1.08860914	0.98808652	1.74221220
1	-2.01883982	-2.04330771	2.99703666
1	-0.18351692	1.54304584	1.49160962
1	-2.43204020	2.59772946	1.25178749
6	-4.87089822	1.51977667	1.85526082
1	-4.27313224	-1.00179043	2.73762247
8	-0.32509563	3.22212230	-3.39268284
8	-1.65956122	1.59619385	-4.90206892
6	-2.93115684	2.92052249	-2.97885134
6	-4.15129764	2.44752085	-3.46639023
6	-5.33741423	2.99167529	-2.96881227
6	-5.32158822	4.00159168	-1.99469766
6	-4.07764515	4.46680943	-1.53346093
6	-2.88344161	3.93330758	-2.01597832
1	-4.16449377	1.68658869	-4.24602356
1	-6.29339174	2.63303374	-3.35445735
6	-6.60622609	4.57042453	-1.44723482
1	-4.04466195	5.26927865	-0.79403727
1	-1.91907959	4.31424173	-1.67987421
1	-5.66713948	0.77361607	1.73420501

1	-5.09905760	2.10082724	2.76256745
1	-4.91229732	2.21494550	1.00558174
1	-6.51518820	5.64652683	-1.24789011
1	-7.44191439	4.41540875	-2.14140082
1	-6.87303943	4.08552742	-0.49495463
1	-0.73895281	1.30301550	-1.62752534

Energy = -8524.643386 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 19

Atomic N.	X	Y	Z
8	2.65888018	-2.87347461	1.58171123
8	2.77612179	-0.15466095	-1.09104615
6	3.23265266	0.13548739	-2.40774166
1	4.01180518	-0.59385995	-2.69433544
1	3.67331079	1.14593049	-2.45883110
1	2.43150119	0.09210253	-3.16688424
8	3.26616792	-0.83055286	2.14907835
6	3.52364400	-2.00353647	1.53123518
6	4.84652521	-2.20764683	0.82464628
1	4.91901939	-1.46220528	0.01539840
1	4.77980827	-3.19709187	0.35717051
6	6.08491101	-2.13385076	1.74250345
1	5.89140606	-2.69983953	2.66803031
1	6.90975913	-2.65321663	1.23194474
6	6.53472107	-0.70809790	2.07664773
1	6.81657461	-0.19799111	1.13950766
1	7.44676449	-0.75205340	2.69201565
6	5.47897345	0.13582427	2.79769399
1	5.24835234	-0.28607755	3.78940118
1	5.88552802	1.14449556	2.97668402
6	4.17461038	0.30744569	2.02862599
1	4.33047366	0.51839290	0.95943943
1	3.58395070	1.12741212	2.45477969
50	0.87279777	0.18052932	-0.36381462
7	0.16575852	-2.30939140	-1.17715632
6	1.25382779	-2.78422510	-2.05702617
1	0.98378286	-3.74476654	-2.53584942
1	1.46478765	-2.04415747	-2.83501589
1	2.16376062	-2.91655295	-1.46160323
7	-0.29516880	0.22144089	-2.25422621
6	-1.06211540	-2.04449783	-1.96571071
1	-1.37852287	-2.96263479	-2.50013971
1	-1.85786158	-1.77109716	-1.25894736
6	-0.88877629	-0.90067403	-2.96786911
1	-1.88980767	-0.65235118	-3.36341552
1	-0.27409048	-1.21412199	-3.82880398
16	-0.19169444	1.69986822	-2.93196630
7	-0.18796291	-2.07062838	1.94282114
6	-0.08936217	-3.36762380	-0.16166849
1	-0.58591199	-4.22502205	-0.65776873
1	0.88895820	-3.71954957	0.19219309
6	-0.92893842	-2.98050508	1.05451699
1	-1.20560620	-3.91498641	1.57033563
1	-1.86946422	-2.49197746	0.75583407
16	-0.89354200	-1.78379219	3.46498587
8	0.21039673	-1.33220165	4.33288413

8	-1.76621214	-2.91480916	3.85670442
6	-1.97941495	-0.37831534	3.13254569
6	-3.36271660	-0.55974187	3.14020041
6	-4.19262993	0.54186197	2.91846216
6	-3.65731034	1.81985719	2.69715507
6	-2.25964478	1.96990843	2.69132674
6	-1.41722539	0.88101480	2.90920392
1	-3.77277200	-1.55089003	3.33115305
1	-0.33473831	1.00116158	2.91019605
1	-1.82497511	2.95534611	2.51343570
6	-4.55992696	3.01342477	2.50700033
1	-5.27572140	0.40589492	2.92620629
8	0.61296542	2.44686589	-1.90423757
8	0.25688222	1.69376806	-4.34410210
6	-1.86307923	2.40170816	-2.93299872
6	-2.41343282	2.86530620	-4.12720808
6	-3.70076624	3.40981655	-4.11801572
6	-4.44370146	3.49588625	-2.93251554
6	-3.86514680	3.01389404	-1.74422337
6	-2.58290013	2.46951023	-1.73600830
1	-1.83130306	2.79603961	-5.04537853
1	-4.13459148	3.77289737	-5.05156146
6	-5.82286975	4.10629198	-2.92116843
1	-4.43107837	3.06501441	-0.81179553
1	-2.14413750	2.09670150	-0.80935175
1	-4.79102494	3.48413703	3.47536803
1	-4.08637550	3.77970254	1.87872811
1	-5.51590908	2.72559932	2.04928448
1	-5.79546747	5.12640108	-2.50762717
1	-6.24158884	4.16993890	-3.93353656
1	-6.51378557	3.52323780	-2.29652507
1	0.79989232	-2.35144692	2.08901912

Energy = -8524.648523 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 20

Atomic N.	X	Y	Z
8	4.16019243	0.32698242	0.70547134
8	3.11054939	-1.67154671	-1.48344843
6	4.31074777	-1.28505299	-2.13958670
1	5.19252736	-1.67401191	-1.59791191
1	4.43643383	-0.18953358	-2.22586936
1	4.33616345	-1.70293672	-3.16210273
8	5.86874885	0.33238469	2.08399136
6	4.88918016	-0.34087088	1.43116819
6	4.75077706	-1.83516768	1.62399960
1	5.70135194	-2.32207695	1.34471952
1	3.99325776	-2.16041558	0.89998468
6	4.35116995	-2.25239630	3.05660701
1	3.54799714	-1.59189741	3.41399780
1	3.91423751	-3.25982737	2.99943372
6	5.51408229	-2.27019305	4.05213716
1	6.26036963	-3.01589177	3.72495727
1	5.14354407	-2.61287071	5.03054764
6	6.21509603	-0.91893880	4.22506725
1	5.52260058	-0.16849355	4.63908029
1	7.03523805	-1.02469097	4.95414698

6	6.82132426	-0.35702723	2.94355751
1	7.33948833	-1.13850501	2.36426403
1	7.54785625	0.43150656	3.17472689
50	1.88538791	-0.21731968	-0.66005215
7	0.12865025	-1.70542856	-1.91654660
6	0.45817347	-1.85436115	-3.34582226
1	-0.19918432	-2.59356291	-3.84102984
1	0.36902281	-0.88943912	-3.85810854
1	1.49938873	-2.19055704	-3.41656908
7	-0.94154990	1.05012492	-2.47056013
6	-1.27383548	-1.28919807	-1.68961516
1	-1.95376943	-2.14758732	-1.86652694
1	-1.37348109	-1.01454571	-0.62933286
6	-1.79399799	-0.14249750	-2.55774293
1	-2.83239962	0.05210287	-2.23062160
1	-1.83172013	-0.43383514	-3.61495134
16	-1.32955491	2.36746506	-3.47566270
7	1.00474766	-1.69210348	0.77213374
6	0.39972985	-2.98525249	-1.21144579
1	-0.27555506	-3.78067746	-1.58411895
1	1.43660919	-3.25486771	-1.45356585
6	0.24849695	-2.86205685	0.30338599
1	0.62451076	-3.79065207	0.76274039
1	-0.82086694	-2.78723271	0.57459200
16	0.64442920	-1.17025041	2.29179184
8	1.59465683	-0.06456529	2.57412555
8	0.52253455	-2.31811974	3.22325792
6	-1.00861295	-0.41649470	2.20152061
6	-2.14326317	-1.16944110	2.51010472
6	-3.40892541	-0.59173011	2.36695597
6	-3.55871511	0.73297108	1.93226004
6	-2.39893535	1.47477572	1.64342754
6	-1.13033116	0.91080626	1.77444646
1	-2.02718012	-2.18833020	2.87881717
1	-0.23090941	1.49364198	1.57089116
1	-2.49421926	2.51416456	1.32182222
6	-4.92413651	1.36423990	1.81721516
1	-4.29614628	-1.18077562	2.60767863
8	-0.33566418	3.40334445	-3.15089422
8	-1.48635276	1.80265497	-4.82907733
6	-2.94879452	2.97099728	-2.94148286
6	-4.10668809	2.48806575	-3.55375017
6	-5.34975371	2.95267181	-3.11702165
6	-5.45117890	3.89233357	-2.08045440
6	-4.26656876	4.37053817	-1.49242833
6	-3.01785001	3.91651864	-1.91315941
1	-4.02788062	1.78069020	-4.37862818
1	-6.25731091	2.58543668	-3.59929596
6	-6.79549452	4.37776610	-1.60015983
1	-4.32420105	5.11995905	-0.70061722
1	-2.09930034	4.30909925	-1.47678750
1	-5.70781556	0.60528527	1.69490920
1	-5.16402061	1.94426317	2.72209025
1	-4.97435394	2.05709031	0.96582879
1	-6.79325220	5.46417715	-1.43670709
1	-7.58916452	4.13805254	-2.31877034
1	-7.06080329	3.90734786	-0.64051822
1	-0.77553418	1.38576910	-1.51690903

Energy = -8524.643391 Hartree
 Number of imaginary frequencies = 0.

Compound I2a isomer 21

Atomic N.	X	Y	Z
8	-0.90545246	0.83141239	-0.02942461
8	1.84705355	0.50620581	-0.84571611
6	3.24246211	0.28277783	-0.68995369
1	3.69520121	-0.16775615	-1.59222818
1	3.48495140	-0.38314005	0.16413305
1	3.74571784	1.24851998	-0.50400934
8	0.14538273	0.99054799	1.90300561
6	-0.47283449	1.56660650	0.86174082
6	-0.59499584	3.06907045	0.78312886
1	-1.03857187	3.46790823	1.70973454
1	-1.28835772	3.27126446	-0.04088947
6	0.77206599	3.74078208	0.51405135
1	1.30703154	3.15626923	-0.25093062
1	0.57811546	4.73490386	0.08529712
6	1.63497816	3.90067895	1.77017554
1	1.11410334	4.56702115	2.48014956
1	2.57080068	4.41285827	1.49880287
6	1.97494178	2.58716907	2.48463611
1	2.58695123	1.93703429	1.84049998
1	2.58277711	2.81072322	3.37649356
6	0.76751764	1.78688609	2.95844398
1	0.00216787	2.42616932	3.42567307
1	1.06685540	1.02263666	3.68525854
50	0.61912456	-1.17948062	-0.62193271
7	-2.62798339	-2.14596450	-1.08653358
6	-2.56623994	-3.41326754	-1.82453160
1	-3.48760075	-3.60214117	-2.41585232
1	-1.70836597	-3.42018378	-2.50779255
1	-2.43731524	-4.23513778	-1.10903459
7	-0.37668915	-0.98164676	-2.61168083
6	-2.80164814	-0.99507106	-1.98252485
1	-3.79548502	-1.02991564	-2.48618408
1	-2.77759047	-0.08161167	-1.37374956
6	-1.75672748	-0.87665500	-3.09980012
1	-1.92727535	0.09903652	-3.58961820
1	-1.93613868	-1.65610791	-3.85684215
16	0.72931277	-1.64924863	-3.60447232
7	-2.39841933	-1.36408449	1.89786083
6	-3.71841343	-2.19774566	-0.09822381
1	-4.70762627	-2.05303453	-0.58880606
1	-3.72414576	-3.20542219	0.34096315
6	-3.58344607	-1.17867028	1.03685714
1	-4.47321148	-1.23014395	1.67816765
1	-3.51992834	-0.15343329	0.64410360
16	-2.50437937	-2.61757385	3.05507141
8	-1.93922682	-3.88307167	2.53457991
8	-3.88116865	-2.57014983	3.59287262
6	-1.36644929	-2.00473940	4.31719800
6	-1.84185954	-1.14360355	5.30803417
6	-0.96143124	-0.69184541	6.29055216
6	0.38665699	-1.08960859	6.29709184
6	0.83350894	-1.95558911	5.28683497

6	-0.03549933	-2.42211520	4.29822625
1	-2.89103531	-0.84960718	5.31011395
1	0.30632644	-3.10880445	3.52436213
1	1.87661306	-2.27723767	5.27640022
6	1.32019859	-0.62776755	7.38833017
1	-1.32854258	-0.02524963	7.07333974
8	1.83725050	-1.99126235	-2.62190783
8	0.21195300	-2.72790468	-4.47735239
6	1.38379105	-0.36554291	-4.70003988
6	1.42020387	-0.58959879	-6.07554939
6	1.92289119	0.41225627	-6.91057479
6	2.38619533	1.62704375	-6.38644287
6	2.32911058	1.82237008	-4.99427090
6	1.83079588	0.83743297	-4.14410672
1	1.05830185	-1.53536818	-6.47690213
1	1.95423956	0.24469097	-7.98880387
6	2.94797385	2.69863478	-7.28742004
1	2.68138328	2.76545817	-4.57068830
1	1.78282940	0.98656238	-3.05985264
1	1.25890154	-1.29556028	8.26175343
1	2.36486191	-0.62746827	7.05054261
1	1.06542027	0.38279174	7.73501425
1	4.04108253	2.76991017	-7.17710882
1	2.73198237	2.48977836	-8.34290030
1	2.53469963	3.68659712	-7.03945953
1	-1.56062921	-1.54047790	1.32461697

Energy = -8524.638851 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 22

Atomic N.	X	Y	Z
8	4.15853602	-1.86838312	-0.11193023
8	4.07649930	-1.08086376	2.89555199
6	3.14319440	-1.52891144	3.87338303
1	2.74971568	-0.70302780	4.48865113
1	3.65506024	-2.23908500	4.54610566
1	2.27876151	-2.05104131	3.42378679
8	6.25206275	-1.63163905	0.54235238
6	5.20125812	-2.41889285	0.23332416
6	5.32698674	-3.92177501	0.34577322
1	6.24158067	-4.27159175	-0.15956954
1	4.46404929	-4.33486112	-0.18914088
6	5.32055338	-4.39451095	1.81788883
1	4.53094080	-3.85279905	2.36030960
1	5.04548386	-5.45955616	1.82782518
6	6.66675340	-4.21915183	2.52848916
1	7.41653829	-4.86684735	2.04047386
1	6.57303654	-4.58283319	3.56318052
6	7.19328607	-2.77902104	2.54977277
1	6.49540818	-2.11324142	3.08313290
1	8.14905748	-2.75526715	3.09780283
6	7.45091120	-2.18343633	1.17026853
1	7.91934765	-2.90730751	0.48379275
1	8.10478784	-1.30632418	1.24055950
50	3.68896017	0.36019493	1.48024910
7	0.05197281	-0.60571505	-1.76915962
6	0.42567562	-0.61138813	-3.18461496

8	0.20491863	3.34032745	1.34761425
8	0.14825638	-0.82304673	0.25544920
6	1.19250710	-1.78755015	0.41093292
1	1.75087488	-1.56429363	1.33472006
1	1.89384863	-1.75160557	-0.43936944
1	0.80931909	-2.82214158	0.49524300
8	1.97344245	3.04714909	2.64158587
6	1.41302690	3.18071947	1.40488320
6	2.30154861	3.09707676	0.17903999
1	3.11620021	3.83738611	0.25045029
1	1.66877824	3.38033896	-0.66958102
6	2.88760586	1.68768639	-0.05698276
1	2.09393243	0.94087061	0.10048243
1	3.15941824	1.61415124	-1.11898568
6	4.11366878	1.37083615	0.80354970
1	4.92893994	2.06651544	0.53599172
1	4.47771101	0.36239083	0.55252482
6	3.87571179	1.45768727	2.31517394
1	3.14220523	0.70266491	2.64134059
1	4.81580079	1.22902451	2.84380819
6	3.40182513	2.82379550	2.80266393
1	3.96236534	3.64139307	2.32051510
1	3.54046990	2.91337562	3.88724908
50	-1.38651432	-1.34034644	-1.08019401
7	-2.81972218	0.56890290	-0.16038992
6	-4.04662586	0.42821587	-0.98225161
1	-4.70373155	1.30762770	-0.86241245
1	-3.78526428	0.31913675	-2.04181481
1	-4.59156755	-0.46855608	-0.66246331
7	-1.13419531	0.47380773	-2.33611276
6	-2.07221347	1.80372508	-0.53293887
1	-2.69317695	2.69549708	-0.32359966
1	-1.17892683	1.86128353	0.09836595
6	-1.64479396	1.80047016	-2.00261041
1	-0.86845719	2.57212233	-2.12652528
1	-2.49097197	2.07383583	-2.65778896
16	0.20234625	0.28843656	-3.25241280
7	-1.28483284	-0.38271118	2.57006334
6	-3.25558264	0.62874191	1.26848230
1	-3.93626336	1.49704524	1.37495055
1	-3.85199629	-0.27310033	1.46429873
6	-2.17841186	0.76456917	2.35422716
1	-2.71983815	0.95618617	3.29112947
1	-1.52839524	1.63366226	2.17836909
16	-2.03504356	-1.81662511	3.04659222
8	-2.25942185	-2.71037916	1.87683117
8	-3.18030876	-1.44392069	3.90830460
6	-0.76416759	-2.59171115	4.06748565
6	-0.41598698	-2.00697750	5.28859155
6	0.53476432	-2.63235159	6.09056574
6	1.14214738	-3.83789204	5.69347033
6	0.77063975	-4.40028443	4.46460838
6	-0.18228540	-3.78583065	3.64722315
1	-0.88819293	-1.07631742	5.60149344
1	-0.48150500	-4.22245468	2.69515519
1	1.23104252	-5.33502297	4.13975387
6	2.15311547	-4.51442260	6.58500480
1	0.81181244	-2.17981944	7.04458957

8	1.19897616	1.37335131	-3.07874029
8	0.58532476	-1.13739315	-2.96470407
6	-0.30634148	0.34409206	-4.98977535
6	-1.05825073	-0.70928019	-5.51934507
6	-1.46455891	-0.65319214	-6.85018313
6	-1.13318384	0.44352158	-7.66657250
6	-0.37881424	1.48491025	-7.10895171
6	0.04010039	1.44229876	-5.77594023
1	-1.30704943	-1.56803807	-4.89561049
1	-2.04705231	-1.47697699	-7.26747760
6	-1.56246955	0.47941069	-9.11203432
1	-0.10823029	2.34281165	-7.72735132
1	0.64099978	2.24235427	-5.34531020
1	2.88984627	-3.79584511	6.97082497
1	1.66132017	-4.97163935	7.45739052
1	2.69121376	-5.30794709	6.05131113
1	-0.97832339	-0.23497583	-9.71239239
1	-2.62041563	0.20229414	-9.22186569
1	-1.42013300	1.47632703	-9.54803519
1	-0.66280832	-0.57537835	1.73842206

Energy = -8524.653379 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 24

Atomic N.	X	Y	Z
8	4.23383440	-1.68293499	-0.07147461
8	3.96087673	-1.18344324	2.98697769
6	2.99674703	-1.75615302	3.86467005
1	2.17438249	-2.25582806	3.32066460
1	2.54443043	-1.00883071	4.53723377
1	3.49932318	-2.51516111	4.48938422
8	6.27738341	-1.42271317	0.71811013
6	5.28132252	-2.22005270	0.28013329
6	5.47069278	-3.72039544	0.26155273
1	6.42559908	-3.98283646	-0.22170242
1	4.65699018	-4.11685033	-0.35663335
6	5.40978198	-4.32976517	1.68120863
1	4.56805415	-3.87572450	2.22573259
1	5.18531141	-5.40165838	1.57754719
6	6.70696271	-4.16574397	2.48018256
1	7.51078305	-4.73341074	1.97870205
1	6.57575284	-4.62804084	3.47048231
6	7.16407171	-2.71331893	2.66236561
1	6.40882954	-2.12973764	3.21357189
1	8.08754889	-2.70131857	3.26356978
6	7.46583672	-1.98122651	1.35960011
1	8.00236315	-2.61791768	0.63748151
1	8.07409771	-1.08847791	1.54626094
50	3.58541305	0.36938184	1.69156001
7	0.17339718	-0.42322814	-1.83226553
6	0.63515700	-0.26960807	-3.21300675
1	0.56214665	-1.21329358	-3.79924473
1	0.05778795	0.50850524	-3.72668830
1	1.68736039	0.04294610	-3.20241328
7	-2.10878599	1.36978292	-2.36419210
6	-1.21609352	-0.87559159	-1.76444997
1	-1.31501835	-1.93733327	-2.09733293

1	-1.53835226	-0.84859226	-0.71201825
6	-2.21474641	-0.07757427	-2.60547905
1	-3.22069798	-0.46985559	-2.36700016
1	-2.04545858	-0.24065227	-3.67737870
16	-3.22957809	2.36334716	-3.14615258
7	1.46259675	-0.21404771	1.07553275
6	1.05375965	-1.35726592	-1.12058639
1	0.90329535	-2.39855676	-1.49517340
1	2.09218411	-1.08725301	-1.35477638
6	0.91414091	-1.40203346	0.40472715
1	1.46936017	-2.29224172	0.74462459
1	-0.13009423	-1.56330528	0.71439189
16	0.62408641	0.49771619	2.26630564
8	1.75268718	1.20608263	3.02051413
8	-0.28409320	-0.37744417	3.04254372
6	-0.40036662	1.84616915	1.62641928
6	-1.53718766	2.21394892	2.34829225
6	-2.27219927	3.32739277	1.93469323
6	-1.89260862	4.07353289	0.80836119
6	-0.76237014	3.65573549	0.08132465
6	-0.01091277	2.55206176	0.48499715
1	-1.83105173	1.63642098	3.22384723
1	0.85720887	2.22620165	-0.08744786
1	-0.47617876	4.19803377	-0.82083212
6	-2.66320811	5.29712701	0.38350540
1	-3.15301825	3.62775480	2.50556049
8	-2.95307037	3.72855296	-2.65796816
8	-3.16468368	2.01518219	-4.57757370
6	-4.87244624	1.88761725	-2.55246541
6	-5.70393084	1.12000777	-3.36852010
6	-6.96793479	0.75364053	-2.89863282
6	-7.41028769	1.14207407	-1.62613823
6	-6.54777481	1.91074631	-0.82384930
6	-5.28560928	2.28790183	-1.27721060
1	-5.36308805	0.83120942	-4.36210761
1	-7.62267222	0.15641577	-3.53577922
6	-8.78546240	0.76908121	-1.13278437
1	-6.87488471	2.22274913	0.16981585
1	-4.62923995	2.89647738	-0.65482390
1	-3.56983230	5.42970541	0.98798978
1	-2.04777204	6.20236983	0.49745211
1	-2.94791612	5.23052947	-0.67586007
1	-9.47099918	1.62772226	-1.20360875
1	-9.21598245	-0.04898001	-1.72399449
1	-8.76219838	0.46052512	-0.07856028
1	-2.01375165	1.64374800	-1.38176427

Energy = -8524.636834 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 25

Atomic N.	X	Y	Z
8	4.09593987	0.32594162	-2.32120941
8	1.82178356	2.30022361	-0.91324415
6	1.46520485	2.82238129	-2.19288506
1	0.37166761	2.83374448	-2.34851044
1	1.91512430	2.24758686	-3.01946213
1	1.82866588	3.86256107	-2.25787340

8	5.27047019	1.86710961	-3.38593515
6	4.95260889	1.18879439	-2.24601913
6	5.66200627	1.54864036	-0.95178129
1	6.75429591	1.47190021	-1.08402128
1	5.36293442	0.77441676	-0.23523044
6	5.29458533	2.94744543	-0.40980027
1	4.20306605	3.08053263	-0.48610870
1	5.53941480	2.96575615	0.66333829
6	6.03755420	4.09679628	-1.09847645
1	7.11911727	3.99344492	-0.90028048
1	5.73148719	5.04999405	-0.63981837
6	5.82685811	4.17827651	-2.61444153
1	4.77084190	4.38142163	-2.85496689
1	6.40681368	5.02708312	-3.01234397
6	6.26038579	2.93128810	-3.38043711
1	7.22315844	2.54340361	-3.00866656
1	6.37812640	3.15906575	-4.44696400
50	1.66976472	0.31841614	-0.36945649
7	0.20552263	1.46970327	1.75467141
6	1.11010813	2.51293903	2.26578070
1	0.57576327	3.23284067	2.91608350
1	1.91457915	2.04906862	2.85287165
1	1.55730305	3.04578323	1.41593694
7	0.16430493	-1.73183854	2.17846851
6	-0.33240638	0.64904990	2.87048646
1	-0.34297917	1.25514659	3.79569794
1	-1.37627606	0.38579356	2.65373475
6	0.46041561	-0.63923693	3.11809941
1	0.27137666	-1.01850152	4.13183054
1	1.54059335	-0.42818369	3.05878460
16	-0.81193743	-3.02016768	2.67352358
7	-0.61932545	0.13347477	-0.54483757
6	-0.86582615	2.06725257	0.92942139
1	-1.59032662	2.63132511	1.55148426
1	-0.37320308	2.77085491	0.24394876
6	-1.60380529	1.00820451	0.10257366
1	-2.22469921	1.53199403	-0.64227513
1	-2.28545529	0.41819414	0.74045415
16	-0.76719769	-0.19909934	-2.13767607
8	0.68497351	-0.47294634	-2.49964920
8	-1.52081292	0.81054940	-2.91706943
6	-1.64104700	-1.76813671	-2.33495955
6	-2.85023781	-1.79039022	-3.02980799
6	-3.54094520	-2.99960402	-3.14865057
6	-3.04049980	-4.18067387	-2.58186639
6	-1.81879902	-4.12540442	-1.88696836
6	-1.11529305	-2.93024851	-1.76238478
1	-3.23242077	-0.87132640	-3.47206511
1	-0.17096611	-2.90653212	-1.21902006
1	-1.41765236	-5.02598884	-1.41998761
6	-3.78012519	-5.48719229	-2.72275675
1	-4.48656820	-3.02322516	-3.69354177
8	-0.77839307	-3.97351968	1.54934784
8	-0.36576933	-3.37550379	4.03444482
6	-2.51529445	-2.42173891	2.81324578
6	-3.01166524	-2.03979114	4.06126828
6	-4.31871758	-1.55646623	4.15377428
6	-5.13740988	-1.45367553	3.01872198

6	-4.61180649	-1.85106545	1.77701550
6	-3.30946258	-2.33663129	1.66523479
1	-2.38380193	-2.14272216	4.94577047
1	-4.71187375	-1.26042916	5.12813765
6	-6.55837302	-0.96112379	3.13001298
1	-5.23358865	-1.78165769	0.88236538
1	-2.91127754	-2.65420714	0.70114812
1	-4.80536830	-5.33231582	-3.08226342
1	-3.27050813	-6.14947165	-3.43935152
1	-3.82411392	-6.02462056	-1.76521360
1	-7.26014896	-1.80748254	3.19112994
1	-6.70196064	-0.34890177	4.02962524
1	-6.84548374	-0.36484430	2.25348776
1	-0.08299351	-1.43353366	1.22635629

Energy = -8524.638053 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 26

Atomic N.	X	Y	Z
8	2.60122680	-0.53692606	1.28301080
8	0.14059285	0.45883997	-0.24130747
6	-0.31909920	-0.87556523	-0.06772260
1	-1.23095772	-1.04060777	-0.67062053
1	-0.56032265	-1.09861071	0.98560029
1	0.44411386	-1.60183475	-0.39657861
8	3.79544399	-1.92102759	0.05306739
6	3.48597327	-0.65917263	0.44420812
6	4.21773424	0.51157412	-0.17663490
1	5.30592162	0.36912007	-0.07015463
1	3.94164747	1.38793056	0.42251970
6	3.85675286	0.74304995	-1.66115746
1	2.76722953	0.66346808	-1.79470542
1	4.11129266	1.78293813	-1.91097539
6	4.58815351	-0.19036424	-2.62959484
1	5.67182034	0.01523130	-2.57630726
1	4.27696138	0.05024368	-3.65699023
6	4.36357397	-1.68454821	-2.37090936
1	3.30493829	-1.95361448	-2.51835986
1	4.93815437	-2.26815957	-3.10861403
6	4.79003579	-2.16287211	-0.98600839
1	5.75422789	-1.72485748	-0.68227886
1	4.89313336	-3.25457181	-0.96889821
50	0.90296346	1.72183853	1.26378806
7	-1.38564716	2.97528584	1.09836008
6	-1.34751211	3.94629732	2.21397235
1	-2.34390972	4.39320607	2.38587904
1	-1.01167343	3.46132569	3.13795855
1	-0.64047440	4.74792231	1.96548747
7	-0.50479389	0.86273123	2.72992102
6	-2.31864565	1.86303755	1.38701105
1	-3.35829307	2.23626194	1.47801805
1	-2.27568721	1.17376080	0.53472866
6	-1.95173382	1.10717994	2.67210203
1	-2.52188743	0.16036351	2.66735415
1	-2.27476563	1.67718366	3.55752670
16	0.17465554	0.71708149	4.23108961
7	-0.55364463	2.45703259	-1.90154943

6	-1.76360377	3.72267174	-0.13274922
1	-2.74758223	4.20500945	0.03906254
1	-1.01914982	4.52092650	-0.26201866
6	-1.85846269	2.94652812	-1.44824013
1	-2.22878296	3.66720655	-2.19177110
1	-2.60446220	2.13577680	-1.38027992
16	-0.27369503	2.38936995	-3.55755647
8	1.09759064	1.86018173	-3.69814301
8	-0.67243973	3.69178740	-4.13073049
6	-1.40531333	1.14617115	-4.23577120
6	-2.53415545	1.55223308	-4.94706324
6	-3.40526446	0.58311033	-5.45343864
6	-3.16489582	-0.78364109	-5.25576722
6	-2.01599161	-1.16367927	-4.53848115
6	-1.13669201	-0.21115357	-4.02859351
1	-2.70814233	2.61441800	-5.11618208
1	-0.23977991	-0.51130260	-3.48638146
1	-1.80610400	-2.22385669	-4.38326955
6	-4.11195553	-1.82770654	-5.79271407
1	-4.28470199	0.89729302	-6.01859983
8	1.62260294	0.98059878	3.99708688
8	-0.56744743	1.50299841	5.24979592
6	0.01187226	-1.02427591	4.69432235
6	-0.84721907	-1.38521309	5.73117920
6	-0.96717874	-2.73493896	6.07571121
6	-0.23810681	-3.72237087	5.39941328
6	0.62172280	-3.32590625	4.35869675
6	0.75400626	-1.98634696	3.99986595
1	-1.40024148	-0.61237436	6.26378341
1	-1.63634133	-3.02270851	6.88884935
6	-0.35323766	-5.17651832	5.78441245
1	1.19967575	-4.08090276	3.82171667
1	1.42780068	-1.68669416	3.19572987
1	-4.87312249	-1.38084805	-6.44449634
1	-3.57427878	-2.59467446	-6.36832103
1	-4.63223974	-2.34637510	-4.97312565
1	0.57872242	-5.53580810	6.24701104
1	-1.16774636	-5.33807983	6.50191413
1	-0.53917951	-5.80878095	4.90431057
1	-0.26397887	1.55770372	-1.43140325

Energy = -8524.652040 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 27

Atomic N.	X	Y	Z
8	4.02652927	0.48115620	-2.32916204
8	1.82911520	2.36998647	-0.73649084
6	1.40815889	2.98720849	-1.95227657
1	1.83078876	2.48984012	-2.84119536
1	1.75107670	4.03631196	-1.94715822
1	0.30875260	2.99016687	-2.06192722
8	5.10693834	2.10474955	-3.37023301
6	4.87713554	1.35053398	-2.25757760
6	5.67222580	1.63716653	-0.99533690
1	6.75259808	1.57981397	-1.21033552
1	5.42959813	0.81651565	-0.30986329
6	5.33516780	2.99560091	-0.34252813

1	4.24036689	3.12355318	-0.33682521
1	5.65202676	2.94899424	0.71065491
6	6.02347965	4.19276396	-1.00596321
1	7.11663002	4.08663130	-0.88979662
1	5.74576925	5.11228080	-0.46745298
6	5.70686907	4.36811306	-2.49527685
1	4.63593236	4.57819134	-2.64785461
1	6.25466721	5.24480039	-2.87805198
6	6.08943234	3.17588087	-3.36801774
1	7.07842898	2.77397832	-3.09254125
1	6.12832084	3.47182726	-4.42354742
50	1.67758183	0.35541545	-0.33172954
7	0.21288453	1.35624876	1.89002776
6	1.11891721	2.36418605	2.46457967
1	0.58652388	3.04181672	3.16055840
1	1.92458224	1.86403007	3.01927621
1	1.56504676	2.94971427	1.64953791
7	0.20801564	-1.86236017	2.12338960
6	-0.32288481	0.46691590	2.95201931
1	-0.34719377	1.01757461	3.91140229
1	-1.36194457	0.20485551	2.71206829
6	0.48302698	-0.82476471	3.12931042
1	0.28996165	-1.26652156	4.11661871
1	1.56119791	-0.59914254	3.09243425
16	-0.76591567	-3.18416572	2.52644300
7	-0.61049294	0.18484986	-0.50023333
6	-0.86053593	2.00593774	1.10867541
1	-1.58618163	2.52441538	1.76819776
1	-0.37120146	2.75695054	0.47300130
6	-1.59707924	1.00476121	0.21154610
1	-2.22389834	1.57663189	-0.49195755
1	-2.27295630	0.36738236	0.80878386
16	-0.77341625	-0.05814563	-2.10691760
8	0.67797594	-0.29433186	-2.49855375
8	-1.54762550	0.98425063	-2.82003591
6	-1.62944376	-1.62507140	-2.38387946
6	-2.85642395	-1.62273164	-3.04720256
6	-3.53240055	-2.83303649	-3.22516829
6	-2.99977149	-4.03958404	-2.74840365
6	-1.76093174	-4.00874974	-2.08297696
6	-1.07200459	-2.81257136	-1.90033871
1	-3.26309819	-0.68388657	-3.42082503
1	-0.11350297	-2.80754076	-1.38184901
1	-1.33465678	-4.93057365	-1.68486883
6	-3.72341857	-5.34635781	-2.95445460
1	-4.49175828	-2.83745082	-3.74600231
8	-0.71002287	-4.06767996	1.34744403
8	-0.33532982	-3.61824109	3.86943924
6	-2.47580210	-2.60751594	2.67814044
6	-2.99579552	-2.31479705	3.94061430
6	-4.30869468	-1.84988702	4.04372310
6	-5.11004536	-1.67770249	2.90465083
6	-4.56079327	-1.98580400	1.64796875
6	-3.25231839	-2.45197468	1.52548196
1	-2.38106536	-2.47178804	4.82640666
1	-4.72015184	-1.62356084	5.02915590
6	-6.53747230	-1.20647763	3.02550869
1	-5.16859325	-1.86139149	0.74967207

1	-2.83616906	-2.70057952	0.54874074
1	-4.76168779	-5.18558909	-3.27149082
1	-3.22656164	-5.95007808	-3.72941221
1	-3.72895089	-5.94762089	-2.03467965
1	-7.23032420	-2.06231607	3.03459004
1	-6.69745937	-0.64404170	3.95443571
1	-6.82177564	-0.56803876	2.17831051
1	-0.02797248	-1.50993153	1.18758421

Energy = -8524.638073 Hartree
Number of imaginary frequencies = 0.

Compound I2a isomer 28

Atomic N.	X	Y	Z
8	3.74766207	2.38998479	0.54909983
8	0.93041004	0.90883542	-0.84731943
6	1.80318488	0.74485550	-1.97863521
1	2.44836003	-0.13262149	-1.81750828
1	2.46211617	1.61650509	-2.13443111
1	1.20402387	0.60378743	-2.89077211
8	4.63336736	0.44969841	-0.01474192
6	4.48821036	1.45422441	0.86429695
6	5.27032925	1.45263645	2.15864936
1	4.92969844	0.59739150	2.76388822
1	4.96281140	2.36198990	2.68718813
6	6.80311813	1.41722682	1.98616878
1	7.10455906	2.12084268	1.19314840
1	7.25017727	1.79589997	2.91742957
6	7.37005726	0.02222719	1.70249911
1	7.12692398	-0.63590487	2.55421896
1	8.46884114	0.07892689	1.65821985
6	6.84650368	-0.62408308	0.41600135
1	7.17456456	-0.05577466	-0.46972822
1	7.28028178	-1.63241555	0.31544010
6	5.33130383	-0.77749684	0.35819179
1	4.90534913	-1.14917539	1.30118956
1	5.04446533	-1.46924090	-0.44291942
50	1.16172096	2.59924566	0.33912650
7	-1.57389177	2.85983943	0.94383990
6	-1.62272439	4.32667570	1.10096099
1	-2.59290437	4.65370623	1.52186490
1	-0.81974278	4.66989818	1.76565703
1	-1.47840383	4.80421242	0.12356403
7	0.73401316	1.57244475	2.24391876
6	-1.66313318	2.20117929	2.26769623
1	-2.45473708	2.68138400	2.87860046
1	-1.95075121	1.15363020	2.11363091
6	-0.33034446	2.22103244	3.02207774
1	-0.45258835	1.72777816	3.99801138
1	-0.03033721	3.25849745	3.24952392
16	1.32224146	0.14579311	2.83149722
7	-1.75770139	0.73921005	-1.56755212
6	-2.70518421	2.45557157	0.06947629
1	-3.65492678	2.59907023	0.62678227
1	-2.73132838	3.13424031	-0.79255486
6	-2.67103011	1.01391336	-0.45884458
1	-3.69276486	0.76197984	-0.78115349
1	-2.42428833	0.30176057	0.34283585

16	-2.21376421	1.18267061	-3.11414695
8	-0.97162794	1.19546153	-3.91492026
8	-3.11646582	2.35961961	-3.08915972
6	-3.22365999	-0.21473913	-3.66507692
6	-4.59167129	-0.04250551	-3.86925042
6	-5.35490801	-1.12541362	-4.31666037
6	-4.76703183	-2.37228440	-4.56840539
6	-3.38312579	-2.51475419	-4.35663595
6	-2.60949957	-1.44733647	-3.90861010
1	-5.04163349	0.93272442	-3.68702650
1	-1.53625956	-1.55915923	-3.75532624
1	-2.90656058	-3.47758874	-4.55117551
6	-5.58670531	-3.53100646	-5.07874315
1	-6.42667914	-0.99451971	-4.47708179
8	2.51844406	-0.17764831	2.01314533
8	1.44068800	0.20256342	4.31044167
6	0.09510658	-1.14684659	2.48145530
6	-0.58084364	-1.76048762	3.53635655
6	-1.52308406	-2.75450766	3.25505763
6	-1.79282112	-3.14583538	1.93592511
6	-1.09538385	-2.50821145	0.89378378
6	-0.15455947	-1.51304421	1.15487901
1	-0.35736651	-1.46377564	4.56058133
1	-2.05496644	-3.23610113	4.07807895
6	-2.78731037	-4.24047874	1.63799376
1	-1.29850326	-2.79148292	-0.14131148
1	0.37130662	-1.00328683	0.34314736
1	-6.66166019	-3.34483194	-4.96014581
1	-5.39411964	-3.70523433	-6.14864585
1	-5.33635935	-4.46186173	-4.55085173
1	-2.27277119	-5.19527071	1.44714941
1	-3.47512007	-4.39824438	2.47884194
1	-3.38053211	-4.00983173	0.74244471
1	-0.72806336	0.84386654	-1.38464128

Energy = -8524.647948 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 29

Atomic N.	X	Y	Z
8	5.51285857	-1.09468059	-1.11483398
8	4.39935671	1.83862272	-0.57235744
6	3.84649917	2.89516174	-1.34516963
1	3.09042685	3.47392028	-0.78419659
1	3.37126153	2.53996821	-2.27640359
1	4.65766823	3.59291150	-1.61866226
8	5.43855606	-0.45974584	-3.23048910
6	6.11524087	-0.62104342	-2.07301925
6	7.56324471	-0.18553325	-1.98333493
1	8.15778780	-0.65374821	-2.78503203
1	7.92727497	-0.57165947	-1.02454511
6	7.71811561	1.35150516	-2.03708222
1	6.93824384	1.80788392	-1.40649384
1	8.68681793	1.60844608	-1.58300197
6	7.67321634	1.92420575	-3.45785874
1	8.52845309	1.52343913	-4.03043228
1	7.81954987	3.01450153	-3.41122603
6	6.38322634	1.62618011	-4.23113814

1	5.51644032	2.11064629	-3.75564470
1	6.46483348	2.05597841	-5.24296285
6	6.06739330	0.14387071	-4.39791379
1	6.96227250	-0.43688471	-4.67503047
1	5.31145175	-0.00158323	-5.17854889
50	3.37584541	0.18647136	0.07389529
7	-0.20001015	1.05527765	2.52937322
6	0.41949728	0.76004781	3.82085957
1	0.32295297	1.59470397	4.55076472
1	-0.02906327	-0.13941771	4.26098576
1	1.48711445	0.55503483	3.66875043
7	-2.35106312	-1.01365434	2.61420820
6	-1.62255934	1.36498695	2.66330313
1	-1.78042459	2.28823547	3.27144787
1	-2.02032013	1.58397176	1.65945892
6	-2.48571861	0.27831996	3.30599404
1	-3.52662743	0.65177308	3.29502361
1	-2.20808460	0.12016975	4.35587107
16	-3.39515857	-2.25535078	3.09914794
7	1.24682914	1.10908789	-0.24681415
6	0.48727258	2.15862432	1.84464477
1	0.12635256	3.14590174	2.21119703
1	1.55672846	2.10642679	2.09884885
6	0.36208568	2.13041515	0.31661652
1	0.62201036	3.13166984	-0.06980984
1	-0.68821997	1.94616970	0.03042605
16	0.98216990	0.54309184	-1.72749510
8	2.28268162	-0.25597684	-1.93748494
8	0.61719935	1.51135627	-2.78665925
6	-0.34179337	-0.69029288	-1.68291351
6	-1.28193079	-0.73057603	-2.71363194
6	-2.27619819	-1.71118800	-2.68579172
6	-2.34119347	-2.65043312	-1.64473688
6	-1.39028674	-2.57438715	-0.61098968
6	-0.39325501	-1.59945808	-0.62302367
1	-1.22584986	0.00024816	-3.51943727
1	0.32835609	-1.53379297	0.19221075
1	-1.44657695	-3.27571310	0.22261755
6	-3.38861781	-3.73545768	-1.63853803
1	-3.01305818	-1.74790728	-3.49064381
8	-3.13978025	-3.36894443	2.16387891
8	-3.22182380	-2.39377877	4.55618863
6	-5.08525371	-1.67368037	2.81216239
6	-5.83823038	-1.18718563	3.88176418
6	-7.13652277	-0.72824949	3.64585819
6	-7.69184744	-0.74940724	2.35818500
6	-6.90894105	-1.24393362	1.29991859
6	-5.61274688	-1.70678467	1.51731624
1	-5.41126914	-1.18723284	4.88403978
1	-7.72955845	-0.34987789	4.48037609
6	-9.10467006	-0.28267849	2.11432841
1	-7.32564729	-1.27198300	0.29136527
1	-5.01742199	-2.10454616	0.69524615
1	-3.02530270	-4.62499047	-2.17684047
1	-3.62783502	-4.05103395	-0.61442527
1	-4.31055962	-3.40809525	-2.13819291
1	-9.79342570	-1.14008730	2.06007218
1	-9.45597933	0.37280128	2.92131437

1 -9.18901306 0.26066792 1.16340103
 1 -2.33544689 -0.95172080 1.59174555
 Energy = -8524.631699 Hartree
 Number of imaginary frequencies = 0.

Compound I2a isomer 30

Atomic N.	X	Y	Z
8	2.94391638	-0.02299084	0.37679715
8	3.59251579	-3.14815273	1.07021503
6	3.85326384	-3.36335983	2.45173954
1	3.01505505	-3.85338249	2.97634953
1	4.07996600	-2.41662648	2.97605462
1	4.73532523	-4.01876445	2.54091281
8	3.60558012	1.96679264	-0.27008463
6	3.34909097	0.67412132	-0.55398704
6	3.60393315	0.15055145	-1.94878632
1	2.98779922	0.72149137	-2.66073461
1	3.23404518	-0.88233725	-1.95921000
6	5.09034468	0.19005345	-2.36579820
1	5.71727911	-0.15889986	-1.52993599
1	5.22665246	-0.54149743	-3.17585766
6	5.56183724	1.56265828	-2.85696797
1	4.98336554	1.83258832	-3.75713693
1	6.61371594	1.49251253	-3.17438368
6	5.41945317	2.68850260	-1.82736980
1	6.07624862	2.51345497	-0.95966838
1	5.75152395	3.63637039	-2.28130848
6	3.99844385	2.90496686	-1.31986242
1	3.25111484	2.87103393	-2.12623296
1	3.91356691	3.87503723	-0.81581332
50	1.87797410	-2.43872355	0.25871655
7	0.40645425	1.50024074	2.23693465
6	1.50525900	2.39681854	2.59431265
1	1.30068194	2.96409518	3.52814022
1	2.42952773	1.82241551	2.73323796
1	1.68296464	3.10941707	1.77914750
7	0.86402243	-1.69691232	2.14876644
6	0.19882096	0.47561118	3.27034475
1	0.27693826	0.93109939	4.28280603
1	-0.82347568	0.08257146	3.18044764
6	1.18586907	-0.70118269	3.18331184
1	1.24103357	-1.19570435	4.16719489
1	2.19412361	-0.32417726	2.96171957
16	0.01937496	-3.02035864	2.59811221
7	-0.83394892	0.95161941	-0.22071975
6	-0.81762187	2.23543598	1.90254129
1	-1.42744448	2.48496384	2.79666068
1	-0.52787416	3.18274654	1.42673802
6	-1.66489617	1.43649222	0.90090245
1	-2.48465256	2.05879758	0.51897582
1	-2.11289398	0.55137695	1.37697412
16	-0.68348755	1.95744436	-1.57429983
8	0.65882385	1.66136303	-2.13335299
8	-1.07555575	3.35609398	-1.28161867
6	-1.92338133	1.28327251	-2.69984352
6	-2.93663597	2.11334990	-3.17499974
6	-3.86888809	1.59532644	-4.07878512

6	-3.79652224	0.26439859	-4.51259750
6	-2.76195259	-0.54849609	-4.01319034
6	-1.82476148	-0.04929733	-3.11270185
1	-2.98725791	3.14747881	-2.83626992
1	-1.02588114	-0.68300969	-2.72764611
1	-2.69225231	-1.58889532	-4.33610939
6	-4.78852298	-0.28507870	-5.50658448
1	-4.66646219	2.24000828	-4.45223017
8	0.34236690	-3.97541238	1.46183399
8	0.24514033	-3.45733264	3.99450966
6	-1.75915194	-2.69835739	2.45231284
6	-2.55889125	-2.73817285	3.59404794
6	-3.92690551	-2.47682974	3.47629442
6	-4.50604509	-2.18376597	2.23361455
6	-3.67428177	-2.15178406	1.09954701
6	-2.30813381	-2.40455069	1.20057969
1	-2.10775972	-2.97886038	4.55592817
1	-4.55521006	-2.50636597	4.36845709
6	-5.98788164	-1.93374783	2.10570376
1	-4.10429862	-1.92106182	0.12287928
1	-1.67202859	-2.37326166	0.31548594
1	-5.66599895	0.36704226	-5.60066043
1	-4.33165717	-0.37590357	-6.50414111
1	-5.13115130	-1.28820190	-5.21717066
1	-6.50360406	-2.82848008	1.72364983
1	-6.43733588	-1.68138255	3.07463140
1	-6.19674205	-1.11579013	1.40247566
1	0.11803389	0.77749383	0.14605478

Energy = -8524.642039 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 31

Atomic N.	X	Y	Z
8	3.67303917	-1.04920774	-1.80927660
8	2.24886136	1.79213356	-0.79451112
6	2.33822023	2.23959396	-2.14756005
1	2.65619146	1.43881500	-2.83494784
1	3.08362448	3.05211982	-2.19243580
1	1.37694299	2.63865720	-2.51672898
8	5.53765919	-0.24294639	-2.68094236
6	4.80167841	-0.63868034	-1.60331460
6	5.41061688	-0.53513893	-0.21564134
1	6.36617881	-1.08479657	-0.18173106
1	4.70895514	-1.05537552	0.44716907
6	5.62040130	0.91820694	0.26297181
1	4.71965892	1.50531075	0.01988702
1	5.69690935	0.90139168	1.36094019
6	6.87786729	1.58537595	-0.30351716
1	7.76637146	1.03915050	0.05941115
1	6.95856940	2.60592513	0.10208828
6	6.93610293	1.64698141	-1.83386196
1	6.11982978	2.26966112	-2.23431292
1	7.87762007	2.13301980	-2.13779822
6	6.88232846	0.28657954	-2.52377092
1	7.51680929	-0.45319220	-2.00842458
1	7.23374716	0.36867876	-3.55958854
50	1.26912834	0.08579188	-0.19459108

7	0.27224463	1.88094878	1.63728316
6	1.39282422	2.72986152	2.08826627
1	1.02472271	3.63102526	2.61537440
1	2.04634820	2.17062689	2.76829617
1	1.98118834	3.02170813	1.20936060
7	0.30518393	-0.96769503	3.20997475
6	-0.53334712	1.40716176	2.78934365
1	-0.83307859	2.28472671	3.39997450
1	-1.45334666	0.95267282	2.40040683
6	0.16228928	0.40011155	3.71515879
1	-0.40663389	0.33588390	4.65359532
1	1.16222709	0.75978208	4.00112790
16	-0.82863932	-2.14946925	3.62258823
7	-0.84862081	0.69366233	-0.68344179
6	-0.57715863	2.67322135	0.70875201
1	-1.12017038	3.46508189	1.26364794
1	0.10829349	3.15443625	-0.00208535
6	-1.56777164	1.81471897	-0.08378144
1	-2.02014445	2.45906080	-0.85567600
1	-2.38520774	1.44860941	0.56119848
16	-0.94111406	0.38412512	-2.27749143
8	0.37481846	-0.34311124	-2.49439725
8	-1.28387301	1.55465674	-3.11777827
6	-2.22680074	-0.85440006	-2.56994199
6	-3.47408919	-0.44560614	-3.04326132
6	-4.47586101	-1.40117713	-3.23334353
6	-4.24646608	-2.75857104	-2.96341285
6	-2.97376839	-3.14198736	-2.50398857
6	-1.96497914	-2.20153026	-2.30364310
1	-3.64465679	0.60407496	-3.27992405
1	-0.97461725	-2.50684732	-1.96639697
1	-2.76854874	-4.19551923	-2.30534784
6	-5.33567605	-3.78472393	-3.14983404
1	-5.45060235	-1.08579453	-3.61014585
8	-0.37732454	-3.35938358	2.91287760
8	-0.97117550	-2.08690289	5.09032107
6	-2.43317829	-1.67157672	2.93272650
6	-3.40135094	-1.11199674	3.76814228
6	-4.63027560	-0.73079957	3.22341786
6	-4.90468323	-0.90458348	1.85886531
6	-3.91178747	-1.47543329	1.04256175
6	-2.68037945	-1.85983096	1.56939982
1	-3.19259787	-0.99717786	4.83118623
1	-5.39149940	-0.29594344	3.87378279
6	-6.24024793	-0.51340805	1.27763514
1	-4.10321769	-1.62008986	-0.02231241
1	-1.92036768	-2.31008930	0.93123227
1	-6.16038719	-3.38959814	-3.75640025
1	-4.95144212	-4.69155347	-3.63670383
1	-5.75277412	-4.09336376	-2.17858916
1	-6.85650286	-1.40395354	1.07974271
1	-6.80234185	0.13471865	1.96190746
1	-6.11921573	0.01283200	0.32059273
1	0.62846927	-1.06964600	2.23964436

Energy = -8524.639620 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 32

Atomic N.	X	Y	Z
8	2.94923177	0.04390302	0.37480824
8	3.66045482	-3.08953818	0.97298202
6	3.94306295	-3.31038107	2.34904757
1	4.19669977	-2.36744638	2.86791373
1	4.81447980	-3.98182132	2.42214531
1	3.10637134	-3.78506911	2.89004417
8	3.54768192	2.07046602	-0.21770387
6	3.32950828	0.77906131	-0.53698892
6	3.59551284	0.30284362	-1.94660193
1	2.95765574	0.87244925	-2.64024631
1	3.26030443	-0.74113826	-1.98417092
6	5.07787312	0.40376469	-2.36756096
1	5.72020816	0.05447346	-1.54357382
1	5.23535723	-0.30109497	-3.19721491
6	5.50024689	1.80399502	-2.82430539
1	4.90805881	2.07737199	-3.71443985
1	6.55213002	1.77770531	-3.14834905
6	5.32592100	2.89729266	-1.76502162
1	5.99521073	2.72332784	-0.90667164
1	5.62094246	3.86767840	-2.19643992
6	3.90217127	3.05063560	-1.24262846
1	3.15081959	3.01442866	-2.04511007
1	3.78822732	4.00261775	-0.71063475
50	1.93138383	-2.38961883	0.18546016
7	0.37718905	1.45540388	2.28384153
6	1.45518606	2.36848906	2.66195736
1	1.24099670	2.90428662	3.61207880
1	2.39380068	1.81323773	2.78133749
1	1.61182983	3.10771110	1.86641167
7	0.90524814	-1.72448214	2.09635423
6	0.19997241	0.39705715	3.28859273
1	0.27645600	0.82430133	4.31335995
1	-0.81414847	-0.01573828	3.19486154
6	1.21187232	-0.75455585	3.15971061
1	1.28415901	-1.27794869	4.12742384
1	2.21014708	-0.34876049	2.94393237
16	0.08644547	-3.07676047	2.50746050
7	-0.86261142	0.93464261	-0.17867182
6	-0.86595126	2.16868782	1.97329850
1	-1.47684552	2.38223953	2.87600573
1	-0.60122114	3.13377290	1.51902203
6	-1.69949906	1.37390418	0.95687633
1	-2.53469370	1.98618542	0.59274513
1	-2.12495395	0.46801506	1.41415406
16	-0.74559467	1.96839047	-1.51397902
8	0.60850367	1.73184670	-2.07331239
8	-1.19093966	3.34553793	-1.19727199
6	-1.95465809	1.26909529	-2.65764769
6	-3.00185108	2.06618524	-3.11552660
6	-3.91038575	1.52987057	-4.03269825
6	-3.78150920	0.21336888	-4.49635521
6	-2.71441040	-0.56646768	-4.01294613
6	-1.80001160	-0.04855768	-3.09966118
1	-3.09619150	3.08945213	-2.75394567
1	-0.97565523	-0.65678195	-2.72729314
1	-2.60071808	-1.59558184	-4.35867984

6	-4.74817896	-0.35433793	-5.50490848
1	-4.73393855	2.14868829	-4.39329910
8	0.42595963	-3.99179959	1.34370442
8	0.32265445	-3.54902084	3.89060041
6	-1.69817408	-2.78524801	2.37230101
6	-2.49388586	-2.86346768	3.51471041
6	-3.86712510	-2.62611771	3.40525245
6	-4.45497452	-2.31923618	2.17021686
6	-3.62693301	-2.24886256	1.03496772
6	-2.25605545	-2.47712454	1.12782584
1	-2.03607494	-3.11558244	4.47049860
1	-4.49251018	-2.68626361	4.29790163
6	-5.94118255	-2.09217535	2.05017727
1	-4.06391735	-2.00765096	0.06391776
1	-1.62307411	-2.41673653	0.24206502
1	-5.65067639	0.26419328	-5.58846630
1	-4.28540543	-0.40614882	-6.50253228
1	-5.05147185	-1.37613961	-5.23775784
1	-6.43479976	-2.96456004	1.59470394
1	-6.40184398	-1.92468616	3.03202649
1	-6.16339565	-1.22635186	1.41087602
1	0.09553291	0.77667582	0.17904385

Energy = -8524.642008 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 33

Atomic N.	X	Y	Z
8	2.90364517	-0.95163461	3.24019790
8	2.96474436	-0.54636609	-1.10225461
6	3.38181296	-1.18382935	-2.30337624
1	2.54990035	-1.64011671	-2.86869696
1	4.11442905	-1.97713577	-2.06860149
1	3.87099332	-0.45601025	-2.97318101
8	4.91126587	-0.79011690	2.35514563
6	3.85134207	-0.22025676	2.96973987
6	3.86737770	1.25923542	3.29490992
1	4.77922051	1.49980546	3.86697655
1	3.00290556	1.43264579	3.94697566
6	3.77647286	2.17379636	2.05389052
1	2.97922235	1.80282768	1.38961990
1	3.45044696	3.16587994	2.39924072
6	5.08785199	2.31813026	1.27598290
1	5.83011313	2.82415398	1.91862023
1	4.92027451	2.98287759	0.41475657
6	5.67942173	0.99396889	0.77980682
1	4.98886049	0.49360071	0.07958166
1	6.60542145	1.20280781	0.21964423
6	6.03815807	0.01412573	1.89148215
1	6.50276446	0.51941232	2.75405375
1	6.73746825	-0.74734115	1.52628336
50	1.05767088	-0.04681327	-0.54314566
7	0.65662720	-2.52891441	0.46536061
6	1.87450147	-3.29663941	0.12478978
1	1.76555316	-4.35772097	0.41866736
1	2.06805064	-3.24331324	-0.95106782
1	2.73399628	-2.85933384	0.64544641
7	-0.10362901	-1.30559595	-1.94459758

6	-0.50799875	-3.02695273	-0.30768007
1	-0.62767992	-4.11793233	-0.15283539
1	-1.40473417	-2.52765942	0.08490824
6	-0.40684519	-2.72378435	-1.80316466
1	-1.37881844	-2.97979665	-2.26034491
1	0.35201626	-3.35924649	-2.29083204
16	-0.27442417	-0.54382186	-3.37816085
7	0.10096130	-0.38691515	2.74143154
6	0.40531156	-2.69654807	1.92412393
1	0.01131107	-3.71655434	2.10054857
1	1.37705437	-2.63348429	2.43248717
6	-0.54946890	-1.69932022	2.58305821
1	-0.84939827	-2.12121558	3.55668960
1	-1.46829482	-1.56855807	1.99058665
16	-0.69429717	0.73709692	3.73747776
8	0.34914030	1.72146360	4.09853423
8	-1.49411382	0.06115428	4.78440926
6	-1.86323085	1.51653594	2.60366935
6	-3.23155999	1.31955257	2.78820306
6	-4.13014195	1.96055527	1.93130103
6	-3.67777131	2.79618890	0.89933810
6	-2.29183377	2.96927907	0.73464488
6	-1.38224126	2.33788710	1.58020429
1	-3.57721859	0.68159643	3.60085770
1	-0.31002482	2.47711029	1.45009085
1	-1.92032879	3.60615087	-0.07022075
6	-4.65131765	3.52096329	0.00405527
1	-5.20226769	1.81272834	2.07303925
8	0.32331773	0.80208130	-3.08216378
8	0.21449592	-1.32067984	-4.54107092
6	-2.05417606	-0.31282793	-3.63557852
6	-2.64166736	-0.76639678	-4.81590015
6	-4.01393452	-0.58282498	-5.00842311
6	-4.80511593	0.04604057	-4.03721840
6	-4.18592342	0.48780155	-2.85379106
6	-2.81903910	0.31473721	-2.64728693
1	-2.02227517	-1.25648325	-5.56615510
1	-4.47682894	-0.93818158	-5.93092141
6	-6.28128271	0.26337496	-4.25761846
1	-4.78683325	0.97150502	-2.08096291
1	-2.34898099	0.65923085	-1.72512119
1	-4.79178877	4.55926318	0.34263544
1	-4.28690250	3.56688196	-1.03128106
1	-5.63727594	3.03802747	0.00766805
1	-6.48537780	1.30961211	-4.53364553
1	-6.66413567	-0.37313927	-5.06542170
1	-6.85795152	0.05135227	-3.34658158
1	1.07300768	-0.46797739	3.09616694

Energy = -8524.648984 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 34

Atomic N.	X	Y	Z
8	4.12495255	0.45052882	-0.03448348
8	3.04842615	-2.62519980	-0.11848075
6	4.42435311	-2.69579220	-0.46521234
1	4.70210672	-3.75613008	-0.59306493

1	5.06064634	-2.26504798	0.32761558
1	4.66420407	-2.17202663	-1.40879555
8	4.38008880	0.03053384	2.11854479
6	4.42242554	0.88489103	1.07833784
6	4.86221737	2.31675337	1.28822206
1	4.11795986	2.80891490	1.93581877
1	4.79058023	2.78968238	0.30218031
6	6.28029788	2.48480356	1.87058451
1	6.97472561	1.80116643	1.35548923
1	6.62013379	3.50360108	1.63088448
6	6.36665792	2.28414876	3.38725447
1	5.72952988	3.03920130	3.87912516
1	7.39708132	2.48368915	3.72063270
6	5.94017813	0.89337586	3.86779110
1	6.62601523	0.11950830	3.48564601
1	6.00892051	0.85437362	4.96721721
6	4.51488227	0.50577727	3.49248164
1	3.79730778	1.32222866	3.65987772
1	4.17950266	-0.35727274	4.07893313
50	1.90885491	-0.95721494	-0.52085989
7	0.12151072	-2.80820996	-0.16735430
6	0.35766653	-3.99155334	-1.01705425
1	-0.32213502	-4.82250895	-0.75155905
1	0.21874793	-3.73022266	-2.07232670
1	1.39832158	-4.30393709	-0.87188887
7	-1.00047315	-1.39556704	-2.57503545
6	-1.26464516	-2.29502807	-0.26487420
1	-1.94922531	-2.95636183	0.30373389
1	-1.28834250	-1.31011521	0.22429252
6	-1.85577212	-2.17517848	-1.67022785
1	-2.85896336	-1.72626274	-1.54448551
1	-1.99419487	-3.16320018	-2.12715242
16	-1.56603499	-1.13577754	-4.15679173
7	1.06384539	-0.80346243	1.55898398
6	0.43826243	-3.14551456	1.24649419
1	-0.24739163	-3.93428720	1.61353004
1	1.46503410	-3.53425593	1.24452577
6	0.35142492	-1.93233303	2.17225936
1	0.79486448	-2.20975016	3.14241487
1	-0.70774780	-1.67960711	2.36791836
16	0.79540194	0.66060191	2.24569797
8	1.66725302	1.62717991	1.52482573
8	0.85575792	0.57938846	3.72741834
6	-0.91546956	1.11890256	1.83539222
6	-1.94671511	0.88037171	2.74453715
6	-3.26390224	1.18198665	2.38076035
6	-3.56489204	1.72472937	1.12425803
6	-2.50422026	1.97364632	0.23347847
6	-1.18839844	1.67191317	0.57854253
1	-1.71083585	0.48594189	3.73249699
1	-0.36456502	1.88192886	-0.10504019
1	-2.71586055	2.41658992	-0.74213075
6	-4.98706505	2.03526912	0.72759998
1	-4.07068911	0.99886290	3.09315741
8	-0.52452539	-0.32845311	-4.81264773
8	-1.98668951	-2.45912458	-4.65331113
6	-3.04845012	-0.10852194	-4.01302584
6	-4.30564342	-0.70982534	-3.93662672

6	-5.43813286	0.09849818	-3.80402235
6	-5.33137693	1.49569645	-3.75051102
6	-4.05201367	2.07316232	-3.84364692
6	-2.91167608	1.28318401	-3.97296256
1	-4.39210057	-1.79358687	-4.00765846
1	-6.42393329	-0.36689288	-3.75124613
6	-6.55395506	2.36599031	-3.60274255
1	-3.95050832	3.16015882	-3.82641348
1	-1.92332130	1.73256361	-4.07041665
1	-5.66678250	1.96548858	1.58629934
1	-5.07089707	3.04612727	0.30360729
1	-5.34384322	1.33162863	-0.04054066
1	-6.59115699	3.13530801	-4.38719704
1	-7.47644992	1.77486194	-3.65852368
1	-6.54800136	2.89272203	-2.63628658
1	-0.64314292	-0.51765860	-2.18426383

Energy = -8524.644928 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 35

Atomic N.	X	Y	Z
8	2.95039500	-0.94659705	2.98015921
8	2.81189164	-0.15204572	-0.99174554
6	3.34764838	-0.61270044	-2.22596757
1	4.20248168	-1.28449766	-2.02872124
1	3.71140662	0.23480143	-2.83200233
1	2.61478895	-1.16383157	-2.84230336
8	5.09604623	-0.75503643	2.53566732
6	3.90834698	-0.19066856	2.85632301
6	3.80913599	1.30907653	3.03599157
1	4.54552416	1.63757681	3.78882055
1	2.81009427	1.49958568	3.44731623
6	4.01121462	2.10413933	1.72606102
1	3.45043896	1.61949969	0.91115006
1	3.56330779	3.09840437	1.86994545
6	5.47616526	2.27254804	1.31352328
1	6.00476084	2.85846532	2.08627628
1	5.52099339	2.86775761	0.38877059
6	6.22387863	0.95285187	1.09665876
1	5.76922705	0.37934595	0.27324140
1	7.26190275	1.16995651	0.79618249
6	6.28938619	0.05773912	2.32945486
1	6.49970439	0.63582952	3.24375841
1	7.07570749	-0.69840935	2.21732869
50	0.83365224	0.12660487	-0.52912043
7	0.67099868	-2.45549065	0.29028704
6	1.93080224	-3.10072291	-0.13775815
1	1.90415126	-4.18900730	0.06053805
1	2.09570722	-2.93725168	-1.20729953
1	2.76769324	-2.64914297	0.40654294
7	-0.13736626	-1.15938334	-2.05335061
6	-0.47623153	-2.96911559	-0.49706786
1	-0.54322790	-4.07118624	-0.39846375
1	-1.39147571	-2.53390395	-0.07106790
6	-0.40261841	-2.58922086	-1.97753181
1	-1.37313171	-2.85070580	-2.43541457
1	0.36728037	-3.17972406	-2.50282757

16	-0.31343353	-0.33471829	-3.44883546
7	0.09472240	-0.51197323	2.69207429
6	0.47011589	-2.75186345	1.73547259
1	0.11965586	-3.79702228	1.84204026
1	1.45314750	-2.69002687	2.22116918
6	-0.49861345	-1.84489705	2.49494810
1	-0.72624428	-2.33332657	3.45711292
1	-1.45168837	-1.73153404	1.95461980
16	-0.68817337	0.51665356	3.79245305
8	0.31743025	1.55206731	4.11642407
8	-1.36084062	-0.25163290	4.86460217
6	-1.98792749	1.25962909	2.78381420
6	-3.31720369	0.89492101	2.99954647
6	-4.31768726	1.49231415	2.22906752
6	-4.00608638	2.45122471	1.25335845
6	-2.65731588	2.79658258	1.05860800
6	-1.64658045	2.20869928	1.81677962
1	-3.55501850	0.16260272	3.77029352
1	-0.60341033	2.48146218	1.66494587
1	-2.39462962	3.53490033	0.29876608
6	-5.09331981	3.12324160	0.45259044
1	-5.35949674	1.21221725	2.39511096
8	0.21430787	1.02014778	-3.06911292
8	0.23548838	-1.02706285	-4.63788723
6	-2.09544586	-0.16470268	-3.73744935
6	-2.64723635	-0.62403627	-4.93209632
6	-4.02243420	-0.48624967	-5.14517487
6	-4.85083912	0.10247514	-4.18051377
6	-4.26619364	0.55407798	-2.98276206
6	-2.89836032	0.42499931	-2.75544550
1	-1.99830190	-1.07891587	-5.67961246
1	-4.45717968	-0.84436903	-6.08019906
6	-6.33242591	0.26018265	-4.41538741
1	-4.89533350	1.01281664	-2.21696386
1	-2.45439026	0.77873008	-1.82376886
1	-5.38174184	4.08038741	0.91438150
1	-4.75928364	3.34615879	-0.56981961
1	-5.99609220	2.50060368	0.39891176
1	-6.61000674	1.32312835	-4.48040402
1	-6.64430934	-0.22673030	-5.34777386
1	-6.91498333	-0.17404400	-3.58993767
1	1.09667847	-0.55265875	2.96269850

Energy = -8524.648736 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 36

Atomic N.	X	Y	Z
8	3.23639178	-2.36896080	3.20922960
8	3.51660706	0.10966164	-0.44328640
6	4.64471645	0.50159039	-1.21321103
1	5.36393789	1.06051268	-0.58769292
1	4.38771559	1.15098260	-2.07422423
1	5.16711185	-0.38579487	-1.61465731
8	5.43940028	-2.18468811	3.27865399
6	4.19085771	-1.65771433	3.47020400
6	4.06292251	-0.23132376	3.96803644
1	4.61494307	-0.11434397	4.91627880

1	2.99886797	-0.07869262	4.18181378
6	4.54130944	0.82678269	2.94966716
1	4.16670339	0.56577458	1.94652174
1	4.06261390	1.78010916	3.21540510
6	6.06012390	1.02088039	2.92196501
1	6.39278090	1.39481526	3.90691400
1	6.30963418	1.81004647	2.19545046
6	6.85861545	-0.24367548	2.58717412
1	6.62941102	-0.59448161	1.56784364
1	7.93560888	-0.00736744	2.60215190
6	6.63487816	-1.40484239	3.55236665
1	6.62304493	-1.06033095	4.59955117
1	7.43780213	-2.14604576	3.45095133
50	1.64797681	0.87558973	-0.94312781
7	0.96729891	-1.63292744	-0.87406758
6	1.87511871	-2.37158756	-1.77593557
1	1.79281340	-3.46183266	-1.61581749
1	1.63620608	-2.14610868	-2.82309447
1	2.90305742	-2.04823949	-1.57247966
7	-1.35825515	0.08364195	-2.07273159
6	-0.44396129	-2.00044238	-1.13751606
1	-0.51619028	-3.09808811	-1.26170470
1	-1.03372263	-1.74619013	-0.24556068
6	-1.09147758	-1.33507165	-2.35232580
1	-2.01307320	-1.89639554	-2.59174957
1	-0.43737734	-1.37905125	-3.23316462
16	-1.95544153	1.04874468	-3.34797505
7	0.82448467	0.36796565	1.02148588
6	1.32026322	-1.94169743	0.54523319
1	1.07304928	-2.99106772	0.78849014
1	2.40618446	-1.81440143	0.63435649
6	0.63457705	-0.99079957	1.52517986
1	1.11007759	-1.13821452	2.50670445
1	-0.43953774	-1.23547218	1.64022064
16	0.56544040	1.66451247	1.98365876
8	1.15485098	2.79620317	1.20669096
8	0.97510036	1.42191721	3.38788881
6	-1.22985069	1.92771522	2.01424415
6	-1.96945902	1.54641480	3.13339741
6	-3.35667102	1.72566039	3.12851416
6	-4.01305874	2.28254528	2.02235584
6	-3.24048217	2.66540491	0.91017602
6	-1.85766382	2.49161645	0.89773167
1	-1.45523060	1.13522767	4.00154916
1	-1.26992927	2.81076089	0.03622514
1	-3.72308668	3.12303367	0.04390054
6	-5.51003436	2.47146490	2.01775241
1	-3.93628974	1.43573941	4.00708895
8	-2.19517517	2.36708175	-2.73520711
8	-1.02904193	0.84322795	-4.47466620
6	-3.55686672	0.35434832	-3.81870862
6	-3.63433879	-0.53809790	-4.89023641
6	-4.87492353	-1.07838337	-5.23382449
6	-6.03779820	-0.73711889	-4.52563027
6	-5.92808174	0.16519004	-3.45362045
6	-4.69778679	0.71448745	-3.09568126
1	-2.73538681	-0.78389789	-5.45455770
1	-4.94147082	-1.77298215	-6.07308002

6	-7.37881498	-1.29604696	-4.92735169
1	-6.82314349	0.44812554	-2.89676318
1	-4.61991257	1.43162840	-2.27846520
1	-5.93776323	2.30621418	3.01469907
1	-5.78262181	3.48465671	1.68991506
1	-5.99629868	1.76740118	1.32457007
1	-7.86157893	-0.64633545	-5.67408010
1	-7.28102527	-2.29234114	-5.37759009
1	-8.05890369	-1.36588950	-4.06849343
1	-1.94077180	0.23926725	-1.24392896

Energy = -8524.644668 Hartree
Number of imaginary frequencies = 0.

Compound I2a isomer 37

Atomic N.	X	Y	Z
8	3.02228031	-2.68644519	0.29401785
8	0.83053337	1.41512690	-0.69463558
6	1.96973819	1.81375300	0.06676462
1	2.12053780	2.90342744	-0.02341538
1	2.90689476	1.32489526	-0.26776272
1	1.82683759	1.56156711	1.13034342
8	5.06258309	-3.46206968	0.58729787
6	4.07743884	-2.58595430	0.90840417
6	4.31176569	-1.56419010	1.99972064
1	5.21156538	-0.97077013	1.76625026
1	3.44813971	-0.88972073	1.98125893
6	4.44886001	-2.18882136	3.40604231
1	3.67195435	-2.95757218	3.54046288
1	4.22390209	-1.40173065	4.13953068
6	5.83535028	-2.76885141	3.70066396
1	6.57543167	-1.94994816	3.67679913
1	5.85042312	-3.16646044	4.72718283
6	6.28800324	-3.86514530	2.72987724
1	5.63329448	-4.74895654	2.80087131
1	7.29801791	-4.20365210	3.01305437
6	6.35044073	-3.43182876	1.26854563
1	6.80114875	-2.43254933	1.15932159
1	6.94890715	-4.13961752	0.68232447
50	1.11285973	0.09982454	-2.26327712
7	-0.51618334	-2.12209347	-2.09009952
6	-0.30679232	-2.66503246	-3.44408354
1	-1.04410470	-3.45510833	-3.68363486
1	-0.38422612	-1.86975532	-4.19561393
1	0.70126765	-3.09534724	-3.50483414
7	-0.96988069	0.49721920	-2.89506005
6	-1.86471061	-1.54196460	-1.93561801
1	-2.65211260	-2.31387127	-2.06006108
1	-1.93513837	-1.13896709	-0.91721695
6	-2.11840912	-0.40384762	-2.92733372
1	-3.04489138	0.10810653	-2.61103742
1	-2.29805306	-0.79399199	-3.94277613
16	-0.88151147	1.72795663	-3.96723302
7	0.30524021	-1.75616007	0.81154638
6	-0.24505688	-3.20723767	-1.11866819
1	-0.86294551	-4.09386898	-1.37203409
1	0.80815474	-3.49895225	-1.24728370
6	-0.49998051	-2.90028753	0.35516282

1	-0.27332281	-3.81941223	0.92167054
1	-1.56131251	-2.67515543	0.53534726
16	0.05799389	-1.32156390	2.43773103
8	1.19849670	-0.43964334	2.77836848
8	-0.22439554	-2.50256670	3.28911806
6	-1.45980344	-0.35205776	2.33938964
6	-2.50819951	-0.66294401	3.20617344
6	-3.66878169	0.11283834	3.16683472
6	-3.79128066	1.18624840	2.27178924
6	-2.71883318	1.46538333	1.40606186
6	-1.54696179	0.70910098	1.43224528
1	-2.40917091	-1.50450351	3.89090328
1	-0.72389081	0.93173755	0.74355072
1	-2.80260570	2.28619895	0.69049303
6	-5.03674614	2.03655206	2.24820843
1	-4.49491827	-0.12516765	3.83931688
8	0.58624125	2.07284775	-3.90972902
8	-1.50731751	1.42968241	-5.27631518
6	-1.77569303	3.13337034	-3.26044821
6	-2.81193325	3.72492926	-3.98116144
6	-3.48654972	4.81572541	-3.42516203
6	-3.13447198	5.31894313	-2.16487066
6	-2.08876882	4.69369261	-1.46074430
6	-1.40485446	3.60391726	-1.99641598
1	-3.07615798	3.33268430	-4.96258017
1	-4.29889499	5.28441508	-3.98386980
6	-3.84071431	6.51852463	-1.58363563
1	-1.80525959	5.07019495	-0.47540328
1	-0.59784386	3.10975857	-1.44686040
1	-5.89177170	1.51052940	2.69212777
1	-4.88434074	2.96432711	2.82149852
1	-5.30093051	2.32956797	1.22310480
1	-3.23547345	7.42905910	-1.71481448
1	-4.80798353	6.69122521	-2.07286712
1	-4.01319866	6.39934417	-0.50502023
1	1.32207504	-1.93889061	0.70220074

Energy = -8524.651044 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 38

Atomic N.	X	Y	Z
8	3.69296745	-2.33742454	-0.33614581
8	3.35169519	-2.28989964	2.91415096
6	2.46132543	-3.08856648	3.68902550
1	1.62259484	-3.48096869	3.08646688
1	2.03410261	-2.53246823	4.53970056
1	3.02297758	-3.94834686	4.09233052
8	5.60396571	-2.11142807	0.74434692
6	4.60139372	-2.89232686	0.26967483
6	4.65333239	-4.39012039	0.48539199
1	4.57193096	-4.57807859	1.56921683
1	3.74090276	-4.78226551	0.02136759
6	5.89843430	-5.09595106	-0.08921482
1	6.10905463	-4.70760020	-1.09884461
1	5.65024726	-6.16042096	-0.21597918
6	7.14685984	-4.98592682	0.79213870
1	6.93329199	-5.45871677	1.76634745

1	7.96332458	-5.56874958	0.33805980
6	7.62568452	-3.55141632	1.03471150
1	7.96052716	-3.08665149	0.09295378
1	8.50437198	-3.57178144	1.69993421
6	6.59026239	-2.63846132	1.68074492
1	6.05969834	-3.11863140	2.51671881
1	7.06865527	-1.72856709	2.06331441
50	2.84009903	-0.50982480	2.03441054
7	0.09578248	-0.49586158	-1.34445208
6	1.10584102	-0.34111631	-2.39345502
1	0.99813942	-1.09085402	-3.20876619
1	1.04476579	0.66192404	-2.83459652
1	2.10359622	-0.45565525	-1.95253941
7	-1.42443921	2.04993704	-1.82682345
6	-1.26168266	-0.43375703	-1.88153516
1	-1.45485466	-1.27905139	-2.58584427
1	-1.96921229	-0.56037191	-1.04600150
6	-1.62620069	0.84136617	-2.64297464
1	-2.67760642	0.72866802	-2.96685541
1	-1.01554552	0.95003320	-3.54812081
16	-1.95522908	3.51667222	-2.48493513
7	0.62282210	-0.94926482	1.70830531
6	0.28494852	-1.75350328	-0.60775040
1	-0.19473923	-2.60528068	-1.14129354
1	1.35995025	-1.97837902	-0.57421255
6	-0.25067081	-1.73480601	0.82757126
1	-0.31852352	-2.77756637	1.18273540
1	-1.27664638	-1.32817783	0.84457207
16	0.03545764	-0.37523614	3.09978622
8	1.33861615	0.10983460	3.75425911
8	-0.82719709	-1.27646006	3.89388318
6	-0.93392166	1.11770913	2.77901992
6	-2.11243076	1.33678295	3.49416432
6	-2.82525800	2.51821744	3.27849307
6	-2.37503004	3.48140022	2.36198020
6	-1.19412230	3.22413062	1.64221763
6	-0.47270167	2.04789438	1.84404914
1	-2.45564205	0.58724627	4.20615584
1	0.43003021	1.84611273	1.26596082
1	-0.84907986	3.94603950	0.90076768
6	-3.12092079	4.77705778	2.16478802
1	-3.74655287	2.69545084	3.83684829
8	-1.76475703	4.51731074	-1.41543634
8	-1.30598454	3.63861692	-3.80235264
6	-3.73495167	3.35875334	-2.77827221
6	-4.19907791	3.08198201	-4.06503120
6	-5.57336278	2.94842309	-4.27800811
6	-6.48876446	3.08783373	-3.22471773
6	-5.99182144	3.36522272	-1.93882873
6	-4.62444211	3.50297416	-1.70878285
1	-3.48784476	2.99085898	-4.88520981
1	-5.94009860	2.73514929	-5.28364122
6	-7.97286716	2.97394356	-3.46539099
1	-6.68937980	3.48148291	-1.10724110
1	-4.24727683	3.73564560	-0.71282772
1	-4.19897152	4.65105927	2.33417150
1	-2.76668215	5.53755660	2.87834387
1	-2.95998628	5.17882476	1.15572698

1	-8.43321974	3.97171634	-3.53576992
1	-8.18827378	2.44349378	-4.40159263
1	-8.47263195	2.44439393	-2.64288743
1	-1.74904766	1.96821593	-0.85847542

Energy = -8524.635452 Hartree
Number of imaginary frequencies = 0.

Compound I2a isomer 39

Atomic N.	X	Y	Z
8	3.17152373	-2.51703353	0.04460813
8	0.68107578	1.51054569	-0.59601435
6	1.79101066	1.94332949	0.18982950
1	1.68688142	1.59124059	1.22932746
1	1.84284727	3.04578091	0.19111581
1	2.76318408	1.57098842	-0.19135758
8	5.26801456	-3.16875702	0.21978709
6	4.24106795	-2.38063283	0.62638516
6	4.45076962	-1.40864622	1.76703553
1	5.30041840	-0.74411414	1.53731301
1	3.54500119	-0.79390899	1.81853035
6	4.68229318	-2.10104235	3.12850100
1	3.96264407	-2.92642897	3.24424936
1	4.43496908	-1.37351936	3.91439236
6	6.11383116	-2.60253995	3.34005399
1	6.79782066	-1.73591362	3.33911643
1	6.19406991	-3.05597645	4.34006938
6	6.59878785	-3.60924774	2.29097303
1	6.00581515	-4.53740435	2.33231593
1	7.63875635	-3.89503184	2.51831684
6	6.57649836	-3.09054424	0.85654372
1	6.95656681	-2.05861901	0.79096664
1	7.19678699	-3.72207290	0.20908741
50	1.05412411	0.32893596	-2.24954530
7	-0.42037684	-2.00625739	-2.21410683
6	-0.17814906	-2.45020117	-3.59851687
1	-0.86290874	-3.27026456	-3.88807189
1	-0.30838543	-1.61695158	-4.29982989
1	0.85565051	-2.80936915	-3.68327163
7	-1.05159116	0.62133041	-2.85981044
6	-1.80442993	-1.52691700	-2.02837172
1	-2.53836312	-2.34145251	-2.19921740
1	-1.89972091	-1.19003280	-0.98811243
6	-2.13568233	-0.35213042	-2.95171308
1	-3.09545602	0.07530973	-2.61024859
1	-2.28736438	-0.69279345	-3.98931120
16	-1.05343940	1.92614649	-3.84434285
7	0.42187996	-1.78303389	0.70327087
6	-0.08130408	-3.13127421	-1.31141170
1	-0.65217357	-4.03334214	-1.61542873
1	0.98511882	-3.35624590	-1.46248592
6	-0.34025582	-2.92812287	0.17947862
1	-0.07411048	-3.87086700	0.68675390
1	-1.40865095	-2.75493121	0.37422410
16	0.20747213	-1.49200960	2.36553994
8	1.30954649	-0.57606876	2.74151470
8	0.02011450	-2.75010425	3.12794233
6	-1.36318740	-0.60588081	2.39386700

6	-2.34496207	-1.02212429	3.29426671
6	-3.54466374	-0.31100706	3.36153963
6	-3.77237422	0.80265781	2.53888824
6	-2.76605317	1.18737701	1.63563060
6	-1.55594170	0.49730177	1.55619854
1	-2.16530373	-1.89519537	3.92082657
1	-0.78844965	0.80326448	0.83593371
1	-2.93262423	2.03999417	0.97370176
6	-5.05972959	1.58289850	2.63184925
1	-4.31892036	-0.63200855	4.06077101
8	0.38595260	2.37007090	-3.75808053
8	-1.65792542	1.67557953	-5.17325050
6	-2.04608038	3.21035045	-3.04452976
6	-3.11606798	3.78268648	-3.73068388
6	-3.86735635	4.78011411	-3.10244432
6	-3.55863070	5.20941197	-1.80401186
6	-2.47656803	4.60575579	-1.13701044
6	-1.71592013	3.60866488	-1.74491887
1	-3.34715278	3.44792669	-4.74132433
1	-4.70682537	5.23284357	-3.63354100
6	-4.34957378	6.31044392	-1.14242041
1	-2.22546894	4.92573073	-0.12327455
1	-0.87945189	3.13133393	-1.22525464
1	-5.87027555	0.97354931	3.05220939
1	-4.93480013	2.46163423	3.28379711
1	-5.37497799	1.95243718	1.64682740
1	-3.81101979	7.26899512	-1.20388590
1	-5.32620559	6.44858596	-1.62398726
1	-4.51426003	6.10156465	-0.07630550
1	1.44263957	-1.90476136	0.55254261

Energy = -8524.651050 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 40

Atomic N.	X	Y	Z
8	4.12793461	-1.50832851	1.24120731
8	2.59942441	-2.52383309	3.93597487
6	1.46263227	-3.38128079	3.95107199
1	1.10466556	-3.62190476	2.93289114
1	0.61709583	-2.94501935	4.50756853
1	1.74451030	-4.32636393	4.44490916
8	5.78723871	-2.34419090	0.06947084
6	4.97330900	-2.39532965	1.15195858
6	5.11941097	-3.51711341	2.15403692
1	6.15242139	-3.53477684	2.54031654
1	4.44086662	-3.26977093	2.98342329
6	4.75383941	-4.90438833	1.58000243
1	3.82296237	-4.82231369	0.99616189
1	4.52152816	-5.56163685	2.43067580
6	5.85620533	-5.55408929	0.73807342
1	6.73480399	-5.73168301	1.38228752
1	5.51806235	-6.54585114	0.40010957
6	6.29838999	-4.73136416	-0.47664952
1	5.47441897	-4.62141567	-1.20043470
1	7.10327160	-5.26926238	-1.00345451
6	6.82952829	-3.34228663	-0.13964553
1	7.49786220	-3.36319199	0.73557409

1	7.39056292	-2.92820475	-0.98596816
50	2.62195644	-0.56676447	3.33336842
7	0.84500670	0.44056949	-1.25117766
6	1.74486899	1.12289232	-2.18338992
1	1.98303513	0.50688120	-3.07951117
1	1.30599282	2.07149006	-2.51515474
1	2.68666134	1.34778784	-1.66656470
7	-1.26788797	2.41305850	-1.82790164
6	-0.42296377	0.07126181	-1.88094763
1	-0.28495860	-0.75693601	-2.61770610
1	-1.09756996	-0.31500693	-1.10126801
6	-1.13800610	1.19196652	-2.63853231
1	-2.11953258	0.79079738	-2.95220714
1	-0.58995587	1.46425246	-3.54933346
16	-2.17598909	3.67746708	-2.48595909
7	0.98112837	-0.65635980	1.75012947
6	1.51423182	-0.74616238	-0.70608956
1	1.62396949	-1.52823861	-1.49631572
1	2.53085031	-0.45552873	-0.40846129
6	0.84517396	-1.41659122	0.49875811
1	1.33550698	-2.39662675	0.62528265
1	-0.21598451	-1.63889411	0.30676392
16	-0.31834555	-0.41866054	2.69153925
8	0.35609488	-0.19278380	4.04791427
8	-1.38150114	-1.44607148	2.61083189
6	-1.11312169	1.16507465	2.32358817
6	-2.45997327	1.32120376	2.65607724
6	-3.05628947	2.57417805	2.49706367
6	-2.33028512	3.66954308	2.00434069
6	-0.98475736	3.47003016	1.64414856
6	-0.36937005	2.22876461	1.80584447
1	-3.02385562	0.47239268	3.04088674
1	0.67029489	2.07692059	1.51713899
1	-0.41558465	4.29895227	1.22123430
6	-2.96346410	5.03002518	1.86532338
1	-4.10477378	2.70512653	2.77186013
8	-2.18559491	4.73377000	-1.45545085
8	-1.64098545	3.90733733	-3.84066327
6	-3.87198755	3.07328039	-2.67254627
6	-4.32707222	2.67321797	-3.92919859
6	-5.63416431	2.19532502	-4.05834697
6	-6.48956134	2.11151361	-2.95087352
6	-6.00252649	2.52145044	-1.69640880
6	-4.70341201	3.00178378	-1.54960074
1	-3.66594126	2.75447505	-4.79123288
1	-5.99558431	1.88562004	-5.04056193
6	-7.90580744	1.61448529	-3.09562541
1	-6.65541884	2.46752995	-0.82312407
1	-4.33722381	3.33071703	-0.57686273
1	-4.03153780	5.00245984	2.11699737
1	-2.47776547	5.75495578	2.53571118
1	-2.85041897	5.40858997	0.83975521
1	-8.62444781	2.43899481	-2.97178503
1	-8.07547172	1.16790603	-4.08331746
1	-8.14440145	0.86210099	-2.33067623
1	-1.52222396	2.26207532	-0.84732466

Energy = -8524.636449 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 41

Atomic N.	X	Y	Z
8	5.44835173	1.46747051	0.54054386
8	3.18783182	2.56777643	2.46045113
6	2.38522849	3.73392076	2.34237569
1	1.35029925	3.57098351	2.69404755
1	2.32721908	4.10449491	1.30376363
1	2.82665771	4.52888644	2.96840683
8	5.01750215	3.51488557	-0.16753775
6	5.75484079	2.65464734	0.56822644
6	6.92745959	3.17048177	1.37769614
1	6.55337544	3.89284177	2.12299028
1	7.30189557	2.30154222	1.93060149
6	8.05705538	3.80688924	0.54170225
1	8.26489353	3.17127590	-0.33412952
1	8.97254622	3.79719284	1.15197786
6	7.77891231	5.24681201	0.09806595
1	7.67701096	5.87989580	0.99667728
1	8.65264793	5.63073720	-0.45114350
6	6.52522931	5.41529438	-0.76630728
1	6.63342346	4.88121860	-1.72423996
1	6.40084921	6.48129002	-1.01720773
6	5.23294541	4.95245030	-0.10184750
1	5.17023524	5.28360811	0.94679306
1	4.36145107	5.35074844	-0.63485516
50	2.89419576	0.81564462	1.44992471
7	-0.91108055	-1.24361142	2.47826170
6	-0.32877923	-2.25118516	3.36423503
1	-0.79814730	-2.26675419	4.37327035
1	-0.42655443	-3.24991058	2.92047754
1	0.74308623	-2.04724510	3.48448798
7	-2.08174380	-3.10616664	0.46485066
6	-2.34799578	-1.44182780	2.29485782
1	-2.90006783	-1.32071268	3.25802465
1	-2.71841360	-0.65045411	1.62378577
6	-2.76797128	-2.79970782	1.73023996
1	-3.86721162	-2.76889429	1.61282185
1	-2.53873213	-3.61009396	2.43383049
16	-2.59654243	-4.48478722	-0.37216700
7	0.59898792	1.14114899	1.12042232
6	-0.65485748	0.11590139	2.97303491
1	-1.39404925	0.40484007	3.75378649
1	0.33061296	0.12201840	3.46273834
6	-0.64873969	1.19577840	1.88449102
1	-0.76648302	2.17869421	2.37380281
1	-1.52334797	1.06745941	1.22314885
16	0.67822785	1.80422834	-0.34123859
8	2.19963055	1.73855970	-0.57528040
8	0.02887140	3.11916568	-0.54492573
6	-0.04592484	0.68111227	-1.56236428
6	-0.80789104	1.20076785	-2.60985806
6	-1.32784320	0.32736004	-3.56778698
6	-1.09507674	-1.05479747	-3.49309116
6	-0.33871122	-1.55131294	-2.41607464
6	0.18517271	-0.69241413	-1.45018293
1	-0.98487185	2.27428615	-2.66301088

1	0.75353482	-1.08608535	-0.60663405
1	-0.17757984	-2.62628568	-2.32408860
6	-1.61920591	-1.99125856	-4.55269067
1	-1.92300476	0.72928827	-4.39018996
8	-1.84268530	-4.47637884	-1.64166011
8	-2.51633292	-5.60211564	0.58571725
6	-4.34617941	-4.24501420	-0.77024269
6	-5.32164662	-4.86429456	0.01151801
6	-6.66975111	-4.66476246	-0.29908547
6	-7.05473691	-3.85588429	-1.37724671
6	-6.04877293	-3.24566123	-2.14875909
6	-4.70062291	-3.43437314	-1.85419325
1	-5.02041446	-5.50784932	0.83731913
1	-7.43553900	-5.15272533	0.30637553
6	-8.50926469	-3.64712591	-1.71560193
1	-6.32876434	-2.61992923	-2.99840561
1	-3.92597761	-2.97390913	-2.46761619
1	-0.88885825	-2.09520580	-5.37048981
1	-1.79469421	-2.99538808	-4.14455692
1	-2.55152273	-1.61603659	-4.99633224
1	-8.73611044	-4.01774711	-2.72619519
1	-9.16458444	-4.16955197	-1.00778222
1	-8.77042851	-2.57884274	-1.69915374
1	-2.00246829	-2.31529723	-0.18156914

Energy = -8524.631030 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 42

Atomic N.	X	Y	Z
8	3.09327504	1.33357836	2.81062676
8	2.49067005	2.02555627	-0.07886649
6	2.39802174	2.22721942	-1.48620270
1	1.71986145	3.05880947	-1.74554268
1	2.04725794	1.31790926	-1.99953767
1	3.40265044	2.48306486	-1.86508159
8	3.91253186	-0.36164031	1.67128306
6	4.03240052	0.88534064	2.14456914
6	5.28595907	1.68669116	1.87620501
1	5.31401722	1.90273307	0.79428727
1	5.13603418	2.64557424	2.38543388
6	6.60272408	1.02667785	2.33285104
1	6.47373957	0.61396486	3.34673957
1	7.35932513	1.82104820	2.42027209
6	7.13558356	-0.05490062	1.38675536
1	7.33270508	0.40415737	0.40243764
1	8.10761706	-0.41319657	1.76054437
6	6.19504851	-1.24869076	1.19329417
1	6.06574181	-1.80239865	2.13765551
1	6.64915958	-1.95545820	0.47964612
6	4.81849901	-0.88495776	0.65263769
1	4.87371243	-0.15943119	-0.17272684
1	4.27697706	-1.76619241	0.29289425
50	0.97681948	1.92512424	1.29427126
7	-1.76505813	0.77252760	2.94135233
6	-1.40533120	1.36656166	4.22513831
1	-2.02322565	0.97723395	5.06309571
1	-0.35031444	1.16227320	4.45239199

1	-1.52762024	2.45740367	4.17634178
7	0.15275773	-0.25898701	1.01797598
6	-1.43465303	-0.65874325	2.88174858
1	-1.55341695	-1.14534660	3.87236421
1	-2.12603839	-1.16593767	2.19485466
6	-0.00472411	-0.87043057	2.36344428
1	0.22532191	-1.94662219	2.34769640
1	0.72371840	-0.42482946	3.06296182
16	0.61160926	-1.30973994	-0.18578968
7	-2.41657765	0.93280072	0.12178562
6	-3.12788194	1.12459034	2.55090618
1	-3.89916161	0.68208138	3.22370653
1	-3.21364413	2.21792932	2.63781850
6	-3.48273277	0.71708296	1.10815586
1	-4.38171701	1.26688990	0.79996070
1	-3.73171665	-0.35361429	1.05288053
16	-2.17033344	2.44770822	-0.52803181
8	-0.68745030	2.68998552	-0.47420372
8	-3.10930641	3.42512154	0.05835209
6	-2.55348077	2.28095782	-2.27921632
6	-3.66430261	2.94429105	-2.79723627
6	-3.95066652	2.81482415	-4.15898599
6	-3.14226686	2.03579313	-4.99853649
6	-2.02905901	1.38035358	-4.44084700
6	-1.72258778	1.49689026	-3.08728045
1	-4.28369505	3.55661107	-2.14308823
1	-0.85685565	0.98480863	-2.66260088
1	-1.38849496	0.76882129	-5.07904914
6	-3.44126493	1.91382644	-6.47166531
1	-4.81694822	3.33263791	-4.57439424
8	0.58836737	-0.51673045	-1.44213361
8	1.82416925	-2.10107954	0.14693421
6	-0.72535918	-2.54410639	-0.30446046
6	-0.55021263	-3.80154106	0.27686078
6	-1.56968779	-4.75191999	0.17805401
6	-2.76098513	-4.46989283	-0.50618986
6	-2.90681918	-3.20113454	-1.09314776
6	-1.90039418	-2.24019366	-0.99848945
1	0.38815691	-4.03140204	0.78054388
1	-1.43226230	-5.73415235	0.63460939
6	-3.84507149	-5.51023175	-0.64121156
1	-3.82242414	-2.96391696	-1.63905223
1	-2.02187681	-1.26177720	-1.46156444
1	-4.43073984	2.32026205	-6.71608917
1	-2.69592684	2.46153992	-7.06840334
1	-3.40680852	0.86534158	-6.79970017
1	-3.79694956	-6.00037636	-1.62614334
1	-3.74688625	-6.29305013	0.12197704
1	-4.84449661	-5.06264762	-0.55176897
1	-1.49700588	0.51067219	0.40292230

Energy = -8524.631696 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 43

Atomic N.	X	Y	Z
8	3.76511801	-0.19169183	3.07628319
8	1.62659045	2.52691937	0.96684998

6	1.00015754	3.79101828	0.75742017
1	1.35459315	4.48871928	1.53507567
1	-0.10173970	3.74229554	0.82204326
1	1.25200843	4.21250988	-0.22947704
8	4.62019549	0.57111836	1.18469612
6	4.25002487	0.75745448	2.48224217
6	4.45948154	2.11770521	3.12152948
1	3.87529268	2.86326575	2.55645025
1	4.01506584	2.03955753	4.12074038
6	5.93492159	2.55636150	3.23087783
1	6.54560625	1.70645257	3.57643343
1	6.00047635	3.32113706	4.01950676
6	6.51669952	3.13561316	1.93753640
1	5.95074865	4.04521395	1.67221531
1	7.55364614	3.45839558	2.11984995
6	6.48820671	2.17534043	0.74427831
1	7.13236496	1.30015069	0.92893289
1	6.90484783	2.68679888	-0.13871786
6	5.09596239	1.68041982	0.36682143
1	4.34550750	2.48662888	0.38411567
1	5.10490886	1.24844865	-0.64167370
50	1.13021909	0.76935289	0.01996450
7	-0.20293210	0.13595018	2.16906632
6	0.54134124	0.60507215	3.36128308
1	-0.10169229	0.56079052	4.25890874
1	1.43520996	-0.00579703	3.52571018
1	0.86797456	1.63728890	3.18496744
7	0.96791840	-2.74774573	0.88425214
6	-0.57422009	-1.29896965	2.32432791
1	-1.06027684	-1.41911278	3.31266105
1	-1.32421520	-1.54356490	1.56177757
6	0.59137054	-2.30233213	2.22482086
1	0.32454999	-3.20668741	2.78912498
1	1.49885811	-1.90173580	2.70052311
16	0.24673146	-4.07733771	0.15091036
7	-1.02776112	1.03693436	-0.36464857
6	-1.42845165	0.97312679	2.02349417
1	-2.16027428	0.71351763	2.81266985
1	-1.11578136	2.01475768	2.17914989
6	-2.07191246	0.86283716	0.63973717
1	-2.83660873	1.65308886	0.56151191
1	-2.58213783	-0.10790727	0.51327831
16	-1.20963276	2.03302664	-1.64694424
8	0.22065543	2.22575913	-2.07687985
8	-2.07315757	3.20328445	-1.36610001
6	-2.01674595	1.11197510	-2.97988214
6	-3.37353833	1.31528959	-3.23143722
6	-3.99323071	0.58742152	-4.25157893
6	-3.27482759	-0.33454893	-5.02653415
6	-1.90463098	-0.50809368	-4.75801955
6	-1.27298440	0.20544931	-3.74173054
1	-3.92561197	2.05182689	-2.64868641
1	-0.20721104	0.08072396	-3.55047419
1	-1.32379332	-1.21060471	-5.35871814
6	-3.94572257	-1.12508105	-6.12151916
1	-5.05354927	0.74855650	-4.45482102
8	0.94329850	-4.21144856	-1.14121931
8	0.21861885	-5.14843839	1.16547572

6	-1.48295407	-3.67306098	-0.20611983
6	-2.49166046	-4.17632673	0.61697973
6	-3.82113740	-3.84483344	0.34344701
6	-4.15572477	-3.02126441	-0.74176842
6	-3.11880300	-2.53261159	-1.55665387
6	-1.78760887	-2.85388617	-1.29740366
1	-2.22991211	-4.82968847	1.44859072
1	-4.61288232	-4.23951237	0.98295817
6	-5.59367690	-2.68647115	-1.04952249
1	-3.35523374	-1.88872789	-2.40588312
1	-0.99139604	-2.48136180	-1.94173844
1	-3.39448537	-1.03937655	-7.06869919
1	-3.98229914	-2.19561701	-5.86836538
1	-4.97432917	-0.78311201	-6.29117800
1	-5.70341399	-1.63478615	-1.34797160
1	-5.96744522	-3.29964008	-1.88412908
1	-6.24378198	-2.87254996	-0.18511305
1	1.29021377	-2.04363074	0.21411863

Energy = -8524.644313 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 44

Atomic N.	X	Y	Z
8	2.73878291	1.20664290	1.59615926
8	2.64887448	2.29520057	-1.26316043
6	4.01902233	1.95551789	-1.39527639
1	4.45008958	2.46355520	-2.27491232
1	4.18348381	0.86735368	-1.53948689
1	4.60005340	2.26595603	-0.50590874
8	3.87419853	-0.66548296	1.33728239
6	3.47785375	0.35619261	2.10545307
6	3.93235383	0.46624619	3.54091792
1	5.03159943	0.38570779	3.58437772
1	3.65454686	1.47582437	3.86423479
6	3.28843637	-0.58573059	4.47287781
1	2.20607254	-0.62308274	4.28196846
1	3.41367050	-0.22633104	5.50512466
6	3.91029646	-1.98063776	4.35460769
1	4.96251916	-1.93782682	4.68864862
1	3.39317849	-2.65849133	5.05059351
6	3.86394658	-2.58325131	2.94541607
1	2.82469682	-2.69832112	2.60126490
1	4.30984972	-3.59089856	2.97103873
6	4.62990973	-1.78838712	1.89555814
1	5.59332683	-1.41316000	2.27689507
1	4.82563450	-2.39936810	1.00695980
50	1.34912463	0.75552175	-0.43534063
7	0.11567480	3.03838636	-0.23650783
6	0.85037151	3.78848504	0.81001349
1	0.35336203	4.75290222	1.02261582
1	0.90354397	3.19699489	1.72964251
1	1.87099691	3.96074013	0.45115826
7	-0.34694685	0.75195998	1.21258829
6	-1.26492932	2.73460942	0.20537216
1	-1.81858368	3.67290555	0.40441394
1	-1.76817376	2.20478788	-0.61556162
6	-1.27904741	1.84803092	1.44966418

1	-2.31654099	1.49157405	1.59072560
1	-1.02077719	2.43041509	2.35105122
16	-0.31851561	-0.43307318	2.32438275
7	0.55874244	2.04634006	-3.03467272
6	0.11008368	3.87187057	-1.46873701
1	-0.53555809	4.75669965	-1.30732046
1	1.14111289	4.22089108	-1.60965146
6	-0.34007581	3.17292113	-2.74854027
1	-0.32466581	3.92205518	-3.55721524
1	-1.37385528	2.80185665	-2.66970494
16	0.51424853	1.38851997	-4.60035243
8	1.79389114	0.66956193	-4.75083481
8	0.08448346	2.41094395	-5.58124946
6	-0.82161049	0.17911621	-4.47622235
6	-2.03104509	0.42112772	-5.12566178
6	-3.05179022	-0.52973581	-5.03465756
6	-2.87502658	-1.71523218	-4.30780976
6	-1.64178085	-1.93137463	-3.66584199
6	-0.61424623	-0.99492568	-3.74561995
1	-2.15811108	1.33774937	-5.70063658
1	0.34178617	-1.16830816	-3.25135537
1	-1.48451926	-2.84995750	-3.09693559
6	-3.96962866	-2.74979955	-4.22943025
1	-4.00056595	-0.34662482	-5.54218065
8	0.78315583	-1.35160876	1.90814079
8	-0.31588710	0.06182039	3.73005242
6	-1.87627799	-1.35090671	2.12268771
6	-2.76220814	-1.46995004	3.19194504
6	-3.95106370	-2.18640550	3.01894560
6	-4.26455111	-2.78624382	1.79191402
6	-3.35460766	-2.64495750	0.72813725
6	-2.16825378	-1.93205688	0.88480748
1	-2.51163266	-1.00438202	4.14465171
1	-4.64731095	-2.27901245	3.85487612
6	-5.53563616	-3.57936912	1.61395448
1	-3.58261232	-3.10320862	-0.23684171
1	-1.46833130	-1.82202305	0.05539215
1	-4.91946156	-2.35921676	-4.61568946
1	-3.70851926	-3.64194305	-4.81890468
1	-4.12980530	-3.08451028	-3.19454031
1	-5.32336957	-4.65912172	1.57682989
1	-6.23505028	-3.40622278	2.44179496
1	-6.04299832	-3.31854520	0.67432096
1	1.55059674	2.22270085	-2.73269579

Energy = -8524.637899 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 45

Atomic N.	X	Y	Z
8	3.65191215	2.82469298	2.78073291
8	3.03986818	1.35044399	-0.42675885
6	3.56510896	2.51495976	-1.05767951
1	3.72670486	3.30374672	-0.30206564
1	2.90569097	2.91796884	-1.84587518
1	4.53570036	2.28235877	-1.52772529
8	3.20250582	0.66577036	2.97719011
6	4.03732233	1.68174890	2.60841443

6	5.40375517	1.34161091	2.04180177
1	5.27051614	0.75991887	1.11540193
1	5.84582093	2.30483051	1.76130206
6	6.33312944	0.59394266	3.02054896
1	6.26412268	1.05728408	4.01836394
1	7.36969456	0.74490194	2.68269630
6	6.06527035	-0.91188751	3.11624687
1	6.24084286	-1.36378495	2.12451248
1	6.80036622	-1.36850396	3.79772019
6	4.65136196	-1.27840666	3.57846214
1	4.47686057	-0.94123405	4.61328074
1	4.54714031	-2.37558291	3.58783953
6	3.53501047	-0.72378890	2.69926288
1	3.76392535	-0.83536106	1.62746184
1	2.59384061	-1.25032489	2.90040004
50	1.36455327	0.30523591	-0.92664426
7	-0.14519344	1.92145207	0.45521950
6	0.35383211	2.18601302	1.82303848
1	-0.29035838	2.91560314	2.34735625
1	0.39784280	1.25747849	2.40072005
1	1.37180732	2.58764855	1.76560883
7	-0.97239000	-0.80532281	1.40080754
6	-1.54256158	1.42485339	0.44411809
1	-2.24028519	2.26464664	0.63557147
1	-1.75829973	1.05344824	-0.57010349
6	-1.88320565	0.34264627	1.47381926
1	-2.93896388	0.06107851	1.30477475
1	-1.80674375	0.74397108	2.49191793
16	-1.00461610	-1.94205166	2.66571066
7	0.38764335	1.76774890	-2.26119597
6	-0.04354499	3.17130675	-0.34692853
1	-0.71912576	3.94522777	0.06641382
1	0.98945418	3.52677056	-0.23719146
6	-0.34395878	2.95293589	-1.83074365
1	-0.01452221	3.85068112	-2.37975178
1	-1.43144686	2.84362394	-1.99966512
16	0.89908219	1.59615612	-3.80577683
8	1.84500461	0.43837972	-3.69528986
8	1.34005425	2.87437459	-4.41035700
6	-0.51435496	1.02876811	-4.78645731
6	-1.19236620	1.93233945	-5.60551248
6	-2.29803861	1.49157451	-6.33730012
6	-2.72974472	0.15897577	-6.26931668
6	-2.02432002	-0.72992873	-5.43921432
6	-0.92292742	-0.30506351	-4.69842000
1	-0.84102883	2.96113881	-5.67693773
1	-0.36637270	-1.00191828	-4.07136688
1	-2.33973569	-1.77358025	-5.38006944
6	-3.89807831	-0.32122590	-7.09365541
1	-2.82890171	2.19598122	-6.98051397
8	0.02872907	-2.92953532	2.30689413
8	-0.95381606	-1.15449302	3.91096320
6	-2.61011990	-2.76723928	2.59767901
6	-3.66401325	-2.29218766	3.37972002
6	-4.90501189	-2.92958813	3.30337346
6	-5.10488004	-4.03270397	2.46074263
6	-4.02138017	-4.49218810	1.69026928
6	-2.77678851	-3.86967666	1.75254237

1	-3.50254709	-1.45196006	4.05416913
1	-5.73066121	-2.56708584	3.91807870
6	-6.44098589	-4.72772714	2.39048532
1	-4.15371131	-5.35891980	1.03994113
1	-1.93129291	-4.24421618	1.17558361
1	-4.56154045	0.50801238	-7.37129872
1	-3.54993497	-0.79161680	-8.02654876
1	-4.48912903	-1.07296191	-6.55308883
1	-7.19606909	-4.20835037	2.99333373
1	-6.80622070	-4.78205232	1.35473984
1	-6.36549940	-5.76171739	2.75880746
1	-0.94978707	-1.29006422	0.49941427

Energy = -8524.643457 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 46

Atomic N.	X	Y	Z
8	2.67631909	1.23121525	1.68000447
8	2.57139854	2.46408569	-1.12249373
6	3.95711473	2.19194124	-1.24903038
1	4.51369958	2.50306191	-0.34447562
1	4.37338742	2.74383740	-2.10919456
1	4.17339180	1.11689473	-1.42121528
8	3.89468024	-0.57623811	1.35024491
6	3.44254359	0.38808155	2.16062792
6	3.86841338	0.44505216	3.60801941
1	4.96943889	0.41183559	3.66690888
1	3.53998576	1.42355682	3.97625346
6	3.25906717	-0.68042132	4.47503504
1	2.18239550	-0.75599428	4.26418589
1	3.35242412	-0.36830590	5.52591251
6	3.94560875	-2.03833228	4.29852265
1	4.98986325	-1.96506909	4.65186622
1	3.44994729	-2.77272057	4.95143732
6	3.94732152	-2.57102301	2.86076922
1	2.91954561	-2.71478921	2.49367850
1	4.43794676	-3.55787008	2.84406088
6	4.69193728	-1.69118111	1.86478172
1	5.63190195	-1.29338393	2.28033892
1	4.92784814	-2.24745006	0.95037036
50	1.33255056	0.82710364	-0.39343061
7	-0.00386514	3.04055395	-0.09009067
6	0.68646471	3.76590527	1.00302756
1	0.14547865	4.69543746	1.25920628
1	0.75625015	3.12991663	1.89131725
1	1.70217819	4.00062458	0.66632396
7	-0.38286010	0.65972264	1.22772765
6	-1.37404679	2.65400669	0.31838944
1	-1.96998091	3.55558913	0.56040475
1	-1.84564731	2.14783754	-0.53562364
6	-1.36147359	1.70231260	1.51338384
1	-2.38437439	1.29634666	1.62429717
1	-1.13523566	2.24572208	2.44715173
16	-0.31121372	-0.57733427	2.27932997
7	0.51383421	2.21648546	-2.92729835
6	-0.03587282	3.93742751	-1.27638698
1	-0.72775804	4.77888609	-1.07789153

1	0.97680747	4.34711497	-1.38284407
6	-0.43617276	3.28760479	-2.59789373
1	-0.44242368	4.07806809	-3.36640648
1	-1.45380816	2.86896357	-2.55480808
16	0.50905266	1.63189871	-4.52244819
8	1.81436804	0.96503638	-4.69070687
8	0.05445058	2.68373372	-5.46000924
6	-0.78558664	0.37348197	-4.46916405
6	-2.00110011	0.60908752	-5.10981009
6	-2.98947359	-0.37871731	-5.07328115
6	-2.77435932	-1.59497836	-4.41009465
6	-1.53609449	-1.80353383	-3.77561083
6	-0.54051113	-0.83003641	-3.80109552
1	-2.15765345	1.55007793	-5.63609748
1	0.41971675	-0.99716618	-3.31287055
1	-1.34880194	-2.74543217	-3.25611002
6	-3.83283170	-2.66919860	-4.39463951
1	-3.94295083	-0.20053421	-5.57371934
8	0.82723093	-1.43022144	1.82456718
8	-0.33267249	-0.15345039	3.70805615
6	-1.83256218	-1.54172787	2.02449826
6	-2.71224548	-1.75379155	3.08424752
6	-3.87188434	-2.50662389	2.87079650
6	-4.16354764	-3.04834286	1.61197933
6	-3.25779666	-2.81794589	0.55999225
6	-2.10065082	-2.06830118	0.75694687
1	-2.47811073	-1.33390234	4.06202080
1	-4.56132488	-2.67553104	3.70039528
6	-5.42045445	-3.84987733	1.37906667
1	-3.46527448	-3.23668972	-0.42734051
1	-1.40302742	-1.89073879	-0.06261732
1	-4.80521198	-2.27932851	-4.72103459
1	-3.56062169	-3.49637050	-5.06811947
1	-3.95223040	-3.09891477	-3.39000132
1	-5.19646167	-4.81177417	0.89567280
1	-5.94472722	-4.05448562	2.32113008
1	-6.11617443	-3.31141254	0.71742408
1	1.49451199	2.42063277	-2.60651725

Energy = -8524.637906 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 47

Atomic N.	X	Y	Z
8	2.56740716	-2.35759590	2.38008112
8	2.86817423	0.25979716	-0.50112429
6	3.58542155	0.41711220	-1.71994426
1	2.94898273	0.31989137	-2.61716664
1	4.38235694	-0.34617929	-1.78514163
1	4.05982749	1.41269304	-1.76238093
8	4.58929563	-1.77706375	1.73085320
6	3.42704636	-1.48118786	2.35438721
6	3.24765996	-0.12877630	3.01065684
1	3.32511968	0.65072398	2.23411940
1	2.22110856	-0.11339963	3.39709530
6	4.24638974	0.15708909	4.15336509
1	4.34791038	-0.73881691	4.78669226
1	3.80241272	0.93365134	4.79331714

6	5.62256793	0.63446383	3.67920573
1	5.49685395	1.58378959	3.13073936
1	6.24867417	0.86380497	4.55550086
6	6.36140950	-0.35939816	2.77718030
1	6.61320249	-1.27890736	3.33054479
1	7.31932546	0.08413226	2.45970135
6	5.60286556	-0.74885075	1.51339756
1	5.12892364	0.11351095	1.02069486
1	6.27885894	-1.22655458	0.79369924
50	0.82958000	0.35395152	-0.24987279
7	0.63381730	-2.29473054	-0.86186271
6	1.94571879	-2.69049787	-1.41743041
1	1.91210116	-3.72309225	-1.81391775
1	2.23649760	-2.00936406	-2.22327138
1	2.70398976	-2.62784090	-0.62886270
7	0.11915598	0.02956776	-2.32532353
6	-0.40351378	-2.28943502	-1.92143134
1	-0.47297619	-3.29039007	-2.39265097
1	-1.36807053	-2.07335132	-1.44018413
6	-0.14999223	-1.23293599	-2.99941123
1	-1.05647130	-1.17649866	-3.62798331
1	0.68013426	-1.53135515	-3.66192286
16	0.14097821	1.44229736	-3.13879517
7	-0.26394419	-1.78500354	2.09236607
6	0.27159846	-3.27058872	0.20264233
1	-0.06698201	-4.21212958	-0.27223038
1	1.18982055	-3.50075947	0.75997184
6	-0.79709476	-2.82973355	1.20297114
1	-1.11184275	-3.72312613	1.76796578
1	-1.69021510	-2.43677951	0.69206868
16	-1.19980102	-1.39262219	3.45551503
8	-0.27607874	-0.65313860	4.34167701
8	-1.95320091	-2.56792949	3.94839542
6	-2.41229772	-0.23809653	2.77950315
6	-3.73068925	-0.65672167	2.59525792
6	-4.66615971	0.25055422	2.09272248
6	-4.30199589	1.56941013	1.78081721
6	-2.96637865	1.96092610	1.97685635
6	-2.01925232	1.06735115	2.47421476
1	-4.01290970	-1.67555047	2.85852417
1	-0.98700973	1.37623222	2.63138910
1	-2.66305615	2.98122232	1.73494997
6	-5.32645075	2.55683532	1.28044450
1	-5.69928228	-0.07088842	1.94866056
8	0.58994812	2.39730793	-2.06757471
8	0.87215361	1.39241303	-4.42609665
6	-1.57843751	1.84707862	-3.54552095
6	-1.93676286	2.07164224	-4.87381154
6	-3.26462870	2.38680041	-5.17740885
6	-4.23637648	2.48000515	-4.17199179
6	-3.84628657	2.24346427	-2.84081728
6	-2.52767434	1.92881531	-2.52153371
1	-1.17674149	2.00067508	-5.65101032
1	-3.54823462	2.56325076	-6.21659160
6	-5.66432279	2.83922497	-4.49889422
1	-4.59006438	2.30654754	-2.04371858
1	-2.23508793	1.74723970	-1.48632455
1	-5.76799113	3.11760835	2.11902844

1	-4.87614085	3.29297165	0.60099557
1	-6.14900178	2.05216960	0.75653767
1	-5.90075396	3.85802951	-4.15546640
1	-5.85027973	2.79939190	-5.57951203
1	-6.37107619	2.15970264	-4.00180808
1	0.69823844	-1.99405638	2.42428293

Energy = -8524.649434 Hartree
Number of imaginary frequencies = 0.

Compound I2a isomer 48

Atomic N.	X	Y	Z
8	4.04918402	0.62327317	1.19931930
8	3.63338347	-1.58967491	-1.13397085
6	5.02021515	-1.28957074	-1.16279714
1	5.50522682	-1.91631122	-1.93112129
1	5.49811352	-1.50886719	-0.19109706
1	5.23584749	-0.23372141	-1.41148283
8	4.23795171	-1.18960317	2.44960467
6	4.35750671	0.14064041	2.28774945
6	4.85824888	1.00274384	3.42681338
1	5.84304056	0.63744416	3.76412957
1	5.00182930	2.00082438	2.99764586
6	3.88469206	1.06753666	4.62486875
1	2.85972866	1.19570184	4.24664136
1	4.13023937	1.97111257	5.20297691
6	3.96379963	-0.14976068	5.55155609
1	4.97495982	-0.19610383	5.99447525
1	3.26602144	-0.00605562	6.39085567
6	3.65593410	-1.48898157	4.87285827
1	2.61481358	-1.52806498	4.51758312
1	3.76076940	-2.29779231	5.61496795
6	4.57980557	-1.83895202	3.71333748
1	5.63602829	-1.62856882	3.94930121
1	4.49161388	-2.90200246	3.46046729
50	2.22970586	-0.18345729	-0.58083036
7	0.83060355	-1.90764806	-1.95650615
6	1.40617809	-2.17193504	-3.28900674
1	0.88871892	-3.00799512	-3.79571291
1	1.34082070	-1.27237377	-3.91170277
1	2.46475351	-2.42133101	-3.15153705
7	-0.25932226	0.67927155	-3.02868023
6	-0.60974723	-1.56803935	-2.00727396
1	-1.20575778	-2.48591439	-2.18627623
1	-0.89531181	-1.18698965	-1.01573450
6	-1.04093329	-0.56366725	-3.07708573
1	-2.12179876	-0.39021546	-2.91790854
1	-0.92160589	-0.98229776	-4.08439009
16	-0.68437328	1.91574271	-4.11349273
7	1.12848129	-1.55592948	0.81020945
6	1.04177972	-3.09358663	-1.08453901
1	0.49641636	-3.96864391	-1.48982553
1	2.11982856	-3.30047904	-1.10694478
6	0.59851281	-2.84770697	0.35794856
1	0.97435839	-3.67809739	0.97786625
1	-0.50543196	-2.87414746	0.42576641
16	0.49160990	-0.96098602	2.19732406
8	1.21310472	0.31019806	2.47128971

8	0.41434548	-2.00704147	3.24993979
6	-1.22723452	-0.50184513	1.82153721
6	-2.27214727	-1.38056820	2.10951016
6	-3.57953268	-1.02963997	1.75491253
6	-3.85888853	0.18961821	1.12296011
6	-2.78948407	1.06606994	0.86120563
6	-1.48147019	0.72733381	1.20167952
1	-2.06016107	-2.31571799	2.62702114
1	-0.65486848	1.41466159	1.01602264
1	-2.98908856	2.03028221	0.38867386
6	-5.26716476	0.56060474	0.72864443
1	-4.39782603	-1.71545376	1.98298062
8	0.24950334	3.01776541	-3.83021737
8	-0.78601373	1.27050111	-5.43570812
6	-2.34299380	2.46686919	-3.64530884
6	-3.46217754	1.89920664	-4.25700716
6	-4.73607169	2.32263875	-3.86930148
6	-4.90626837	3.30499391	-2.88262476
6	-3.75966530	3.86913746	-2.29538794
6	-2.48129201	3.45686823	-2.66709317
1	-3.32994491	1.15853490	-5.04503784
1	-5.61358046	1.88836377	-4.35165546
6	-6.28306678	3.74661648	-2.45465331
1	-3.87135071	4.65306624	-1.54372772
1	-1.59309714	3.91306375	-2.22972959
1	-5.99956415	-0.13614861	1.15569600
1	-5.52108190	1.57575669	1.06595184
1	-5.38676430	0.54409612	-0.36581842
1	-6.33296357	4.83726309	-2.33257783
1	-7.04610229	3.44461680	-3.18302473
1	-6.55349212	3.30027421	-1.48482785
1	-0.12003542	1.06919454	-2.09067343

Energy = -8524.644658 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 49

Atomic N.	X	Y	Z
8	2.57513305	-2.40763892	2.32696388
8	2.87253426	0.39300510	-0.38350103
6	3.62570108	0.64531239	-1.56394081
1	3.02382177	0.58436267	-2.48780992
1	4.44849553	-0.08837431	-1.64598596
1	4.06923500	1.65532955	-1.52926284
8	4.59202099	-1.71065617	1.78568465
6	3.39901775	-1.49897697	2.38491766
6	3.14326727	-0.19782676	3.11535756
1	3.21318520	0.63067044	2.39056777
1	2.10506915	-0.24675776	3.46635420
6	4.09219289	0.05587044	4.30701402
1	4.20971542	-0.87256493	4.88862773
1	3.59647375	0.77390194	4.97665364
6	5.46236843	0.61446826	3.91052519
1	5.31582558	1.59001996	3.41588496
1	6.04985120	0.81380433	4.82027298
6	6.26998578	-0.29277527	2.97676906
1	6.54064691	-1.23429036	3.48215028
1	7.21899849	0.20593554	2.72031635

6	5.56940610	-0.63250900	1.66610093
1	5.07680092	0.23949667	1.21001137
1	6.28724681	-1.03836699	0.94283217
50	0.82465735	0.39728532	-0.20176273
7	0.75180345	-2.21307934	-0.97794716
6	2.09687645	-2.52442344	-1.50746877
1	2.11812200	-3.53143526	-1.96578171
1	2.38765899	-1.78489001	-2.26004736
1	2.82437346	-2.48146583	-0.68918483
7	0.19935029	0.17572670	-2.31750770
6	-0.24792936	-2.18130335	-2.07268822
1	-0.26193493	-3.15336005	-2.60528489
1	-1.23611365	-2.03107324	-1.61486303
6	0.00085221	-1.05193762	-3.07523985
1	-0.88570614	-0.98969880	-3.73109017
1	0.86328964	-1.27902241	-3.72465356
16	0.19435387	1.63534438	-3.04421069
7	-0.26436239	-1.92075837	1.96706977
6	0.39220324	-3.26548218	0.01181517
1	0.10747072	-4.18786911	-0.53108535
1	1.29921285	-3.49541092	0.58733586
6	-0.72628175	-2.92719209	0.99728139
1	-1.02562216	-3.86476955	1.49504344
1	-1.61580342	-2.53577345	0.47895250
16	-1.25978788	-1.64787664	3.31716022
8	-0.39562551	-0.92987253	4.27796141
8	-1.98197989	-2.87855687	3.71176581
6	-2.49404378	-0.50033896	2.66928559
6	-3.78776611	-0.95639307	2.41249878
6	-4.74158716	-0.05566707	1.93361357
6	-4.42056206	1.29323052	1.71686213
6	-3.10920130	1.72216599	1.98436034
6	-2.14387255	0.83561853	2.45913643
1	-4.03755978	-1.99967376	2.60258801
1	-1.13062335	1.17290205	2.67184666
1	-2.83945268	2.76652310	1.81694732
6	-5.46730352	2.26985696	1.24203072
1	-5.75548446	-0.40663647	1.73292342
8	0.57322173	2.53901252	-1.90377834
8	0.96678848	1.68814405	-4.30704533
6	-1.52521617	2.00456585	-3.48278160
6	-1.85489001	2.27699758	-4.80994363
6	-3.18338276	2.56299492	-5.13699568
6	-4.18453824	2.58165265	-4.15586800
6	-3.82311369	2.29732704	-2.82643266
6	-2.50374386	2.00975347	-2.48400864
1	-1.07220680	2.26502702	-5.56758742
1	-3.44458859	2.77560850	-6.17533183
6	-5.61116438	2.92117313	-4.50818196
1	-4.58984134	2.30076674	-2.04893194
1	-2.23349358	1.79059734	-1.45000312
1	-5.98377858	2.73265780	2.09746660
1	-5.02072172	3.08325124	0.65465296
1	-6.23206230	1.77329710	0.62999053
1	-5.83189721	3.97340674	-4.26999039
1	-5.80493001	2.77760791	-5.57886672
1	-6.32230022	2.30499156	-3.94116076
1	0.69324523	-2.11496617	2.32063158

Energy = -8524.649443 Hartree
 Number of imaginary frequencies = 0.

Compound I2a isomer 50

Atomic N.	X	Y	Z
8	4.01255809	0.72857185	1.22781222
8	3.68916547	-1.40130921	-1.19393010
6	5.06165540	-1.04074303	-1.21376124
1	5.55450074	-1.28658072	-0.25592413
1	5.23057213	0.03427414	-1.41105917
1	5.56862599	-1.60758175	-2.01381647
8	4.27600490	-1.12814525	2.39760907
6	4.34128954	0.21156288	2.29433047
6	4.80758073	1.04270838	3.47041983
1	5.80671321	0.70339064	3.79234723
1	4.91007850	2.06361507	3.08544063
6	3.83309185	1.01541367	4.66918321
1	2.80352857	1.11836845	4.29580517
1	4.04218997	1.90201032	5.28657592
6	3.96202460	-0.23712418	5.54173757
1	4.97450573	-0.26187224	5.98336108
1	3.25954155	-0.15866996	6.38573243
6	3.70820623	-1.55670361	4.80469663
1	2.66928343	-1.62223128	4.44687073
1	3.84612649	-2.39232997	5.51081372
6	4.64484449	-1.81778785	3.63208214
1	5.69172199	-1.57487001	3.87823070
1	4.59996140	-2.87143151	3.33274890
50	2.22916122	-0.07740333	-0.58712744
7	0.90176273	-1.79511514	-2.03909616
6	1.48883206	-1.98089927	-3.37981317
1	1.00538314	-2.81495919	-3.92215300
1	1.38868257	-1.05952903	-3.96482602
1	2.55624244	-2.19403853	-3.24984428
7	-0.28237220	0.78897277	-3.01005419
6	-0.55053293	-1.50891971	-2.07924711
1	-1.11108859	-2.44057083	-2.29715881
1	-0.85100168	-1.17987119	-1.07357646
6	-1.01883011	-0.47839953	-3.10792976
1	-2.10496768	-0.35046647	-2.94175336
1	-0.88631991	-0.85190592	-4.13121310
16	-0.75917447	2.05511916	-4.03729612
7	1.18295496	-1.55002552	0.74150611
6	1.15802431	-3.00769036	-1.21727661
1	0.64786957	-3.88545628	-1.66075364
1	2.24337836	-3.17127051	-1.24531952
6	0.70376390	-2.84073504	0.23296990
1	1.11052463	-3.68170482	0.81813686
1	-0.39842855	-2.91253474	0.29630986
16	0.52160386	-1.04073988	2.15127511
8	1.19408113	0.24348296	2.48293374
8	0.48264750	-2.13426834	3.15659363
6	-1.21274443	-0.63107386	1.79006282
6	-2.22387219	-1.56083941	2.03515468
6	-3.54290174	-1.24484381	1.69091243
6	-3.86719737	-0.01063740	1.11169300
6	-2.83153317	0.91663298	0.89275360

6	-1.51233911	0.61345413	1.22334173
1	-1.97747756	-2.50907201	2.51202758
1	-0.71214458	1.33908259	1.07067544
1	-3.06665524	1.89216677	0.46162870
6	-5.28767434	0.32341389	0.72824231
1	-4.33485170	-1.97075850	1.88532318
8	0.14095103	3.17475837	-3.71644457
8	-0.85404450	1.46318190	-5.38472515
6	-2.42983602	2.53108365	-3.53092700
6	-3.53634358	1.94949644	-4.15267790
6	-4.81917050	2.31486677	-3.73659559
6	-5.01096787	3.25343914	-2.71191240
6	-3.87731195	3.83358118	-2.11530379
6	-2.59009201	3.47867237	-2.51485127
1	-3.38839776	1.24437574	-4.96997284
1	-5.68707847	1.86980992	-4.22645428
6	-6.39695989	3.63150090	-2.25381983
1	-4.00661795	4.58486504	-1.33373031
1	-1.71276348	3.94775769	-2.06931746
1	-5.99326888	-0.42240086	1.11569232
1	-5.58329363	1.30944741	1.11449601
1	-5.40226342	0.35730617	-0.36633639
1	-6.47950036	4.71302057	-2.07974027
1	-7.15644586	3.34047319	-2.99037119
1	-6.64534426	3.13131453	-1.30457304
1	-0.14782650	1.14231838	-2.05684352

Energy = -8524.644658 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 51

Atomic N.	X	Y	Z
8	0.90153938	-0.68026847	-0.20137689
8	2.22846644	1.24584696	-1.90570716
6	3.20741460	1.79747220	-2.77932576
1	2.79748737	2.61950870	-3.39286888
1	3.63662207	1.05169474	-3.47990601
1	4.04386334	2.19965345	-2.18086150
8	1.76166049	-0.33889968	1.78075862
6	1.91854433	-0.72858907	0.50566976
6	3.26421829	-1.20340668	0.01925241
1	3.49186980	-2.14137236	0.55377278
1	3.13134578	-1.46488511	-1.03707194
6	4.41693116	-0.18995872	0.17436367
1	4.06311298	0.79657911	-0.15808729
1	5.20867352	-0.49098896	-0.52756738
6	5.01095071	-0.11457578	1.58314807
1	5.41870179	-1.10265896	1.85800121
1	5.86378542	0.58166279	1.57758030
6	4.01209153	0.32215090	2.65826041
1	3.66249639	1.35105196	2.47504375
1	4.51198831	0.33201024	3.64062458
6	2.79828009	-0.58753929	2.78660427
1	3.06307014	-1.65438334	2.75446934
1	2.26563401	-0.39283536	3.72514100
50	0.95398985	-0.18151051	-2.75667904
7	-1.88092799	-1.83309674	-2.25167179
6	-2.43136148	-1.67200585	-3.60281984

8	4.35827478	-1.00644072	-1.76496661
8	4.57875514	-2.30103227	1.11770656
6	3.85081550	-3.30544501	1.81559189
1	3.63019974	-3.01858135	2.85694450
1	4.46007981	-4.22587757	1.84111327
1	2.88939056	-3.54489750	1.32538593
8	3.63682872	-3.03571732	-2.25741354
6	4.64514532	-2.14057993	-2.13439462
6	6.06687203	-2.56838365	-2.42981007
1	6.13388616	-2.98054316	-3.45066145
1	6.66014867	-1.64731751	-2.40289232
6	6.61602206	-3.59101658	-1.40857381
1	6.31720577	-3.27608258	-0.39596081
1	7.71442554	-3.54550226	-1.45018072
6	6.17236278	-5.03203200	-1.67983947
1	6.56718544	-5.35116600	-2.66076690
1	6.63304350	-5.69619652	-0.93251374
6	4.65451684	-5.24588367	-1.66906228
1	4.23547449	-5.04652927	-0.67055283
1	4.43858576	-6.30320430	-1.89413681
6	3.88953643	-4.40760115	-2.68679778
1	4.39173103	-4.39541639	-3.66747546
1	2.87699453	-4.80417408	-2.82891313
50	4.00082323	-0.34289897	0.93727176
7	0.06571799	0.65761837	-1.63261176
6	0.43046520	1.49216473	-2.77880278
1	0.18208173	1.01720954	-3.75452845
1	-0.07751834	2.46278907	-2.72269736
1	1.51213149	1.67567926	-2.75466271
7	-2.01084915	2.57085176	-0.74882087
6	-1.36022808	0.33352110	-1.62423770
1	-1.62493368	-0.35287209	-2.46498356
1	-1.58482373	-0.21309864	-0.69491191
6	-2.31374484	1.52443932	-1.73775679
1	-3.33895438	1.12573402	-1.62471863
1	-2.25077703	1.98632364	-2.73119237
16	-3.08359009	3.87376451	-0.65591341
7	1.75348794	-0.67895270	0.69907310
6	0.86755261	-0.57263728	-1.63072456
1	0.50760569	-1.27811256	-2.41645904
1	1.89988617	-0.30906150	-1.89854584
6	0.90950729	-1.34198657	-0.30626753
1	1.31459390	-2.34393307	-0.52582722
1	-0.10309121	-1.50397351	0.09558576
16	1.32249134	-0.70899766	2.25854739
8	2.67034251	-0.39172747	2.91976777
8	0.59578705	-1.91108797	2.72539007
6	0.26915082	0.70707964	2.65896671
6	-0.67468195	0.57228379	3.67845298
6	-1.42267857	1.68808604	4.06117163
6	-1.24299746	2.93299117	3.43882597
6	-0.30579013	3.02919871	2.39330293
6	0.45325081	1.92657605	2.00151770
1	-0.81140188	-0.39425813	4.16174280
1	1.16664795	2.00291277	1.18092061
1	-0.18365213	3.97866272	1.87056459
6	-2.01565739	4.14873159	3.88311598
1	-2.15466253	1.58999214	4.86521793

8	-2.59996324	4.70086465	0.46730553
8	-3.20927577	4.40549057	-2.02522928
6	-4.69990095	3.20223003	-0.19226883
6	-5.68710188	3.04944270	-1.16612772
6	-6.92747556	2.52013789	-0.79962277
6	-7.19328802	2.14183461	0.52394807
6	-6.17791043	2.30556151	1.48355298
6	-4.93640007	2.83336316	1.13624663
1	-5.48312911	3.35818590	-2.19077046
1	-7.70363797	2.40276105	-1.55795285
6	-8.54076074	1.59405702	0.92127954
1	-6.36735020	2.01961705	2.51993030
1	-4.15962315	2.97065270	1.88869552
1	-2.87462199	3.87226877	4.50862072
1	-1.37392539	4.81688377	4.47820386
1	-2.37152855	4.72632275	3.01906248
1	-9.11697036	2.34475637	1.48374096
1	-9.13299043	1.30891189	0.04272353
1	-8.43830042	0.71349270	1.57068317
1	-1.78481749	2.22977388	0.19037565

Energy = -8524.636346 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 53

Atomic N.	X	Y	Z
8	1.26311346	-0.81456535	0.21205773
8	2.52792439	1.41755292	-1.34269381
6	2.23040953	2.74424037	-0.94562674
1	3.15004896	3.20966538	-0.54980433
1	1.46972359	2.77056078	-0.14291792
1	1.87551569	3.36440205	-1.78616958
8	2.32563235	-0.33266094	2.07061967
6	2.32832074	-0.86772767	0.83421423
6	3.58752740	-1.49480858	0.28170583
1	3.82569218	-2.37177234	0.90612560
1	3.31478884	-1.88173606	-0.70802810
6	4.80642918	-0.55511172	0.16833535
1	4.48076103	0.39495717	-0.28242582
1	5.50417375	-1.01761135	-0.54598914
6	5.54595615	-0.31813889	1.48786176
1	5.94159365	-1.27977964	1.85872579
1	6.42081663	0.32337104	1.29966777
6	4.68746005	0.31351440	2.58766940
1	4.35525776	1.32308021	2.29659054
1	5.29542535	0.43508162	3.49919825
6	3.46286620	-0.50681796	2.97294037
1	3.68724828	-1.58106833	3.05284674
1	3.05724343	-0.16836651	3.93391320
50	1.44989635	0.11027146	-2.48894209
7	-1.18915418	-2.03974693	-2.33553888
6	-1.48067952	-1.97792198	-3.77224360
1	-2.54300735	-2.21454196	-3.99732924
1	-1.25265307	-0.98765803	-4.18301445
1	-0.85149264	-2.71363468	-4.29116769
7	-0.71797604	0.92772086	-2.36308554
6	-1.99130790	-1.09216409	-1.55050746
1	-3.05303036	-1.42336368	-1.47127821

1	-1.58540082	-1.06340429	-0.52838397
6	-2.04347940	0.33444123	-2.10502207
1	-2.59391336	0.93578146	-1.35909149
1	-2.64169939	0.34342319	-3.02976708
16	-0.64994884	1.97752160	-3.60533976
7	0.09959553	-3.53368288	0.07004389
6	-1.41467207	-3.43098434	-1.90270685
1	-2.44546468	-3.74985252	-2.18355225
1	-0.71218644	-4.06844757	-2.45982290
6	-1.27484849	-3.72965350	-0.41245299
1	-1.52282272	-4.79132983	-0.27480012
1	-2.00682087	-3.14344976	0.17064869
16	0.44693435	-4.16121300	1.59874172
8	1.79018516	-3.64210027	1.93958548
8	0.17451413	-5.60983799	1.54612057
6	-0.74371565	-3.44697874	2.76454626
6	-1.71377239	-4.27202493	3.33424184
6	-2.63365203	-3.72247389	4.23097844
6	-2.59960198	-2.36020925	4.56094280
6	-1.61536593	-1.55216118	3.96436088
6	-0.68623750	-2.08297629	3.07113628
1	-1.73311246	-5.33080590	3.07858107
1	0.07126245	-1.44239799	2.61805846
1	-1.57611660	-0.48770855	4.20402409
6	-3.58054422	-1.77331686	5.54471588
1	-3.39179173	-4.36611065	4.68088318
8	0.85065096	2.03732992	-3.86173145
8	-1.51505125	1.66216893	-4.76721738
6	-1.16258670	3.62015123	-3.04215046
6	-1.59432313	4.55078982	-3.99156072
6	-1.97553517	5.82287412	-3.56804536
6	-1.94272173	6.17797098	-2.20873274
6	-1.52471872	5.21533930	-1.27765595
6	-1.13032953	3.93925217	-1.68474543
1	-1.64066840	4.27055865	-5.04316757
1	-2.31242073	6.55309821	-4.30619972
6	-2.33164059	7.56644655	-1.76720530
1	-1.50700033	5.46732503	-0.21572637
1	-0.80808525	3.19133371	-0.96109909
1	-4.42357795	-2.45241296	5.72436915
1	-3.09480056	-1.58054590	6.51370877
1	-3.97904669	-0.81358208	5.18730210
1	-1.48843768	8.26391246	-1.89088124
1	-3.16640970	7.95825570	-2.36388819
1	-2.62219176	7.58497763	-0.70890979
1	0.43704699	-2.56051234	0.01115708

Energy = -8524.638001 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 54

Atomic N.	X	Y	Z
8	2.97783196	-0.93831901	-2.72681808
8	1.43172553	-3.44134853	0.92050538
6	2.50411330	-3.71243376	1.81249231
1	2.85496728	-4.74448348	1.64622921
1	2.18924880	-3.61942232	2.86674646
1	3.37276948	-3.03948782	1.66177662

8	5.08837692	-1.37072523	-2.27927173
6	4.07086104	-0.48497604	-2.40530563
6	4.31416098	0.98288179	-2.12777932
1	5.15039201	1.34421819	-2.74921543
1	3.40867039	1.51347996	-2.44651716
6	4.60240527	1.28384993	-0.63984473
1	3.88806260	0.72679726	-0.01232289
1	4.38887371	2.34930764	-0.47164924
6	6.04208352	0.99021529	-0.20736097
1	6.72361169	1.65505670	-0.76641375
1	6.16068658	1.25207722	0.85530127
6	6.48989148	-0.46007819	-0.42036529
1	5.89830757	-1.15062424	0.20240978
1	7.53701414	-0.56572416	-0.09319494
6	6.41812661	-0.93911496	-1.86679325
1	6.79129977	-0.17582203	-2.56811582
1	7.01766094	-1.84726417	-2.00215274
50	0.94244305	-1.47978600	0.48965567
7	-0.44839302	-2.66747773	-1.25468633
6	0.41285671	-3.62715553	-1.98635987
1	-0.19171117	-4.26054775	-2.66003437
1	1.16888904	-3.09112653	-2.57165882
1	0.93184304	-4.24815863	-1.24745707
7	0.31319205	0.10041214	-2.54416284
6	-1.24093518	-1.82486441	-2.19232101
1	-1.91416844	-2.49046050	-2.76883596
1	-1.86895345	-1.15414938	-1.59160044
6	-0.45007822	-0.97930826	-3.19111950
1	-1.17323063	-0.54656103	-3.89862483
1	0.22881564	-1.59605886	-3.79605972
16	0.02430824	1.68484107	-3.07062321
7	-1.14972441	-1.62675822	1.25949024
6	-1.38079709	-3.42811072	-0.36691431
1	-2.10326844	-3.99710838	-0.98264907
1	-0.75837629	-4.13055501	0.20287218
6	-2.11848394	-2.51813913	0.61895501
1	-2.60984268	-3.16626659	1.36209707
1	-2.90773498	-1.93574879	0.11247539
16	-1.07460565	-1.55837839	2.89611834
8	0.35681100	-1.18358926	3.15547510
8	-1.67442672	-2.74026101	3.55777248
6	-2.05778320	-0.12837261	3.42385537
6	-3.41296706	-0.29722667	3.71438037
6	-4.17348582	0.81148693	4.09169148
6	-3.59677462	2.08663567	4.19842403
6	-2.22809219	2.22443933	3.91234125
6	-1.45655366	1.12825659	3.52505144
1	-3.85822325	-1.29048535	3.66254434
1	-0.39293691	1.23425307	3.31328318
1	-1.75817530	3.20660940	3.99503710
6	-4.41495690	3.27391954	4.64204083
1	-5.23355596	0.68111489	4.31788997
8	1.18731486	2.45662290	-2.57675851
8	-0.34939245	1.74042637	-4.50294571
6	-1.44891610	2.14209000	-2.13220182
6	-2.53470562	2.69471513	-2.81103262
6	-3.66158594	3.08413281	-2.08240127
6	-3.71557898	2.92478754	-0.69022095

6	-2.60664270	2.35978977	-0.03454237
6	-1.47277755	1.97208238	-0.74473791
1	-2.49051432	2.80724310	-3.89365938
1	-4.51573971	3.51394566	-2.60871413
6	-4.92709441	3.35818109	0.09659990
1	-2.63336040	2.21367432	1.04673271
1	-0.61927140	1.52699068	-0.23247468
1	-5.48537790	3.11567661	4.45658656
1	-4.29076262	3.45434612	5.72119598
1	-4.10471936	4.19132647	4.12330988
1	-4.72392473	4.29303920	0.64160076
1	-5.78965442	3.53517760	-0.55837244
1	-5.20656147	2.60311046	0.84441631
1	1.33720007	-0.06073212	-2.57306391

Energy = -8524.651502 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 55

Atomic N.	X	Y	Z
8	5.38178642	-0.39020863	-0.83487248
8	2.82128001	2.11189701	-0.00096947
6	3.79910785	2.82431800	-0.76150165
1	3.37363117	3.72227172	-1.24080761
1	4.26197095	2.20092633	-1.54606825
1	4.60008402	3.14833209	-0.07639933
8	3.58746877	-1.16801248	0.34186593
6	4.80408767	-0.50112730	0.22249247
6	5.31766929	-0.03963642	1.56555456
1	6.35657022	0.28688160	1.42609715
1	4.73056728	0.83821842	1.87741247
6	5.20886650	-1.17306030	2.61356630
1	4.21683399	-1.14539310	3.08831405
1	5.94145074	-0.96278680	3.40765155
6	5.44943726	-2.60077740	2.06701219
1	6.29708946	-2.59460178	1.35982657
1	5.76160625	-3.24164929	2.90590323
6	4.21487903	-3.25991529	1.41562679
1	3.38610500	-3.25551875	2.14180834
1	4.43431738	-4.31845472	1.19663617
6	3.73903989	-2.60441353	0.12247884
1	4.44429562	-2.75931899	-0.70889805
1	2.75093593	-2.97342620	-0.17672774
50	1.27550042	1.08167651	-0.89869995
7	0.28544349	1.38733382	1.44663593
6	1.21824617	0.91560096	2.49054026
1	0.83542403	1.13537728	3.50413571
1	1.39054111	-0.16159365	2.38635205
1	2.17275207	1.43295717	2.33929727
7	-0.44267389	-1.51521709	0.88486768
6	-1.07095249	0.79878555	1.57332130
1	-1.61859609	1.30750455	2.39124563
1	-1.61390718	1.01539889	0.64046499
6	-1.14990182	-0.69739767	1.87834212
1	-2.22557658	-0.94615179	1.94382394
1	-0.70230253	-0.91995301	2.85527127
16	-0.32686895	-3.18517316	1.18896096
7	-0.19556803	2.80397344	-0.88771797

6	0.19417238	2.87577599	1.50621700
1	-0.23836005	3.18733395	2.47682845
1	1.22622484	3.24325828	1.43049537
6	-0.62329926	3.45491955	0.34872432
1	-0.43629937	4.54051546	0.31827677
1	-1.70576848	3.31081838	0.51752244
16	0.17702282	3.70701140	-2.19664908
8	1.14508083	2.81430671	-2.93028107
8	0.56006866	5.10191915	-1.87290280
6	-1.29840443	3.80893694	-3.24209269
6	-2.00589227	5.00862476	-3.31539705
6	-3.15874353	5.07231478	-4.10274073
6	-3.60865682	3.95681883	-4.82310784
6	-2.87198604	2.76223858	-4.73346719
6	-1.72297157	2.68077823	-3.94981413
1	-1.64229205	5.88034679	-2.77249546
1	-1.14563862	1.75769348	-3.89680270
1	-3.20172286	1.88500515	-5.29377683
6	-4.83257256	4.04034385	-5.70085523
1	-3.71304397	6.01079244	-4.16433901
8	0.34808088	-3.74025691	0.00187760
8	0.23238114	-3.30572774	2.54872452
6	-2.00939490	-3.84159283	1.22594708
6	-2.67754124	-3.96616204	2.44570658
6	-3.98364731	-4.46031860	2.45490583
6	-4.62775575	-4.83429864	1.26571314
6	-3.92738762	-4.70035963	0.05400425
6	-2.62379040	-4.20851327	0.02449931
1	-2.16911241	-3.69938445	3.37155194
1	-4.50940637	-4.56376482	3.40571969
6	-6.02511067	-5.39967365	1.28589289
1	-4.40889884	-4.99506386	-0.88014616
1	-2.07406172	-4.13009253	-0.91337459
1	-5.46482260	4.89486369	-5.42741000
1	-4.54814382	4.16318808	-6.75756080
1	-5.43783853	3.12581126	-5.63377969
1	-5.99871932	-6.49989729	1.25064882
1	-6.56212103	-5.11163202	2.19852979
1	-6.60662071	-5.06165131	0.41771728
1	-0.73364687	-1.36289213	-0.08535319

Energy = -8524.629425 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 56

Atomic N.	X	Y	Z
8	3.13098755	0.02771595	1.48337702
8	3.69451343	-2.10928110	-0.63983985
6	3.56644534	-3.50154502	-0.37221872
1	3.05231575	-3.70093364	0.58583721
1	4.57748983	-3.94110368	-0.31290989
1	3.01276439	-4.03148373	-1.16501213
8	4.77880442	0.79532358	0.23509382
6	4.33686787	0.24863616	1.38344441
6	5.31712608	-0.09854803	2.48050035
1	5.98880262	0.75153390	2.68083282
1	4.71382012	-0.27384814	3.37872161
6	6.14431002	-1.35923642	2.13739014

1	5.46981174	-2.12514974	1.72542608
1	6.54948171	-1.76160801	3.07758399
6	7.30088017	-1.09422513	1.16768454
1	8.02846164	-0.42053517	1.65392987
1	7.83324255	-2.03965056	0.98238395
6	6.88106119	-0.48409213	-0.17525401
1	6.19820448	-1.15754927	-0.71835093
1	7.77639166	-0.35338808	-0.80424225
6	6.20728765	0.87882617	-0.06323732
1	6.69554715	1.52717207	0.68211135
1	6.21560435	1.39938201	-1.02780455
50	2.11485941	-0.81937046	-0.89413122
7	-0.49521966	0.22292753	2.59964522
6	0.45021755	0.61582722	3.64500899
1	0.09423356	0.34230466	4.66239925
1	1.42200091	0.13675155	3.47392580
1	0.60492483	1.70199382	3.60980326
7	0.59912581	-1.82068871	0.47294909
6	-0.68824198	-1.23272633	2.56925128
1	-0.83888640	-1.62649215	3.60086573
1	-1.60940355	-1.45206370	2.01113335
6	0.46816644	-2.01049506	1.92298993
1	0.34129097	-3.08219164	2.15230606
1	1.42447869	-1.70671046	2.37283786
16	-0.04180316	-2.93016322	-0.53244101
7	-1.57882206	1.61491713	0.34191241
6	-1.76732240	0.94529858	2.72783243
1	-2.44886967	0.47354043	3.46874625
1	-1.54881275	1.96167091	3.08464851
6	-2.47471038	1.05939775	1.37246592
1	-3.36095542	1.69948857	1.47245020
1	-2.81606967	0.07516457	1.01702823
16	-1.58200917	3.29877400	0.11232859
8	-0.19752592	3.64326622	-0.27174374
8	-2.26968438	3.98608159	1.23051217
6	-2.63551770	3.48809323	-1.34420460
6	-3.90998440	4.03503935	-1.20686672
6	-4.70839263	4.18949345	-2.34394860
6	-4.24613751	3.81036036	-3.61199117
6	-2.95311864	3.26616738	-3.71841738
6	-2.14481268	3.10467194	-2.59574247
1	-4.25988326	4.34211970	-0.22193584
1	-1.13891674	2.69422489	-2.68289100
1	-2.57472319	2.96768348	-4.69795768
6	-5.09853666	4.00495454	-4.84095277
1	-5.70717846	4.61791436	-2.24203773
8	0.69002905	-2.59008743	-1.82524123
8	-0.00708490	-4.32382699	-0.03370029
6	-1.78369405	-2.56260227	-0.87108877
6	-2.76411538	-3.46843336	-0.46548311
6	-4.10648122	-3.17765171	-0.72271430
6	-4.48020298	-1.99964780	-1.38542195
6	-3.46947853	-1.10615670	-1.78306735
6	-2.12731498	-1.37783798	-1.52824938
1	-2.46903321	-4.38995627	0.03477955
1	-4.87647266	-3.88334398	-0.40533686
6	-5.92779700	-1.70376428	-1.68808572
1	-3.73763246	-0.17858659	-2.29255248

1	-1.35525964	-0.67178857	-1.83329089
1	-6.15180401	4.16547855	-4.57784524
1	-4.76169936	4.88195895	-5.41509639
1	-5.03667187	3.13754140	-5.51263537
1	-6.16050076	-1.92818657	-2.74067845
1	-6.59984953	-2.30683025	-1.06421162
1	-6.16096107	-0.64245479	-1.52586558
1	-0.60795687	1.33253915	0.54455932

Energy = -8524.640530 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 57

Atomic N.	X	Y	Z
8	4.17726206	-1.51786974	0.18442252
8	2.72898152	0.30160943	2.32276926
6	3.40488291	-0.55395561	3.24102346
1	4.31020968	-0.03958169	3.60583985
1	3.72482894	-1.50852102	2.78909043
1	2.77701556	-0.78728414	4.12220872
8	6.27925974	-1.27767063	0.80968084
6	5.21824749	-0.88956853	0.04828427
6	5.36905473	0.28545464	-0.89090439
1	6.24288653	0.13425246	-1.54627187
1	4.47051516	0.28136436	-1.51890626
6	5.49849750	1.63396218	-0.14771104
1	4.76447076	1.66335544	0.67342959
1	5.20974688	2.43066145	-0.84861370
6	6.91011838	1.91761712	0.37591032
1	7.59767940	1.99989198	-0.48429606
1	6.92261303	2.89978417	0.87386463
6	7.46111145	0.85980347	1.33958340
1	6.86152042	0.81996022	2.26356635
1	8.48189301	1.14537783	1.64279561
6	7.53877831	-0.55077039	0.76074987
1	7.92448995	-0.54437168	-0.27145590
1	8.20423716	-1.17769587	1.36703366
50	1.54862383	-0.51224392	0.83159646
7	-0.22342507	0.98709742	2.02477867
6	-0.35596030	0.64258484	3.45249902
1	-1.00634522	1.36014364	3.98662923
1	-0.76503448	-0.36836106	3.56311843
1	0.64497988	0.66608395	3.89956671
7	-1.88026045	-1.41468375	1.28287428
6	-1.52706759	1.04736536	1.32484218
1	-2.06579028	1.97176247	1.61670482
1	-1.32331957	1.12139366	0.24670104
6	-2.49106794	-0.11216370	1.57833206
1	-3.38901340	0.08590462	0.96392200
1	-2.81025555	-0.13772364	2.62783336
16	-2.79167361	-2.80651387	1.65016837
7	1.43942155	1.46435443	-0.19102022
6	0.48279806	2.28945029	1.89451576
1	-0.12572307	3.10212204	2.33708158
1	1.41696611	2.18856945	2.46346173
6	0.81217367	2.63107760	0.44247218
1	1.48804120	3.50152797	0.43832387
1	-0.10376471	2.93866692	-0.09562636

16	1.52992838	1.49006828	-1.83290141
8	2.27741269	0.26095120	-2.20790188
8	1.96781345	2.82097999	-2.31664793
6	-0.16669285	1.25928833	-2.44559241
6	-0.95886954	2.36541259	-2.75913149
6	-2.28449768	2.16753613	-3.15893363
6	-2.82809518	0.87916332	-3.26306896
6	-2.00393277	-0.21874918	-2.95629956
6	-0.68258384	-0.03765329	-2.54929990
1	-0.52920733	3.36558192	-2.70894595
1	-0.03755583	-0.89020725	-2.33193299
1	-2.40348854	-1.23096472	-3.04966070
6	-4.24632342	0.66867438	-3.73248956
1	-2.90415375	3.03256105	-3.40342822
8	-1.95147182	-3.93759197	1.22538072
8	-3.25003784	-2.62470718	3.04011811
6	-4.24848612	-2.76838481	0.57945102
6	-5.42805549	-2.17552798	1.03243453
6	-6.53739193	-2.13659043	0.18368763
6	-6.48430605	-2.68236913	-1.10714271
6	-5.28549615	-3.28410936	-1.53077006
6	-4.16835052	-3.33026611	-0.69922656
1	-5.47967389	-1.77722762	2.04520977
1	-7.46478725	-1.68234383	0.53669654
6	-7.68004957	-2.63098598	-2.02426021
1	-5.23186933	-3.73442939	-2.52390728
1	-3.24887561	-3.82171055	-1.01750407
1	-4.86121367	1.56256163	-3.56537064
1	-4.27213172	0.44659042	-4.81079047
1	-4.71715106	-0.17932177	-3.21607652
1	-7.89533198	-3.61974071	-2.45334990
1	-8.57642965	-2.28322403	-1.49602596
1	-7.49900333	-1.94694321	-2.86749732
1	-1.50224442	-1.49854095	0.33430922

Energy = -8524.642216 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 58

Atomic N.	X	Y	Z
8	3.26383453	1.63837372	-2.07477063
8	-0.87737409	-0.06335916	0.09204780
6	-0.20198413	-0.08832313	-1.17351573
1	-0.00045950	-1.12649111	-1.48814837
1	0.75844526	0.45640365	-1.16095180
1	-0.84322489	0.38556199	-1.93322274
8	5.15688318	0.56191720	-2.46739186
6	4.18383030	0.99015187	-1.60939573
6	4.28272270	0.62200871	-0.13964379
1	5.24515070	0.96906836	0.27204982
1	3.48832320	1.19011269	0.35917241
6	4.11239769	-0.88742076	0.13742841
1	3.27424674	-1.27918687	-0.46036420
1	3.81189501	-1.00773025	1.18859047
6	5.37513245	-1.71708260	-0.11218822
1	6.16197089	-1.38435404	0.58736390
1	5.16735890	-2.76902896	0.13565628
6	5.92305503	-1.63187883	-1.54067673

1	5.20527800	-2.05368777	-2.26294909
1	6.83490006	-2.24698927	-1.61364366
6	6.28784181	-0.22175859	-1.99633663
1	6.82070697	0.33242228	-1.20634936
1	6.93987068	-0.26159661	-2.87776370
50	0.31311752	-0.15802921	1.82095649
7	-1.65581696	0.75303433	3.31435873
6	-0.97825318	0.79804167	4.63111377
1	-1.70153335	0.98405884	5.44560790
1	-0.45881893	-0.14809016	4.82645779
1	-0.23635610	1.60583287	4.62295538
7	-0.92334155	-1.80071592	2.61366559
6	-2.68403840	-0.32084617	3.29211805
1	-3.45285413	-0.12677578	4.06539472
1	-3.16566271	-0.29238782	2.30641618
6	-2.07721198	-1.71279826	3.49150729
1	-2.85122157	-2.45587976	3.23168721
1	-1.81174807	-1.88584858	4.54882778
16	-0.29300035	-3.21374195	2.11031855
7	-2.07967695	2.42869143	0.54146225
6	-2.28008694	2.08740237	3.08694408
1	-3.05000063	2.24861177	3.86916655
1	-1.49870981	2.84223220	3.24738045
6	-2.94375133	2.35276089	1.72645275
1	-3.46634532	3.31437978	1.82890810
1	-3.71117453	1.59974821	1.49657424
16	-0.88721093	3.63520992	0.60349884
8	0.38604701	3.07434149	1.13398296
8	-1.50578134	4.79822926	1.28107959
6	-0.63015047	4.02256573	-1.13462625
6	-1.58020253	4.79921167	-1.80512860
6	-1.36507236	5.11617187	-3.14384921
6	-0.21503195	4.66986170	-3.82094049
6	0.71899413	3.89497577	-3.11917284
6	0.52265597	3.57054352	-1.77459179
1	-2.46619664	5.15245386	-1.27859656
1	1.26337802	2.97413515	-1.24411183
1	1.61710216	3.52717353	-3.61764616
6	0.01610570	5.04186718	-5.26409163
1	-2.10113842	5.72217237	-3.67557051
8	0.85653781	-2.72538575	1.26171651
8	-0.01587145	-4.19583019	3.18214966
6	-1.51337910	-3.97904529	1.01134687
6	-1.80751760	-5.33472429	1.15281379
6	-2.73074678	-5.92191436	0.28335547
6	-3.36367566	-5.17065759	-0.71708730
6	-3.04982828	-3.80390234	-0.82911453
6	-2.13037014	-3.20016638	0.02666440
1	-1.31575835	-5.91255768	1.93449556
1	-2.96270722	-6.98358739	0.38614734
6	-4.36917552	-5.80302431	-1.64679492
1	-3.53381190	-3.20353781	-1.60241444
1	-1.89076408	-2.13550413	-0.05576727
1	-0.91622021	4.99957984	-5.84396297
1	0.40114522	6.07050931	-5.34419760
1	0.75029603	4.37615483	-5.73503070
1	-4.13078313	-5.58464781	-2.69760659
1	-4.40165791	-6.89261562	-1.52147505

1 -5.38055053 -5.41157813 -1.45865990
 1 -1.63297575 1.50670877 0.29991543
 Energy = -8524.651073 Hartree
 Number of imaginary frequencies = 0.

Compound I2a isomer 59

Atomic N.	X	Y	Z
8	3.86843300	0.70331063	1.28721471
8	1.68950763	2.76692806	-2.18384272
6	1.17258494	3.34855833	-3.37492200
1	1.13974986	2.63060718	-4.21180249
1	1.82845561	4.18619429	-3.66619068
1	0.14843555	3.74757555	-3.24582246
8	5.78447603	0.70140109	0.20617203
6	4.73560460	0.03107343	0.73947344
6	4.66845849	-1.47662226	0.62206717
1	5.59479318	-1.92098549	1.02262091
1	3.84017530	-1.80139127	1.26379562
6	4.43870963	-1.96722979	-0.82493959
1	3.65067155	-1.35638330	-1.29416506
1	4.03753984	-2.98945868	-0.76728101
6	5.70081957	-1.97637176	-1.69274613
1	6.42086749	-2.69580653	-1.26492052
1	5.44710738	-2.35449341	-2.69499412
6	6.39226658	-0.61524409	-1.82938909
1	5.74008024	0.10917269	-2.34350297
1	7.28916426	-0.72908272	-2.45966845
6	6.84366315	0.00024189	-0.50868662
1	7.30192722	-0.74970230	0.15573027
1	7.57964305	0.79381689	-0.68480070
50	0.96290800	1.10717130	-1.21057018
7	0.45394441	2.79754659	0.67089054
6	1.65429175	3.64034120	0.87638769
1	1.42938205	4.49463060	1.54054488
1	2.46770367	3.04691440	1.30916673
1	1.98539110	4.00342842	-0.10434235
7	1.20045583	0.14958631	2.17648079
6	-0.08391423	2.28129334	1.95723794
1	-0.40937790	3.14527077	2.57209336
1	-0.97369034	1.67893979	1.73081747
6	0.86486953	1.43633097	2.80826784
1	0.36186403	1.25319195	3.76939359
1	1.78664584	1.98293641	3.05179667
16	0.96901819	-1.25109191	3.09973277
7	-1.21133454	1.61398342	-1.26326755
6	-0.59481027	3.60680927	-0.01399626
1	-0.97054229	4.39429703	0.66774145
1	-0.10240664	4.08965015	-0.86829181
6	-1.75839464	2.75595084	-0.53203483
1	-2.36942979	3.39348446	-1.19177422
1	-2.40513907	2.42150847	0.29817165
16	-1.81221025	1.19891273	-2.72723473
8	-0.65497476	0.48445802	-3.36611905
8	-2.47743859	2.32555061	-3.42360112
6	-3.08936171	-0.06231300	-2.47422926
6	-4.41775610	0.33066351	-2.29821850
6	-5.39446796	-0.64351359	-2.08211000

6	-5.06706289	-2.00817915	-2.05527600
6	-3.72426749	-2.37477815	-2.24641195
6	-2.73465097	-1.41311633	-2.45299953
1	-4.68207970	1.38647827	-2.35106383
1	-1.69548782	-1.69937904	-2.61249260
1	-3.44862680	-3.43122760	-2.23431889
6	-6.13267459	-3.05813000	-1.86111894
1	-6.43329795	-0.33773508	-1.94364698
8	1.73448759	-2.29698540	2.38406122
8	1.20103878	-1.02203494	4.54482050
6	-0.80129119	-1.54864627	2.90085448
6	-1.57370324	-1.79054681	4.03671792
6	-2.93627852	-2.05923543	3.88486810
6	-3.53283608	-2.08553193	2.61595615
6	-2.72906844	-1.83234521	1.48978678
6	-1.36742445	-1.56895112	1.62281448
1	-1.10638629	-1.75837649	5.02024759
1	-3.54585824	-2.24530171	4.77091570
6	-5.00057639	-2.39211131	2.45283414
1	-3.17549784	-1.83511347	0.49381530
1	-0.75007229	-1.36564217	0.74739531
1	-7.00806524	-2.65043549	-1.33880840
1	-6.48010495	-3.44721445	-2.83090524
1	-5.75282504	-3.91410778	-1.28686609
1	-5.14639657	-3.42816416	2.10951896
1	-5.54320646	-2.27711407	3.39980926
1	-5.46392012	-1.73513138	1.70391410
1	2.17177371	0.12701620	1.81324540

Energy = -8524.650287 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 60

Atomic N.	X	Y	Z
8	2.51195349	0.74275065	-1.11474837
8	0.25322792	2.45226159	-2.27840630
6	0.97072126	2.18076639	-3.47021459
1	0.58408475	2.80856417	-4.29254226
1	0.88364444	1.12250947	-3.79582054
1	2.04814918	2.39596966	-3.35198174
8	3.71820165	0.83040584	0.72595380
6	3.37780101	0.20736781	-0.41331596
6	4.06762768	-1.07040243	-0.82329392
1	3.86384638	-1.83306429	-0.05479150
1	3.55761143	-1.39272173	-1.73792194
6	5.58393260	-0.92775430	-1.06486966
1	5.78146474	-0.01748496	-1.65426495
1	5.90156501	-1.77333925	-1.69305014
6	6.42619240	-0.92522472	0.21523678
1	6.28428113	-1.88944152	0.73260557
1	7.49266469	-0.87145067	-0.05347779
6	6.09300165	0.20799466	1.19119934
1	6.32462299	1.18995863	0.74664509
1	6.73242146	0.11376575	2.08399195
6	4.64920161	0.21888037	1.67692950
1	4.27646513	-0.78017966	1.94155033
1	4.53677996	0.85567855	2.56130419
50	0.00591405	0.81622229	-0.87721544

7	-0.30004469	2.98726586	0.47449469
6	1.06353847	3.55383320	0.60724821
1	1.05374414	4.45758797	1.24364557
1	1.73989874	2.80911779	1.04022272
1	1.42519625	3.80703036	-0.39580339
7	0.33752748	0.51850317	1.45885452
6	-0.84813595	2.58992932	1.79247076
1	-0.93893981	3.47494767	2.45178283
1	-1.85402133	2.18181243	1.62187205
6	0.01210911	1.52201126	2.46693887
1	-0.57453411	1.10551844	3.30619367
1	0.91813830	1.97012400	2.91052457
16	0.90328518	-0.90516161	2.00473202
7	-2.41592848	2.39038375	-1.49634559
6	-1.15673895	4.01506173	-0.17241729
1	-1.27157473	4.87958906	0.50975197
1	-0.61307023	4.34842147	-1.06561607
6	-2.54865116	3.54788664	-0.59047627
1	-3.04373348	4.40740148	-1.07495383
1	-3.17223021	3.25190821	0.26244328
16	-3.88275766	1.90815625	-2.24896611
8	-4.11439684	2.69881926	-3.47728378
8	-4.89638707	1.87510891	-1.17424488
6	-3.46680281	0.22573838	-2.73371801
6	-3.70063421	-0.81862815	-1.83660346
6	-3.35606388	-2.11617241	-2.21073751
6	-2.77256997	-2.38199629	-3.46112990
6	-2.56240752	-1.31135931	-4.34369944
6	-2.90887088	-0.00605847	-3.99119591
1	-4.15486386	-0.60892932	-0.86863273
1	-2.75886883	0.82365269	-4.68117598
1	-2.12172757	-1.50143853	-5.32377453
6	-2.35487829	-3.78231758	-3.83042581
1	-3.53906214	-2.94051898	-1.51887583
8	1.35165708	-1.65387478	0.79357366
8	1.85998269	-0.75921453	3.13881560
6	-0.52250524	-1.81012545	2.67967279
6	-0.56813613	-2.13525314	4.03397193
6	-1.67669166	-2.82682516	4.53503106
6	-2.73795833	-3.19878258	3.69999112
6	-2.66419172	-2.85943934	2.33584135
6	-1.56976467	-2.16750662	1.82388492
1	0.26428955	-1.85275152	4.67766497
1	-1.71385877	-3.08241613	5.59585231
6	-3.93386214	-3.94329102	4.23983165
1	-3.48175547	-3.14271587	1.66897710
1	-1.51877646	-1.90828404	0.76490997
1	-1.36024091	-4.00729624	-3.41458154
1	-3.05258393	-4.52918700	-3.42874247
1	-2.29548903	-3.91084889	-4.91874489
1	-4.07250592	-4.90275933	3.71983554
1	-3.82523983	-4.15074741	5.31185947
1	-4.85899418	-3.36480154	4.09807167
1	-1.67429450	2.56685967	-2.21031708

Energy = -8524.635446 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 61

Atomic N.	X	Y	Z
8	2.53626719	0.62516357	-1.10612063
8	0.34698959	2.40008481	-2.29895948
6	1.05526469	2.08573838	-3.48584838
1	0.69279547	2.71569200	-4.31750102
1	0.92986626	1.02689960	-3.79683459
1	2.13976115	2.26308728	-3.36926439
8	3.70807985	0.72801137	0.75707771
6	3.38854405	0.09673559	-0.38330981
6	4.08920050	-1.18325349	-0.77184265
1	3.86680830	-1.94034088	-0.00250143
1	3.60084419	-1.51368502	-1.69533633
6	5.61187549	-1.04765900	-0.98109125
1	5.82436760	-0.14488895	-1.57673223
1	5.93926931	-1.90139759	-1.59303232
6	6.42627502	-1.03398705	0.31651022
1	6.27281258	-1.99377531	0.83880120
1	7.49831349	-0.98297001	0.07041457
6	6.07235273	0.10722355	1.27564416
1	6.31299997	1.08559933	0.82800577
1	6.69296084	0.02065182	2.18235403
6	4.61870158	0.12142671	1.73099994
1	4.24012791	-0.87602768	1.99329140
1	4.48749896	0.76286194	2.60934652
50	0.04005872	0.78995462	-0.87884928
7	-0.21006326	2.98514708	0.44266289
6	1.16913898	3.51081098	0.58276494
1	1.18091629	4.42181168	1.20870453
1	1.81770268	2.75054077	1.03085106
1	1.54798529	3.74159860	-0.41940234
7	0.35091667	0.51207266	1.46152665
6	-0.78256589	2.61891734	1.75934248
1	-0.85399341	3.51369041	2.40778499
1	-1.79828598	2.23867669	1.58263483
6	0.03942885	1.53447508	2.45489300
1	-0.56887398	1.14278535	3.29068464
1	0.95157988	1.96243614	2.90587153
16	0.86861249	-0.92116830	2.03080975
7	-2.32924891	2.43604126	-1.53935125
6	-1.02791711	4.03279372	-0.22244717
1	-1.11991968	4.90794672	0.44954876
1	-0.46628546	4.33871997	-1.11438160
6	-2.43099147	3.60747791	-0.64780309
1	-2.89251939	4.47774873	-1.14608374
1	-3.07157115	3.34244809	0.20271778
16	-3.80372206	1.99624789	-2.30178913
8	-3.99600477	2.78019848	-3.54117914
8	-4.82885838	2.01016772	-1.23757795
6	-3.44124981	0.29505795	-2.76362565
6	-3.72200602	-0.73062020	-1.85826398
6	-3.42003225	-2.04341194	-2.21499636
6	-2.83231232	-2.34325597	-3.45585687
6	-2.57381626	-1.29040209	-4.34664176
6	-2.87785411	0.03027308	-4.01198405
1	-4.17910992	-0.49434170	-0.89779712
1	-2.69069960	0.84656948	-4.70882903
1	-2.12894276	-1.50664172	-5.31933081

6	-2.46308383	-3.76210976	-3.80572252
1	-3.64040386	-2.85329080	-1.51691344
8	1.32202961	-1.69260938	0.83598439
8	1.80409927	-0.78706541	3.18374191
6	-0.59503196	-1.78113588	2.68284725
6	-0.69157526	-2.06894672	4.04301940
6	-1.83180309	-2.72124322	4.52537433
6	-2.87474902	-3.09041706	3.66616963
6	-2.74841736	-2.79117010	2.29666764
6	-1.62202904	-2.13831517	1.80292703
1	0.12704518	-1.79034386	4.70585944
1	-1.90844755	-2.94852387	5.59052586
6	-4.10874718	-3.78407118	4.18768607
1	-3.54946046	-3.07577837	1.61059043
1	-1.52997942	-1.91113314	0.73937805
1	-1.50534852	-4.03584220	-3.33616811
1	-3.21743541	-4.47432494	-3.44506566
1	-2.35070222	-3.89310459	-4.88944370
1	-4.31441700	-4.70718365	3.62651656
1	-4.00280799	-4.04532299	5.24819524
1	-4.99664090	-3.14169870	4.08568792
1	-1.57356663	2.57767354	-2.24653625

Energy = -8524.635253 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 62

Atomic N.	X	Y	Z
8	3.14700612	0.02559022	-1.26149151
8	1.21477153	1.59715369	-2.98548937
6	2.04942458	1.07025329	-4.00800555
1	1.80334282	1.54860494	-4.97119334
1	1.92559412	-0.02284579	-4.14507539
1	3.11563811	1.25825894	-3.78925869
8	4.07874629	0.67434066	0.62714561
6	3.92303788	-0.24427883	-0.33712352
6	4.71117819	-1.53141343	-0.30668588
1	4.42456967	-2.08466047	0.60243656
1	4.35080173	-2.11411390	-1.16167565
6	6.24217425	-1.35265903	-0.37618688
1	6.49333224	-0.61433561	-1.15499200
1	6.67210229	-2.30855518	-0.71047701
6	6.89055507	-0.96112337	0.95553354
1	6.70704686	-1.76597371	1.68772438
1	7.98225333	-0.90492445	0.82367655
6	6.38320477	0.36014824	1.54257462
1	6.64294838	1.20707686	0.88630305
1	6.89087252	0.54580847	2.50309768
6	4.88532209	0.39479226	1.81780852
1	4.51300018	-0.52631256	2.28669766
1	4.62542247	1.22758740	2.48032625
50	0.67989072	0.27170228	-1.36448033
7	0.17409436	2.69623440	-0.60532498
6	1.50417186	3.31895174	-0.39918727
1	1.40086223	4.33948358	0.01330434
1	2.10294489	2.70830443	0.28526232
1	2.01473631	3.35490773	-1.36794137
7	0.66756014	0.52939802	0.99357068

6	-0.56404493	2.58141362	0.67325773
1	-0.75244100	3.58641512	1.09891448
1	-1.53390094	2.11247718	0.45500039
6	0.18892146	1.72133810	1.68715252
1	-0.51554701	1.47849994	2.50374692
1	1.01483589	2.29147221	2.14681571
16	1.14918998	-0.70538462	1.93854764
7	-1.53941810	1.68624310	-2.85351317
6	-0.57332687	3.53786190	-1.57815270
1	-0.82273068	4.50666828	-1.10386428
1	0.11422015	3.73063885	-2.41158489
6	-1.85580449	2.93268612	-2.14164918
1	-2.30639578	3.68154968	-2.81349175
1	-2.59162146	2.72335331	-1.34966709
16	-2.71013366	1.08249206	-3.92999526
8	-1.96486712	0.20801250	-4.85545531
8	-3.56841646	2.18192543	-4.42629658
6	-3.73375193	0.05158489	-2.85778597
6	-4.99997098	0.49640320	-2.47796579
6	-5.78914380	-0.32016415	-1.66427209
6	-5.32921678	-1.57214901	-1.23015105
6	-4.05329943	-1.99713468	-1.64040386
6	-3.25147863	-1.19475574	-2.44954988
1	-5.36133608	1.45988645	-2.83580923
1	-2.26788076	-1.53168569	-2.77649825
1	-3.68636284	-2.97686081	-1.32830875
6	-6.17589251	-2.43802482	-0.33138215
1	-6.78400699	0.01900915	-1.36996424
8	1.74556834	-1.71474646	1.01552742
8	1.95139425	-0.26199218	3.11430739
6	-0.35855320	-1.45126013	2.63019873
6	-0.57251892	-1.44611344	4.00731456
6	-1.73658037	-2.02772118	4.52162947
6	-2.68701775	-2.61614407	3.67748133
6	-2.44486956	-2.60763296	2.29110312
6	-1.29386254	-2.02741255	1.76443848
1	0.17570815	-0.99820154	4.66042419
1	-1.90467217	-2.02602275	5.60042232
6	-3.94155531	-3.24510676	4.23172737
1	-3.17048285	-3.06723779	1.61638313
1	-1.11248613	-2.02634212	0.68842885
1	-7.24444016	-2.21775078	-0.45214216
1	-6.01600354	-3.50511390	-0.53583252
1	-5.92265581	-2.26586207	0.72684114
1	-4.02941177	-4.29661138	3.92098823
1	-3.95441448	-3.21252655	5.32846946
1	-4.84096290	-2.72589356	3.86739436
1	-0.59496754	1.70851977	-3.31365183

Energy = -8524.636346 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 63

Atomic N.	X	Y	Z
8	3.82337311	0.82669569	1.34675866
8	1.61762382	2.86564772	-2.10228176
6	1.09819286	3.44458262	-3.29365808
1	1.73045129	4.30649707	-3.56570388

1	0.05996414	3.80863436	-3.17420926
1	1.10001216	2.73631355	-4.13933293
8	5.72931990	0.91631038	0.25192968
6	4.71674773	0.19672753	0.79091714
6	4.71892870	-1.31220430	0.67018450
1	5.66782272	-1.71392277	1.06290150
1	3.91092732	-1.67623724	1.31666612
6	4.50156522	-1.81027787	-0.77628374
1	3.68201113	-1.23634709	-1.23810404
1	4.14956523	-2.85044602	-0.71787038
6	5.75597221	-1.75804147	-1.65371437
1	6.51244540	-2.44371722	-1.23333764
1	5.51247447	-2.14550580	-2.65494064
6	6.38121743	-0.36547187	-1.79217971
1	5.69093948	0.32849037	-2.29851301
1	7.27710105	-0.43499760	-2.43032736
6	6.81417924	0.26730113	-0.47350947
1	7.31254433	-0.46199859	0.18503129
1	7.51062266	1.09495017	-0.65344951
50	0.93752700	1.16449578	-1.16721647
7	0.34756879	2.80390860	0.73506809
6	1.51484695	3.68487618	0.96922777
1	1.25293886	4.51745366	1.64726484
1	2.34488535	3.11246755	1.39866399
1	1.84190874	4.07866661	-0.00091388
7	1.17419570	0.16088198	2.21276574
6	-0.18675641	2.24682288	2.00579001
1	-0.55292233	3.08786255	2.62951827
1	-1.04995096	1.61485093	1.75808559
6	0.78249212	1.42542414	2.85689939
1	0.27483038	1.20977859	3.80875504
1	1.67985730	2.00276009	3.11987706
16	0.98571866	-1.25973699	3.11473355
7	-1.25419274	1.59310949	-1.23616930
6	-0.72112458	3.58715704	0.05073695
1	-1.13190546	4.34990896	0.74032787
1	-0.23617155	4.10061107	-0.78988195
6	-1.84819418	2.70499367	-0.49432025
1	-2.47314639	3.33131601	-1.15167935
1	-2.49261408	2.33547557	0.32265961
16	-1.81624727	1.19125595	-2.71928779
8	-0.62430744	0.53055056	-3.35294256
8	-2.50656222	2.31047707	-3.40319485
6	-3.05416171	-0.11712315	-2.51707539
6	-4.39962843	0.22618597	-2.37603256
6	-5.34708809	-0.78544975	-2.20091611
6	-4.97220443	-2.13717318	-2.18064686
6	-3.61157481	-2.45376093	-2.33789118
6	-2.65193570	-1.45529910	-2.50201688
1	-4.69995681	1.27247539	-2.42533547
1	-1.59926219	-1.70252986	-2.63643047
1	-3.29879476	-3.49996531	-2.33316367
6	-6.00083123	-3.22896667	-2.02035020
1	-6.39994444	-0.51879435	-2.09114458
8	1.80867245	-2.26336325	2.40237649
8	1.18010061	-1.03794973	4.56651587
6	-0.76612448	-1.63111402	2.87854021
6	-1.54553652	-1.93173689	3.99550222

6	-2.89205603	-2.25716121	3.81424292
6	-3.46605859	-2.28159586	2.53494934
6	-2.65603349	-1.96832424	1.42863129
6	-1.30975286	-1.64818270	1.59076371
1	-1.09659813	-1.89995115	4.98756911
1	-3.50761427	-2.48916714	4.68521363
6	-4.91585485	-2.64915989	2.34016279
1	-3.08569863	-1.96816051	0.42527622
1	-0.68773743	-1.39829197	0.73083827
1	-6.97267056	-2.82247629	-1.71273181
1	-6.14963449	-3.77164145	-2.96635516
1	-5.68433021	-3.96992090	-1.27230714
1	-5.00972577	-3.68511263	1.97877089
1	-5.47955965	-2.57311500	3.27873752
1	-5.39430634	-2.00116193	1.59299650
1	2.14922600	0.17963704	1.85957003

Energy = -8524.650281 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 64

Atomic N.	X	Y	Z
8	3.14475834	0.19518937	-1.24854532
8	1.17377179	1.83234960	-2.86168370
6	2.01910160	1.39837657	-3.91849637
1	3.08092898	1.59527424	-3.68663648
1	1.76076579	1.93755314	-4.84566452
1	1.92048760	0.31506820	-4.13233135
8	4.06172558	0.72592422	0.68369118
6	3.92773474	-0.12284696	-0.34556872
6	4.74731325	-1.38892771	-0.40906799
1	4.47758848	-2.01337907	0.45809440
1	4.39892446	-1.91720860	-1.30346622
6	6.27309029	-1.16690832	-0.46751597
1	6.50311996	-0.36836913	-1.19149741
1	6.72604448	-2.08503297	-0.87026903
6	6.91534742	-0.85599644	0.88820057
1	6.75564078	-1.71655435	1.56014012
1	8.00474716	-0.76148422	0.75925079
6	6.37560458	0.40503172	1.57107958
1	6.61109432	1.30426918	0.97833156
1	6.88153457	0.53303435	2.54188045
6	4.87826333	0.38054840	1.85008051
1	4.53075230	-0.58174544	2.25027113
1	4.59893908	1.15557415	2.57211528
50	0.67287492	0.38337569	-1.33800876
7	0.10951084	2.73475182	-0.40962402
6	1.42448982	3.37230885	-0.15709056
1	1.29706077	4.35832507	0.32646749
1	2.03720897	2.72885943	0.48350387
1	1.93443143	3.48889742	-1.11980674
7	0.65619165	0.47292532	1.03209088
6	-0.62587905	2.51132921	0.85613061
1	-0.83909691	3.47860735	1.35170957
1	-1.58379587	2.03506587	0.60372220
6	0.14800215	1.60018659	1.80790104
1	-0.55035842	1.28249766	2.60376707
1	0.95944454	2.15645151	2.30848070

16	1.16806178	-0.81400667	1.88715275
7	-1.57996727	1.84720504	-2.72562378
6	-0.65714891	3.62606349	-1.32124933
1	-0.92906364	4.55252441	-0.77951309
1	0.02593051	3.89371460	-2.13748942
6	-1.92513990	3.03345581	-1.92926873
1	-2.39083316	3.81723508	-2.54904918
1	-2.65736275	2.75322307	-1.15616968
16	-2.73543509	1.29468059	-3.84514113
8	-1.96978117	0.50338269	-4.82716053
8	-3.61714613	2.40707600	-4.26549813
6	-3.73736519	0.16847595	-2.85110889
6	-5.00778478	0.56334071	-2.43211388
6	-5.77970879	-0.32519306	-1.67956497
6	-5.29888939	-1.59987580	-1.34576657
6	-4.01944921	-1.97271471	-1.79414584
6	-3.23427673	-1.09815397	-2.54261543
1	-5.38606620	1.54547761	-2.71364791
1	-2.24798234	-1.39377917	-2.89992539
1	-3.63747443	-2.96879952	-1.56233195
6	-6.12725427	-2.54528456	-0.51249210
1	-6.77768471	-0.02487756	-1.35513098
8	1.79043456	-1.73915998	0.89557182
8	1.95734846	-0.43641839	3.09420341
6	-0.32092069	-1.64568477	2.51965094
6	-0.53096003	-1.75306460	3.89323406
6	-1.68037603	-2.39879233	4.36177702
6	-2.61969380	-2.94102856	3.47527730
6	-2.38295458	-2.81678992	2.09354645
6	-1.24642791	-2.17181284	1.61258438
1	0.20820677	-1.33933464	4.57842684
1	-1.84615109	-2.48387170	5.43756483
6	-3.85176260	-3.65048741	3.98053437
1	-3.10167652	-3.23530055	1.38555797
1	-1.07012207	-2.07986221	0.53962715
1	-7.19917675	-2.32756864	-0.60437037
1	-5.95883600	-3.59043445	-0.80477348
1	-5.86435774	-2.45723058	0.55366950
1	-3.83719502	-4.71500705	3.70181747
1	-3.92859935	-3.58965647	5.07347157
1	-4.76679201	-3.21809804	3.54952273
1	-0.63552954	1.92311137	-3.18067562

Energy = -8524.636354 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 65

Atomic N.	X	Y	Z
8	3.34686682	-0.83543960	0.29332810
8	3.66440729	1.68133320	-1.42152505
6	3.75851819	1.64759131	-2.84161994
1	3.12133990	2.40904478	-3.32136192
1	3.47722988	0.66380966	-3.25966779
1	4.80510900	1.85153711	-3.12806339
8	4.57517836	0.57648952	1.45957971
6	4.46646215	-0.53105485	0.70182460
6	5.69982068	-1.33382432	0.35655696
1	6.29665119	-1.53235464	1.26115913

1	5.33611343	-2.29369518	-0.02797641
6	6.56933706	-0.62597079	-0.70840549
1	5.91269545	-0.23766263	-1.50172665
1	7.21733545	-1.38458173	-1.17168967
6	7.44244846	0.49994575	-0.14431423
1	8.17750087	0.06609883	0.55650270
1	8.02545325	0.94327540	-0.96598799
6	6.66665657	1.61003440	0.57527976
1	5.96253948	2.10791144	-0.11109423
1	7.37829253	2.37635630	0.92262673
6	5.88169799	1.13975957	1.79458271
1	6.44525514	0.41183219	2.40024194
1	5.61444363	1.98626845	2.43757345
50	1.92962117	1.39091257	-0.35828094
7	0.05943006	-2.66871000	-0.18901727
6	1.15982481	-3.55276700	0.19624219
1	1.06750459	-4.56500071	-0.25482641
1	2.11835337	-3.11823514	-0.11284030
1	1.18008299	-3.65806406	1.28869892
7	0.88224376	-0.06917917	-1.75136054
6	0.03053787	-2.44764344	-1.64071877
1	0.15733410	-3.41245497	-2.18379874
1	-0.96018721	-2.05935458	-1.91600971
6	1.09603791	-1.46560196	-2.15109873
1	1.14349647	-1.53961018	-3.25086329
1	2.08779227	-1.75741291	-1.77640026
16	0.16861288	0.95513015	-2.79720880
7	-1.64277158	-0.91689461	1.30356350
6	-1.22710980	-3.16013199	0.32052938
1	-1.67108246	-3.94133825	-0.33420011
1	-1.05204350	-3.61819761	1.30426735
6	-2.22360954	-2.00924495	0.50247921
1	-3.13126757	-2.38275881	0.99406717
1	-2.52307353	-1.58445500	-0.46782443
16	-1.89253076	-0.94198476	2.98396698
8	-0.66433138	-0.36748692	3.57106378
8	-2.42033301	-2.25570844	3.42088480
6	-3.23034974	0.25510783	3.19543493
6	-4.50887105	-0.19094493	3.52574955
6	-5.53097427	0.74655105	3.69939623
6	-5.28860473	2.11975963	3.55300057
6	-3.98664126	2.53860553	3.22395244
6	-2.95658314	1.61772339	3.04683706
1	-4.68986585	-1.25767505	3.65279410
1	-1.94610646	1.94611470	2.80387727
1	-3.77823133	3.60386666	3.10777816
6	-6.38663933	3.13020272	3.77241689
1	-6.53396971	0.40247726	3.95856418
8	0.54958224	2.29467762	-2.17826318
8	0.47688529	0.71074153	-4.22461515
6	-1.63581127	0.87011380	-2.65331728
6	-2.38701377	0.41976660	-3.73932905
6	-3.77752197	0.34886679	-3.62139737
6	-4.42616941	0.72883846	-2.43747628
6	-3.64251693	1.17948220	-1.36018069
6	-2.25485226	1.24976556	-1.45914543
1	-1.88115125	0.14115677	-4.66292822
1	-4.36822247	-0.00451111	-4.46861926

6	-5.92942178	0.68072056	-2.32509987
1	-4.12522293	1.47226168	-0.42577388
1	-1.65928795	1.59198691	-0.61315703
1	-7.37914266	2.66896748	3.68993729
1	-6.31112469	3.57663944	4.77613253
1	-6.32449783	3.95350506	3.04770611
1	-6.36366608	1.68271275	-2.46647777
1	-6.36790935	0.01988531	-3.08383460
1	-6.24486683	0.32958533	-1.33307920
1	-0.62511593	-0.87746299	1.14197893

Energy = -8524.640524 Hartree
Number of imaginary frequencies = 0.

Compound I2a isomer 66

Atomic N.	X	Y	Z
8	3.41872249	-1.13947247	-0.70431332
8	3.30282892	1.47326452	0.29434601
6	3.30828035	2.88847705	0.44647103
1	2.84024912	3.41828171	-0.40675090
1	4.35541289	3.23488990	0.50591898
1	2.78184816	3.20369505	1.36270914
8	3.95507331	-1.33116439	1.42618739
6	4.31768100	-1.19437563	0.14609314
6	5.77654690	-1.13079905	-0.23509004
1	6.32824862	-1.96072522	0.23652527
1	5.80932973	-1.27128881	-1.32152656
6	6.42489343	0.22019259	0.14734024
1	5.73744228	1.02795448	-0.14445723
1	7.34002263	0.33048375	-0.45294810
6	6.78272260	0.33268221	1.63274012
1	7.55765084	-0.41634138	1.87510846
1	7.23987863	1.31736168	1.81462594
6	5.59879971	0.14765535	2.58981353
1	4.82547882	0.91132161	2.41477537
1	5.95070295	0.27367674	3.62637253
6	4.93196764	-1.21930220	2.51124967
1	5.66446039	-2.03767240	2.41872506
1	4.31575138	-1.40287613	3.39859297
50	1.62618311	0.59236726	-0.55729889
7	0.38533224	-2.47415395	-0.80038445
6	0.95405963	-3.45133278	-1.73268260
1	0.58045639	-4.48126442	-1.54825543
1	0.72401318	-3.16939694	-2.76705307
1	2.04582823	-3.45171431	-1.62005087
7	-0.83321750	-1.09151521	-2.99744768
6	-1.07541580	-2.38379012	-0.89111965
1	-1.56952090	-3.31001926	-0.51916042
1	-1.39538956	-1.55844290	-0.23821902
6	-1.60641841	-2.13327637	-2.30719210
1	-2.67082873	-1.85826028	-2.21279245
1	-1.56706698	-3.05137527	-2.91001827
16	-1.54748519	-0.20061321	-4.22891279
7	0.67560145	-0.40600828	1.21172443
6	0.82737822	-2.78791875	0.56518215
1	0.45437089	-3.78611972	0.88898358
1	1.92327881	-2.84124074	0.53789277
6	0.40423226	-1.77769394	1.63681416

1	0.95318985	-2.03593197	2.55959097
1	-0.67157204	-1.90058827	1.86044793
16	0.11882456	0.82271072	2.11978587
8	0.41476783	2.00796497	1.22551470
8	0.60135663	0.85286668	3.51927547
6	-1.68528486	0.66822732	2.21669946
6	-2.28406364	0.34118275	3.43288196
6	-3.67423720	0.20642856	3.49362313
6	-4.47162289	0.39395456	2.35614442
6	-3.84110393	0.72955687	1.14393727
6	-2.45655075	0.86534960	1.06710061
1	-1.66174861	0.21148854	4.31755466
1	-1.97916928	1.13990581	0.12596879
1	-4.44175235	0.88770647	0.24589860
6	-5.97055875	0.23825530	2.42055143
1	-4.14622047	-0.04601401	4.44493483
8	-0.47097958	0.63726584	-4.78546934
8	-2.31300877	-1.16532699	-5.04205398
6	-2.74688462	0.91580066	-3.45681775
6	-4.10480010	0.59621830	-3.47057868
6	-5.01599566	1.47338437	-2.87370914
6	-4.58833602	2.66165278	-2.26456031
6	-3.21311128	2.95973731	-2.27078890
6	-2.29202961	2.09802623	-2.86164365
1	-4.43793105	-0.31361768	-3.96886113
1	-6.08058251	1.23235553	-2.89246956
6	-5.57095565	3.60468761	-1.61660912
1	-2.86072231	3.88467098	-1.81045854
1	-1.23008648	2.34409163	-2.88470786
1	-6.31359272	0.08292843	3.45106160
1	-6.47988195	1.12639754	2.01944175
1	-6.30348146	-0.62156533	1.81973536
1	-5.44038798	4.63128537	-1.98729730
1	-6.60718300	3.29941297	-1.80928557
1	-5.42445511	3.63819663	-0.52600962
1	-0.20923239	-0.52281586	-2.41134642

Energy = -8524.633301 Hartree

Number of imaginary frequencies = 0.

Compound I2a isomer 67

Atomic N.	X	Y	Z
8	3.64693021	-1.49776426	1.49163860
8	2.41710202	-0.19536159	-1.98980457
6	3.16582579	0.90608192	-2.49331057
1	3.40719160	1.65722004	-1.71490531
1	2.63232698	1.42615491	-3.30755398
1	4.12026964	0.52788199	-2.89874899
8	3.85258753	0.74381532	1.18065202
6	4.27218254	-0.55446337	1.03385434
6	5.58877567	-0.66310549	0.31051404
1	5.95315518	-1.69102261	0.43625891
1	5.40321125	-0.50642355	-0.76418936
6	6.60141979	0.37875508	0.84175734
1	6.47693981	1.32469824	0.29490308
1	7.60916318	0.00940770	0.60016375
6	6.51726333	0.66743400	2.35911865
1	6.37019586	-0.27347436	2.91750009

1	7.49072128	1.06125040	2.68812413
6	5.44087998	1.69768950	2.76113138
1	5.60898576	2.62347138	2.18757349
1	5.55700076	1.95839204	3.82631055
6	4.00213279	1.23948181	2.55241962
1	3.69929535	0.44833159	3.25354959
1	3.28823594	2.06584680	2.64370421
50	0.77494039	0.20481796	-0.79764906
7	0.54284273	-2.40725145	-0.87438330
6	1.36452725	-2.88206282	-2.01379257
1	1.15038860	-3.94651406	-2.22442615
1	1.16937160	-2.27548557	-2.90231135
1	2.42324508	-2.75574431	-1.76692663
7	-0.90253907	-0.40855468	-2.16213110
6	-0.90007719	-2.59529065	-1.17359406
1	-1.11582563	-3.66795436	-1.34490947
1	-1.47100979	-2.26532935	-0.29492197
6	-1.35412211	-1.77537708	-2.38304890
1	-2.45612615	-1.84469088	-2.43446021
1	-0.95770589	-2.19686514	-3.32153220
16	-1.01704754	0.70528289	-3.34512986
7	0.73795762	-1.50380764	2.10157322
6	0.94344359	-3.20388426	0.31837675
1	0.71632634	-4.27082609	0.12448406
1	2.03518719	-3.11701703	0.40966240
6	0.31046107	-2.84030530	1.66031500
1	0.60410018	-3.62374555	2.37900385
1	-0.78793593	-2.85750566	1.60611130
16	0.18667170	-1.01716542	3.63742726
8	1.09908506	0.07332083	4.04117595
8	-0.03754292	-2.18505869	4.51937035
6	-1.43293163	-0.32232691	3.25087158
6	-2.58276972	-0.96967803	3.70236240
6	-3.83114772	-0.41144871	3.41487630
6	-3.94108057	0.78066915	2.68418722
6	-2.76204909	1.41390561	2.25219252
6	-1.50922026	0.87186519	2.52845664
1	-2.49017334	-1.88836126	4.28067563
1	-0.59863046	1.36434390	2.18873867
1	-2.82788232	2.34834038	1.69162054
6	-5.29058255	1.36400342	2.34908729
1	-4.73483286	-0.91053358	3.76909353
8	-0.12469359	1.80132124	-2.82862425
8	-0.80691452	0.17047761	-4.71104145
6	-2.71093719	1.35103572	-3.30404680
6	-3.53134577	1.21045681	-4.42182157
6	-4.83710572	1.70915402	-4.37628781
6	-5.33056441	2.34756717	-3.23074600
6	-4.47988047	2.47351141	-2.11673967
6	-3.17799817	1.98026475	-2.14579380
1	-3.13971581	0.72240794	-5.31362433
1	-5.48159883	1.60175142	-5.25078995
6	-6.73134999	2.90587231	-3.19157635
1	-4.84616473	2.97095826	-1.21597636
1	-2.52088225	2.08448988	-1.28189202
1	-6.07192073	0.97921825	3.01679430
1	-5.28171332	2.46018228	2.42009017
1	-5.57956298	1.10660114	1.31787808

1	-6.71578660	4.00654531	-3.19852785
1	-7.31875793	2.57455744	-4.05718327
1	-7.26030260	2.59745908	-2.27843697
1	1.76808768	-1.39189442	2.08723927

Energy = -8524.633619 Hartree
Number of imaginary frequencies = 0.

Compound I2a isomer 68

Atomic N.	X	Y	Z
8	3.82083236	1.87798472	1.32577611
8	3.47892919	-0.49416378	-0.73590848
6	4.49214034	0.21772918	-1.44259919
1	4.58982683	1.26740606	-1.11641518
1	4.31126073	0.21477940	-2.53459757
1	5.46211091	-0.27733712	-1.26603589
8	5.98100509	1.73573571	1.75086096
6	4.69220730	1.40170582	2.04040413
6	4.40978746	0.46262527	3.19089672
1	4.90006387	0.83027369	4.10760155
1	3.32557771	0.50245178	3.34799330
6	4.85805406	-0.98784974	2.90298542
1	4.56668251	-1.25612939	1.87483681
1	4.28834947	-1.65207065	3.56903762
6	6.35546444	-1.22644581	3.12283371
1	6.58747132	-1.06535050	4.19038052
1	6.58968074	-2.28211019	2.91407785
6	7.27746435	-0.33323137	2.28416103
1	7.15351815	-0.54089374	1.20882074
1	8.32655229	-0.56885182	2.52785228
6	7.08707299	1.16542128	2.50480246
1	6.97172754	1.40618765	3.57390922
1	7.95252051	1.72166670	2.12393537
50	1.75566406	0.48759112	-0.14443916
7	0.70600188	-1.41409317	-1.59255773
6	1.23133382	-1.39670111	-2.97029197
1	0.89210377	-2.27713684	-3.54738243
1	0.91554630	-0.48253392	-3.48628765
1	2.32631148	-1.40615471	-2.91366092
7	-1.11641588	0.89936292	-2.22849580
6	-0.77300629	-1.46633951	-1.54243851
1	-1.12036806	-2.48337339	-1.81635869
1	-1.07785789	-1.29311562	-0.50014049
6	-1.52059693	-0.49414302	-2.45548147
1	-2.59914870	-0.65903815	-2.27531468
1	-1.32644514	-0.71693533	-3.51220649
16	-1.74641081	2.07819039	-3.28504033
7	1.20085666	-1.22507653	1.16959234
6	1.27883392	-2.57460841	-0.85983647
1	0.93390102	-3.52391426	-1.31422675
1	2.36897796	-2.49798753	-0.97060219
6	0.92166120	-2.56006078	0.62538250
1	1.52266799	-3.33284837	1.13140674
1	-0.13860885	-2.84057879	0.76741081
16	0.54218957	-0.88753591	2.63835711
8	1.05343744	0.46001099	3.00227790
8	0.70113485	-2.03461913	3.56356724
6	-1.24626755	-0.69504778	2.36973271

6	-2.10777655	-1.77730659	2.55859521
6	-3.46980937	-1.62593459	2.27829197
6	-3.98772189	-0.40451281	1.82450380
6	-3.10067959	0.67460007	1.65799504
6	-1.73917214	0.53757771	1.92594144
1	-1.71283078	-2.71803425	2.94137163
1	-1.05563105	1.38092560	1.81774394
1	-3.48796442	1.64022812	1.32548007
6	-5.46348451	-0.23435950	1.56155032
1	-4.14339657	-2.47243797	2.42568507
8	-1.20832047	3.35741064	-2.79530351
8	-1.49161636	1.56837271	-4.64530714
6	-3.53668031	2.09786564	-3.03047341
6	-4.36099918	1.30767425	-3.83299736
6	-5.74015226	1.31996579	-3.60870886
6	-6.30482603	2.11026079	-2.59707049
6	-5.44964362	2.90554568	-1.81287489
6	-4.07185745	2.90479877	-2.02071746
1	-3.92616057	0.71508308	-4.63723240
1	-6.38968750	0.71074840	-4.23955844
6	-7.79238871	2.11455067	-2.35090788
1	-5.87287452	3.54440690	-1.03523683
1	-3.41296994	3.54324731	-1.43204275
1	-5.95282108	-1.20032050	1.38148182
1	-5.96272355	0.23384389	2.42421757
1	-5.64351714	0.41415897	0.69282311
1	-8.18568535	3.14002959	-2.30760126
1	-8.33116256	1.57299552	-3.13822833
1	-8.03237822	1.63721336	-1.38850367
1	-1.22886430	1.21855648	-1.26149143

Energy = -8524.642216 Hartree

Number of imaginary frequencies = 0.

Intermediate 2b (I2b)

Compound I2b isomer 1

Atomic N.	X	Y	Z
50	2.07658231	-2.35131503	1.12549345
7	0.41137668	-1.20454327	2.50804520
6	0.90356798	-1.00734347	3.88986895
1	0.08452546	-0.67503165	4.55114905
1	1.69990519	-0.25455677	3.90807645
1	1.31143078	-1.96088417	4.24516763
7	1.70805768	1.21329819	0.81577311
6	-0.19703424	0.04625174	1.95797385
1	-1.07374024	0.30019639	2.58011519
1	-0.56404563	-0.17966395	0.94968155
6	0.69102669	1.28532213	1.87867231
1	1.13281751	1.52269663	2.86575172
6	2.41706642	2.41517583	0.52833929
6	1.76497827	3.48058120	-0.13467826
6	2.48676162	4.64538465	-0.42659919
6	3.84157372	4.78470343	-0.11079136
6	4.47747101	3.70572368	0.51533097
6	3.79367068	2.53037450	0.84236652
7	0.22346857	-3.03281586	0.35053012
6	-0.61780663	-2.29379129	2.51914084

1	-1.51616040	-1.94442036	3.06008641
1	-0.16698451	-3.13146411	3.06903949
6	-0.98800425	-2.75872597	1.11285726
1	-1.60166889	-3.67292348	1.23262861
1	-1.64939753	-2.01289948	0.62846953
6	0.07825513	-3.64891242	-0.91960310
6	-0.54143035	-2.97903978	-2.00878251
6	-0.67006525	-3.62952515	-3.24247507
6	-0.19289117	-4.92700098	-3.45345173
6	0.44353046	-5.56586392	-2.38400747
6	0.58658508	-4.95867449	-1.13021409
6	0.32925971	3.36326247	-0.58261784
1	1.97202251	5.46097531	-0.94140333
6	4.60646279	6.03570393	-0.47167190
1	5.53857544	3.78215279	0.76654196
6	4.53127343	1.39771556	1.51737859
6	-1.00470765	-1.54907827	-1.88435743
1	-1.13974580	-3.09273339	-4.07163435
6	-0.37092018	-5.62015045	-4.78302271
1	0.83494744	-6.57731253	-2.52323235
6	1.28345722	-5.71154424	-0.02237610
1	0.14015410	4.03213887	-1.43316888
1	-0.38677226	3.63127515	0.21037576
1	0.10415817	2.33004472	-0.88307730
1	4.58736830	0.49950230	0.88100023
1	4.04883775	1.09102977	2.45902384
1	5.56079205	1.69531518	1.75297718
1	5.16693129	5.90394119	-1.41089866
1	5.33742252	6.29746004	0.30637649
1	3.93199597	6.89143027	-0.60882726
1	-1.07729573	-1.08069497	-2.87513862
1	-0.30193296	-0.96528740	-1.27133552
1	-1.99623554	-1.46944760	-1.40939270
1	0.83624355	-5.50240086	0.95732760
1	2.34500671	-5.42439571	0.06020287
1	1.25808296	-6.79251910	-0.21579792
1	0.48577114	-6.26754251	-5.01669222
1	-0.48537465	-4.89467485	-5.60004653
1	-1.26915378	-6.25834288	-4.78313116
1	2.36906714	0.45905624	1.01513707
8	2.17957161	-3.66094807	2.73989409
6	3.43725725	-4.01277089	3.29440834
1	3.60857036	-5.10028018	3.20173987
1	3.47409118	-3.75938107	4.37045645
1	4.29228722	-3.50112474	2.80814118
1	0.00761836	2.11157696	1.64778685
8	-2.79732374	1.91471522	1.15109452
8	-4.91893903	2.45538971	0.82328442
6	-3.69612455	2.07764572	0.34682841
6	-3.51142001	1.90234119	-1.15113021
1	-4.24131563	1.17275019	-1.53958554
1	-2.51383738	1.46524837	-1.27282278
6	-3.61705431	3.21958444	-1.94934070
1	-3.06184724	4.01051025	-1.41996890
1	-3.10277223	3.07384615	-2.91086051
6	-5.05507324	3.67119234	-2.22361646
1	-5.55018065	2.91139905	-2.85304932
1	-5.03570432	4.59736338	-2.81853603

6	-5.90419495	3.89590782	-0.96787249
1	-5.49963333	4.72275050	-0.36168579
1	-6.91910762	4.20056274	-1.27095794
6	-6.04585340	2.66967322	-0.07048320
1	-6.23274512	1.75701745	-0.65958694
1	-6.88538302	2.79983845	0.62338915

Energy = -7584.965620 Hartree
Number of imaginary frequencies = 0.

Compound I2b isomer 2

Atomic N.	X	Y	Z
8	-0.30301990	-3.19973165	-1.73859865
8	0.16295564	-0.50980721	0.96743949
6	1.38026794	-1.21017805	1.17487456
1	1.44031080	-1.59293191	2.21056474
1	2.28088899	-0.58539205	1.00820537
1	1.45442995	-2.07843526	0.49224639
8	-1.26433043	-5.17871556	-1.52126292
6	-0.92677699	-3.95651270	-1.01376812
6	-1.31782082	-3.61101680	0.41087200
1	-2.41093109	-3.70159627	0.53043232
1	-1.04995343	-2.55402330	0.54929414
6	-0.61075307	-4.47365378	1.47901958
1	0.45564820	-4.57110709	1.21960617
1	-0.64407938	-3.91962978	2.42861446
6	-1.23390434	-5.85688586	1.68929996
1	-2.26744176	-5.72768734	2.05532054
1	-0.68856970	-6.38246534	2.48851845
6	-1.26476701	-6.73758918	0.43587270
1	-0.24341565	-6.97661622	0.09734334
1	-1.74342288	-7.69944162	0.68231981
6	-2.02998670	-6.13683526	-0.73962512
1	-2.97596785	-5.67627090	-0.41128085
1	-2.27061367	-6.91387988	-1.47567726
50	0.28452744	1.54505310	0.54365056
7	-1.45661309	1.14714986	-1.14212947
6	-1.82448048	2.42456431	-1.78729610
1	-2.71477334	2.29826309	-2.42902644
1	-0.99223956	2.78994623	-2.39880356
1	-2.03555390	3.17168388	-1.01413880
7	1.31393992	0.22532826	-2.18290256
6	-1.15462943	0.09338421	-2.14846362
1	-2.02617809	-0.01703851	-2.82142357
1	-1.03351259	-0.85245819	-1.60179697
6	0.09178846	0.31800443	-2.99939401
1	0.07363202	-0.44844939	-3.79779195
1	0.06743288	1.29262144	-3.50345903
6	2.55326484	0.39999113	-2.87349747
6	2.94618000	1.68090248	-3.32052784
6	4.17547897	1.82523998	-3.97850779
6	5.04038918	0.74870207	-4.19086344
6	4.64537357	-0.50644855	-3.71162494
6	3.42166255	-0.70369463	-3.06431506
7	-1.58210361	2.06422642	1.47034785
6	-2.56364849	0.66113115	-0.26636137
1	-2.22993334	-0.30891293	0.12734212
1	-3.47922076	0.51143263	-0.86951843

6	-2.83622679	1.60876024	0.90012353
1	-3.46764962	2.46014213	0.56220345
1	-3.46386676	1.04790163	1.61941469
6	-1.63381140	2.64753394	2.76483736
6	-1.88072789	1.85824528	3.91955260
6	-1.90239918	2.46611545	5.18186726
6	-1.67827248	3.83589042	5.35261196
6	-1.41550691	4.60053609	4.20995135
6	-1.39333445	4.03633985	2.92890447
6	2.10144794	2.90410376	-3.06328252
1	4.47151812	2.82232066	-4.31433358
6	6.35676186	0.92716146	-4.90854664
1	5.30615715	-1.36584279	-3.85177858
6	3.05247071	-2.08165129	-2.56707267
6	-2.07619354	0.36534067	3.81243747
1	-2.08133326	1.84150568	6.06172934
6	-1.73514417	4.47306663	6.72057187
1	-1.22774074	5.67247171	4.31637378
6	-1.11451636	4.91671976	1.73412198
1	2.72354600	3.80853999	-3.07398311
1	1.60517221	2.83754436	-2.08376339
1	1.32039130	3.04247647	-3.82926316
1	3.05755909	-2.13504560	-1.46581057
1	3.77640047	-2.82259726	-2.92874036
1	2.05225690	-2.40024237	-2.89558179
1	6.57106120	1.98875362	-5.08867872
1	6.35225325	0.41670896	-5.88416751
1	7.19113739	0.50555885	-4.32904204
1	-1.79752336	-0.12736405	4.75384436
1	-1.47121655	-0.05246119	2.99400161
1	-3.12831359	0.10357064	3.61102527
1	-1.87747751	4.78630640	0.95327751
1	-0.14491226	4.68086056	1.26900986
1	-1.09761233	5.97422286	2.02982075
1	-1.52374741	3.74086167	7.51184152
1	-2.73310587	4.89430588	6.92246085
1	-1.01184710	5.29538696	6.81163543
1	1.30481595	-0.68426748	-1.71670288

Energy = -7584.971578 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 3

Atomic N.	X	Y	Z
8	-1.43011449	-3.51254327	-0.82456136
8	-3.39767658	-3.59591299	0.18394949
6	-2.61837234	-3.24610948	-0.87870735
6	-3.25656650	-2.52812756	-2.05448213
1	-4.09601342	-3.12413095	-2.45020236
1	-2.48291180	-2.49695130	-2.83064447
6	-3.73786141	-1.09886019	-1.71791903
1	-2.96899059	-0.58742525	-1.11516042
1	-3.81691693	-0.54021338	-2.66295827
6	-5.09742026	-1.05388181	-1.01292249
1	-5.86595404	-1.46331033	-1.69227489
1	-5.37339222	-0.00352165	-0.83316073
6	-5.15872824	-1.82150031	0.31233281
1	-4.48911719	-1.36862050	1.06054657

1	-6.17918851	-1.74678413	0.72258739
6	-4.82452564	-3.30611973	0.20379360
1	-5.30759444	-3.76780435	-0.67286078
1	-5.16718337	-3.84134838	1.09784282
8	-1.00302632	0.16086268	0.30918341
6	-1.48711458	-0.30758113	1.55865104
1	-2.38868986	0.25430721	1.86840909
1	-0.74997728	-0.20889642	2.38125573
1	-1.76494937	-1.37647346	1.49568563
50	0.83924010	1.17131175	0.30181171
7	1.34269166	-0.06977739	-1.75634930
6	2.66445512	0.34551969	-2.27006709
1	2.84287251	-0.07121649	-3.27746815
1	3.45496374	-0.00093199	-1.59525954
1	2.70713146	1.43948507	-2.31520283
7	1.70461747	-1.86124121	0.74121697
6	1.23286023	-1.55105537	-1.66639601
1	1.46097773	-1.98646448	-2.65789717
1	0.18438779	-1.78757910	-1.43714078
6	2.12030234	-2.22459095	-0.62418867
1	2.04425665	-3.31495794	-0.79889311
1	3.17683475	-1.96055708	-0.76128556
6	2.44403515	-2.46000536	1.80860422
6	1.84305708	-3.45645721	2.61658857
6	2.57297390	-4.00849249	3.67478543
6	3.88545954	-3.61409070	3.95988035
6	4.45480004	-2.62313165	3.15511461
6	3.75895158	-2.02908888	2.09386433
7	0.35590363	2.48468669	-1.32884438
6	0.25002780	0.43185421	-2.64115601
1	-0.68281445	0.03683178	-2.21566639
1	0.38111911	0.02814182	-3.66312891
6	0.18332498	1.95751336	-2.66948272
1	0.94606227	2.36107512	-3.37179426
1	-0.79419024	2.22035730	-3.11862935
6	-0.03162505	3.83379543	-1.10989578
6	-1.40032601	4.21203004	-1.08288294
6	-1.74474040	5.54853651	-0.84048601
6	-0.78116844	6.53607928	-0.61300855
6	0.56399536	6.14859507	-0.62244769
6	0.95315771	4.82662355	-0.86840463
6	0.42831517	-3.92080323	2.36178586
1	2.10006315	-4.77876655	4.28945916
6	4.64222572	-4.21064719	5.12233073
1	5.47011032	-2.27920380	3.36855976
6	4.41504021	-0.91632459	1.31431300
6	-2.49244355	3.18631505	-1.26654607
1	-2.80378988	5.82024182	-0.81000290
6	-1.17567648	7.97527828	-0.38148800
1	1.33723045	6.89940470	-0.43801303
6	2.42116938	4.47286240	-0.87559453
1	0.19747718	-4.79492204	2.98342935
1	0.24826717	-4.19786674	1.31266239
1	-0.31001208	-3.14203230	2.61401422
1	4.89356742	-1.27866671	0.38933356
1	5.20012988	-0.43876239	1.91488489
1	3.67878568	-0.14838552	1.03441289
1	4.43102810	-5.28390199	5.22999270

1	4.35905815	-3.72799525	6.07119840
1	5.72641959	-4.08530192	5.00076524
1	-3.41761320	3.51737550	-0.77527553
1	-2.19055292	2.21380801	-0.85020067
1	-2.73202561	3.02858168	-2.33143473
1	2.69812834	3.92953927	-1.79049194
1	2.68941605	3.82167401	-0.02943907
1	3.03697751	5.37986841	-0.81119894
1	-2.20365621	8.05172715	-0.00168106
1	-1.12731944	8.55712224	-1.31594855
1	-0.50623322	8.46475524	0.33966673
1	0.71460337	-2.09682525	0.83623248

Energy = -7584.971844 Hartree
Number of imaginary frequencies = 0.

Compound I2b isomer 4

Atomic N.	X	Y	Z
8	0.34882318	-2.43456260	2.82762420
8	0.38676576	0.38636992	4.64263166
6	-0.51905710	1.32221214	5.21927029
1	-0.55532873	2.28062003	4.67527627
1	-0.19715237	1.53308507	6.25322249
1	-1.54633945	0.91963240	5.25543749
8	0.40132886	-4.55490690	3.40604987
6	0.40247146	-3.24327714	3.74995515
6	0.49220514	-2.84692196	5.20648699
1	-0.32761453	-3.32365237	5.76970866
1	0.33494831	-1.75866317	5.23396987
6	1.84722042	-3.20617634	5.85581287
1	2.66344210	-2.93243426	5.16792964
1	1.96963159	-2.56548772	6.74120173
6	1.97509128	-4.67218341	6.28106025
1	1.21894892	-4.88187640	7.05758794
1	2.95538565	-4.82836253	6.75727421
6	1.80111615	-5.68411307	5.14335546
1	2.60453798	-5.57970406	4.39608510
1	1.88845550	-6.70417717	5.55156656
6	0.46096175	-5.60014142	4.41993413
1	-0.37553058	-5.47620896	5.12590143
1	0.28108656	-6.51088891	3.83621612
50	1.06581196	0.23165655	2.71537018
7	-0.97837301	0.39213320	-2.14690638
6	-1.56785320	1.60647358	-2.68528884
1	-0.98283493	2.53471490	-2.51863826
1	-2.55930818	1.75847174	-2.23247428
1	-1.70432462	1.49357750	-3.77187068
7	2.51972220	0.24647405	-3.77146360
6	0.18663743	-0.11331000	-2.85730200
1	-0.09857730	-0.23721543	-3.91712205
1	0.40933288	-1.12112771	-2.46533124
6	1.49026682	0.72900205	-2.83280720
1	1.25841284	1.77472692	-3.06662177
1	1.93880213	0.71982250	-1.82817643
6	2.31088864	0.36501142	-5.16861441
6	2.23779013	1.64037783	-5.78172980
6	2.07042703	1.72112872	-7.16961482
6	2.00312664	0.58819907	-7.98709221

6	2.13378637	-0.66124216	-7.36999226
6	2.28140842	-0.79432700	-5.98570043
7	-0.49748181	1.11721614	1.60234225
6	-1.03192309	0.24562222	-0.69829921
1	-0.71949561	-0.78055669	-0.44263086
1	-2.08855350	0.34390122	-0.39607738
6	-0.20772953	1.23762159	0.16462220
1	0.86963691	1.04549659	0.01407918
1	-0.39243566	2.26469716	-0.19143751
6	-1.73782432	1.66942136	2.03300701
6	-2.77306943	0.83215791	2.52336054
6	-3.98388459	1.40196322	2.93579173
6	-4.21556125	2.78079394	2.89070060
6	-3.17493667	3.59701626	2.43701060
6	-1.94625783	3.07524904	2.01307329
6	2.41657316	2.91243570	-4.98876742
1	2.02119142	2.71255591	-7.62801616
6	1.79174218	0.70807984	-9.47714770
1	2.11094477	-1.56611619	-7.98283515
6	2.41355817	-2.17082967	-5.37819443
6	-2.58988545	-0.66025009	2.63198734
1	-4.77297058	0.74069422	3.30329217
6	-5.54515019	3.36438015	3.30379128
1	-3.31264460	4.68173247	2.42794588
6	-0.85455178	4.03510161	1.60631454
1	2.79193576	3.71442594	-5.63818834
1	3.12962320	2.76366283	-4.16541987
1	1.47450637	3.27226117	-4.54467714
1	3.38495698	-2.31650349	-4.87600074
1	2.33491507	-2.94189495	-6.15474114
1	1.62874034	-2.36910916	-4.63033289
1	0.72097546	0.66631860	-9.73404981
1	2.28790550	-0.10792976	-10.02060549
1	2.18116972	1.66112282	-9.86098859
1	-3.55359554	-1.15260434	2.81808406
1	-1.91425344	-0.91878260	3.46203014
1	-2.14247769	-1.08864556	1.72571938
1	-0.86118451	4.24113206	0.52410652
1	0.13834122	3.63345954	1.85242512
1	-0.98311014	4.99848384	2.11771992
1	-6.00939838	2.77693320	4.10794195
1	-6.25301056	3.37704613	2.45958058
1	-5.43646960	4.40017434	3.65348314
1	2.77459950	-0.71066340	-3.53218149

Energy = -7584.949135 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 5

Atomic N.	X	Y	Z
8	0.30918518	-0.57491803	0.40428382
8	2.22415500	1.48351099	1.90402283
6	3.54990789	1.30449616	2.36112061
1	3.92980205	2.21963477	2.85428554
1	4.27126892	1.04826355	1.55518835
1	3.59718653	0.49095450	3.11005058
8	-0.65996492	-1.35900359	2.21846929
6	0.45118823	-1.16933242	1.46927220

6	1.77264055	-1.73462893	1.93611711
1	2.03078047	-1.30142166	2.91530172
1	2.51809497	-1.37365357	1.21968392
6	1.79751451	-3.27739750	2.00800741
1	1.31451033	-3.69647002	1.11084700
1	2.85012140	-3.59403212	1.96517509
6	1.16217878	-3.85674614	3.27614211
1	1.73272568	-3.50088611	4.15147262
1	1.26622878	-4.95268852	3.26521179
6	-0.31317902	-3.49265971	3.47099376
1	-0.93439985	-3.93016342	2.67258115
1	-0.67106827	-3.92889876	4.41778668
6	-0.59076037	-1.99469409	3.52894925
1	0.14495684	-1.46254261	4.15129200
1	-1.58794672	-1.80285828	3.94272211
50	1.89590338	1.70719430	-0.14185267
7	0.32079407	2.08359455	-2.68549002
6	1.26395053	2.03045879	-3.80202221
1	0.88611314	2.55620759	-4.70483548
1	1.48247702	0.98865816	-4.06339909
1	2.20836407	2.50068394	-3.49539988
7	-0.33612977	-0.89840853	-2.64467616
6	-0.97779068	1.48346993	-3.02684986
1	-1.50158706	2.10969972	-3.78541747
1	-1.60207358	1.49680778	-2.12068701
6	-0.94501747	0.05745642	-3.57722761
1	-1.99643199	-0.20461411	-3.81636921
1	-0.40307427	0.02964537	-4.53460710
6	-0.52018601	-2.27741943	-2.94815178
6	0.27772148	-2.88918573	-3.94262404
6	0.11027478	-4.25293229	-4.21362109
6	-0.81296070	-5.04187410	-3.51885947
6	-1.58250936	-4.42315338	-2.52642356
6	-1.46387926	-3.05832185	-2.23714749
7	0.26386072	2.99766776	0.22020291
6	0.14522651	3.47307151	-2.23271187
1	-0.44770508	4.05953691	-2.96965406
1	1.14767294	3.92963386	-2.18511872
6	-0.50611207	3.61701035	-0.85895256
1	-0.59804301	4.70415834	-0.67153359
1	-1.54664471	3.23946339	-0.89224850
6	-0.21355862	3.34336170	1.52345115
6	-1.40368807	2.77989942	2.04251667
6	-1.84785773	3.16153138	3.31728108
6	-1.15589918	4.08916897	4.09928093
6	0.01313608	4.64668169	3.56707751
6	0.49605090	4.29070230	2.30370164
6	1.33786787	-2.10352513	-4.67146187
1	0.74118779	-4.71563952	-4.97720073
6	-0.99202655	-6.50500201	-3.84712820
1	-2.31288179	-5.01603151	-1.96921371
6	-2.35413935	-2.43294900	-1.18838171
6	-2.21133307	1.77538947	1.25791092
1	-2.76588456	2.71284453	3.70716170
6	-1.63732836	4.46721478	5.47995630
1	0.56885600	5.38346136	4.15337617
6	1.76649956	4.92385883	1.79402511
1	2.08983952	-2.77444558	-5.10698977

1	1.83453633	-1.40491445	-3.98281616
1	0.91863277	-1.50532654	-5.49679282
1	-1.78882657	-2.03767255	-0.33083546
1	-3.06977834	-3.17114694	-0.80419650
1	-2.93059140	-1.58956140	-1.59916118
1	-1.75000567	-6.64692185	-4.63410839
1	-1.32365458	-7.07628736	-2.96925408
1	-0.05682535	-6.95071809	-4.21323775
1	-2.77135667	1.11567662	1.93396122
1	-1.56593659	1.15417343	0.62431049
1	-2.94963702	2.27267711	0.60728468
1	1.67169513	5.24750334	0.74826113
1	2.60046348	4.20670553	1.83326962
1	2.03923751	5.79255706	2.40795720
1	-1.02896318	3.98408439	6.26092373
1	-2.68074924	4.16245029	5.63681670
1	-1.56949924	5.55220844	5.64577955
1	-0.62492239	-0.69438245	-1.68682455

Energy = -7584.956774 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 6

Atomic N.	X	Y	Z
8	4.23016665	-3.68489805	-0.91043869
8	-0.41197380	-0.17367361	0.80985972
6	-0.04039546	-0.02904644	2.16903486
1	0.99550708	0.34738005	2.30697442
1	-0.10607583	-1.00397157	2.68704931
1	-0.71620411	0.67158652	2.69046302
8	2.19830459	-4.16606444	-0.16832744
6	3.39021350	-3.51160620	-0.04772418
6	3.61920508	-2.62416538	1.16575488
1	2.84419450	-1.84052208	1.21035523
1	4.57802651	-2.12580324	0.98174412
6	3.66113595	-3.39283928	2.50339773
1	4.25616369	-4.31187686	2.37625081
1	4.20420580	-2.77384605	3.23375158
6	2.28009163	-3.72726976	3.07703818
1	1.75333725	-2.78283161	3.29751868
1	2.40524741	-4.24314405	4.04219907
6	1.39469251	-4.57763489	2.15967348
1	1.83260035	-5.57839949	2.01030592
1	0.41961418	-4.73436989	2.64931855
6	1.12003227	-3.96377865	0.78998752
1	0.87675585	-2.89167953	0.85849159
1	0.26965396	-4.46078788	0.30830579
50	0.86148439	0.50810587	-0.67953693
7	0.65693100	2.34821255	-2.69957413
6	1.89194412	2.18670363	-3.48199596
1	1.87065162	2.78717998	-4.41190615
1	2.03368227	1.13337574	-3.75148509
1	2.75228400	2.49661839	-2.87438430
7	-0.46581239	-0.28142374	-2.15845620
6	-0.51567381	1.82415617	-3.42700624
1	-0.56163156	2.25108492	-4.45028236
1	-1.41703721	2.13579003	-2.88176251
6	-0.50875804	0.29881507	-3.49462707

1	-1.44176710	-0.00583862	-4.00335824
1	0.31171902	-0.04193863	-4.16144033
6	-0.88941862	-1.65008460	-2.11116366
6	-0.08524302	-2.69448137	-2.63250534
6	-0.56204464	-4.01427590	-2.59976490
6	-1.81164997	-4.33893662	-2.06712802
6	-2.59406029	-3.29624586	-1.55380092
6	-2.15958545	-1.96656196	-1.56484853
7	0.02996841	3.28860082	0.07465754
6	0.48984875	3.75893094	-2.30416474
1	0.14856655	4.37092219	-3.16391081
1	1.48573747	4.13994097	-2.02496824
6	-0.46241695	3.98242183	-1.13249979
1	-0.54438691	5.07320057	-0.96861596
1	-1.46976090	3.62184420	-1.37316678
6	-0.56916332	3.63315533	1.32811110
6	-1.92952458	3.35936388	1.58823817
6	-2.45546010	3.69564176	2.84295177
6	-1.68064704	4.26923177	3.85507410
6	-0.32569152	4.49553058	3.58590924
6	0.24191041	4.19341838	2.34460011
6	1.27934125	-2.43904061	-3.22591845
1	0.07651249	-4.80983712	-2.99205999
6	-2.29393140	-5.76945254	-2.01642682
1	-3.57877622	-3.52244352	-1.13576207
6	-3.04377794	-0.88675500	-0.99781176
6	-2.81058678	2.66034569	0.58369976
1	-3.50689013	3.47142193	3.03871782
6	-2.28299878	4.63966198	5.18859391
1	0.31180342	4.92332918	4.36347740
6	1.71356272	4.45211675	2.11425950
1	1.94145616	-3.29941163	-3.06586273
1	1.75733006	-1.55614611	-2.77783740
1	1.22012454	-2.26302701	-4.31237019
1	-2.58358205	-0.46571003	-0.09206107
1	-4.03324604	-1.29041494	-0.74415167
1	-3.17453416	-0.05852931	-1.70939831
1	-3.37122225	-5.83705228	-2.22424345
1	-2.12932287	-6.21124301	-1.02047336
1	-1.76347666	-6.39689619	-2.74502780
1	-3.65620395	2.17885348	1.09101932
1	-2.25264975	1.88112266	0.04697598
1	-3.23333205	3.35635763	-0.15865504
1	1.89073182	5.13272266	1.26527274
1	2.27324014	3.52299414	1.91507492
1	2.16378666	4.91540156	3.00062820
1	-1.58028638	4.45390712	6.01265373
1	-3.20013645	4.06850900	5.38468571
1	-2.54746803	5.70845792	5.22197047
1	1.03503851	3.45754172	0.14285764

Energy = -7584.961392 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 7

Atomic N.	X	Y	Z
8	0.54491391	-0.55886062	-0.10232621
8	1.08459431	0.68263985	-3.03404261

6	1.42113031	-0.02384071	-4.21207859
1	0.65773818	-0.77055918	-4.52034130
1	2.37522664	-0.56904800	-4.08119497
1	1.55818545	0.66730912	-5.06548116
8	2.56750247	-0.31974985	0.73389320
6	1.73488625	-0.84368021	-0.19712373
6	2.28548354	-1.77527323	-1.25224256
1	3.04765171	-1.24548904	-1.84561309
1	1.44754215	-1.98611144	-1.92463777
6	2.86341995	-3.08990117	-0.68384032
1	2.18373828	-3.48860974	0.08619390
1	2.86913686	-3.82852857	-1.49900000
6	4.28491507	-2.96378331	-0.12636731
1	4.96077188	-2.66283333	-0.94551064
1	4.63077409	-3.95307629	0.21087717
6	4.42932272	-1.96060739	1.02240408
1	3.85325016	-2.28673666	1.90364893
1	5.48469815	-1.92147377	1.33776114
6	4.00780018	-0.53793439	0.67236868
1	4.37941785	-0.22974173	-0.31700295
1	4.39097699	0.17188784	1.41523782
50	-0.87154658	0.55140736	-2.32789911
7	-3.23759955	1.03312476	-0.52799319
6	-4.37903420	0.31475939	-1.09350316
1	-5.35313935	0.73853346	-0.76819106
1	-4.33983477	-0.74294288	-0.80881605
1	-4.32641682	0.36515767	-2.18974066
7	-2.20985071	-1.23288230	1.24139885
6	-3.24582788	1.01822952	0.94228011
1	-4.10400050	1.61603293	1.32718143
1	-2.33014487	1.52140783	1.28801087
6	-3.32859790	-0.35602893	1.60741090
1	-3.37191773	-0.16773298	2.70019495
1	-4.27767619	-0.84980746	1.34979259
6	-2.06343671	-2.41862495	2.01715327
6	-2.88743449	-3.53630511	1.75096892
6	-2.71649343	-4.70804411	2.49906298
6	-1.74183284	-4.81857695	3.49640917
6	-0.92372166	-3.70754924	3.73467666
6	-1.07306873	-2.50971600	3.02561780
7	-0.74706772	2.49238186	-1.50264274
6	-3.20392835	2.41497409	-1.03317749
1	-4.01342540	3.02626283	-0.57512303
1	-3.40414605	2.37051477	-2.11645272
6	-1.87380438	3.13567473	-0.82556136
1	-2.00973903	4.15863777	-1.22598526
1	-1.68240596	3.27092856	0.25671870
6	0.43353927	3.30017646	-1.52061422
6	1.21709290	3.48019081	-0.35561326
6	2.35709566	4.29578817	-0.41089912
6	2.74879525	4.94826462	-1.58215230
6	1.95561548	4.77172360	-2.72239969
6	0.81469755	3.96264784	-2.71491140
6	-3.90600581	-3.49571710	0.64048793
1	-3.35284646	-5.56848024	2.27577525
6	-1.59388413	-6.08438822	4.30659634
1	-0.15422093	-3.76655471	4.50917095
6	-0.19259221	-1.32672772	3.35573462

6	0.85711488	2.81715094	0.95125212
1	2.95549084	4.42009448	0.49609130
6	3.99508699	5.80013128	-1.62738521
1	2.23231305	5.28043983	-3.64979066
6	0.00994433	3.81070323	-3.98117562
1	-4.17573929	-4.51099596	0.32149518
1	-3.50732105	-2.94133777	-0.22123446
1	-4.83744821	-2.99368112	0.94919093
1	0.44871299	-1.02573396	2.51354202
1	0.46127782	-1.56166064	4.20540945
1	-0.78986895	-0.44239763	3.62715641
1	-2.19972204	-6.04190072	5.22593124
1	-0.55111471	-6.24698751	4.61237614
1	-1.92602832	-6.96426786	3.73868678
1	1.75376871	2.65692678	1.56458015
1	0.37394583	1.84611700	0.78523234
1	0.16877059	3.44264681	1.54333247
1	-1.06935439	3.89386036	-3.79256604
1	0.18203758	2.82147913	-4.43159988
1	0.29865173	4.57299228	-4.71703534
1	4.82394771	5.26822753	-2.12099822
1	4.33082719	6.07160296	-0.61748236
1	3.82694002	6.72799958	-2.19293251
1	-1.33650522	-0.70414731	1.21937558

Energy = -7584.956766 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 8

Atomic N.	X	Y	Z
8	0.13424198	-3.11432981	-1.35747923
8	0.40414287	0.43804594	-1.09037840
6	1.38182223	0.54733418	-2.12076554
1	1.58526694	1.60784851	-2.35203516
1	1.07333982	0.06045778	-3.06697273
1	2.32760568	0.07689017	-1.79950550
8	2.15419797	-2.54798017	-0.65458856
6	1.26189958	-3.48223686	-1.05098899
6	1.67105932	-4.94137766	-1.09966302
1	2.56198315	-5.05662761	-1.73993556
1	0.84061350	-5.46006585	-1.59184381
6	1.93945017	-5.55818350	0.29011948
1	1.14185382	-5.24737004	0.98238996
1	1.85964212	-6.65124700	0.19145658
6	3.31610558	-5.21526475	0.86833518
1	4.09541430	-5.64405526	0.21376303
1	3.42905427	-5.71137216	1.84477276
6	3.58324885	-3.71525021	1.03420156
1	2.88336769	-3.26946838	1.75870975
1	4.59577095	-3.57435776	1.44639109
6	3.50887290	-2.91189244	-0.25953327
1	4.00641599	-3.43227766	-1.09414330
1	3.99040906	-1.93476096	-0.13380835
50	-1.28279494	-0.70963163	-1.52338527
7	-3.19039711	1.08721975	-1.02201318
6	-4.28446688	0.48476690	-1.81058966
1	-5.24991961	0.98055486	-1.59436786
1	-4.38005936	-0.58436197	-1.58576414

1	-4.05944700	0.58560949	-2.88015202
7	-1.84945546	-0.97301432	0.55195028
6	-3.43103814	0.89204887	0.42663207
1	-4.45583389	1.22542729	0.69100920
1	-2.71067554	1.51214759	0.97350383
6	-3.21779803	-0.55978614	0.85461786
1	-3.38780869	-0.60475191	1.94472075
1	-4.01072046	-1.19752340	0.40789769
6	-1.32118032	-1.98798032	1.39702073
6	-1.88684624	-3.28705991	1.47760636
6	-1.36097143	-4.22279908	2.38179767
6	-0.27622828	-3.92601748	3.21096214
6	0.29694180	-2.65192257	3.09784501
6	-0.19818400	-1.68574589	2.21438178
7	-0.69907322	3.16855405	-1.29726092
6	-3.13010939	2.52936868	-1.39124610
1	-4.11221914	2.98488336	-1.14384944
1	-3.00820536	2.57380842	-2.48349623
6	-2.04166037	3.39903424	-0.76137879
1	-2.32513909	4.43564054	-0.99226063
1	-2.07625385	3.33039870	0.34427029
6	0.20301691	4.26677026	-1.21628090
6	1.26112274	4.28821474	-0.27433553
6	2.15480720	5.36584522	-0.27141038
6	2.02704731	6.44265896	-1.15689703
6	0.97692991	6.40472852	-2.08000976
6	0.07134917	5.33767876	-2.13359490
6	-3.02463042	-3.70239559	0.57874510
1	-1.81149945	-5.21849144	2.42686724
6	0.25151244	-4.93273001	4.20603960
1	1.14384494	-2.38828812	3.73832492
6	0.43889358	-0.32172527	2.16250664
6	1.42868056	3.17385682	0.73063050
1	2.96861684	5.36804766	0.45875674
6	2.97872578	7.61397061	-1.10296708
1	0.87086257	7.21815051	-2.80282759
6	-0.99205299	5.31353035	-3.20328293
1	-3.07264092	-4.79631359	0.49568086
1	-2.90156030	-3.28280930	-0.43064643
1	-4.00058546	-3.35917212	0.95744658
1	0.79565109	-0.08225755	1.15048359
1	1.27767310	-0.25977057	2.86966474
1	-0.29053009	0.46104681	2.41956768
1	-0.05634310	-4.68069462	5.23320756
1	1.35125326	-4.96834024	4.20309758
1	-0.12303574	-5.94240578	3.98918865
1	2.23675677	3.41167440	1.43440135
1	1.66015020	2.20945234	0.25485888
1	0.50875001	3.01383751	1.31300111
1	-1.97399002	5.64736169	-2.82964940
1	-1.12555128	4.29154504	-3.58618057
1	-0.72074749	5.97776555	-4.03439117
1	3.99330098	7.29529367	-0.82596537
1	2.65647322	8.35679634	-0.35558376
1	3.03391683	8.12903837	-2.07182290
1	-0.29240286	2.28680342	-0.95357297

Energy = -7584.965911 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 9

Atomic N.	X	Y	Z
8	2.44942074	0.85112665	-0.50006526
8	0.51956161	2.86243316	1.51619357
6	1.34253022	3.39391099	2.53907102
1	0.74171425	3.93576220	3.29560786
1	2.06467074	4.11894395	2.11818642
1	1.93067746	2.62347295	3.07917444
8	4.32979955	1.34583979	-1.52765829
6	3.15063798	1.73574678	-0.97513721
6	2.76688105	3.19911776	-0.98071204
1	3.56115680	3.78694803	-0.48918954
1	1.86553325	3.26946717	-0.35570274
6	2.49877731	3.76705776	-2.39159387
1	1.88018690	3.05487097	-2.95922180
1	1.88806207	4.67434279	-2.27146882
6	3.76247941	4.12578946	-3.17906342
1	4.30330974	4.92654626	-2.64433759
1	3.47276376	4.54792172	-4.15393421
6	4.72303696	2.95354093	-3.40381618
1	4.24962453	2.16947193	-4.01659344
1	5.59952930	3.30701368	-3.97130090
6	5.24273485	2.31146497	-2.12154411
1	5.51601447	3.07083042	-1.37091955
1	6.13251950	1.70451292	-2.32905052
50	0.33730360	0.78342953	1.32388286
7	-1.99392656	0.92104836	2.47894988
6	-2.06185215	2.26710686	3.08737261
1	-3.09108073	2.49422931	3.42151569
1	-1.71536976	3.02238190	2.37406406
1	-1.39287773	2.30176795	3.95762491
7	-1.07311121	1.02020695	-0.28087194
6	-2.91105246	0.81457733	1.31888743
1	-3.91994541	1.18604262	1.59089862
1	-2.98072110	-0.24412197	1.04246815
6	-2.36537226	1.57713780	0.11062879
1	-3.09194212	1.44968019	-0.71000643
1	-2.34448978	2.66009719	0.34023823
6	-0.76526394	0.97332411	-1.65640868
6	-0.93706525	2.09743726	-2.51163328
6	-0.68181425	1.97216678	-3.88533929
6	-0.22377456	0.78217552	-4.45697235
6	-0.00643384	-0.30173745	-3.59692388
6	-0.26648092	-0.23403792	-2.22478887
7	-1.33266953	-2.08636797	2.42344254
6	-2.27857895	-0.06945289	3.55285194
1	-3.19505935	0.23785676	4.09502237
1	-1.44545748	0.00281070	4.27105823
6	-2.47771354	-1.52969032	3.15131061
1	-2.67159018	-2.07789797	4.09478607
1	-3.39207963	-1.62994361	2.54992729
6	-1.19388271	-3.49719298	2.34802085
6	-2.15499003	-4.28867867	1.67716423
6	-1.96913971	-5.67591916	1.61211152
6	-0.85047656	-6.30934026	2.16131735
6	0.11232370	-5.50217591	2.77917335

6	-0.03819874	-4.11635440	2.88705367
6	-1.29512585	3.45932306	-1.96363161
1	-0.82155766	2.85045566	-4.52281088
6	0.01630141	0.66253344	-5.94328738
1	0.36139339	-1.24506596	-4.00986825
6	-0.02650665	-1.45025614	-1.36820182
6	-3.33340611	-3.67020073	0.96582889
1	-2.71624268	-6.27475425	1.08474262
6	-0.68895338	-7.80907133	2.09824481
1	1.00983461	-5.96440051	3.19799435
6	1.03552832	-3.29532712	3.56174492
1	-1.00799200	4.24205033	-2.67910503
1	-0.77731188	3.64552141	-1.01071529
1	-2.37310013	3.57768929	-1.77132471
1	0.91646852	-1.36512059	-0.80314742
1	0.04825587	-2.35384696	-1.98772798
1	-0.82831896	-1.58426445	-0.62858428
1	-0.80825479	0.12886130	-6.44277183
1	0.93782566	0.10294339	-6.16015056
1	0.09848897	1.65170766	-6.41471995
1	-3.72347247	-4.35878845	0.20523470
1	-3.04066099	-2.73524077	0.46588838
1	-4.16604222	-3.43503193	1.64791841
1	0.64063124	-2.71412162	4.41087927
1	1.50612201	-2.57635328	2.87095126
1	1.83035147	-3.94581389	3.94738466
1	0.36695822	-8.09566243	1.99679479
1	-1.24216970	-8.23524610	1.25027365
1	-1.07036717	-8.29066253	3.01294877
1	-0.46751639	-1.65855542	2.75546717

Energy = -7584.966297 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 10

Atomic N.	X	Y	Z
8	2.53001355	0.64601216	-0.36142454
8	0.79812970	2.51273972	1.95365380
6	1.64879229	2.78171705	3.05369647
1	2.13846646	1.87561493	3.46649621
1	1.09156654	3.25858777	3.88376336
1	2.45389437	3.48125943	2.75917495
8	4.46250522	1.08591145	-1.31410649
6	3.33192568	1.51117511	-0.69084774
6	3.11952568	2.98920860	-0.44770539
1	3.97010786	3.38923390	0.13077707
1	2.22461857	3.05761290	0.18680238
6	2.93778933	3.81461621	-1.74018096
1	2.24958411	3.28478892	-2.41677208
1	2.43373656	4.75297872	-1.46454705
6	4.24500666	4.15283138	-2.46297525
1	4.86792766	4.78163250	-1.80249517
1	4.01948365	4.76647199	-3.34904464
6	5.06560928	2.93219842	-2.89181126
1	4.51259131	2.32540027	-3.62688649
1	5.98507715	3.27242445	-3.39584075
6	5.48945610	2.02411876	-1.74189289
1	5.84061104	2.60699801	-0.87486613

1	6.30443817	1.36089686	-2.05676863
50	0.39611664	0.52324591	1.43093646
7	-1.93002974	0.73171209	2.58818281
6	-1.86395257	1.96362609	3.40357452
1	-2.86891946	2.24647785	3.76772115
1	-1.42431763	2.77973057	2.82048000
1	-1.21212087	1.78637367	4.26945056
7	-0.94919942	1.16286649	-0.11835085
6	-2.83014338	0.91214454	1.42404565
1	-3.79771734	1.34547263	1.74944518
1	-3.00943189	-0.07526946	0.98245788
6	-2.18064200	1.79064123	0.35368283
1	-2.90023095	1.87542899	-0.47852664
1	-2.04664553	2.81487602	0.75246696
6	-0.62278141	1.29797435	-1.48382343
6	-0.65154639	2.55497822	-2.15021537
6	-0.38468552	2.61971979	-3.52566898
6	-0.05246764	1.49007949	-4.27835175
6	0.02591306	0.26694503	-3.60104979
6	-0.25076104	0.14672944	-2.23555350
7	-1.59562222	-2.28435386	2.05727547
6	-2.34162923	-0.37880008	3.48961231
1	-3.23072572	-0.06244344	4.07083482
1	-1.52057128	-0.51249729	4.21287993
6	-2.68861563	-1.72671888	2.86050164
1	-2.95969892	-2.39198639	3.70442372
1	-3.59595044	-1.63038376	2.24794923
6	-1.60683438	-3.67261811	1.76109636
6	-2.63468330	-4.24097502	0.97327912
6	-2.59667273	-5.61290512	0.69129714
6	-1.56202852	-6.44159042	1.13514266
6	-0.52984464	-5.84974658	1.87310107
6	-0.53363914	-4.48973176	2.19726589
6	-0.86715637	3.84484122	-1.39326023
1	-0.41236519	3.59745270	-4.01604387
6	0.19756023	1.57975462	-5.76458358
1	0.29403555	-0.63486872	-4.15816683
6	-0.16302066	-1.20825323	-1.58221139
6	-3.72753495	-3.39534466	0.36676820
1	-3.39386074	-6.03771885	0.07573675
6	-1.56039313	-7.92169100	0.83761994
1	0.30550356	-6.46604457	2.21510613
6	0.60913867	-3.90511913	2.99379010
1	-0.48123217	4.69340205	-1.97461052
1	-0.35098727	3.81884138	-0.42181986
1	-1.92909139	4.05139663	-1.18670982
1	0.77375665	-1.31989365	-1.01150994
1	-0.17892283	-2.00588029	-2.33680731
1	-0.98731874	-1.36535813	-0.87248567
1	-0.69069778	1.27539627	-6.34136073
1	1.02265730	0.92288511	-6.07570804
1	0.44585331	2.60680311	-6.06667343
1	-4.17631448	-3.91128103	-0.49183495
1	-3.32750155	-2.43174101	0.01856776
1	-4.54149527	-3.17947015	1.07714760
1	0.26316617	-3.42473198	3.92348056
1	1.16586883	-3.14192503	2.42531961
1	1.32314288	-4.68987637	3.27298537

1	-0.53959977	-8.30109408	0.69122084
1	-2.14254829	-8.14838687	-0.06593198
1	-2.00511033	-8.49601631	1.66615700
1	-0.69630993	-2.00950977	2.45405650

Energy = -7584.966293 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 11

Atomic N.	X	Y	Z
8	2.58278459	-0.80912502	1.98087955
8	0.38230555	0.81475043	0.08079159
6	1.25044107	1.92612443	-0.13645186
1	0.72396854	2.89309904	-0.03648826
1	1.66341224	1.87298783	-1.15895368
1	2.10594728	1.94768706	0.56626299
8	4.73730066	-1.03914954	1.60554424
6	3.46466315	-0.93934018	1.13989253
6	3.20288079	-1.00854991	-0.34794346
1	3.77859133	-0.21743186	-0.85827815
1	2.13804612	-0.77214876	-0.47055465
6	3.53630739	-2.37956405	-0.97488644
1	3.15000567	-3.17992969	-0.32568733
1	2.97416830	-2.45739744	-1.91688204
6	5.02439164	-2.59385965	-1.26646845
1	5.35712140	-1.84179386	-2.00340825
1	5.16142679	-3.57565699	-1.74602813
6	5.93044152	-2.50504251	-0.03420724
1	5.69414217	-3.30523555	0.68584765
1	6.97758947	-2.66082753	-0.34141941
6	5.86772715	-1.16824446	0.69711113
1	5.87184697	-0.32101990	-0.00748135
1	6.72861812	-1.05599282	1.36745597
50	0.05267243	0.33404365	2.11020911
7	-2.52641238	0.62493437	2.22002758
6	-2.90034736	1.74720386	3.09382175
1	-3.97955798	1.73734430	3.33690223
1	-2.64409564	2.69573646	2.60865990
1	-2.32732516	1.67475665	4.02763204
7	-2.08445158	2.50843278	-0.15420671
6	-3.28324671	0.61672816	0.94355509
1	-4.31796090	0.26740930	1.13849132
1	-2.80076293	-0.12566612	0.29236244
6	-3.39046197	1.94565716	0.20019187
1	-4.01131108	1.73748894	-0.69542643
1	-3.96199235	2.67317140	0.79866756
6	-2.09836370	3.52313093	-1.15549465
6	-2.46995538	4.84324802	-0.81354698
6	-2.45773312	5.83706872	-1.80100578
6	-2.07381007	5.57028134	-3.11903087
6	-1.69534484	4.25991710	-3.43609877
6	-1.71186837	3.23161022	-2.48682495
7	-0.81425959	-1.57963166	1.67214897
6	-2.72665700	-0.66233898	2.92814453
1	-3.80277508	-0.82443882	3.13674360
1	-2.20371572	-0.57895946	3.89458791
6	-2.16249622	-1.85139295	2.15200222
1	-2.19576739	-2.72089799	2.84035987

1	-2.85188192	-2.11527973	1.32076914
6	-0.17067623	-2.72667902	1.12560007
6	-0.30278125	-3.03738147	-0.25150915
6	0.27834716	-4.20802291	-0.75714673
6	1.00057654	-5.08869429	0.05618180
6	1.13558731	-4.76450602	1.41099528
6	0.56758671	-3.60533688	1.95781602
6	-2.82714240	5.20253707	0.60650987
1	-2.73593159	6.85649680	-1.52099542
6	-2.08843131	6.65271487	-4.17190699
1	-1.39030472	4.02410852	-4.45908941
6	-1.33996157	1.82568515	-2.89662573
6	-1.06846393	-2.12261001	-1.17511231
1	0.15909714	-4.43775985	-1.81980289
6	1.64184591	-6.33010830	-0.51755478
1	1.69422036	-5.43679419	2.06797348
6	0.75037472	-3.30689785	3.42536897
1	-2.74029852	6.28491515	0.76793775
1	-2.16235507	4.68216844	1.31109601
1	-3.86055171	4.91684382	0.86167954
1	-0.45944906	1.44573435	-2.35698040
1	-1.12253218	1.78577314	-3.97166746
1	-2.15855590	1.11807402	-2.69260741
1	-3.02669834	6.63393292	-4.74918215
1	-1.26465398	6.52789417	-4.88841222
1	-2.00205261	7.65048219	-3.72069199
1	-0.92341264	-2.41888215	-2.22279092
1	-0.74437977	-1.08008938	-1.04700874
1	-2.15083401	-2.15771116	-0.97104686
1	-0.20835213	-3.11793298	3.92908005
1	1.36922748	-2.40957314	3.57171750
1	1.24486471	-4.14672314	3.93136507
1	2.64171275	-6.11094656	-0.92701945
1	1.04229974	-6.75000403	-1.33709476
1	1.76758877	-7.10725434	0.24857468
1	-1.40975628	1.76265031	-0.36993928

Energy = -7584.967518 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 12

Atomic N.	X	Y	Z
8	2.58551168	-0.46648860	2.07096464
8	0.34268015	0.83035576	-0.01555600
6	1.16106508	1.95132862	-0.34722399
1	0.59306143	2.89978204	-0.34246141
1	1.57570197	1.81365704	-1.36109570
1	2.01506219	2.08033207	0.34569239
8	4.75310306	-0.63770134	1.74280961
6	3.48387725	-0.65002381	1.25777795
6	3.24641711	-0.89877928	-0.21488988
1	3.79630548	-0.14715197	-0.80683956
1	2.17449308	-0.72361521	-0.37359270
6	3.64513707	-2.31701791	-0.67708154
1	3.28224371	-3.05361628	0.05569321
1	3.10093324	-2.52575182	-1.60967326
6	5.14500254	-2.49996587	-0.92698488
1	5.45735879	-1.82473422	-1.74300251

1	5.32947928	-3.52393659	-1.28768234
6	6.02857272	-2.23027545	0.29536190
1	5.81498908	-2.95080889	1.10148389
1	7.08556301	-2.37606559	0.01847422
6	5.90015506	-0.82153311	0.86524098
1	5.87814145	-0.06232839	0.06688642
1	6.74643034	-0.59496984	1.52523274
50	0.00702271	0.56724356	2.05295545
7	-2.58365558	0.75238735	2.10883721
6	-3.01633530	1.94638759	2.85055367
1	-4.09720681	1.91592883	3.08442325
1	-2.79433104	2.84620216	2.26594528
1	-2.45283069	2.00198363	3.79127438
7	-2.18887830	2.38109876	-0.45281104
6	-3.32275582	0.57145215	0.83478449
1	-4.34443891	0.20148730	1.05827242
1	-2.80129808	-0.21651240	0.27330617
6	-3.47529287	1.80513509	-0.05112350
1	-4.07465651	1.47388681	-0.92402232
1	-4.08463225	2.56863710	0.45865541
6	-2.23134494	3.27984301	-1.55873459
6	-2.65756838	4.61346335	-1.36448084
6	-2.67372005	5.49422773	-2.45375017
6	-2.26548788	5.10176246	-3.73257687
6	-1.83238866	3.78115452	-3.90295768
6	-1.81900055	2.86168304	-2.84770407
7	-0.76842597	-1.42098609	1.82813988
6	-2.73857100	-0.45686063	2.95273524
1	-3.80965549	-0.64288672	3.16720617
1	-2.23408024	-0.24451783	3.90918126
6	-2.11182246	-1.69754421	2.31862961
1	-2.11889505	-2.48696076	3.09821886
1	-2.77583419	-2.08143635	1.51387488
6	-0.06645963	-2.59251236	1.42395978
6	-0.16669085	-3.06721011	0.09133014
6	0.47314986	-4.26020342	-0.26975950
6	1.22426130	-5.00570590	0.64661100
6	1.32704052	-4.52013488	1.95492216
6	0.69986048	-3.33277481	2.35852541
6	-3.04331058	5.10935386	0.00611303
1	-2.99424248	6.52611164	-2.28783579
6	-2.31151975	6.06271900	-4.89656417
1	-1.50664443	3.44865418	-4.89213392
6	-1.38763424	1.43569126	-3.09979029
6	-0.96014846	-2.30150697	-0.93842735
1	0.37833677	-4.61718864	-1.29925463
6	1.92659858	-6.27534172	0.22656111
1	1.90712452	-5.08468294	2.69004834
6	0.84998568	-2.85716536	3.78242806
1	-3.00051481	6.20542191	0.05011365
1	-2.36601406	4.69485086	0.76678278
1	-4.06733024	4.81168237	0.28433466
1	-0.50577491	1.14823872	-2.50769702
1	-1.14577275	1.29124600	-4.16053524
1	-2.18470691	0.72281059	-2.83696807
1	-3.25390737	5.96244407	-5.45856564
1	-1.49096834	5.87744362	-5.60349343
1	-2.24306805	7.10531892	-4.55739401

1	-0.78664368	-2.70873917	-1.94365993
1	-0.68591056	-1.23706528	-0.92823500
1	-2.04262170	-2.36372806	-0.74150984
1	-0.12142283	-2.62858560	4.24315148
1	1.44887508	-1.93569248	3.82913952
1	1.35089584	-3.61921256	4.39418510
1	2.88656059	-6.05627696	-0.26916054
1	1.32116897	-6.85348008	-0.48555890
1	2.14427937	-6.91672083	1.09119884
1	-1.48203136	1.64499035	-0.58122848

Energy = -7584.967539 Hartree
Number of imaginary frequencies = 0.

Compound I2b isomer 13

Atomic N.	X	Y	Z
8	0.61896443	-0.11658616	-0.97177067
8	0.10969781	2.94127064	-0.26794332
6	1.20220726	3.80287571	-0.01184157
1	1.85079097	3.46702617	0.82419212
1	0.85568589	4.82452118	0.23388372
1	1.84392366	3.88877274	-0.90983145
8	2.68237039	0.57051172	-1.33610209
6	1.38221255	0.49702125	-1.71185603
6	0.93762916	1.14185138	-3.00394069
1	1.17618043	2.21711361	-2.96678480
1	-0.15440412	1.06361570	-3.01098244
6	1.53709590	0.49593441	-4.27119683
1	1.48346586	-0.60125945	-4.18388613
1	0.89301609	0.76821484	-5.12036726
6	2.97174342	0.93369199	-4.58295243
1	2.97471019	2.01954984	-4.78085298
1	3.30394263	0.44982056	-5.51442459
6	3.98367606	0.63542456	-3.47170891
1	4.08453519	-0.45013175	-3.31024543
1	4.97740467	0.99619670	-3.78322538
6	3.66458768	1.29441050	-2.13408779
1	3.33255696	2.33672078	-2.26098801
1	4.54821551	1.29539498	-1.48470583
50	-0.41568662	1.53408706	1.17015461
7	-1.65746085	-1.08870394	1.99144219
6	-1.96275969	-0.73368861	3.38143764
1	-2.75655200	-1.37693444	3.81435497
1	-2.29392300	0.31171813	3.44974522
1	-1.05518612	-0.83852455	3.98990921
7	-2.38911772	1.44517069	0.43667034
6	-2.84033058	-0.94290331	1.12872448
1	-3.67514557	-1.57244371	1.51215566
1	-2.57247758	-1.31847358	0.13157830
6	-3.36050733	0.48884607	0.98002030
1	-4.23263685	0.43272211	0.30853258
1	-3.76817500	0.83807185	1.94994095
6	-2.93448660	2.37823470	-0.49666928
6	-3.14935766	3.73059807	-0.13441686
6	-3.69993745	4.61631848	-1.06832995
6	-4.04577888	4.21371180	-2.36293101
6	-3.81852534	2.87884294	-2.71090372
6	-3.27356902	1.95771319	-1.80695139

7	1.06850212	-2.65020837	0.70352795
6	-1.15925013	-2.48136107	1.93838483
1	-2.01670205	-3.17802449	2.06952266
1	-0.49545966	-2.63764877	2.80125400
6	-0.38218174	-2.86396572	0.66152571
1	-0.59329048	-3.91868919	0.44304732
1	-0.75219924	-2.28836027	-0.19778495
6	1.86536031	-3.24299938	1.70505727
6	1.91244218	-4.65093585	1.87431886
6	2.73417117	-5.19582454	2.86984273
6	3.54690488	-4.40852996	3.69035853
6	3.53484368	-3.02635962	3.46868580
6	2.71512289	-2.43189716	2.50464348
6	-2.78873779	4.24419422	1.23771492
1	-3.86445081	5.65552162	-0.77122930
6	-4.66813130	5.18222212	-3.34019033
1	-4.06391997	2.54059936	-3.72149486
6	-3.03438588	0.53636104	-2.25285115
6	1.16956892	-5.59003138	0.95543811
1	2.75794856	-6.28327912	2.98177340
6	4.39822432	-5.02190793	4.77598130
1	4.17772868	-2.38157706	4.07390826
6	2.74598815	-0.93551734	2.31818327
1	-3.31379549	5.18503813	1.45017570
1	-1.70810211	4.44484124	1.30954456
1	-3.03777771	3.51873266	2.02436310
1	-2.08840190	0.15017229	-1.84737380
1	-3.01013295	0.47320588	-3.34926391
1	-3.83078844	-0.14385721	-1.90888723
1	-4.51028177	4.85950650	-4.37833426
1	-4.24991626	6.19218263	-3.22717409
1	-5.75583872	5.26206212	-3.18367157
1	1.63592610	-6.58398411	0.97348803
1	1.18219906	-5.21808385	-0.07952258
1	0.11343175	-5.72346635	1.24172218
1	1.75266382	-0.47952282	2.46055555
1	3.07776451	-0.64480914	1.30789675
1	3.43286228	-0.47124829	3.03736009
1	5.34152101	-4.47310584	4.90624807
1	4.64079481	-6.06948861	4.55007768
1	3.87889833	-5.00942554	5.74792748
1	1.28228214	-1.66685566	0.54240497

Energy = -7584.958147 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 14

Atomic N.	X	Y	Z
8	3.36470894	0.15409825	0.51935493
8	0.35848526	0.87766034	-0.63172092
6	0.08422204	2.23358656	-0.94437611
1	-0.96681489	2.35594945	-1.25949438
1	0.72761742	2.57695014	-1.77687934
1	0.25885398	2.92633547	-0.09493223
8	5.33271238	0.29412400	-0.44269609
6	3.97840211	0.32762317	-0.53008927
6	3.31257694	0.56178208	-1.86606143
1	3.66370953	1.52308747	-2.28001308

1	2.23924035	0.65398460	-1.64270729
6	3.54421162	-0.56666647	-2.89394409
1	3.39430508	-1.54029616	-2.40318644
1	2.75144853	-0.48539430	-3.65199447
6	4.90543176	-0.52175325	-3.59374291
1	4.98148796	0.41466370	-4.17429244
1	4.96382307	-1.34268095	-4.32548894
6	6.10670991	-0.60606012	-2.64661059
1	6.12082902	-1.57076560	-2.11391351
1	7.03782679	-0.56069782	-3.23503103
6	6.17071221	0.51392257	-1.61353225
1	5.92672882	1.49084403	-2.06101901
1	7.17569952	0.58094365	-1.17919233
50	0.80134465	0.39889179	1.34735922
7	-1.14811337	-0.56968280	3.22591151
6	-1.21556206	0.15113821	4.49930653
1	-1.70402270	-0.44804217	5.29497786
1	-1.76956070	1.09163408	4.39035893
1	-0.19603654	0.39908851	4.82435447
7	-2.70346369	1.34930593	1.58556025
6	-2.47444905	-0.87787073	2.66851597
1	-3.02566824	-1.58138332	3.33128369
1	-2.31288705	-1.37585485	1.70331320
6	-3.36061806	0.34710940	2.43666578
1	-4.26971322	-0.00480336	1.93290803
1	-3.69419821	0.77737930	3.40169095
6	-3.50954451	2.40085681	1.06829592
6	-3.31685676	3.73436617	1.50254479
6	-4.08603046	4.75880232	0.93964892
6	-5.05561861	4.50672917	-0.03760108
6	-5.21289700	3.18569161	-0.47101587
6	-4.45329763	2.13082528	0.04912741
7	0.54770886	-1.69634943	1.05643804
6	-0.32564838	-1.78170539	3.39930887
1	-0.81096669	-2.48449482	4.11051837
1	0.62323227	-1.45585054	3.85708125
6	-0.01476485	-2.53627023	2.10994737
1	0.67685844	-3.35097236	2.40025880
1	-0.92997357	-3.05178949	1.75001157
6	1.02337503	-2.45357082	-0.05670498
6	0.24034065	-2.56629194	-1.23518669
6	0.71034732	-3.33730578	-2.30547792
6	1.93362042	-4.01683321	-2.25412518
6	2.68809110	-3.91109124	-1.08213741
6	2.25873250	-3.14830759	0.01471225
6	-2.28308139	4.06441458	2.55422090
1	-3.92483003	5.78419469	1.28208310
6	-5.90811515	5.61934146	-0.59870694
1	-5.93224393	2.96647365	-1.26446297
6	-4.60100792	0.74654883	-0.53254952
6	-1.10582637	-1.89466133	-1.33651664
1	0.09216402	-3.41747231	-3.20381657
6	2.43034731	-4.81310315	-3.43736732
1	3.64553987	-4.43537348	-1.01314825
6	3.12326079	-3.09640358	1.25029483
1	-2.30355174	5.13574649	2.79011276
1	-1.25848463	3.82346010	2.22525468
1	-2.45919753	3.51542880	3.49290008

1	-3.63066458	0.23059757	-0.55504808
1	-4.99537129	0.80184646	-1.55563413
1	-5.29586967	0.11640666	0.04606030
1	-6.84676678	5.72759726	-0.03194085
1	-6.18184024	5.42523841	-1.64504264
1	-5.38721003	6.58546403	-0.55435160
1	-1.57609924	-2.12012998	-2.30313215
1	-1.00610854	-0.80525802	-1.22689029
1	-1.78260099	-2.24259180	-0.54108939
1	2.82101100	-3.85957703	1.98618199
1	3.05695588	-2.11861156	1.74244689
1	4.17430019	-3.29150319	0.99845111
1	2.89080583	-4.15775232	-4.19466454
1	1.60902910	-5.34868507	-3.93410873
1	3.18716846	-5.54999614	-3.13628450
1	-1.89840065	1.73377065	2.08046087

Energy = -7584.961190 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 15

Atomic N.	X	Y	Z
8	3.28635838	0.24746094	0.55151512
8	0.05635893	0.89294507	0.08822946
6	0.27936574	2.27190539	-0.20302757
1	-0.39560559	2.93692653	0.36703391
1	0.09887808	2.45180662	-1.27713303
1	1.31531029	2.59471917	0.01748074
8	4.97314085	0.91410501	-0.69147814
6	3.67820364	0.51871852	-0.57762868
6	2.81230182	0.41939810	-1.81348710
1	2.78828547	1.39805287	-2.32293443
1	1.79841893	0.21407967	-1.44615090
6	3.26692459	-0.67176231	-2.80669796
1	3.51155084	-1.59000175	-2.25155438
1	2.40304216	-0.92275751	-3.43931529
6	4.43575930	-0.25835411	-3.70571552
1	4.12341130	0.59836199	-4.32851667
1	4.66326136	-1.07905961	-4.40383247
6	5.71108465	0.12655307	-2.94907305
1	6.11118396	-0.73460405	-2.38965651
1	6.48952767	0.41700066	-3.67354253
6	5.53955573	1.29054781	-1.97882641
1	4.93887116	2.10128604	-2.42174095
1	6.51576624	1.70542495	-1.69957933
50	0.87160106	0.24135683	1.92549923
7	-1.29852211	-0.56487339	3.10418908
6	-1.61095410	0.26630359	4.27654744
1	-2.38476515	-0.19869425	4.91600383
1	-1.95305253	1.25446097	3.94927591
1	-0.69642519	0.39971895	4.86936458
7	-2.66322047	1.43153782	1.23136405
6	-2.48853563	-0.83328483	2.25903323
1	-3.12684923	-1.58873131	2.76146395
1	-2.12089761	-1.27996259	1.32447265
6	-3.37978407	0.36164633	1.93080356
1	-4.21584119	-0.04585218	1.32580103
1	-3.84038434	0.75840118	2.84975185

6	-3.48005019	2.40062868	0.57843455
6	-4.08481808	3.43156872	1.33268378
6	-4.86439643	4.39415517	0.67788467
6	-5.05672694	4.37697550	-0.70737064
6	-4.43991242	3.35510954	-1.43967178
6	-3.66792496	2.36256312	-0.82494206
7	0.64351339	-1.84177581	1.46310508
6	-0.69145258	-1.84694248	3.53529212
1	-1.42490874	-2.44728562	4.10930643
1	0.14105656	-1.59361336	4.21143312
6	-0.15488648	-2.66459466	2.36168013
1	0.43313403	-3.49683403	2.80060383
1	-0.99960885	-3.15655512	1.83220776
6	1.33615573	-2.60048892	0.47656293
6	0.72050275	-2.89566112	-0.76632877
6	1.38756513	-3.70458701	-1.69578244
6	2.65927962	-4.23171429	-1.44230974
6	3.26242537	-3.92199759	-0.21810263
6	2.62840145	-3.11944041	0.74089989
6	-3.85692067	3.53910566	2.81918213
1	-5.31619943	5.19382268	1.27065655
6	-5.92008380	5.41126441	-1.38953006
1	-4.57401864	3.31853456	-2.52404543
6	-3.06568054	1.25536906	-1.65832477
6	-0.64735131	-2.34984343	-1.09403239
1	0.89495501	-3.93044484	-2.64583313
6	3.36982353	-5.07912926	-2.47121808
1	4.25513836	-4.32272770	0.00456250
6	3.33172301	-2.81555971	2.04073721
1	-4.09046445	4.55037020	3.17673513
1	-2.80999720	3.30746217	3.06294359
1	-4.48731389	2.83788584	3.38979969
1	-1.96624217	1.24199822	-1.61494120
1	-3.36250413	1.36332220	-2.70942687
1	-3.40211219	0.26515446	-1.31386551
1	-6.94827740	5.04104827	-1.52994526
1	-5.52961050	5.66870779	-2.38390541
1	-5.98307361	6.33371219	-0.79648813
1	-0.89250947	-2.52551774	-2.15018551
1	-0.69561650	-1.27130277	-0.88705231
1	-1.43088825	-2.83546834	-0.49018511
1	2.68678509	-3.00371914	2.91040103
1	3.62905082	-1.75743408	2.08756077
1	4.23753552	-3.42793909	2.14241823
1	3.89568352	-4.45331873	-3.21095526
1	2.66430104	-5.71167023	-3.02780358
1	4.12010389	-5.73136045	-2.00413324
1	-1.94690888	1.04338726	0.60334950

Energy = -7584.967552 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 16

Atomic N.	X	Y	Z
8	1.71368769	0.57172128	3.03961232
8	2.18407494	0.76072414	-1.11878590
6	3.09100344	-0.11515977	-1.76447705
1	3.00426853	-0.06986408	-2.86705973

1	2.95670734	-1.18144786	-1.47817754
1	4.13334397	0.15947561	-1.51030308
8	3.28959361	1.87651084	2.20866487
6	2.78744812	0.63738301	2.45858058
6	3.57659279	-0.58503606	2.03717321
1	3.68745801	-0.57333308	0.94082463
1	2.94154839	-1.44253130	2.28793532
6	4.95936711	-0.72062005	2.70887156
1	4.87518679	-0.48415790	3.78203397
1	5.25663434	-1.77828350	2.65036645
6	6.05394139	0.13278810	2.06049014
1	6.17992095	-0.19247610	1.01357799
1	7.01325398	-0.06417605	2.56384442
6	5.77588514	1.63914733	2.07720013
1	5.75758530	2.02251733	3.11065825
1	6.60077821	2.16285968	1.56696104
6	4.48230117	2.05455457	1.38550142
1	4.32739193	1.54248793	0.42389608
1	4.48458548	3.13512797	1.19586964
50	0.28688394	-0.09986721	-0.66085648
7	-0.39149015	2.14938035	0.12942809
6	0.72071676	3.09894586	-0.13773077
1	0.37156246	4.13627014	0.00948511
1	1.09664363	2.96642326	-1.15551631
1	1.54341215	2.88836372	0.55323174
7	-0.85687819	0.72310002	-2.29430619
6	-1.54771874	2.45972436	-0.76123773
1	-1.81433310	3.52805115	-0.65154931
1	-2.39592751	1.84743148	-0.43042401
6	-1.24870487	2.12019237	-2.21782355
1	-2.17795218	2.29786625	-2.79249349
1	-0.50491631	2.83808474	-2.61934235
6	-0.80160956	0.10492088	-3.57196000
6	0.03752176	0.57435587	-4.61836209
6	0.04079114	-0.08841337	-5.85369513
6	-0.74165666	-1.22054259	-6.09762319
6	-1.54369562	-1.69097262	-5.05122685
6	-1.59367916	-1.05202125	-3.80759737
7	-1.46500161	-0.00563165	2.13209439
6	-0.75971159	2.31042283	1.57200968
1	-1.07420788	3.35996161	1.72738626
1	0.16038078	2.15349482	2.15335812
6	-1.85667987	1.40941448	2.13321426
1	-2.05818564	1.78166235	3.15819880
1	-2.79511737	1.52891220	1.57745250
6	-2.37443490	-0.93567325	2.71509730
6	-3.61548396	-1.21540885	2.09755516
6	-4.47529854	-2.15261017	2.68549289
6	-4.14328344	-2.84315189	3.85424569
6	-2.89475868	-2.57922420	4.42973982
6	-2.01004212	-1.64003123	3.89015406
6	0.97843717	1.73706060	-4.41406440
1	0.69994727	0.28379652	-6.64321463
6	-0.73631090	-1.90267202	-7.44475096
1	-2.16382750	-2.57739108	-5.21019641
6	-2.50834657	-1.58853349	-2.73442968
6	-4.01214596	-0.57697257	0.79020329
1	-5.42744750	-2.36435658	2.19205142

6	-5.09874531	-3.83006514	4.48057554
1	-2.59805522	-3.11561738	5.33471124
6	-0.67758290	-1.40030140	4.55923571
1	1.80433505	1.69125635	-5.13669007
1	1.39882084	1.72764147	-3.39708245
1	0.47755307	2.70839408	-4.55668839
1	-1.94941257	-2.01268405	-1.88515241
1	-3.15344706	-2.38055900	-3.13761459
1	-3.14045567	-0.79008586	-2.32162384
1	-1.59123557	-1.57911088	-8.06005031
1	-0.80664391	-2.99486661	-7.34314490
1	0.17817930	-1.66919349	-8.00691238
1	-4.72107141	-1.21786049	0.24996081
1	-3.13414008	-0.41748096	0.14889545
1	-4.50570112	0.39883862	0.93138882
1	-0.51611060	-0.33943670	4.80261044
1	0.16821183	-1.70448913	3.92287349
1	-0.61144033	-1.97320858	5.49267173
1	-4.56474341	-4.68747295	4.91347291
1	-5.81873692	-4.21143633	3.74398316
1	-5.67718573	-3.36383296	5.29415825
1	-0.54240184	-0.09100248	2.56516541

Energy = -7584.967757 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 17

Atomic N.	X	Y	Z
8	1.94054027	-1.32149876	1.20468617
8	1.59361969	2.36081904	0.66847847
6	2.97750984	2.52616407	0.40954865
1	3.20691149	3.59561339	0.24982583
1	3.32738810	1.97872883	-0.48895650
1	3.58570001	2.17548850	1.26438497
8	3.06583918	-0.25567525	2.78431084
6	2.70423127	-1.40066906	2.15632885
6	3.24341356	-2.72955924	2.65106798
1	4.34632291	-2.70665451	2.65513409
1	2.93101058	-3.46582271	1.90192290
6	2.72144729	-3.13209821	4.04707894
1	1.63972740	-2.93361375	4.09856636
1	2.84561075	-4.22056996	4.15001090
6	3.44788210	-2.44186975	5.20577703
1	4.50849640	-2.74940644	5.19681462
1	3.03135403	-2.80446381	6.15833459
6	3.37883594	-0.91117472	5.17911976
1	2.33880212	-0.56573082	5.28907642
1	3.93596671	-0.51117827	6.04206500
6	3.96825330	-0.27044850	3.92680441
1	4.92072243	-0.74374857	3.63692686
1	4.15820577	0.79650680	4.09489474
50	0.55197097	0.78783303	-0.21469552
7	-1.09212095	2.59283475	-0.82693121
6	-0.44974944	3.72819642	-1.51476695
1	-1.14708110	4.57743765	-1.63460704
1	-0.08621457	3.40832164	-2.49862025
1	0.40822869	4.04349692	-0.90841072
7	-1.02476527	1.11409726	-3.50766066

6	-2.27645815	2.06078705	-1.55337134
1	-3.14714413	2.71596413	-1.35548454
1	-2.50589789	1.07566791	-1.11872768
6	-2.15668737	1.94239381	-3.07263068
1	-3.12113566	1.52661649	-3.42284700
1	-2.07892115	2.94826417	-3.51086096
6	-1.07900649	0.49465975	-4.78147651
6	-1.14990224	1.26786251	-5.96394213
6	-1.18634885	0.61680166	-7.20428501
6	-1.12698608	-0.77466062	-7.32224613
6	-1.01142217	-1.51972507	-6.14227849
6	-0.99174502	-0.91739936	-4.88079192
7	-0.96744318	0.71328293	1.30778238
6	-1.47450020	2.99890325	0.55391138
1	-2.27433213	3.76409292	0.51256495
1	-0.57340983	3.44160629	1.00135373
6	-1.92067082	1.81320411	1.40131480
1	-2.02914227	2.19102014	2.43400021
1	-2.94107561	1.49058828	1.09995609
6	-1.01404752	-0.22770698	2.36543156
6	-1.40715693	-1.57002077	2.12010890
6	-1.48026579	-2.48145680	3.18036558
6	-1.17691833	-2.11667804	4.49764831
6	-0.75029082	-0.80344741	4.72348277
6	-0.65118685	0.13929036	3.69080649
6	-1.10876988	2.77607630	-5.92534426
1	-1.23495222	1.22791124	-8.10941633
6	-1.19454909	-1.45175032	-8.67005735
1	-0.94329692	-2.60904769	-6.20138973
6	-0.87249491	-1.77377577	-3.64252418
6	-1.74836858	-2.02799051	0.72416622
1	-1.79865784	-3.50629445	2.97002697
6	-1.31942065	-3.10202402	5.63383977
1	-0.47262512	-0.50048828	5.73782452
6	-0.10236160	1.51222972	3.99294650
1	-0.79540797	3.17416865	-6.89923877
1	-0.39785233	3.12751617	-5.16282740
1	-2.08835691	3.22201835	-5.69098717
1	0.04958039	-1.56451052	-3.07568403
1	-0.85832753	-2.83739476	-3.91139747
1	-1.71418608	-1.61619578	-2.94896174
1	-2.21878907	-1.78862749	-8.89700574
1	-0.54644251	-2.33851675	-8.70793066
1	-0.88863526	-0.77005188	-9.47527543
1	-2.25911858	-3.00010815	0.74708117
1	-0.84312059	-2.13956691	0.10671792
1	-2.39088629	-1.29831991	0.21185625
1	-0.89920746	2.24231555	4.21156436
1	0.47341709	1.89805410	3.13886934
1	0.54675063	1.48007903	4.87917777
1	-1.03411323	-4.11803988	5.32533073
1	-2.36008774	-3.15444582	5.99181797
1	-0.69539373	-2.81655542	6.49237409
1	-0.77029004	0.44206848	-2.78184759

Energy = -7584.965995 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 18

Atomic N.	X	Y	Z
8	2.20709540	-1.29584587	2.45848647
8	1.87648830	1.70073413	-0.48016719
6	2.72211578	1.65062939	-1.61568453
1	2.42998234	2.38736975	-2.38838965
1	2.73604938	0.65598634	-2.11311824
1	3.76543861	1.88217529	-1.32520890
8	3.44952394	0.52153648	2.63472412
6	3.13631942	-0.64341018	2.00533462
6	3.95176214	-1.08435990	0.80716713
1	3.84210338	-0.33096071	0.01036871
1	3.47188676	-2.00302069	0.45053685
6	5.44646606	-1.33292627	1.09976965
1	5.55195892	-1.88702997	2.04662916
1	5.83464361	-1.99569643	0.31203611
6	6.29699620	-0.05933112	1.13140811
1	6.24698734	0.42238262	0.13988064
1	7.35191544	-0.33170326	1.29081047
6	5.87284850	0.95869615	2.19440711
1	6.01842932	0.55016418	3.20795546
1	6.52220759	1.84646826	2.12187542
6	4.43252745	1.44291349	2.07146033
1	4.14483290	1.67489496	1.03488812
1	4.28551482	2.34834478	2.67337951
50	0.18230312	0.40720073	-0.57432232
7	-0.53100138	1.40567891	1.57814207
6	0.42375047	2.48724028	1.93674668
1	0.01740354	3.08415309	2.77229599
1	0.61503738	3.12716896	1.07148108
1	1.37524716	2.03722178	2.23777391
7	-1.31519695	1.85849550	-1.12442082
6	-1.85601843	1.99555369	1.22762857
1	-2.18973570	2.65491702	2.05121214
1	-2.57064033	1.16968239	1.12347631
6	-1.80557233	2.75701239	-0.09305397
1	-2.83746509	3.08700760	-0.32017003
1	-1.21478276	3.68627711	0.03831354
6	-1.44442710	2.25346314	-2.48280602
6	-0.85738634	3.44053300	-2.99842494
6	-1.02660546	3.76555628	-4.35147418
6	-1.74073566	2.94967926	-5.23353238
6	-2.29046151	1.76849330	-4.72173916
6	-2.16351901	1.41187003	-3.37475809
7	-1.04388559	-1.68076804	1.66619994
6	-0.63383613	0.50717444	2.77181610
1	-0.99431681	1.11388642	3.62417680
1	0.38827627	0.17940593	3.01093399
6	-1.53304306	-0.72160096	2.66455049
1	-1.56394492	-1.16275792	3.68149549
1	-2.56612796	-0.44044504	2.42469862
6	-1.75569393	-2.90977555	1.53906006
6	-3.06452821	-2.93346362	1.00548561
6	-3.72828472	-4.16133726	0.87824402
6	-3.13404240	-5.37386593	1.23683135
6	-1.82682340	-5.33196459	1.73680213
6	-1.13008534	-4.13051980	1.89826778
6	0.00226726	4.33438180	-2.13757904

1	-0.56012756	4.67945593	-4.73036777
6	-1.92885951	3.33586473	-6.68112787
1	-2.85045983	1.10701839	-5.38835715
6	-2.81435258	0.14438889	-2.87868996
6	-3.74616130	-1.67877679	0.52059465
1	-4.73853614	-4.16416309	0.46084234
6	-3.85651048	-6.68724985	1.05567633
1	-1.33225250	-6.26436421	2.02130643
6	0.27633650	-4.15146420	2.44793740
1	0.68123752	4.92890699	-2.76364725
1	0.60260010	3.74040209	-1.43198150
1	-0.59753110	5.04508298	-1.54606107
1	-2.07451257	-0.61173689	-2.57162357
1	-3.44022307	-0.30072263	-3.66363670
1	-3.43866904	0.34269993	-1.99624096
1	-2.89650102	3.83930474	-6.83737651
1	-1.91272887	2.45493955	-7.33812683
1	-1.14333421	4.02729137	-7.01555117
1	-4.49507362	-1.92026098	-0.24490497
1	-3.01843721	-0.98147084	0.08266495
1	-4.27446852	-1.14734695	1.32944939
1	0.39127252	-3.50342528	3.32974343
1	1.01665082	-3.80458331	1.71011999
1	0.55542565	-5.17124356	2.74131013
1	-3.51145577	-7.21079614	0.15002125
1	-4.93979696	-6.53709987	0.95702080
1	-3.68069977	-7.36254666	1.90520680
1	-0.05304979	-1.86167012	1.84389816

Energy = -7584.967746 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 19

Atomic N.	X	Y	Z
8	1.37143492	-3.52516312	-0.09809666
8	2.96678795	0.29893280	-0.76886906
6	3.73159366	0.98489199	-1.74535707
1	3.20102322	1.85424832	-2.17237860
1	4.00591083	0.31082881	-2.58180326
1	4.67400198	1.35491000	-1.30218878
8	2.33874767	-2.49113189	1.60019748
6	2.39998173	-3.05293064	0.36391386
6	3.72652798	-3.07647331	-0.37101273
1	4.03485105	-2.03241786	-0.55354142
1	3.51165388	-3.53257354	-1.34473243
6	4.84846760	-3.85947130	0.34308274
1	4.44476864	-4.80637933	0.73726740
1	5.59593912	-4.13800255	-0.41515884
6	5.55174553	-3.07867539	1.45793167
1	6.02816482	-2.18665360	1.01645114
1	6.36635594	-3.69329752	1.87205338
6	4.62799136	-2.62926324	2.59417923
1	4.21906313	-3.49875880	3.13462412
1	5.21439068	-2.05420526	3.32939247
6	3.46857066	-1.74582617	2.14723734
1	3.77827823	-0.98103759	1.41728542
1	3.02278401	-1.23306700	3.00840400
50	0.99517266	0.64750703	-0.16784151

7	0.18607623	-0.30268501	-2.34317701
6	1.05455650	-1.40879278	-2.80874902
1	0.83226702	-1.65490104	-3.86253322
1	0.90615285	-2.30046177	-2.19024990
1	2.10140147	-1.10020054	-2.71278218
7	-1.84900312	-1.35627915	-0.03690971
6	-1.24812115	-0.71388258	-2.39823360
1	-1.45556061	-1.05251332	-3.43295403
1	-1.85889609	0.17778397	-2.20855010
6	-1.68779866	-1.81509164	-1.42825863
1	-2.65743127	-2.18067953	-1.78794729
1	-1.00446780	-2.67930059	-1.47582960
6	-2.96134207	-1.84307486	0.70477702
6	-2.74359377	-2.59507443	1.88667854
6	-3.84319917	-3.03444750	2.63032666
6	-5.16159539	-2.76471168	2.24372005
6	-5.35305493	-1.99556349	1.09240508
6	-4.28423860	-1.51624067	0.32320611
7	0.50793372	2.39637850	-1.31190889
6	0.39842700	0.88574707	-3.22754821
1	-0.08048578	0.70602160	-4.20839890
1	1.48170440	0.96964663	-3.38773827
6	-0.11076609	2.18649885	-2.61600650
1	0.16562383	2.99746382	-3.31886282
1	-1.21932034	2.18322515	-2.58914892
6	0.13901277	3.58661062	-0.61387375
6	-1.17959614	3.82469077	-0.14199995
6	-1.46846873	5.01695390	0.53780420
6	-0.49637081	5.98771408	0.78972063
6	0.80488814	5.73331554	0.34120467
6	1.13687978	4.56231586	-0.34843244
6	-1.34276723	-2.91048441	2.35421181
1	-3.65960491	-3.61515206	3.53797197
6	-6.33217982	-3.29296550	3.03756859
1	-6.36976920	-1.73140377	0.78974112
6	-4.57409916	-0.60597006	-0.84629068
6	-2.28331348	2.80921680	-0.30603458
1	-2.48837879	5.17799469	0.89766212
6	-0.82469158	7.24823314	1.55317218
1	1.58836533	6.47333873	0.52559348
6	2.55812917	4.35643635	-0.80981557
1	-1.37254938	-3.57189170	3.22920815
1	-0.79370491	-2.00147983	2.65053520
1	-0.73801575	-3.40400479	1.57789757
1	-3.83458844	0.20542306	-0.90323814
1	-5.57056553	-0.15760129	-0.74047757
1	-4.55820783	-1.12960023	-1.81552078
1	-6.57187990	-4.33014366	2.75319248
1	-7.23487937	-2.69045650	2.86764609
1	-6.11928735	-3.29421514	4.11573020
1	-3.05491337	2.95371438	0.46143356
1	-1.90320909	1.78056258	-0.21452731
1	-2.78150433	2.88955482	-1.28591885
1	2.59940239	4.10720938	-1.87885783
1	3.04442759	3.52505808	-0.27758971
1	3.15418843	5.26226099	-0.63633277
1	-0.50503046	7.17096918	2.60454716
1	-1.90454862	7.44760203	1.55088399

1 -0.31366067 8.12196464 1.12426253
 1 -0.98898414 -1.53062647 0.48255567
 Energy = -7584.967623 Hartree
 Number of imaginary frequencies = 0.

Compound I2b isomer 20

Atomic N.	X	Y	Z
8	3.33836578	-3.13734594	-0.94441967
8	2.22147118	0.81697559	-1.33930217
6	2.64301767	1.39044800	-2.56238593
1	1.86281755	2.00880219	-3.04214796
1	2.94758770	0.60903600	-3.28770663
1	3.52170217	2.04108962	-2.39647678
8	3.25676811	-1.81548294	0.83047779
6	3.80120980	-2.16719349	-0.37044813
6	4.96332680	-1.35526398	-0.91288124
1	4.63630111	-0.31049777	-1.03992540
1	5.16295775	-1.76624111	-1.90950530
6	6.23893328	-1.41534952	-0.04615284
1	6.40949023	-2.45223877	0.28659293
1	7.09511543	-1.15433366	-0.68666923
6	6.22258927	-0.46742451	1.15778366
1	6.15599877	0.56991327	0.78688778
1	7.18204771	-0.54440437	1.69319610
6	5.07257901	-0.70949172	2.14108447
1	5.16871374	-1.69742669	2.62082676
1	5.12957511	0.03625167	2.95090535
6	3.68190918	-0.60531420	1.52225678
1	3.58971065	0.25151331	0.83633789
1	2.92187887	-0.49358461	2.30566677
50	0.33631206	0.83277687	-0.43310300
7	-0.43671127	-0.80815469	-2.16359361
6	0.60362232	-1.82627115	-2.43400128
1	0.33372799	-2.43707059	-3.31412234
1	0.74359647	-2.48144522	-1.56897351
1	1.55630178	-1.31821137	-2.61467660
7	-1.69455390	-1.67621147	0.55404646
6	-1.75806852	-1.44724045	-1.91771044
1	-2.04040202	-2.02125382	-2.82168204
1	-2.49817301	-0.64089436	-1.80930193
6	-1.86335828	-2.38820910	-0.71929327
1	-2.85571818	-2.87758521	-0.79301355
1	-1.11973460	-3.19110929	-0.78876352
6	-1.90682113	-2.41011269	1.75781434
6	-1.01729674	-3.43855925	2.14577452
6	-1.25295226	-4.11535086	3.34979934
6	-2.31887035	-3.79595770	4.19688927
6	-3.16011741	-2.74506241	3.81391455
6	-2.97832217	-2.05272778	2.61238259
7	-0.81118681	2.01652725	-1.82765749
6	-0.54770778	0.10956481	-3.33684235
1	-1.00720664	-0.42663071	-4.18884195
1	0.47728425	0.37907289	-3.62000886
6	-1.33650014	1.38093592	-3.02838082
1	-1.22975689	2.04101332	-3.91255044
1	-2.41834784	1.14571708	-2.96917458
6	-1.42606646	3.22693809	-1.40228103

6	-2.79029994	3.30019463	-1.01022955
6	-3.33606563	4.52522503	-0.60043136
6	-2.57780230	5.69570331	-0.53600853
6	-1.22691221	5.60931630	-0.89350595
6	-0.64369806	4.41262153	-1.32212160
6	0.20761827	-3.77718496	1.33480024
1	-0.55602957	-4.90439286	3.64366163
6	-2.56066295	-4.56387574	5.47402158
1	-3.98890414	-2.45642638	4.46529138
6	-3.91465487	-0.92179139	2.25208868
6	-3.66767297	2.07497079	-0.95457112
1	-4.38731059	4.55404756	-0.30041586
6	-3.17752991	6.99893446	-0.06566277
1	-0.60532952	6.50786471	-0.85076922
6	0.81070846	4.41009941	-1.72307803
1	0.95850687	-4.27354433	1.96195564
1	0.66834203	-2.87582511	0.90890196
1	-0.01288601	-4.46395273	0.50180206
1	-3.39607509	0.05071763	2.21023854
1	-4.70993429	-0.82922644	3.00205262
1	-4.40041216	-1.07710782	1.27520904
1	-3.25705668	-5.40144888	5.30860560
1	-3.00061875	-3.92373488	6.25104496
1	-1.62752541	-4.98935457	5.86759920
1	-4.48143456	2.21522472	-0.23088460
1	-3.07862410	1.19698090	-0.65004476
1	-4.13138684	1.83751297	-1.92546144
1	0.93863003	4.03455027	-2.74774025
1	1.42400753	3.76408377	-1.07663942
1	1.22439989	5.42576843	-1.66993271
1	-2.83292361	7.25391013	0.94889150
1	-4.27409391	6.94814819	-0.04072012
1	-2.88924056	7.83301970	-0.72181992
1	-2.30416781	-0.85795280	0.55322907

Energy = -7584.965258 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 21

Atomic N.	X	Y	Z
8	2.17110631	0.30644591	-1.28980650
8	1.36781907	1.93438660	1.31414079
6	1.81844685	1.62299182	2.61723076
1	1.40667242	2.33350288	3.35753751
1	2.92200464	1.69459617	2.67328938
1	1.53792641	0.60187052	2.95228001
8	3.37092625	-0.59815502	0.32785449
6	3.26336384	0.22737682	-0.73644419
6	4.47247447	1.00090155	-1.21843532
1	4.81827159	1.66339532	-0.40693606
1	4.10347384	1.64518012	-2.02440961
6	5.63852514	0.12234198	-1.71817217
1	5.24151334	-0.68041693	-2.36036887
1	6.27346651	0.74642302	-2.36443553
6	6.50536179	-0.47015525	-0.60251777
1	6.97405331	0.35697487	-0.04172002
1	7.33093179	-1.04280892	-1.05249006
6	5.74913045	-1.36603210	0.38384670

1	5.35480514	-2.26295153	-0.12077860
1	6.45049300	-1.72652770	1.15367849
6	4.59877746	-0.67706671	1.10937857
1	4.87546948	0.33111017	1.45506197
1	4.28902332	-1.26089734	1.98422510
50	-0.00719526	0.67684311	0.39035773
7	-0.99193915	-0.42651696	-2.07466121
6	-0.19493171	-1.43151636	-2.78655308
1	-0.63608218	-1.69951619	-3.76859999
1	-0.10173357	-2.33579999	-2.17273384
1	0.80990188	-1.02613753	-2.95177608
7	-1.80146161	-2.66104759	-0.16482050
6	-2.37817905	-0.86743957	-1.82054846
1	-2.99000436	-0.74416858	-2.73991821
1	-2.81155038	-0.19715694	-1.05964777
6	-2.56188640	-2.31858951	-1.37462003
1	-3.64856311	-2.45864452	-1.21829430
1	-2.28198797	-2.98842895	-2.20133691
6	-2.25794638	-3.72686105	0.64746531
6	-2.32387462	-5.04668038	0.13948509
6	-2.76879692	-6.08052571	0.97395531
6	-3.12798912	-5.86525349	2.30755545
6	-3.01479768	-4.56126190	2.80447965
6	-2.59563135	-3.49304823	2.00530014
7	-0.71871686	2.28023248	-0.79954457
6	-0.97856250	0.85182892	-2.80872711
1	-1.56355581	0.76552273	-3.75045818
1	0.06822180	1.06065945	-3.07132797
6	-1.51324777	2.03314658	-2.00153861
1	-1.45863966	2.91562718	-2.66430887
1	-2.59341391	1.88799279	-1.79307834
6	-0.77311683	3.62724544	-0.32417713
6	-1.93030606	4.13145786	0.32006750
6	-1.95771496	5.46552812	0.75033019
6	-0.87282902	6.32641989	0.56337364
6	0.26163619	5.81578161	-0.07799275
6	0.33381342	4.48973702	-0.51964718
6	-1.85129852	-5.37934990	-1.25464780
1	-2.80730465	-7.09476477	0.56757397
6	-3.63096073	-6.99246381	3.17717300
1	-3.27221150	-4.36194402	3.84801124
6	-2.50535250	-2.10763168	2.59782347
6	-3.13733050	3.25961560	0.56741712
1	-2.85488737	5.83677700	1.25337740
6	-0.90861478	7.75006034	1.06606327
1	1.12189768	6.47060257	-0.24169837
6	1.58880416	3.99304216	-1.18942165
1	-1.61868637	-6.44943829	-1.33333396
1	-0.94624334	-4.80666763	-1.50596003
1	-2.60547169	-5.15203856	-2.02456250
1	-1.47281305	-1.72194690	2.60313529
1	-2.86275283	-2.10850936	3.63529026
1	-3.10950659	-1.37794705	2.03514645
1	-4.73230456	-7.01994209	3.19875660
1	-3.28975921	-6.88257031	4.21609706
1	-3.28731493	-7.96757348	2.80574383
1	-3.73138699	3.64674792	1.40580620
1	-2.84113908	2.22533246	0.79605260

1	-3.79991641	3.21842099	-0.31193629
1	1.36544645	3.43306459	-2.10795450
1	2.11628625	3.30308333	-0.51405724
1	2.25446918	4.83202255	-1.43433603
1	-0.48666622	7.82379854	2.08124871
1	-1.93676018	8.13458835	1.11102285
1	-0.31984669	8.41731763	0.42117923
1	-1.59133055	-1.82360214	0.38092181

Energy = -7584.957406 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 22

Atomic N.	X	Y	Z
8	2.49271193	-0.56635378	0.66549501
8	1.72728270	-0.75568891	-2.68352304
6	2.82180143	-0.24798337	-3.42543508
1	2.56848945	-0.15382279	-4.49964159
1	3.68834606	-0.93240368	-3.35513454
1	3.16492323	0.74964509	-3.08165127
8	4.24603443	-1.36917854	1.72241991
6	3.38702520	-1.40312172	0.66954307
6	3.56554048	-2.44650154	-0.41137104
1	4.58201005	-2.36395795	-0.83338038
1	2.85371322	-2.17441710	-1.20343549
6	3.32046757	-3.89274848	0.07145825
1	2.41020336	-3.92111208	0.69004924
1	3.10569590	-4.50544313	-0.81681367
6	4.49963632	-4.51574198	0.82461011
1	5.36650566	-4.58053515	0.14344030
1	4.24596198	-5.55147352	1.09926469
6	4.92303924	-3.75085742	2.08273988
1	4.11306596	-3.74435133	2.82991066
1	5.77644463	-4.26791477	2.55131968
6	5.35176806	-2.30945065	1.82758817
1	5.98988866	-2.22992197	0.93245568
1	5.91768568	-1.92001210	2.68274090
50	0.78197145	0.47799911	-1.27746232
7	-1.15368278	0.86642759	-2.97831526
6	-0.64386038	0.38936175	-4.28187393
1	-1.46306561	0.32046560	-5.02127622
1	-0.15238770	-0.58210607	-4.16315391
1	0.10824340	1.09779893	-4.65408029
7	-0.66119480	-1.05627350	-0.84866126
6	-2.20222393	-0.04045772	-2.45280515
1	-2.95933931	-0.24764316	-3.23620031
1	-2.68800421	0.46237534	-1.60822785
6	-1.59608986	-1.34486150	-1.93309349
1	-2.42865148	-1.96241447	-1.55481072
1	-1.15436589	-1.90601151	-2.77925373
6	-0.59052565	-1.97223509	0.22141949
6	-0.46557680	-3.37430209	0.01372081
6	-0.47088478	-4.24408017	1.11434757
6	-0.55941312	-3.78554757	2.43138138
6	-0.62755073	-2.40018184	2.62609049
6	-0.64717740	-1.49344869	1.56197535
7	-1.63558269	2.95620753	-0.76623215
6	-1.62182169	2.26658208	-3.16713271

1	-2.28017580	2.31071980	-4.05763089
1	-0.72653861	2.86448383	-3.40393498
6	-2.38819552	2.93039194	-2.02473239
1	-2.63172906	3.95180877	-2.37918658
1	-3.35226714	2.42367297	-1.87766986
6	-2.02388523	3.87877655	0.24042167
6	-3.29108857	3.78777517	0.86192614
6	-3.62631729	4.71001511	1.86204852
6	-2.74256294	5.70372180	2.29300235
6	-1.47573850	5.74575823	1.69849487
6	-1.10198675	4.86050822	0.68288116
6	-0.22597965	-3.95025584	-1.36252825
1	-0.37356000	-5.31812657	0.92928185
6	-0.59314355	-4.74264989	3.59922539
1	-0.68770572	-2.00698833	3.64468870
6	-0.74274614	-0.01800707	1.85254321
6	-4.25870708	2.67864579	0.52910485
1	-4.60633929	4.62424225	2.33860501
6	-3.14135214	6.70074776	3.35421377
1	-0.75314632	6.49592268	2.02976442
6	0.28023751	4.95103203	0.08007394
1	0.21742540	-4.95202111	-1.28075550
1	0.45596786	-3.30902216	-1.94100507
1	-1.14901061	-4.05313471	-1.95453552
1	0.23722945	0.47690193	1.75036719
1	-1.08637183	0.15452007	2.88115382
1	-1.42610884	0.48480842	1.15388943
1	-1.61658059	-4.86760300	3.98800097
1	0.02505309	-4.38301061	4.43464150
1	-0.22976666	-5.73834609	3.30938312
1	-4.97532766	2.53953347	1.34881440
1	-3.72543092	1.72937136	0.37322625
1	-4.84362212	2.88393513	-0.38168892
1	0.24741966	5.10873697	-1.01025224
1	0.87190783	4.03738429	0.25520985
1	0.83600025	5.78906015	0.51878025
1	-2.28398544	6.98776239	3.97858463
1	-3.92236955	6.29446294	4.01125195
1	-3.54004322	7.62425999	2.90459242
1	-0.63651551	3.03589772	-0.95925667

Energy = -7584.966268 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 23

Atomic N.	X	Y	Z
8	-0.00264138	-0.70825314	-0.34643106
8	2.40411163	0.39149777	-2.00659629
6	2.75952649	0.21374075	-3.36431265
1	3.48794165	0.97583756	-3.70550766
1	1.89557326	0.25510180	-4.06059659
1	3.24396216	-0.77104849	-3.49975830
8	-0.10172209	-2.13096483	-2.03161379
6	0.33548916	-1.80092070	-0.80098777
6	1.23855745	-2.74731229	-0.04255489
1	0.75549896	-3.73327961	0.06152397
1	1.34428271	-2.31920356	0.96031702
6	2.62412047	-2.90017831	-0.71141330

1	2.96507903	-1.90784696	-1.04776961
1	3.33206589	-3.23481980	0.06083601
6	2.63597577	-3.91006407	-1.86392182
1	2.37261381	-4.90695397	-1.46796773
1	3.66091446	-3.99649076	-2.25626559
6	1.68727638	-3.57610504	-3.02129700
1	2.00294456	-2.65508476	-3.53505734
1	1.73560010	-4.38338285	-3.77063368
6	0.22353073	-3.42499112	-2.62695324
1	-0.10524823	-4.22770239	-1.94821648
1	-0.41897145	-3.44616155	-3.51510186
50	0.73985943	1.58762432	-1.59405113
7	-1.31173376	3.10204597	0.05450838
6	-2.22889002	3.74141526	-0.88818164
1	-2.72743460	4.63667989	-0.45871391
1	-2.99590366	3.02786246	-1.21117720
1	-1.66677451	4.04986754	-1.78031651
7	-2.90264365	0.53313243	0.36970052
6	-1.99200058	2.66924552	1.28315328
1	-2.32922119	3.55483848	1.87008967
1	-1.25509511	2.14016174	1.90629201
6	-3.21357426	1.76874821	1.09913660
1	-3.60334129	1.56423338	2.11739757
1	-4.01308781	2.31306827	0.57369955
6	-3.87351042	-0.50487844	0.44416789
6	-5.03869114	-0.43370184	-0.35362900
6	-5.97647052	-1.47211676	-0.29133333
6	-5.79293701	-2.59351989	0.52468583
6	-4.62496006	-2.65572469	1.29427449
6	-3.67162135	-1.63091852	1.27897029
7	1.63527235	2.30191959	0.18796451
6	-0.19262880	4.00357030	0.37140119
1	-0.52745730	4.83805502	1.02749873
1	0.14287062	4.45247870	-0.57810602
6	1.00867186	3.32426064	1.02633845
1	1.73956054	4.12826964	1.23972945
1	0.72000651	2.92602828	2.01897528
6	2.88408620	1.83856038	0.70598653
6	2.93992020	0.96347578	1.81800726
6	4.18605414	0.54385217	2.30619059
6	5.38871425	0.96691024	1.73503478
6	5.31868028	1.84397633	0.64606383
6	4.09780157	2.28239048	0.12264046
6	-5.25223618	0.71699790	-1.30358283
1	-6.86783412	-1.40976818	-0.92117299
6	-6.83126958	-3.68789823	0.59305072
1	-4.45627658	-3.52064494	1.94147162
6	-2.45277134	-1.72671183	2.16722576
6	1.68552835	0.46726183	2.49520536
1	4.21122756	-0.13698009	3.16186969
6	6.71977479	0.48167485	2.25808337
1	6.24481501	2.20075809	0.18733349
6	4.09495273	3.22289188	-1.05596338
1	-5.96820860	0.44518028	-2.09016275
1	-4.29959045	1.00764977	-1.76923453
1	-5.65174659	1.60852368	-0.79345433
1	-1.51345755	-1.75913700	1.59426511
1	-2.49843241	-2.63230775	2.78553974

1	-2.37688931	-0.86143072	2.84395806
1	-7.55036950	-3.50417538	1.40740937
1	-6.37149712	-4.66796888	0.78111375
1	-7.40675913	-3.75245670	-0.34054692
1	1.86960093	-0.49496982	2.99342253
1	0.87054681	0.34156379	1.77083488
1	1.34048576	1.16773314	3.27333554
1	3.37706663	4.04376732	-0.92170841
1	3.80491455	2.69030705	-1.97414415
1	5.09435494	3.65005452	-1.21290936
1	7.14006097	-0.30461185	1.61095427
1	6.62346223	0.06161010	3.26832554
1	7.45772268	1.29590011	2.29491505
1	-1.97717791	0.18996255	0.62844702

Energy = -7584.956551 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 24

Atomic N.	X	Y	Z
8	0.24385866	-0.31461398	1.14931927
8	1.87178925	-1.10494506	-1.69824158
6	2.04581848	-2.47012807	-2.02918770
1	1.09292149	-3.03640232	-2.09791793
1	2.66976094	-2.97737994	-1.26949666
1	2.56219550	-2.58224585	-3.00157431
8	0.85726126	-2.25975539	1.99503418
6	1.11819682	-0.95758262	1.71701848
6	2.46305182	-0.37219013	2.09635607
1	2.63493322	-0.49863492	3.17898036
1	2.38878870	0.70125108	1.89359356
6	3.63967718	-0.97665514	1.29884592
1	3.34476312	-1.05475631	0.23993336
1	4.46960782	-0.25559024	1.33620150
6	4.12933106	-2.32092258	1.84718062
1	4.51482562	-2.17038053	2.87150223
1	4.98454643	-2.66577549	1.24547354
6	3.06819815	-3.42678504	1.88577883
1	2.74782768	-3.70100162	0.86806860
1	3.50981454	-4.33505397	2.32815001
6	1.82480351	-3.08988079	2.70110649
1	2.08434356	-2.61559412	3.66137772
1	1.24992333	-3.99871283	2.91672289
50	-0.07425323	-0.34374695	-1.86147952
7	-2.31496090	1.48644163	-2.46838696
6	-3.23651706	0.92152948	-3.45359861
1	-3.91260692	1.68942764	-3.88643462
1	-3.84947869	0.13325136	-3.00152275
1	-2.66000313	0.46554286	-4.26983135
7	-2.85878322	0.12253133	0.23069850
6	-3.02602137	2.06543905	-1.32109106
1	-3.76023294	2.83038625	-1.66110245
1	-2.28809639	2.59577269	-0.69992257
6	-3.76980496	1.06499385	-0.43403735
1	-4.36237239	1.65805299	0.29291685
1	-4.50030681	0.49282983	-1.02183651
6	-3.46829939	-0.82751162	1.10310577
6	-4.13541824	-1.95043608	0.56454415

6	-4.71291431	-2.88338569	1.43516633
6	-4.63451099	-2.75355466	2.82558411
6	-3.94357282	-1.64965315	3.33954414
6	-3.36759818	-0.68348302	2.50755569
7	0.65984091	1.65581318	-1.96007127
6	-1.41718035	2.46108079	-3.10515218
1	-1.95494666	3.40175911	-3.36042950
1	-1.07306243	2.01306392	-4.05061478
6	-0.18970610	2.80957832	-2.26905030
1	0.39266602	3.53842607	-2.86235353
1	-0.50243332	3.36135578	-1.36080950
6	1.99131256	2.03151833	-1.59218581
6	2.26100541	2.67266911	-0.35683138
6	3.57815433	3.03402483	-0.03826404
6	4.64578763	2.79404436	-0.90746003
6	4.35942570	2.18696093	-2.13522603
6	3.06180983	1.80382190	-2.49381471
6	-4.18701021	-2.18344459	-0.92449710
1	-5.21795799	-3.75341395	1.00728297
6	-5.28893105	-3.75946692	3.74217801
1	-3.85626298	-1.52948459	4.42258046
6	-2.64504137	0.49691913	3.11389059
6	1.16381700	2.98029630	0.63377941
1	3.76932161	3.52096216	0.92241808
6	6.06177093	3.15863589	-0.52983115
1	5.17223315	2.00722246	-2.84388532
6	2.82875936	1.16543341	-3.83909484
1	-4.31748815	-3.25121510	-1.14441625
1	-3.26104125	-1.83211120	-1.40180633
1	-5.02914247	-1.65227863	-1.39872066
1	-1.57513612	0.50230975	2.85240420
1	-2.71981630	0.47147392	4.20839272
1	-3.06797426	1.45531796	2.77346546
1	-6.30923008	-3.44507058	4.01457911
1	-4.72517853	-3.87744894	4.67789242
1	-5.36882998	-4.74484694	3.26307557
1	1.57573881	3.08831735	1.64681571
1	0.41046342	2.18172346	0.64777665
1	0.65369754	3.92705749	0.39438988
1	1.95018527	1.59113755	-4.34359719
1	2.64181297	0.08845587	-3.71790671
1	3.70630866	1.29719161	-4.48590692
1	6.59698699	2.29253795	-0.10823164
1	6.08318650	3.95665769	0.22481433
1	6.63522474	3.49761106	-1.40399817
1	-2.13362597	0.63471184	0.73432254

Energy = -7584.956412 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 25

Atomic N.	X	Y	Z
8	-0.33454077	-3.38466610	-0.51077007
8	0.70126791	-0.21845898	0.27857036
6	2.10099511	-0.33016757	0.07730292
1	2.61327803	0.58876644	0.41101241
1	2.38328540	-0.50138799	-0.98128251
1	2.51598232	-1.17507508	0.65967873

8	1.43229049	-4.52588752	0.16332223
6	0.26124277	-3.87953781	0.43390988
6	-0.22514035	-3.79921767	1.86658079
1	-0.31523253	-4.81619531	2.28546316
1	-1.23218133	-3.37078774	1.81606435
6	0.66749232	-2.93276412	2.78076391
1	0.91927645	-2.00009793	2.25222142
1	0.05921511	-2.63297406	3.64659415
6	1.92618145	-3.64505267	3.28617548
1	1.62216120	-4.49743032	3.91956140
1	2.48947801	-2.96218047	3.94131341
6	2.85771692	-4.16769392	2.18694973
1	3.27865815	-3.33644690	1.59838086
1	3.71346277	-4.68256769	2.65408835
6	2.20699639	-5.15402765	1.22175631
1	1.58022467	-5.88692198	1.75570316
1	2.97400405	-5.70746180	0.66571885
50	-0.52172300	-0.51652572	-1.37247806
7	-2.09447302	1.38454406	-2.84519946
6	-2.65482824	0.59976901	-3.95181265
1	-3.44363260	1.15524801	-4.49818830
1	-3.08889140	-0.33390188	-3.57359289
1	-1.85373641	0.33259726	-4.65376176
7	-2.30805812	-0.07726070	-0.24630271
6	-3.10838149	1.66265081	-1.81298511
1	-4.02858448	2.07970696	-2.27671500
1	-2.69800367	2.41677492	-1.12726775
6	-3.46393457	0.42302884	-0.99134942
1	-4.25296847	0.72548666	-0.28121960
1	-3.94017133	-0.32772913	-1.65512496
6	-2.64006379	-0.70512467	0.99138050
6	-3.40747599	-1.89824403	1.03954936
6	-3.74976011	-2.45440197	2.28199840
6	-3.35212117	-1.87634502	3.49040735
6	-2.58721375	-0.70446066	3.42848638
6	-2.23033495	-0.10815996	2.21348168
7	0.74391842	2.30092856	-2.32541548
6	-1.47618807	2.61996249	-3.35932937
1	-2.24797117	3.39208987	-3.55977167
1	-1.01697831	2.38098542	-4.33245616
6	-0.40354116	3.21975612	-2.45428419
1	-0.09752711	4.18781833	-2.89358032
1	-0.81917641	3.43772119	-1.46127494
6	2.00676408	2.84454475	-1.95814465
6	2.19195538	3.48478560	-0.71148002
6	3.45956711	3.98718214	-0.39086628
6	4.55957234	3.85569068	-1.24427405
6	4.36385705	3.17708983	-2.45254687
6	3.11329870	2.67511927	-2.82635383
6	-3.83199674	-2.61454336	-0.21844237
1	-4.33360664	-3.37898430	2.29844743
6	-3.74691002	-2.47913900	4.81794238
1	-2.26860069	-0.22491784	4.35825748
6	-1.43709930	1.17218058	2.21814854
6	1.08278151	3.56596074	0.30741242
1	3.59221124	4.47297525	0.57925462
6	5.90651673	4.43221879	-0.88028969
1	5.20844687	3.03648358	-3.13175159

6	2.96288455	1.94779546	-4.14252753
1	-4.06951656	-3.66459351	-0.00249095
1	-3.03349077	-2.59109026	-0.97344652
1	-4.72936813	-2.16271099	-0.67006985
1	-0.44045696	1.00514688	1.78357115
1	-1.32649400	1.55450857	3.24189331
1	-1.92780070	1.94189843	1.60455893
1	-4.50517798	-1.86354436	5.32698873
1	-2.88644079	-2.55474754	5.49914071
1	-4.16942034	-3.48470730	4.68917408
1	1.49894793	3.72985451	1.30983280
1	0.50347807	2.63183689	0.32528605
1	0.38474179	4.39416005	0.10648242
1	2.21860309	2.42643713	-4.80023139
1	2.65329243	0.89821061	-4.00538775
1	3.91648204	1.93494427	-4.68459706
1	6.72647634	3.83522058	-1.30258423
1	6.04107563	4.47714156	0.20909970
1	6.01831908	5.45838123	-1.26560040
1	0.84281348	1.78053114	-3.19667892

Energy = -7584.961369 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 26

Atomic N.	X	Y	Z
8	0.62603560	-0.48316500	-0.01672838
8	1.54320398	1.29705680	-2.42203657
6	2.17662109	0.95877138	-3.64083385
1	2.09571090	1.77176303	-4.38929966
1	1.77122355	0.03975279	-4.11412481
1	3.25621195	0.79124249	-3.46973305
8	2.03663279	-1.90898297	-0.93896824
6	1.77481381	-0.92276342	-0.05927574
6	2.88407381	-0.37296495	0.80898646
1	3.34778862	-1.18531920	1.39332000
1	2.39949061	0.31137961	1.51397061
6	3.95977035	0.37389387	-0.01286619
1	3.45666557	0.98724956	-0.77759858
1	4.47381881	1.07034887	0.66555010
6	4.99921515	-0.55780168	-0.64515496
1	5.53901478	-1.08880173	0.15896944
1	5.75222123	0.04797866	-1.17233336
6	4.42590601	-1.59503484	-1.61804899
1	4.00070559	-1.10635412	-2.50819470
1	5.24337476	-2.24145285	-1.97782579
6	3.36444550	-2.51246040	-1.02434539
1	3.65465842	-2.88910120	-0.03082753
1	3.19166256	-3.37550247	-1.67808721
50	-0.46001394	0.74490310	-2.19132161
7	-3.19730607	0.52563989	-0.90532291
6	-4.04417679	-0.23734966	-1.82143612
1	-5.12537068	-0.02185415	-1.68355206
1	-3.87522935	-1.31183265	-1.68482898
1	-3.76822900	0.01265191	-2.85505445
7	-2.21250253	-1.86971272	0.68381735
6	-3.51493140	0.25155645	0.50314407
1	-4.52299132	0.65386171	0.75686911

8	0.63793713	-0.71337921	-0.54799370
8	1.84363769	0.90028771	-2.94279467
6	2.45544511	0.48288268	-4.14765238
1	2.51283474	1.30574880	-4.88691701
1	1.93426370	-0.36390998	-4.64209486
1	3.49442599	0.15892839	-3.95076870
8	1.93207917	-2.31987162	-1.33752099
6	1.72945131	-1.27785318	-0.50309045
6	2.83917429	-0.82709886	0.41798855
1	3.19532050	-1.67209498	1.03030215
1	2.38707809	-0.09303972	1.09362381
6	4.01834698	-0.19572362	-0.35819539
1	3.61394861	0.44917739	-1.15508657
1	4.56385352	0.45962371	0.33640234
6	4.99282044	-1.23167123	-0.92857527
1	5.44559831	-1.79450713	-0.09305519
1	5.82086430	-0.70882139	-1.43137422
6	4.36763297	-2.23045399	-1.91006811
1	4.02501443	-1.72083924	-2.82394531
1	5.13756093	-2.95350157	-2.22616507
6	3.20365089	-3.03884994	-1.34978172
1	3.41564124	-3.41789073	-0.33739856
1	2.98555979	-3.89756960	-1.99585336
50	-0.20867479	0.58589787	-2.72582868
7	-2.75223931	0.55377311	-1.17820093
6	-3.74899003	-0.20507689	-1.93782114
1	-4.78855964	0.06277111	-1.65281735
1	-3.61123750	-1.28191776	-1.78629035
1	-3.61569967	-0.00078113	-3.00896624
7	-2.63829917	-1.16788517	2.17917039
6	-2.86668579	0.32680019	0.26735022
1	-3.86900436	0.66327839	0.62752259
1	-2.11593174	0.94801984	0.77382836
6	-2.64052811	-1.12302810	0.70223093
1	-3.42564758	-1.78422587	0.29258527
1	-1.67404636	-1.46130749	0.30817157
6	-2.74936410	-2.43234193	2.81449013
6	-1.71869840	-3.39462466	2.69873914
6	-1.84983928	-4.61749671	3.36870118
6	-2.95391886	-4.91927019	4.17256260
6	-3.94338722	-3.93860741	4.30758176
6	-3.86557121	-2.71069702	3.64248072
7	-0.40453488	2.40208542	-1.65332463
6	-2.86342765	1.98788253	-1.49881468
1	-3.78816176	2.42281370	-1.05990416
1	-2.95543976	2.06507348	-2.59457563
6	-1.66856615	2.83031468	-1.05781487
1	-1.89574466	3.87072505	-1.36197787
1	-1.61716245	2.85730375	0.04856876
6	0.67286839	3.30774818	-1.41132414
6	1.27352144	3.41387182	-0.13342536
6	2.31414236	4.33226028	0.06769037
6	2.78615636	5.15712204	-0.95616621
6	2.17899870	5.04624372	-2.21290900
6	1.14147731	4.14084090	-2.45857078
6	-0.45700420	-3.10102371	1.92652979
1	-1.04266126	-5.34896571	3.27506729
6	-3.08098944	-6.25823386	4.85856888

1	-4.81050561	-4.13620290	4.94308167
6	-4.96725997	-1.69184586	3.82198389
6	0.82633698	2.55091143	1.02106650
1	2.77098277	4.39700609	1.05939396
6	3.92894815	6.11740729	-0.72668148
1	2.52277150	5.68596742	-3.03026298
6	0.53747965	4.06687227	-3.83866546
1	0.35852542	-3.75134311	2.27104673
1	-0.15832152	-2.05117550	2.05938254
1	-0.57828423	-3.26697078	0.84477651
1	-4.60883491	-0.77057815	4.31153337
1	-5.76818799	-2.09932145	4.45133111
1	-5.41824654	-1.39557319	2.86121004
1	-3.63597667	-6.97619197	4.23352886
1	-3.62101589	-6.17206943	5.81156118
1	-2.09524334	-6.69851662	5.06252845
1	1.65402575	2.39102457	1.72647516
1	0.46307436	1.57628264	0.66886569
1	0.01112825	3.02402197	1.59267991
1	-0.55985198	4.02553144	-3.80235857
1	0.87373872	3.16049475	-4.36576511
1	0.83918935	4.93428422	-4.44087137
1	4.87867471	5.70377956	-1.10188178
1	4.06267468	6.33234678	0.34213350
1	3.76401060	7.07023410	-1.24973788
1	-3.37912160	-0.55529072	2.52055234

Energy = -7584.957963 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 28

Atomic N.	X	Y	Z
8	0.92575453	-3.07598683	-1.23092233
8	0.74321568	0.17508757	-0.18093645
6	1.65326918	0.80476027	-1.06847139
1	1.80893380	1.85816399	-0.77809182
1	1.31641817	0.79829379	-2.12492079
1	2.63883879	0.30155565	-1.04376068
8	3.03659009	-3.12561478	-1.87943694
6	2.09512216	-3.17940806	-0.89303066
6	2.54005850	-3.34893970	0.54536630
1	3.15578462	-4.25999532	0.63849347
1	1.62347675	-3.50727642	1.12422867
6	3.31106377	-2.13500593	1.10670793
1	2.78141957	-1.21327056	0.81940547
1	3.25249898	-2.18624489	2.20378356
6	4.78570025	-2.08304618	0.69443177
1	5.30406048	-2.96221539	1.11698240
1	5.25802637	-1.19974915	1.15213961
6	5.03314744	-2.05696681	-0.81797179
1	4.63162027	-1.13440613	-1.26764496
1	6.11957813	-2.04695300	-1.00550354
6	4.45331745	-3.24821417	-1.57466764
1	4.63748444	-4.19421048	-1.03961649
1	4.90977902	-3.32869039	-2.56912248
50	-0.92850128	-0.72651650	-1.01976273
7	-3.68606661	0.07628525	-0.89782657
6	-4.37574604	-0.89161829	-1.75921657

1	-5.47787947	-0.83007198	-1.65519554
1	-4.06199943	-1.91278131	-1.51022833
1	-4.10447421	-0.70759792	-2.80725966
7	-1.72201777	-1.26944943	0.91059478
6	-3.92328097	-0.20602861	0.52864135
1	-5.01083097	-0.32923609	0.72310458
1	-3.56654360	0.65533343	1.11012714
6	-3.17105481	-1.44584991	1.01373947
1	-3.44652028	-1.59333923	2.07233644
1	-3.56207214	-2.33806891	0.48268548
6	-0.97683142	-1.96734024	1.90749572
6	-0.97552366	-3.38456620	1.98103116
6	-0.26693029	-4.02632858	3.00905318
6	0.45545473	-3.31513585	3.97044471
6	0.45014334	-1.91679520	3.88331683
6	-0.24919557	-1.23319311	2.88224717
7	-1.79667863	2.33418519	-1.60577971
6	-4.07689462	1.45038374	-1.26118709
1	-5.06082877	1.70969922	-0.81776936
1	-4.21281424	1.47924165	-2.35478692
6	-3.06367799	2.52392703	-0.87339586
1	-3.51564976	3.50827621	-1.09810124
1	-2.87556232	2.49907241	0.20845339
6	-0.93712011	3.45629632	-1.77088184
6	-0.36281086	4.10705595	-0.65536492
6	0.49187858	5.19550109	-0.87325216
6	0.82297603	5.64811159	-2.15407548
6	0.27874793	4.95990303	-3.24473235
6	-0.59442076	3.88053818	-3.07862884
6	-1.68772268	-4.22855170	0.95325589
1	-0.27212323	-5.11931616	3.04482153
6	1.22055655	-4.02289886	5.06377002
1	0.99492243	-1.33306513	4.63071493
6	-0.24500729	0.27287385	2.86819460
6	-0.58377724	3.60794646	0.75067552
1	0.93636733	5.68528872	-0.00307245
6	1.72755467	6.83997065	-2.35502372
1	0.53559058	5.27398589	-4.25955018
6	-1.14871400	3.17372802	-4.29400743
1	-1.28148511	-5.24862081	0.94370281
1	-1.57225423	-3.80314125	-0.05366256
1	-2.76707322	-4.30836121	1.15820407
1	0.27831925	0.64442484	1.97482131
1	0.24872278	0.66631482	3.76702281
1	-1.26993612	0.66955569	2.82535714
1	0.92183353	-3.66367134	6.06006392
1	2.30441526	-3.84971911	4.97379118
1	1.05066879	-5.10725795	5.03111833
1	0.21216630	3.97276240	1.41268997
1	-0.57568646	2.50896990	0.77778188
1	-1.54098996	3.95046653	1.17482279
1	-2.25076852	3.19300606	-4.32044201
1	-0.83748959	2.11665978	-4.33915274
1	-0.79208442	3.65480525	-5.21310691
1	2.35363177	6.72317449	-3.25050755
1	2.38969038	6.98880599	-1.49132013
1	1.14477777	7.76602313	-2.48428108
1	-2.00653776	1.93428105	-2.51994939

Energy = -7584.961356 Hartree
 Number of imaginary frequencies = 0.

Compound I2b isomer 29

Atomic N.	X	Y	Z
8	0.98100496	-2.97362834	-1.42288571
8	0.77326716	0.11365235	0.04325383
6	1.93239950	0.74340500	-0.47831626
1	2.08948564	1.72307004	0.00518822
1	1.88648326	0.91729414	-1.57248513
1	2.83317225	0.12842891	-0.28947681
8	3.17803617	-3.17918542	-1.52122682
6	2.00768324	-3.25374070	-0.82321749
6	2.04171529	-3.66062711	0.63584849
1	2.54011846	-4.64004009	0.73659562
1	0.99537511	-3.78843283	0.93432827
6	2.72653786	-2.62696027	1.55557487
1	2.36406348	-1.62094368	1.29254995
1	2.37553023	-2.81466845	2.58081640
6	4.25717820	-2.69065016	1.53974377
1	4.57624027	-3.67138170	1.93540457
1	4.65764561	-1.93530207	2.23392676
6	4.89748368	-2.49429420	0.16106766
1	4.70077268	-1.48077255	-0.22449800
1	5.99229623	-2.58381952	0.25587406
6	4.44999688	-3.50138751	-0.89415340
1	4.41387245	-4.52451131	-0.48550679
1	5.14597952	-3.50120313	-1.74232610
50	-0.68141840	-0.47359236	-1.31697523
7	-3.30177277	0.61270021	-1.76962157
6	-3.81164105	-0.15557090	-2.91167464
1	-4.89349302	0.01855838	-3.08071652
1	-3.65624261	-1.22886250	-2.74709983
1	-3.25822291	0.12452757	-3.81783683
7	-1.99578765	-1.16464164	0.24712926
6	-3.92861755	0.18351350	-0.50724786
1	-5.03508706	0.16200957	-0.61218128
1	-3.67201012	0.91917280	0.26754633
6	-3.43028659	-1.18485749	-0.04099355
1	-3.98463857	-1.42972295	0.88156023
1	-3.73767556	-1.95376046	-0.77951185
6	-1.59610440	-2.06701748	1.27788208
6	-1.72089007	-3.47262121	1.12716310
6	-1.36033451	-4.31965850	2.18697705
6	-0.86805949	-3.82704363	3.39815629
6	-0.74202103	-2.43801194	3.53070984
6	-1.09790309	-1.55427936	2.50554776
7	-1.12384825	2.71071516	-1.62846673
6	-3.47449214	2.05676069	-2.00982417
1	-4.51794025	2.36904295	-1.79606131
1	-3.31166938	2.23595557	-3.08515378
6	-2.52174446	2.95186277	-1.22210547
1	-2.81964056	4.00142619	-1.40497147
1	-2.63196398	2.77252172	-0.14412880
6	-0.16567495	3.73712112	-1.39639540
6	0.13811207	4.17037674	-0.08580744
6	1.10419780	5.16973224	0.08938774

6	1.80206862	5.73783616	-0.98070346
6	1.51699570	5.26153993	-2.26570953
6	0.54781638	4.27991188	-2.49364478
6	-2.19582076	-4.08858711	-0.16543841
1	-1.45592180	-5.40030284	2.04892519
6	-0.49415835	-4.75348254	4.53111667
1	-0.36934983	-2.02273932	4.47131093
6	-0.97216533	-0.06970649	2.72634607
6	-0.49154038	3.52783222	1.12480246
1	1.33664736	5.49041222	1.10812153
6	2.82121358	6.82977388	-0.76121818
1	2.06113479	5.66865459	-3.12166311
6	0.28536810	3.80166211	-3.90302969
1	-1.87878448	-5.13775889	-0.23173529
1	-1.78642282	-3.55048626	-1.03203529
1	-3.29377371	-4.07281148	-0.25312668
1	-0.20675902	0.35174161	2.05808483
1	-0.70041494	0.14421680	3.76887214
1	-1.91632907	0.44468965	2.49463271
1	-1.15190876	-4.60698324	5.40185314
1	0.53582047	-4.57524257	4.87552660
1	-0.57255193	-5.80586022	4.22730117
1	0.12496171	3.70871112	2.01481411
1	-0.58082891	2.44111545	0.98484310
1	-1.49597816	3.92599495	1.33954771
1	-0.76409974	3.95259887	-4.20539309
1	0.51240137	2.72970780	-4.02816724
1	0.91239215	4.34995271	-4.61687399
1	3.65520966	6.74999267	-1.47229259
1	3.23377696	6.79219298	0.25606399
1	2.37341702	7.82734464	-0.89640226
1	-1.11188349	2.45742059	-2.61609464

Energy = -7584.961380 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 30

Atomic N.	X	Y	Z
8	0.55375702	0.16738088	-0.80033531
8	1.77734615	1.98896065	1.54890344
6	2.33902046	2.84012947	0.56154990
1	2.09971062	3.90137029	0.74706007
1	1.99552267	2.59551065	-0.45993764
1	3.43891945	2.73417823	0.58477136
8	1.30642446	-1.20728418	-2.33831141
6	1.39807047	-0.67402046	-1.09904470
6	2.52043091	-1.10120329	-0.17965292
1	2.46201743	-2.18981466	-0.01353123
1	2.33548668	-0.59945732	0.77806762
6	3.92615041	-0.71919168	-0.69444498
1	3.90553063	0.31232977	-1.08006415
1	4.60168962	-0.70640196	0.17330060
6	4.49135965	-1.67496387	-1.74935267
1	4.59391652	-2.67778312	-1.30008616
1	5.50801929	-1.35222434	-2.02227214
6	3.64054177	-1.79134915	-3.01804890
1	3.60247530	-0.83015649	-3.55610669
1	4.11156118	-2.51359087	-3.70460438

6	2.21215944	-2.26561970	-2.77537194
1	2.16797608	-3.09977980	-2.05836897
1	1.75296443	-2.60002909	-3.71347771
50	-0.04470128	1.05100640	1.65922691
7	-3.03535539	0.00993389	1.52678754
6	-3.58444351	0.50088695	2.79148739
1	-4.67977864	0.67978095	2.74305819
1	-3.09380900	1.43851343	3.08214214
1	-3.38815539	-0.23701681	3.58074998
7	-1.31507608	2.51973766	0.80301230
6	-3.27318917	0.94473763	0.41548685
1	-4.36474651	1.01792376	0.20198778
1	-2.78351619	0.53584425	-0.48057671
6	-2.76396940	2.36956625	0.63127138
1	-3.08553179	2.93153028	-0.26296126
1	-3.31697507	2.83757012	1.47162994
6	-0.86050317	3.83012610	0.45786152
6	-0.52909007	4.77049371	1.46397582
6	-0.10773764	6.05557785	1.09642945
6	0.00893751	6.44529159	-0.24156787
6	-0.31468622	5.50401722	-1.22498408
6	-0.74515518	4.21081923	-0.90467101
7	-1.43453570	-2.27147607	0.48886545
6	-3.58742362	-1.32091615	1.23026736
1	-4.65921265	-1.24954513	0.93619832
1	-3.54664516	-1.90745376	2.16137162
6	-2.84544301	-2.09823067	0.14140494
1	-3.34229552	-3.07836517	0.05368232
1	-2.96303443	-1.59497993	-0.83240763
6	-0.73190282	-3.46343139	0.28027394
6	-0.75248999	-4.13015356	-0.97284086
6	-0.01107126	-5.30953994	-1.12893848
6	0.78290727	-5.84506870	-0.10958582
6	0.82966907	-5.14449890	1.10265889
6	0.08874369	-3.97965044	1.32087199
6	-0.59404508	4.41185742	2.92887601
1	0.13872009	6.77244248	1.88419800
6	0.50348472	7.82300926	-0.61274645
1	-0.21948280	5.77862832	-2.27914566
6	-1.04911574	3.23595925	-2.01580536
6	-1.47211765	-3.55199655	-2.16928146
1	-0.04000736	-5.81176582	-2.09997858
6	1.54498304	-7.13481034	-0.29936666
1	1.44957798	-5.52664282	1.91806970
6	0.15400757	-3.28560807	2.65918100
1	-0.63071389	5.31809160	3.54818094
1	0.29713393	3.83886159	3.23183991
1	-1.47094952	3.79188068	3.16005230
1	-0.72580946	2.21977311	-1.75333085
1	-0.54812571	3.54238454	-2.94374647
1	-2.12876546	3.18482814	-2.23316577
1	0.05785719	8.16952092	-1.55537766
1	1.59703170	7.82914999	-0.74717864
1	0.26749715	8.55744127	0.16950728
1	-1.14280483	-4.05628064	-3.08744616
1	-1.25981997	-2.47752099	-2.27264101
1	-2.56525640	-3.66197831	-2.11283748
1	-0.84240428	-3.20218512	3.12337590

1	0.55173415	-2.25915129	2.58723536
1	0.80001551	-3.84017003	3.35120405
1	2.52416741	-7.10286623	0.19937604
1	1.71110655	-7.34826286	-1.36426622
1	0.99619282	-7.99165005	0.12330844
1	-1.19492598	-1.78296006	1.34910007

Energy = -7584.957687 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 31

Atomic N.	X	Y	Z
8	4.07896391	-0.21001466	3.26720598
8	0.84406297	-0.25116275	-0.59390157
6	0.37298514	-1.01504372	-1.68635261
1	-0.68642917	-1.31441110	-1.58517139
1	0.95395602	-1.94841106	-1.80193956
1	0.47418432	-0.43394511	-2.62186951
8	4.61675882	-0.91345743	1.23522510
6	4.55093255	0.06991581	2.18237500
6	5.05220779	1.46195225	1.82967499
1	6.09623923	1.41050188	1.47762230
1	5.04854326	2.01557911	2.77585573
6	4.18511863	2.19053409	0.78067227
1	3.12075178	2.03535490	1.02028501
1	4.37314659	3.27092984	0.87825195
6	4.46678037	1.76842316	-0.66502990
1	5.50634157	2.04472796	-0.91798195
1	3.81803852	2.34796642	-1.33988172
6	4.26321657	0.27481815	-0.94065071
1	3.20542880	-0.00607656	-0.79775349
1	4.50288587	0.07288197	-1.99797364
6	5.13794135	-0.64763006	-0.09835061
1	6.17318922	-0.27446190	-0.02024907
1	5.17511615	-1.64875276	-0.54575622
50	0.08483485	0.09447456	1.29811974
7	-2.18714263	0.64706536	2.73122152
6	-1.95544152	1.71526659	3.70680901
1	-2.76823376	1.77038748	4.45820105
1	-1.87897121	2.68683407	3.20363891
1	-1.00430761	1.53371425	4.22496310
7	-1.99255925	1.47472905	-0.12799440
6	-3.34791976	0.91575453	1.87495885
1	-4.21887253	1.26119648	2.47009302
1	-3.64437070	-0.02841224	1.39572624
6	-3.05661998	1.94833188	0.78609214
1	-3.99626798	2.15397999	0.24013550
1	-2.73475944	2.90064837	1.22595226
6	-1.68332139	2.36893953	-1.21354509
6	-0.93188134	3.54040633	-0.98216647
6	-0.62846900	4.37261143	-2.06797229
6	-1.03574927	4.07996132	-3.37278073
6	-1.77300095	2.90842846	-3.57783553
6	-2.11185349	2.05340619	-2.52381777
7	-1.11447543	-1.70702291	1.43018495
6	-2.23143174	-0.66632549	3.39601636
1	-3.12783827	-0.76370427	4.04444666
1	-1.34522632	-0.71374336	4.04832377

6	-2.18817397	-1.83495090	2.41358992
1	-2.05322113	-2.74851555	3.02301611
1	-3.18664722	-1.95085794	1.94219625
6	-0.79344871	-2.92929727	0.77213445
6	-1.71400759	-3.55275566	-0.11144865
6	-1.38025071	-4.76489751	-0.73002815
6	-0.15333251	-5.39636039	-0.51251158
6	0.74749364	-4.77462829	0.35941177
6	0.45662435	-3.56563848	1.00285342
6	-0.42605058	3.91390779	0.38928483
1	-0.03488570	5.27129461	-1.88283039
6	-0.71048114	5.00584711	-4.51974174
1	-2.10000773	2.65046160	-4.58799903
6	-2.92429749	0.81064768	-2.80584029
6	-3.03983499	-2.91500659	-0.44668129
1	-2.10165153	-5.21972922	-1.41468981
6	0.20301716	-6.68613777	-1.21210610
1	1.71131953	-5.25100081	0.55820262
6	1.48458089	-2.97659408	1.93633385
1	0.46700851	4.54694289	0.30809318
1	-0.16228246	3.02504598	0.98113207
1	-1.17485872	4.48658629	0.96095635
1	-2.34438456	-0.11195106	-2.64165391
1	-3.25393121	0.80030198	-3.85202059
1	-3.82657796	0.75069256	-2.17710090
1	-1.53979845	5.70479741	-4.71235316
1	-0.53412570	4.44698021	-5.44891832
1	0.18248979	5.60829053	-4.30622356
1	-3.37713038	-3.22260098	-1.44572465
1	-2.95833590	-1.81803002	-0.42534527
1	-3.83227339	-3.19512158	0.26586903
1	1.02627125	-2.56926710	2.84790371
1	2.04965415	-2.15604872	1.46553616
1	2.22325735	-3.73458484	2.22773274
1	0.86984206	-6.50357939	-2.06981084
1	-0.69227732	-7.19548034	-1.59325390
1	0.72856057	-7.37670611	-0.53711084
1	-2.29433372	0.58079797	-0.52393064

Energy = -7584.959542 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 32

Atomic N.	X	Y	Z
8	3.29664892	-1.92332805	3.54104322
8	0.91015091	-0.20896688	-0.54362679
6	0.55259216	-0.48311939	-1.88366945
1	-0.53740129	-0.59668672	-2.03004295
1	1.01716555	-1.42148346	-2.23805149
1	0.89977026	0.33672025	-2.53975711
8	4.15627546	-2.03769608	1.50120929
6	4.00417720	-1.40138373	2.70144444
6	4.70914314	-0.07148775	2.92029438
1	5.79149616	-0.18231410	2.73908049
1	4.57262734	0.15292778	3.98462031
6	4.15205205	1.07992108	2.05603845
1	3.05091539	1.03575656	2.06165888
1	4.42921076	2.02967850	2.53908489

6	4.67178251	1.08868183	0.61477085
1	5.76385118	1.25625670	0.63325043
1	4.23450466	1.94737101	0.08222992
6	4.37388846	-0.19017290	-0.17526164
1	3.28574119	-0.32371363	-0.30283572
1	4.79961634	-0.08932521	-1.18755305
6	4.96022848	-1.45943235	0.43360959
1	5.99153432	-1.30431716	0.79342991
1	4.98275288	-2.26338232	-0.31269121
50	-0.13308548	-0.35461804	1.23593589
7	-2.54238614	0.10636387	2.46244778
6	-2.36327641	0.74841200	3.76712965
1	-3.28655528	0.70364262	4.37852191
1	-2.07764850	1.80007547	3.64308662
1	-1.55234777	0.24571749	4.31099052
7	-1.72996558	1.75844182	0.11401152
6	-3.48547537	0.83497799	1.60669589
1	-4.40198434	1.11936952	2.16460772
1	-3.80189367	0.16164526	0.79709186
6	-2.87697643	2.09354272	0.98812914
1	-3.66950436	2.62516376	0.42891365
1	-2.52711805	2.78258086	1.76713117
6	-1.12074429	2.88478233	-0.54471300
6	-0.28522394	3.76603509	0.17329656
6	0.30979212	4.83651847	-0.50787291
6	0.11228339	5.05798637	-1.87374861
6	-0.71388780	4.16517795	-2.56574989
6	-1.34008401	3.08999723	-1.92676946
7	-1.54924693	-1.86078855	0.58344925
6	-2.86837560	-1.32085839	2.62350520
1	-3.87281990	-1.45984511	3.07660722
1	-2.12811604	-1.73036062	3.32879211
6	-2.79217759	-2.10223506	1.31345952
1	-2.88652889	-3.17124687	1.58265783
1	-3.69360568	-1.87965902	0.70490914
6	-1.26780363	-2.84345056	-0.40907412
6	-2.08211427	-2.97527295	-1.56538195
6	-1.79366109	-3.96249363	-2.51660562
6	-0.71393827	-4.83775441	-2.37422407
6	0.08222180	-4.70082585	-1.23188500
6	-0.16952805	-3.73186748	-0.25273883
6	0.00621137	3.58091381	1.64189451
1	0.96595659	5.50733535	0.05223446
6	0.75138783	6.23106921	-2.57665247
1	-0.88194852	4.30913853	-3.63578254
6	-2.23329497	2.16817882	-2.72461784
6	-3.23565585	-2.03848909	-1.82767317
1	-2.42893036	-4.03679970	-3.40373409
6	-0.39708358	-5.87259289	-3.42714731
1	0.92686239	-5.37977736	-1.08709685
6	0.73531224	-3.66805001	0.95241095
1	0.97040893	4.03722363	1.90080210
1	0.04671320	2.51676116	1.91731565
1	-0.75710686	4.06176088	2.27565253
1	-1.81190955	1.15368924	-2.81238619
1	-2.36209473	2.55100144	-3.74446303
1	-3.23671171	2.07246843	-2.28073213
1	0.05118427	7.07811911	-2.65098279

1	1.05392652	5.96945897	-3.59993190
1	1.63900979	6.58551149	-2.03603446
1	-3.42436293	-1.94745356	-2.90587117
1	-3.02196728	-1.03821639	-1.42233184
1	-4.17158816	-2.38437850	-1.36029284
1	0.17209188	-3.50021794	1.88057475
1	1.47423887	-2.85441573	0.87304690
1	1.30807018	-4.59875282	1.05683803
1	0.37861467	-5.51064833	-4.12083372
1	-1.28394012	-6.11929379	-4.02645988
1	-0.01908048	-6.80084163	-2.97596065
1	-2.06126156	1.10763941	-0.60266733

Energy = -7584.959540 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 33

Atomic N.	X	Y	Z
8	0.07924844	-0.75544598	0.54665002
8	3.16934507	-0.63053849	0.21429133
6	3.10813646	-1.80891679	-0.57613357
1	3.76741060	-1.74594034	-1.45882771
1	2.08748697	-2.03064551	-0.93268818
1	3.44710252	-2.66672386	0.03413373
8	-0.24811041	-2.74256638	1.42774191
6	0.08838209	-1.44096766	1.56642520
6	0.46205111	-0.90198701	2.92891796
1	-0.34750830	-1.11968957	3.64533968
1	0.51272068	0.18738242	2.81294874
6	1.80556821	-1.45110505	3.45947477
1	2.54993971	-1.41882668	2.64760078
1	2.16275526	-0.75691046	4.23467458
6	1.70473362	-2.85478202	4.06469252
1	1.04818518	-2.81608643	4.95174509
1	2.69709492	-3.16148200	4.42946651
6	1.16838052	-3.92762673	3.11002697
1	1.84891912	-4.07036863	2.25513411
1	1.12743445	-4.89310566	3.64022882
6	-0.23064536	-3.65141829	2.56888390
1	-0.90564283	-3.26926276	3.35087976
1	-0.67231578	-4.56487004	2.15345846
50	2.14003439	1.15242172	0.15746493
7	0.06367651	3.28885042	-0.37782466
6	1.03869644	4.37910678	-0.29783248
1	0.68276305	5.29849242	-0.80846332
1	1.99574448	4.08214795	-0.74685382
1	1.22712512	4.61683402	0.75777135
7	1.73154727	1.29009746	-1.93020858
6	-0.21605579	2.90068052	-1.76436573
1	-0.66699626	3.74306105	-2.33755940
1	-0.94896502	2.08142184	-1.74565304
6	1.01559124	2.42047614	-2.53526446
1	0.65397523	2.12994427	-3.53647064
1	1.69441001	3.27909594	-2.71778328
6	2.36372349	0.45926200	-2.90696943
6	3.75030223	0.56301316	-3.17264751
6	4.32651703	-0.25148412	-4.15772305
6	3.57735460	-1.17897948	-4.88796441

6	2.20905020	-1.27604348	-4.60940459
6	1.59155222	-0.47977196	-3.63835025
7	-2.01778313	1.45133092	1.04355173
6	-1.14193283	3.70397816	0.36476829
1	-1.52460128	4.66505219	-0.04964961
1	-0.82543931	3.89677383	1.40140434
6	-2.32149554	2.73360988	0.39602831
1	-3.11066957	3.23142726	0.97709333
1	-2.74315125	2.60248425	-0.62039520
6	-3.13686971	0.71292404	1.53207346
6	-3.66481649	-0.39382263	0.82374388
6	-4.72250314	-1.12204966	1.38419790
6	-5.29584908	-0.77651842	2.61326432
6	-4.76668320	0.32624455	3.29341075
6	-3.69788594	1.07193319	2.78143729
6	4.63353901	1.51454443	-2.40199104
1	5.39710283	-0.15557134	-4.35730525
6	4.22836959	-2.07178713	-5.91723387
1	1.60211127	-2.00222702	-5.15686301
6	0.12074136	-0.65600320	-3.35443785
6	-3.11875067	-0.79140669	-0.52773024
1	-5.12175471	-1.97524909	0.82947572
6	-6.46768323	-1.54793639	3.17213515
1	-5.18441291	0.60728598	4.26383188
6	-3.13219213	2.21983372	3.57984679
1	5.56482707	1.70885605	-2.95065798
1	4.90979085	1.08872619	-1.42374864
1	4.13456269	2.47416424	-2.20948890
1	-0.06592861	-0.69915936	-2.27239131
1	-0.25465058	-1.57763390	-3.81813469
1	-0.47986146	0.17935631	-3.74927873
1	3.53803514	-2.30682452	-6.73908454
1	4.54113139	-3.02919369	-5.47060481
1	5.12524587	-1.60288536	-6.34452540
1	-3.77461828	-1.53343972	-1.00048066
1	-2.11144736	-1.22953592	-0.46050464
1	-3.04618265	0.07274232	-1.20493678
1	-3.51291066	3.19409011	3.23267090
1	-2.03783946	2.25503420	3.48330899
1	-3.40166838	2.12694405	4.64014947
1	-6.46939639	-1.53472608	4.27085755
1	-6.45460968	-2.59521620	2.84080981
1	-7.42414732	-1.11314280	2.84052905
1	-1.42844081	0.87025051	0.44589122

Energy = -7584.955972 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 34

Atomic N.	X	Y	Z
8	0.39254491	-0.88409203	0.22966811
8	2.37787268	1.34335615	1.42757531
6	3.42903839	0.38972193	1.40992634
1	4.33448663	0.78279761	0.91638906
1	3.14881876	-0.54632982	0.89358718
1	3.69661523	0.13629819	2.45187433
8	-0.56435147	-2.73637095	0.91929447
6	-0.10140943	-1.49205209	1.17641672

6	-0.18164839	-0.93788251	2.58128625
1	-1.23480881	-0.92116824	2.90780078
1	0.17314683	0.09820118	2.51976042
6	0.67698571	-1.71378598	3.60494925
1	1.66202276	-1.93285938	3.16351265
1	0.86653561	-1.03995134	4.45318118
6	0.02557312	-2.99781214	4.12729934
1	-0.90832840	-2.73268024	4.65223026
1	0.68439742	-3.45738639	4.88027724
6	-0.29863910	-4.02992590	3.04243254
1	0.62269578	-4.40297612	2.56614270
1	-0.78385539	-4.90346157	3.50754953
6	-1.23439241	-3.52217855	1.95128000
1	-2.07398225	-2.94062660	2.36212239
1	-1.65019947	-4.36087192	1.37993119
50	0.88128217	1.74827039	0.08345367
7	-1.09380460	2.18174275	-2.35765168
6	-0.89029643	3.59752693	-2.66779203
1	-1.08681546	3.83560407	-3.73493442
1	0.13892839	3.89591587	-2.43116830
1	-1.56429815	4.20328836	-2.04752941
7	1.88635026	1.43948303	-1.75996849
6	-0.22962867	1.30464075	-3.16362289
1	-0.51477952	1.36790187	-4.23931409
1	-0.39742641	0.26891920	-2.83336663
6	1.26830162	1.59693085	-3.08082139
1	1.74077229	0.89561227	-3.79057121
1	1.47341809	2.60312614	-3.50094042
6	3.29102777	1.18933340	-1.84364956
6	4.22755950	2.21199710	-1.55553476
6	5.59885159	1.94407251	-1.66657733
6	6.08249498	0.68803261	-2.04552178
6	5.14622539	-0.31509298	-2.32014694
6	3.76732507	-0.09166350	-2.22784690
7	-2.64210222	0.48215995	-0.47075032
6	-2.51304144	1.83543642	-2.53015710
1	-2.78818713	1.81408728	-3.60910436
1	-3.10518055	2.63710179	-2.06187949
6	-2.93162390	0.50331474	-1.90505368
1	-4.01467609	0.39508245	-2.07903444
1	-2.44111388	-0.33354799	-2.42906298
6	-3.51934298	-0.04552830	0.48319283
6	-4.08959541	-1.33708061	0.33604629
6	-4.94453557	-1.82194708	1.33558945
6	-5.23631127	-1.10037185	2.49766579
6	-4.62364049	0.15055713	2.64720860
6	-3.78529765	0.69298400	1.66927151
6	3.78313303	3.58176021	-1.10274047
1	6.30961740	2.74494394	-1.44616143
6	7.56533564	0.41173338	-2.11891951
1	5.49789248	-1.31041198	-2.60550216
6	2.81350285	-1.22707203	-2.50785840
6	-3.72420380	-2.24067543	-0.81885226
1	-5.37702461	-2.81792560	1.20538968
6	-6.18606939	-1.63786689	3.54133423
1	-4.81856515	0.73760700	3.54864643
6	-3.17896121	2.05994225	1.87120227
1	4.58640948	4.31674385	-1.24665883

1	3.52679359	3.57623021	-0.03102022
1	2.89188768	3.92344225	-1.64652650
1	1.95180464	-1.19996727	-1.82753745
1	3.32406651	-2.19335580	-2.40025564
1	2.41486231	-1.18482811	-3.53488370
1	7.80192947	-0.30400690	-2.91844585
1	7.93561510	-0.02014686	-1.17537632
1	8.13545855	1.33265002	-2.30226323
1	-4.04008098	-3.27067998	-0.60644623
1	-2.63692686	-2.24256145	-0.98638110
1	-4.19708144	-1.94535977	-1.76722769
1	-3.45478804	2.75159136	1.05831023
1	-2.07643677	2.03625116	1.90007974
1	-3.52281357	2.49964006	2.81576425
1	-5.85407124	-1.38543739	4.55850223
1	-6.27793561	-2.73062827	3.47353672
1	-7.19715509	-1.21744820	3.41904814
1	-2.14615298	1.31998340	-0.17367168

Energy = -7584.957687 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 35

Atomic N.	X	Y	Z
8	-0.86778601	0.62859188	3.16562604
8	0.88497069	0.23533511	0.15268938
6	2.04958221	-0.01972122	0.93279060
1	2.97150465	0.25431089	0.38635523
1	2.10344982	-1.09416196	1.18011997
1	2.06005926	0.53572648	1.88991590
8	-0.40071932	-1.49468980	2.76486721
6	-1.04066622	-0.54367893	3.47920009
6	-1.90823047	-0.94601083	4.65563992
1	-2.71621301	-1.60675827	4.30140991
1	-2.37623114	-0.01892445	5.00522343
6	-1.13353378	-1.62512160	5.80516208
1	-0.19751507	-1.07416498	5.99151401
1	-1.73604095	-1.52541842	6.72039308
6	-0.83895715	-3.11068736	5.57149804
1	-1.79803496	-3.65116550	5.49007536
1	-0.32759945	-3.52175667	6.45576067
6	-0.00276909	-3.40534807	4.32172064
1	1.00706552	-2.97335606	4.41374911
1	0.13287381	-4.49513434	4.22808393
6	-0.62086147	-2.91111176	3.01796798
1	-1.69884748	-3.12761485	2.96215437
1	-0.13661623	-3.38729842	2.15694049
50	-0.24029499	1.91614569	0.70377189
7	-0.51794635	2.87395888	-1.66924858
6	0.19825962	4.15024107	-1.82364463
1	-0.09045325	4.67321460	-2.75436232
1	1.27881471	3.96820901	-1.82518408
1	-0.04135371	4.79500680	-0.96776712
7	2.09705115	1.37988888	-2.28845414
6	-0.28214944	1.94118975	-2.80294068
1	-0.90770147	2.25602616	-3.66261197
1	-0.63589932	0.95176091	-2.47969294
6	1.15176502	1.82551355	-3.31502295

1	1.10299777	1.12088566	-4.17106341
1	1.48248758	2.78781854	-3.73921232
6	3.34166319	0.88279602	-2.77397304
6	4.35659117	1.78794619	-3.15966126
6	5.58394331	1.29040126	-3.61712450
6	5.84720659	-0.08080183	-3.69361355
6	4.83436272	-0.96294028	-3.29751038
6	3.58663568	-0.51053070	-2.85317677
7	-2.09915928	1.14031187	-0.07130911
6	-1.97322254	3.12288366	-1.52155908
1	-2.38247665	3.56529652	-2.45126217
1	-2.08928490	3.86258198	-0.71305600
6	-2.74765201	1.85763257	-1.15889675
1	-3.77653742	2.18230968	-0.90059464
1	-2.86541356	1.22098333	-2.06327644
6	-2.89719972	0.10745126	0.49348813
6	-2.75497430	-1.23448791	0.05826514
6	-3.58251802	-2.22958968	0.59780983
6	-4.55526184	-1.94571657	1.56383653
6	-4.67996656	-0.61915000	1.99349104
6	-3.87019266	0.40474676	1.48278004
6	4.15062272	3.27646892	-3.03700086
1	6.36470497	2.00139139	-3.90007392
6	7.17046641	-0.59576465	-4.20789588
1	5.01342802	-2.04027321	-3.34875374
6	2.51437875	-1.50934464	-2.48586173
6	-1.72953477	-1.59596782	-0.98668786
1	-3.47124218	-3.25670766	0.23815462
6	-5.42651236	-3.03777742	2.13977889
1	-5.43340647	-0.36930520	2.74604960
6	-4.02854311	1.81070006	2.00692947
1	5.11294980	3.80482375	-3.04161224
1	3.61769309	3.51268202	-2.10479149
1	3.55068773	3.68367499	-3.86707144
1	2.21666786	-1.44083333	-1.42934060
1	2.86440504	-2.53237077	-2.67460734
1	1.59841050	-1.35156558	-3.07586458
1	7.10301525	-0.87582188	-5.27136355
1	7.49529876	-1.49013070	-3.65792280
1	7.95716149	0.16559859	-4.11885388
1	-1.68671933	-2.68480991	-1.12701406
1	-0.73374725	-1.22423582	-0.70364789
1	-1.97868584	-1.14671317	-1.96125152
1	-4.28848793	2.52314034	1.21006932
1	-3.09236629	2.16952778	2.45883260
1	-4.81900803	1.85364345	2.76813844
1	-4.96844486	-3.49204965	3.03414593
1	-5.58777911	-3.84627138	1.41352429
1	-6.40853545	-2.64922165	2.44266090
1	1.64211787	0.73369466	-1.62674991

Energy = -7584.966794 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 36

Atomic N.	X	Y	Z
8	2.52902892	-0.66634729	2.73278730
8	1.85258745	1.85435421	-0.89187710

6	2.64056942	1.62066541	-2.04458623
1	2.26772834	2.18019684	-2.92419649
1	2.68000273	0.55043435	-2.34357067
1	3.68034690	1.95098125	-1.86397797
8	3.59289586	-2.03789442	1.36544306
6	3.55879917	-0.91005964	2.12248389
6	4.77339534	-0.00334463	2.15936300
1	5.66803705	-0.57976615	2.44802822
1	4.57424362	0.72068778	2.95794569
6	5.02610305	0.72784947	0.82186091
1	4.06859472	1.10492918	0.42667051
1	5.64625116	1.61158447	1.03419870
6	5.74104759	-0.13262619	-0.22517396
1	6.74568888	-0.39351691	0.15251792
1	5.90003092	0.46667557	-1.13447800
6	5.00872890	-1.42558241	-0.60110114
1	4.04027826	-1.20599407	-1.07811293
1	5.60709601	-1.97227105	-1.34799618
6	4.76213071	-2.37792098	0.56388543
1	5.64493666	-2.46182598	1.21832568
1	4.51659079	-3.38104529	0.19503134
50	0.21634396	0.53810826	-0.59314643
7	-0.25104755	1.85342174	1.45983092
6	0.76527353	2.93284854	1.56006055
1	0.49053533	3.63408141	2.36778660
1	0.85322866	3.46329538	0.60865308
1	1.74099514	2.48568135	1.77745388
7	-1.36019100	1.89601632	-1.17424625
6	-1.59142100	2.44174504	1.16888887
1	-1.80614577	3.23961968	1.90499207
1	-2.33573956	1.64426152	1.28399854
6	-1.67932821	2.97707416	-0.25657418
1	-2.71799497	3.32660327	-0.41193572
1	-1.04110243	3.87858467	-0.35117736
6	-1.64430948	2.07093729	-2.55494264
6	-1.12935760	3.14966072	-3.32343701
6	-1.46198030	3.25259419	-4.68222826
6	-2.26847726	2.31378972	-5.33002782
6	-2.74597661	1.23835181	-4.57083041
6	-2.45867163	1.10464399	-3.20894643
7	-0.81423908	-1.17858329	2.06021482
6	-0.24682455	1.13721361	2.77457970
1	-0.50525070	1.87168018	3.56131895
1	0.78775140	0.81465741	2.95481794
6	-1.17546097	-0.06270792	2.94319756
1	-1.10953052	-0.34558638	4.01360274
1	-2.22177087	0.21686754	2.76882089
6	-1.56440073	-2.38334483	2.19370344
6	-2.92876537	-2.42996880	1.82364861
6	-3.63005299	-3.63669086	1.94828488
6	-3.02538572	-4.81063538	2.40551933
6	-1.66477705	-4.75315797	2.72943994
6	-0.92654874	-3.56885131	2.63850042
6	-0.17504347	4.16038990	-2.73378354
1	-1.05024214	4.08737828	-5.25668810
6	-2.62157569	2.45404451	-6.79152203
1	-3.37762116	0.48466305	-5.04909524
6	-3.04207552	-0.05375034	-2.43893228

6	-3.63394457	-1.23209954	1.23884101
1	-4.68158859	-3.65840956	1.65029744
6	-3.81088861	-6.09125408	2.55443365
1	-1.15734871	-5.65854120	3.07239961
6	0.53939053	-3.57474389	3.00036014
1	0.41360212	4.63620436	-3.52979183
1	0.51518927	3.68168616	-2.02285807
1	-0.70049585	4.96612982	-2.19567108
1	-2.26788576	-0.75344720	-2.08623924
1	-3.74329808	-0.61999633	-3.06642398
1	-3.57183249	0.29898986	-1.54306920
1	-3.67252557	2.75732253	-6.92238834
1	-2.49178853	1.50435822	-7.33084857
1	-1.99556072	3.21203887	-7.28124766
1	-4.46676742	-1.55255774	0.59932333
1	-2.94553621	-0.62899263	0.63084273
1	-4.06053688	-0.57459151	2.01444557
1	0.78392821	-2.82181501	3.76478569
1	1.18330798	-3.35935139	2.13331474
1	0.83009271	-4.55794484	3.39162819
1	-3.20131718	-6.96910003	2.29838182
1	-4.69994704	-6.09175316	1.90937318
1	-4.15777174	-6.22856479	3.59115617
1	0.18559131	-1.36866687	2.16568371

Energy = -7584.966859 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 37

Atomic N.	X	Y	Z
8	1.68407779	-2.14699287	-0.59373874
8	1.93104910	0.93420321	1.07971789
6	3.07093859	1.35095708	0.34230712
1	3.12837778	2.45426709	0.26307141
1	3.10067751	0.94678952	-0.68810232
1	3.98948572	1.01326920	0.85626947
8	3.81687425	-2.54867670	-0.99538764
6	2.73079112	-2.62003839	-0.17562241
6	2.87191247	-3.25415607	1.19203158
1	3.27244366	-4.27690885	1.09028079
1	1.85436720	-3.33174173	1.59128991
6	3.75647509	-2.43857138	2.15969660
1	3.48225690	-1.37421947	2.08597549
1	3.50094736	-2.75113402	3.18286797
6	5.26166629	-2.63142572	1.94942831
1	5.51676399	-3.68579958	2.15632936
1	5.81011355	-2.03164932	2.69249278
6	5.76524218	-2.27618698	0.54616662
1	5.62754506	-1.20279609	0.33773112
1	6.84975441	-2.46675889	0.49358178
6	5.10967406	-3.07003837	-0.57997942
1	5.01354292	-4.13679101	-0.32000130
1	5.70658523	-2.99825550	-1.49753344
50	0.22588837	0.30389548	0.05763322
7	-0.93370066	2.29278616	1.04882515
6	-0.16556590	3.53854921	0.86122743
1	-0.62083367	4.38307458	1.40947726
1	-0.10774705	3.78074807	-0.20662072

1	0.84952720	3.36765579	1.23995582
7	-1.81148993	2.61121519	-1.87267741
6	-2.34055864	2.39465442	0.56936776
1	-2.94849568	2.90493899	1.34112422
1	-2.72989237	1.36871608	0.47849750
6	-2.57159946	3.15170961	-0.73866175
1	-3.66255130	3.11102131	-0.92356054
1	-2.32546914	4.21357629	-0.59204723
6	-2.28312257	2.85971637	-3.18784083
6	-2.36523533	4.17770455	-3.69417473
6	-2.82218687	4.37818857	-5.00366549
6	-3.17590410	3.31886276	-5.84405720
6	-3.04385828	2.01965054	-5.33877236
6	-2.61169579	1.76951388	-4.03288695
7	-0.69826492	-0.46141600	1.84409072
6	-0.90511014	1.89892764	2.48559103
1	-1.49710430	2.61969832	3.08257996
1	0.14751895	1.95204279	2.79772942
6	-1.40833123	0.47815154	2.70394017
1	-1.26206114	0.25200927	3.77368429
1	-2.50777259	0.43311215	2.54535557
6	-0.60154846	-1.79569504	2.30573142
6	-1.19038445	-2.86119595	1.57192377
6	-1.08388525	-4.17521050	2.04318673
6	-0.41416230	-4.49063141	3.23132788
6	0.17583934	-3.43841966	3.93929724
6	0.10922454	-2.10932928	3.49890163
6	-1.90056040	5.36553942	-2.88729624
1	-2.87454535	5.40183737	-5.38366042
6	-3.68944880	3.56434829	-7.24242360
1	-3.29254081	1.16873021	-5.97804630
6	-2.49140486	0.34587325	-3.54295769
6	-1.93618454	-2.59747080	0.28783149
1	-1.55443936	-4.97706279	1.46765514
6	-0.29836775	-5.91968860	3.70658109
1	0.72864513	-3.65769553	4.85752781
6	0.85811153	-1.04584471	4.26507216
1	-1.68296751	6.21409040	-3.54886638
1	-0.98662970	5.12238200	-2.32526985
1	-2.65360830	5.70587055	-2.15891770
1	-1.45418754	0.07881324	-3.28236141
1	-2.82553001	-0.35591373	-4.31715878
1	-3.10189184	0.16450434	-2.64354678
1	-4.79075065	3.54895312	-7.27189197
1	-3.33620420	2.79369973	-7.94169885
1	-3.36591185	4.54357246	-7.62063290
1	-2.57251859	-3.45338755	0.02551348
1	-1.24385039	-2.43047993	-0.55274459
1	-2.56169813	-1.69752245	0.36847701
1	0.22232048	-0.52443714	4.99933809
1	1.26045800	-0.28699840	3.57770754
1	1.68876127	-1.49265504	4.82826944
1	0.52272895	-6.44769965	3.19509055
1	-1.21886953	-6.48550121	3.50468837
1	-0.09743637	-5.96808046	4.78538360
1	-1.62250801	1.61665673	-1.73501821

Energy = -7584.965741 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 38

Atomic N.	X	Y	Z
8	3.97227837	0.37418039	1.43140515
8	-0.91917864	0.94405682	-3.82237405
6	-0.25380375	0.15897611	-4.79725050
1	-0.43457461	-0.92910619	-4.68542242
1	0.84220837	0.31485453	-4.75687614
1	-0.59323167	0.44693883	-5.80744582
8	5.15626481	-1.21503872	2.41202616
6	5.08012757	-0.03539851	1.73562334
6	6.35951031	0.69560568	1.37344124
1	6.95828333	0.88166920	2.28033466
1	6.03905608	1.66849205	0.98355570
6	7.21825454	-0.04506028	0.32504963
1	6.56444944	-0.42547632	-0.47604914
1	7.88514042	0.69223637	-0.14582111
6	8.06967092	-1.18039953	0.90255674
1	8.79561218	-0.75079296	1.61460118
1	8.66415285	-1.63186939	0.09357089
6	7.27387311	-2.27887372	1.61581688
1	6.60818775	-2.80466988	0.91238893
1	7.97532617	-3.03561806	2.00262968
6	6.43740087	-1.79256143	2.79486526
1	6.99318700	-1.07537323	3.42032727
1	6.14173020	-2.63649784	3.42948017
50	-1.79243149	0.05850741	-2.16222557
7	-0.11719876	1.24696122	-0.75007099
6	0.98469025	1.74355778	-1.60635853
1	1.71278913	2.31061286	-1.00050571
1	0.57276634	2.37364483	-2.40139031
1	1.49371086	0.90322385	-2.09006441
7	-2.79129156	1.84668476	-1.57819034
6	-0.89311387	2.40109329	-0.19852901
1	-0.19044679	3.18856636	0.13085476
1	-1.44640744	2.03307314	0.67622475
6	-1.89958725	2.93895532	-1.21317974
1	-2.46554085	3.75252840	-0.72569602
1	-1.36082916	3.40140178	-2.06424699
6	-4.11550858	2.13842779	-1.99281527
6	-4.40748578	3.04730277	-3.04527812
6	-5.74253712	3.30361071	-3.38447921
6	-6.81289709	2.67432728	-2.74077591
6	-6.51075312	1.75200798	-1.73294521
6	-5.19402056	1.47779703	-1.34534765
7	1.57616989	-1.67599235	1.08134916
6	0.40826261	0.42148184	0.37416050
1	-0.45851269	0.09896669	0.96976496
1	1.04792100	1.05388763	1.01802162
6	1.20078768	-0.82520972	-0.05349205
1	0.61176772	-1.39838036	-0.78436769
1	2.13864890	-0.53527472	-0.54501471
6	0.57419941	-2.24290493	1.90834333
6	-0.34713673	-3.18468713	1.38689592
6	-1.30424282	-3.74806348	2.24074769
6	-1.36840501	-3.44290354	3.60368280
6	-0.41529271	-2.55223297	4.11125405

6	0.54560656	-1.94593562	3.29550953
6	-3.30728947	3.68375972	-3.85999469
1	-5.94727903	4.00046328	-4.20229202
6	-8.24259123	2.99113812	-3.10955351
1	-7.32622617	1.23707787	-1.21779731
6	-4.93911295	0.48809163	-0.23538199
6	-0.27785559	-3.65133536	-0.04602302
1	-2.00626883	-4.47453383	1.82297318
6	-2.43128283	-4.04320099	4.49217736
1	-0.42295442	-2.31010514	5.17731395
6	1.54679682	-0.99276089	3.90385937
1	-3.70665893	4.05217313	-4.81433009
1	-2.50410886	2.96051773	-4.06833268
1	-2.84830805	4.54366706	-3.34609724
1	-4.52328539	-0.46024827	-0.61393536
1	-5.87230888	0.25003549	0.29224997
1	-4.20705250	0.87832040	0.48547856
1	-8.62923714	3.83893707	-2.52112665
1	-8.90508649	2.13507603	-2.92106458
1	-8.33100562	3.26566992	-4.17007232
1	-0.73513815	-4.64479936	-0.14430517
1	0.76541385	-3.70972495	-0.38885050
1	-0.81541986	-2.98091443	-0.73750773
1	1.52787280	-0.00441732	3.41867938
1	2.58100901	-1.36324466	3.81563676
1	1.33719236	-0.84903467	4.97145101
1	-2.06572813	-4.18240103	5.51908732
1	-2.76612603	-5.01836846	4.11258392
1	-3.31924639	-3.39316191	4.54802466
1	2.30367951	-1.20198602	1.61888004

Energy = -7584.970487 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 39

Atomic N.	X	Y	Z
8	2.18740873	0.84054135	1.53610401
8	1.23609394	1.23198444	-1.59265822
6	1.70221427	0.59202175	-2.76533589
1	1.80442342	-0.50896070	-2.66135595
1	2.69547653	0.99012520	-3.04466276
1	1.02868712	0.77713254	-3.62380654
8	3.95536446	-0.13275741	0.63570008
6	3.33329370	0.96913606	1.11608181
6	4.04514122	2.30358402	1.07986556
1	5.02665060	2.23095829	1.57669658
1	3.42375538	2.98937724	1.66623689
6	4.21700695	2.83057949	-0.36381673
1	3.28624411	2.64394114	-0.92413434
1	4.34238461	3.92202823	-0.31051938
6	5.42666657	2.23051565	-1.08878555
1	6.34599234	2.52302786	-0.55104145
1	5.50265620	2.67675135	-2.09222471
6	5.40386662	0.70316421	-1.22436605
1	4.57247958	0.37848579	-1.86913224
1	6.33115068	0.37306061	-1.72088838
6	5.30852841	-0.05678288	0.09341322
1	5.98544483	0.35816096	0.85723822

1	5.56775153	-1.11229899	-0.05234268
50	0.13213130	0.11638029	-0.22287699
7	-1.32345052	-0.27083170	2.41190479
6	-0.53718656	0.44070971	3.42468353
1	-1.15546398	0.74022667	4.29762369
1	-0.07186136	1.33250398	2.99208323
1	0.27012118	-0.21434034	3.77689770
7	-1.02973212	1.81853687	0.23728678
6	-2.43346660	0.54252905	1.89576190
1	-3.18554962	0.73959873	2.69325999
1	-2.93020017	-0.03728438	1.10304987
6	-2.01556211	1.89345315	1.31706780
1	-2.94350510	2.36082544	0.93655993
1	-1.67274279	2.55331104	2.13806971
6	-0.90682801	3.04877536	-0.48465948
6	-0.22649724	4.16049612	0.06382255
6	-0.15449427	5.35569204	-0.66709447
6	-0.73764731	5.49153062	-1.92861479
6	-1.40510111	4.38095015	-2.46043563
6	-1.49696907	3.16962431	-1.76805001
7	-1.90359267	-2.81620507	0.85454457
6	-1.79931650	-1.53852620	2.99501880
1	-2.42112179	-1.33349438	3.89600580
1	-0.90881471	-2.08957467	3.33739979
6	-2.62284078	-2.44305711	2.07901308
1	-2.86818347	-3.34246956	2.66987570
1	-3.58450472	-1.95885720	1.84240703
6	-1.97089362	-4.14031163	0.37259959
6	-3.21838887	-4.72917355	0.05399149
6	-3.25030061	-6.04366218	-0.42906735
6	-2.08885933	-6.79296105	-0.64023130
6	-0.86243542	-6.17538574	-0.36545667
6	-0.77953644	-4.87373817	0.13825351
6	0.44162054	4.08514131	1.41435143
1	0.38294105	6.20365317	-0.23328932
6	-0.66269383	6.79122393	-2.69408570
1	-1.86856834	4.45814599	-3.44766321
6	-2.21446661	2.00652469	-2.40691542
6	-4.50113272	-3.93747794	0.13744794
1	-4.22079926	-6.48214204	-0.67631142
6	-2.15342456	-8.21772210	-1.13607149
1	0.06514778	-6.72769284	-0.53770370
6	0.57119346	-4.26410077	0.42604433
1	1.26638662	4.80881541	1.47704709
1	0.83545302	3.07750334	1.60431477
1	-0.25824111	4.32649121	2.23098355
1	-1.49880204	1.24878217	-2.76343754
1	-2.80036246	2.34178066	-3.27303080
1	-2.88554801	1.49974683	-1.70028776
1	-1.65463300	7.26123741	-2.78219779
1	-0.29016805	6.63431604	-3.71717483
1	0.00300226	7.50875350	-2.19622590
1	-5.29012606	-4.42702250	-0.44804850
1	-4.35376368	-2.92109255	-0.25793236
1	-4.87468629	-3.83145502	1.16768024
1	0.65960927	-3.93235605	1.47337023
1	0.77333188	-3.38107005	-0.20221263
1	1.36965550	-4.99299057	0.23819448

1	-1.31181997	-8.45036601	-1.80353429
1	-3.08639871	-8.40786896	-1.68415229
1	-2.11292678	-8.93513706	-0.30057629
1	-0.95566736	-2.44266798	0.85445755

Energy = -7584.956717 Hartree
Number of imaginary frequencies = 0.

Compound I2b isomer 40

Atomic N.	X	Y	Z
8	1.95497478	-1.12696785	-1.64013501
8	1.77653411	0.27431794	1.56347705
6	2.85687637	1.16249838	1.31626449
1	2.77059894	2.09121074	1.91387790
1	2.94504686	1.46322690	0.25438749
1	3.80818840	0.67796449	1.60274685
8	4.12349643	-0.99374012	-2.02802881
6	3.04943637	-1.65692745	-1.51493714
6	3.25884006	-2.98298105	-0.81506923
1	3.78029474	-3.68281448	-1.48966618
1	2.25595533	-3.38326511	-0.62874420
6	4.03320283	-2.86195395	0.51510622
1	3.63337315	-2.00980949	1.08725791
1	3.81106983	-3.76114511	1.10834783
6	5.55180811	-2.74505535	0.35066955
1	5.93103538	-3.67281531	-0.11302118
1	6.01966351	-2.68593431	1.34581437
6	6.01637978	-1.55416177	-0.49475618
1	5.75063875	-0.60002757	-0.01143591
1	7.11625706	-1.57065084	-0.56721786
6	5.46780370	-1.53824708	-1.91846937
1	5.50041119	-2.54065981	-2.37552374
1	6.05643214	-0.86007524	-2.54853433
50	0.16732322	0.22625838	0.23809148
7	-1.23880610	1.06410309	2.13689685
6	-0.63349253	2.23283784	2.80391323
1	-1.19257320	2.51587343	3.71407592
1	-0.60478239	3.08133640	2.11001247
1	0.39447634	1.96729328	3.07925270
7	-2.14177834	3.01206594	-0.05413938
6	-2.64604195	1.29907480	1.70765228
1	-3.31532809	1.17083608	2.57994268
1	-2.90335069	0.50986631	0.98429888
6	-2.96660362	2.66992842	1.11132847
1	-4.04338459	2.64399505	0.85454340
1	-2.85615810	3.43914128	1.88962631
6	-2.63722871	3.96638272	-0.98034259
6	-2.87779535	5.30365913	-0.58788458
6	-3.35322714	6.21820000	-1.53723716
6	-3.57412942	5.86588599	-2.87165852
6	-3.28599739	4.54883565	-3.24983960
6	-2.82914257	3.59512851	-2.33526133
7	-0.64703310	-1.56164000	1.11776776
6	-1.16438057	-0.12048884	3.03771083
1	-1.84836158	0.02008038	3.89730330
1	-0.12918599	-0.16257805	3.40481553
6	-1.47739559	-1.42040537	2.30822001
1	-1.30724262	-2.23719018	3.02974459

1	-2.56073560	-1.47014768	2.06366569
6	-0.35949142	-2.88173485	0.69775921
6	-0.78435675	-3.34575175	-0.57645685
6	-0.48753365	-4.65458573	-0.97692486
6	0.21477471	-5.54539364	-0.15718682
6	0.65213240	-5.07249389	1.08493025
6	0.39324848	-3.76666012	1.52216480
6	-2.56191651	5.78784638	0.80625208
1	-3.52863940	7.24986802	-1.22116402
6	-4.11134865	6.86465778	-3.86827502
1	-3.42812413	4.24748152	-4.29077805
6	-2.53744643	2.18855459	-2.80188636
6	-1.55045599	-2.44514003	-1.51275505
1	-0.83000122	-4.99093182	-1.95928774
6	0.47685603	-6.96798903	-0.59094357
1	1.23781165	-5.73365653	1.73056549
6	0.99035798	-3.29943598	2.82755016
1	-2.44683897	6.87952701	0.81368595
1	-1.62658934	5.33933601	1.17267963
1	-3.35214225	5.53935788	1.53237906
1	-1.47583426	1.91838101	-2.67928653
1	-2.78259183	2.07848328	-3.86552404
1	-3.12269923	1.43815701	-2.24608938
1	-5.20304907	6.76803755	-3.98160292
1	-3.66838301	6.71809949	-4.86323547
1	-3.90569940	7.89595157	-3.55083444
1	-2.06175987	-3.03367815	-2.28642886
1	-0.88207323	-1.73485336	-2.02520074
1	-2.29383123	-1.84631661	-0.96836468
1	1.28059786	-2.24030690	2.76156276
1	1.87719263	-3.89707288	3.07876374
1	0.29104616	-3.39969675	3.67381477
1	0.61371522	-7.03852418	-1.67908082
1	-0.36475893	-7.62834396	-0.32689553
1	1.37384505	-7.37645759	-0.10480480
1	-1.83197558	2.16496552	-0.53401108

Energy = -7584.965787 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 41

Atomic N.	X	Y	Z
8	2.78106360	-3.24845380	1.21030305
8	1.96741345	0.20690791	-1.61196019
6	2.35420418	-0.17104037	-2.92008891
1	1.55507577	-0.02120556	-3.66832080
1	2.65448967	-1.23696142	-2.95232037
1	3.22619801	0.42561550	-3.24448210
8	4.74990398	-3.06648269	0.21641730
6	3.82674404	-2.63039385	1.12488528
6	4.13723118	-1.39921805	1.95761437
1	5.07375858	-1.55328867	2.52020865
1	3.32169433	-1.33180662	2.68701672
6	4.22441287	-0.09421327	1.13581463
1	3.40268052	-0.06088051	0.40224895
1	4.06089076	0.74752686	1.82554544
6	5.56589550	0.10805016	0.42526285
1	6.36759380	0.18788617	1.18113847

1	5.54546791	1.07106282	-0.10754270
6	5.93370487	-1.00371348	-0.56288177
1	5.21004334	-1.04353678	-1.39260422
1	6.91426804	-0.77702508	-1.01310893
6	6.03000560	-2.39415219	0.05798281
1	6.55725565	-2.36857958	1.02588554
1	6.57967730	-3.07261849	-0.60641309
50	0.11442488	0.78302774	-0.89292526
7	-0.74035712	-1.53334665	-1.17637217
6	0.27027726	-2.55109516	-0.81198154
1	-0.08621496	-3.56809699	-1.05266588
1	0.50732989	-2.48926256	0.25391091
1	1.19167149	-2.34830214	-1.36736487
7	-1.34467996	-0.96477069	1.78223792
6	-2.03683200	-1.76718371	-0.47798429
1	-2.53850745	-2.63444629	-0.94844657
1	-2.67393019	-0.88957938	-0.66428206
6	-1.97610793	-2.05033158	1.02284761
1	-3.02307674	-2.22569862	1.34233336
1	-1.43707411	-2.98929150	1.20313187
6	-1.50827063	-0.94264829	3.19540612
6	-0.97513509	-1.96721419	4.01201314
6	-1.14457637	-1.88174545	5.40079794
6	-1.79605520	-0.80886596	6.01622712
6	-2.27731477	0.21505040	5.19203113
6	-2.15163901	0.16630450	3.80041701
7	-1.06544248	0.89167997	-2.69253316
6	-0.96053317	-1.54704233	-2.65376076
1	-1.49058210	-2.47418256	-2.94219956
1	0.03388121	-1.56410190	-3.11822029
6	-1.72494861	-0.32407089	-3.15225979
1	-1.73058850	-0.38132190	-4.25894466
1	-2.78847245	-0.39854126	-2.84715397
6	-1.63469465	2.13402244	-3.09386231
6	-2.93583647	2.54846078	-2.69839838
6	-3.43535660	3.78532590	-3.12976886
6	-2.68945746	4.65308526	-3.93100249
6	-1.39505937	4.25456246	-4.28351328
6	-0.86020670	3.02413229	-3.88650217
6	-0.17478740	-3.11119584	3.44035256
1	-0.72406077	-2.67706541	6.02167864
6	-1.98367681	-0.75989047	7.51347838
1	-2.77378879	1.07810723	5.64278930
6	-2.69104578	1.30188402	2.96126882
6	-3.78183573	1.72438244	-1.76033665
1	-4.43569046	4.08620235	-2.80623059
6	-3.25933410	5.96715856	-4.40773138
1	-0.78055786	4.91839844	-4.89749684
6	0.53610564	2.65531435	-4.32204235
1	0.43556218	-3.57634529	4.22514001
1	0.50224921	-2.77602906	2.64179412
1	-0.81366933	-3.90473119	3.02068076
1	-1.89632200	1.82169730	2.40076692
1	-3.18055232	2.04943578	3.59769615
1	-3.43597453	0.95713948	2.22558213
1	-2.96937238	-1.15638682	7.80525673
1	-1.92305998	0.26958196	7.89293258
1	-1.22389680	-1.36100220	8.03117559

1	-4.52551995	2.35584750	-1.25696964
1	-3.15511833	1.25011171	-0.98971476
1	-4.33120043	0.92136511	-2.27719997
1	0.54906410	1.68184540	-4.83116761
1	1.22826555	2.57012613	-3.47069716
1	0.93770455	3.41388231	-5.00681688
1	-2.49677812	6.75862338	-4.41084884
1	-4.09250006	6.29586777	-3.77192443
1	-3.64395984	5.88398960	-5.43677536
1	-1.63255700	-0.06630527	1.39354697

Energy = -7584.963379 Hartree
Number of imaginary frequencies = 0.

Compound I2b isomer 42

Atomic N.	X	Y	Z
8	2.77847423	-1.65952726	0.55308114
8	0.57814799	-3.85393423	-0.99487844
6	1.72454866	-4.35215820	-1.66558177
1	1.45790839	-5.25630444	-2.24253513
1	2.51379435	-4.63006468	-0.94386069
1	2.17133487	-3.62707639	-2.37538927
8	4.09028909	-1.20470934	2.26627366
6	3.12975362	-0.83005178	1.37991981
6	2.58189839	0.58171473	1.43257306
1	2.12547652	0.76654231	2.41880890
1	1.77330389	0.61198730	0.69253367
6	3.62907703	1.67060149	1.11455668
1	4.23631726	1.35486583	0.25080570
1	3.08590383	2.57239515	0.79489438
6	4.53370906	2.03703966	2.29563883
1	3.90579881	2.44752954	3.10521744
1	5.21564038	2.84685962	1.99264015
6	5.35273960	0.86935862	2.85508044
1	6.07564108	0.50254766	2.10822660
1	5.94579386	1.22359286	3.71408451
6	4.51602590	-0.31269558	3.33455912
1	3.63548564	0.01540028	3.90910104
1	5.11503975	-0.97050150	3.97618398
50	0.22554164	-1.81899840	-0.93107726
7	-2.16755569	-2.32283633	-1.67658948
6	-2.27786000	-3.79388465	-1.79881407
1	-3.33311290	-4.08793201	-1.94766017
1	-1.86673784	-4.28337783	-0.91174646
1	-1.68106644	-4.13050102	-2.65461769
7	-0.93941953	-1.83710549	0.87426498
6	-2.96558648	-1.81976590	-0.53252464
1	-4.01103504	-2.18201071	-0.60071671
1	-2.96046851	-0.72400034	-0.58933658
6	-2.34331611	-2.22456054	0.80283887
1	-2.93042448	-1.72510684	1.59375669
1	-2.48776547	-3.31323389	0.97420555
6	-0.47288078	-1.44687595	2.15605523
6	0.36365898	-2.30000769	2.92281514
6	0.81158578	-1.87714637	4.18400112
6	0.45484767	-0.63937635	4.72884490
6	-0.36431370	0.19859667	3.96095004
6	-0.83114732	-0.17936345	2.69616473

7	-1.73129108	0.59633406	-2.61049723
6	-2.57551242	-1.73357949	-2.98442451
1	-3.49836830	-2.23853695	-3.32998059
1	-1.78226551	-1.99095587	-3.70480457
6	-2.86144394	-0.23356855	-3.04261894
1	-3.14388558	-0.02337224	-4.09289596
1	-3.75116096	-0.00543410	-2.43767851
6	-1.67209146	1.94820711	-3.03605495
6	-2.66277154	2.87871105	-2.64426165
6	-2.55528347	4.20920925	-3.07072296
6	-1.48695732	4.66288052	-3.84970229
6	-0.49434706	3.73570006	-4.19004518
6	-0.56755908	2.39330086	-3.80594517
6	0.77626806	-3.65599975	2.41028262
1	1.44643156	-2.55233856	4.76462087
6	0.90743735	-0.23175444	6.11159506
1	-0.64358737	1.18047346	4.35416837
6	-1.67883496	0.78405928	1.90308950
6	-3.79046368	2.49093449	-1.71939263
1	-3.32506569	4.91844351	-2.75543634
6	-1.41006994	6.09642889	-4.31703432
1	0.36329708	4.06313948	-4.78331567
6	0.52977186	1.43684282	-4.20955039
1	0.98144860	-4.33802366	3.24683062
1	1.68983370	-3.58801486	1.79976403
1	0.01119483	-4.09094606	1.75698524
1	-1.38718117	0.78220632	0.84286863
1	-1.58753787	1.80366993	2.30053065
1	-2.74781439	0.51693645	1.93543303
1	0.13965785	-0.46214971	6.86731273
1	1.10132134	0.84902239	6.17050198
1	1.82288855	-0.76257879	6.40738632
1	-4.20964975	3.38198960	-1.23434096
1	-3.43565702	1.80542218	-0.93579749
1	-4.61733690	1.98859946	-2.24614317
1	0.14208515	0.58698583	-4.79428753
1	1.05555157	1.00997357	-3.33969667
1	1.27823267	1.94953877	-4.82653114
1	-0.37279677	6.45892246	-4.33496204
1	-1.99364505	6.76101425	-3.66561416
1	-1.80929452	6.20549834	-5.33816118
1	-0.84859330	0.11688409	-2.79422146

Energy = -7584.962164 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 43

Atomic N.	X	Y	Z
8	1.98877435	-0.91572738	1.84931550
8	2.36802315	0.97273573	-1.63287830
6	2.63733381	0.82803916	-3.01491708
1	1.78460162	1.11941491	-3.65404105
1	2.90073506	-0.22058980	-3.26122711
1	3.49842035	1.45787850	-3.30465550
8	3.67476673	-2.03211488	0.95899086
6	3.19014068	-0.95185230	1.62938703
6	4.14072449	0.14676262	2.06356928
1	4.93405216	-0.28251090	2.69943320

1	3.53953433	0.81511838	2.69078961
6	4.77180626	0.93857251	0.89679615
1	3.99724723	1.17087339	0.14812573
1	5.12337609	1.89946539	1.30168364
6	5.94965899	0.22680043	0.22531607
1	6.76448219	0.09681490	0.95993794
1	6.35119622	0.87338939	-0.56991833
6	5.60213501	-1.14161304	-0.36981753
1	4.84937363	-1.03869511	-1.16736322
1	6.50248344	-1.57234691	-0.83789190
6	5.09273199	-2.15822479	0.64645729
1	5.67702907	-2.12627472	1.58055552
1	5.15905719	-3.17533151	0.24125420
50	0.58112322	1.49304033	-0.70148456
7	-0.35928598	-0.72058274	-1.27957733
6	0.64234860	-1.80758240	-1.17711775
1	0.23209376	-2.74954678	-1.57970725
1	0.93378750	-1.96049462	-0.13514619
1	1.53449802	-1.51544151	-1.74237627
7	-0.92803196	-2.31679616	1.61591093
6	-1.59222403	-1.04053590	-0.50399545
1	-1.98740942	-2.00824270	-0.86039235
1	-2.32987470	-0.26597239	-0.75727262
6	-1.45814268	-1.07113850	1.02684868
1	-0.84063658	-0.21318168	1.34806919
1	-2.46108250	-0.89154568	1.43766720
6	-1.65919419	-2.92771914	2.66810712
6	-2.95703152	-3.44791712	2.43992636
6	-3.64609950	-4.05955480	3.49540942
6	-3.08910802	-4.20683819	4.76901309
6	-1.78630981	-3.73286787	4.96109613
6	-1.06608404	-3.09570521	3.94552771
7	-0.67844075	1.91196219	-2.39599223
6	-0.70741588	-0.51178362	-2.71797190
1	-1.31511365	-1.36143145	-3.08137129
1	0.24141092	-0.51161067	-3.27061727
6	-1.43338576	0.80630044	-2.97284430
1	-1.52020035	0.91288483	-4.07279040
1	-2.47635918	0.73985562	-2.60186738
6	-1.23957159	3.21499570	-2.54010951
6	-2.46748543	3.59485123	-1.93397561
6	-2.96306608	4.89349106	-2.11906599
6	-2.28085940	5.85273007	-2.87094615
6	-1.05870901	5.47831817	-3.44132074
6	-0.53088791	4.19142269	-3.29085013
6	-3.58200802	-3.44061728	1.06638002
1	-4.64490878	-4.45891024	3.30042507
6	-3.86541224	-4.84268682	5.89699416
1	-1.31326198	-3.85008394	5.93961570
6	0.33348179	-2.60211058	4.22240795
6	-3.23980179	2.65637949	-1.04012353
1	-3.90770751	5.16499321	-1.63974947
6	-2.81780950	7.25495223	-3.02908315
1	-0.49917661	6.20822075	-4.03266811
6	0.78544427	3.85414248	-3.94555520
1	-4.42689613	-4.14037738	1.02859532
1	-2.84546266	-3.74292700	0.30684823
1	-3.96497709	-2.45244068	0.76794421

1	1.08717142	-3.13481750	3.62028991
1	0.58909586	-2.75513439	5.27852574
1	0.44984024	-1.53216334	3.99468684
1	-4.36321407	-4.08112539	6.51858453
1	-3.20891726	-5.42320526	6.56015501
1	-4.64680912	-5.51423145	5.51570496
1	-3.88111783	3.22188172	-0.35155617
1	-2.55730173	2.03574509	-0.44035554
1	-3.89281304	1.97434949	-1.60803105
1	0.70085641	2.95588030	-4.57235047
1	1.57116059	3.64324261	-3.20454793
1	1.12817301	4.68823912	-4.57219077
1	-2.32466948	7.95081383	-2.33174497
1	-3.89652272	7.29581158	-2.82729699
1	-2.64410844	7.63871685	-4.04444073
1	0.04673627	-2.17648462	1.88285127

Energy = -7584.967024 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 44

Atomic N.	X	Y	Z
8	2.22984790	-3.74731560	0.81412415
8	2.27075078	0.37890707	-1.08547876
6	2.90590196	0.28881751	-2.34722746
1	2.29861159	0.70946843	-3.16892005
1	3.13712141	-0.76468451	-2.60044504
1	3.86372378	0.84001328	-2.32922063
8	4.37329467	-3.57434968	0.29203636
6	3.31075551	-3.26041738	1.09219646
6	3.52279068	-2.31556492	2.26176494
1	4.30522905	-2.71486253	2.92936853
1	2.57758591	-2.32812746	2.81685466
6	3.87383326	-0.87079625	1.84304027
1	3.22997067	-0.55938039	1.00460007
1	3.62829719	-0.20858755	2.68695779
6	5.34608784	-0.66778487	1.47339849
1	5.97341218	-0.87200651	2.35951273
1	5.50665767	0.39072743	1.21753028
6	5.83563802	-1.54324864	0.31508592
1	5.30269759	-1.29273815	-0.61602744
1	6.90253863	-1.33500081	0.13082488
6	5.70149409	-3.04380547	0.55688584
1	6.01271915	-3.31748932	1.57851858
1	6.33061463	-3.60256997	-0.14728747
50	0.34589428	0.97060491	-0.60961140
7	-0.57276146	-1.08550257	-1.65780667
6	0.26782278	-2.27409074	-1.39182931
1	-0.09345825	-3.15034558	-1.95831540
1	0.27350556	-2.50600042	-0.32301984
1	1.29819048	-2.05090531	-1.68690848
7	-1.75224608	-1.21505220	1.17531144
6	-2.00142071	-1.32850202	-1.30636144
1	-2.44818680	-1.98163365	-2.08023740
1	-2.52347147	-0.36151936	-1.36385771
6	-2.28189655	-1.98617197	0.04463875
1	-3.38255124	-2.10508291	0.10302501
1	-1.86110615	-2.99979355	0.05934015

6	-2.21196584	-1.52913654	2.48452575
6	-1.94434915	-2.78649939	3.07484377
6	-2.40056819	-3.03271101	4.37712845
6	-3.08637307	-2.07474009	5.12960465
6	-3.30120518	-0.82265809	4.54196442
6	-2.88448242	-0.53484446	3.23876215
7	-0.40783870	1.65952034	-2.50677093
6	-0.47090611	-0.70775311	-3.09942565
1	-0.98523056	-1.46571087	-3.71964118
1	0.59686895	-0.72674836	-3.35319114
6	-1.03025955	0.68177310	-3.39051211
1	-0.80204713	0.90118428	-4.45249078
1	-2.13698413	0.65975563	-3.32450284
6	-0.79418661	3.02118423	-2.66491301
6	-2.12085733	3.47735923	-2.43422317
6	-2.43283643	4.83281146	-2.60950379
6	-1.47524175	5.77618910	-2.98967888
6	-0.16359576	5.32561462	-3.17644867
6	0.19078866	3.98047931	-3.02532298
6	-1.12788295	-3.84329231	2.37282758
1	-2.18360986	-4.00637108	4.82409704
6	-3.58675423	-2.38139194	6.52060370
1	-3.81603658	-0.04420208	5.11072036
6	-3.14432797	0.83575883	2.65704118
6	-3.20303026	2.55455792	-1.93206150
1	-3.45812707	5.16169599	-2.41842706
6	-1.84152821	7.22525621	-3.20145685
1	0.61202029	6.04215700	-3.45965125
6	1.62180277	3.56684418	-3.26317744
1	-0.73939282	-4.56733251	3.10058852
1	-0.26999613	-3.40899054	1.84003247
1	-1.71861836	-4.41463524	1.63895522
1	-2.21123553	1.37085430	2.41431778
1	-3.69745361	1.45687507	3.37239297
1	-3.74165255	0.78815424	1.73181462
1	-4.63687707	-2.71439579	6.50246059
1	-3.53857103	-1.49610044	7.16977537
1	-2.99877689	-3.18219698	6.98925889
1	-3.99644193	3.12700249	-1.43404770
1	-2.79238983	1.83416976	-1.20817094
1	-3.67667383	1.97471489	-2.74026680
1	1.68297229	2.75497852	-4.00085333
1	2.10393719	3.19196970	-2.34765720
1	2.21168256	4.41757025	-3.62915061
1	-1.04000854	7.89630529	-2.86231019
1	-2.76101250	7.48845632	-2.66124405
1	-2.01451802	7.43997621	-4.26814388
1	-1.88411761	-0.21866599	0.99906768

Energy = -7584.963390 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 45

Atomic N.	X	Y	Z
8	2.20810325	-1.86084103	0.26276953
8	0.94414141	-0.67465246	-2.64835486
6	2.34974935	-0.50246490	-2.67665878
1	2.66690428	-0.17767998	-3.68531422

1	2.88125847	-1.44088369	-2.43701101
1	2.70819585	0.26475030	-1.95676251
8	3.26016424	-2.91914418	1.88941647
6	2.62883359	-1.81068308	1.40839047
6	2.51517443	-0.58378350	2.28979622
1	1.98475516	-0.84144522	3.22109224
1	1.87634119	0.11519305	1.73539974
6	3.87170933	0.07729022	2.61417949
1	4.48836708	0.11704347	1.70172386
1	3.67573557	1.12226732	2.89765137
6	4.64410999	-0.60214822	3.74976511
1	4.04658135	-0.52747362	4.67483265
1	5.57667849	-0.04755545	3.93828605
6	4.97527747	-2.07722016	3.49988045
1	5.66119048	-2.18682186	2.64400384
1	5.50629638	-2.48068238	4.37763426
6	3.75769352	-2.96410566	3.25525400
1	2.93704044	-2.73211103	3.95265583
1	4.02370917	-4.02079880	3.38296049
50	-0.04943109	-0.15388947	-0.81849481
7	-1.74290631	-1.39167771	-2.38255648
6	-1.16213233	-2.70029647	-2.76148777
1	-1.89012958	-3.29666909	-3.34357212
1	-0.88294430	-3.25774551	-1.86139042
1	-0.25353435	-2.51719972	-3.34300840
7	-1.38254407	-1.48590879	0.36057997
6	-2.92173057	-1.58562057	-1.51500539
1	-3.67916070	-2.21571955	-2.02348422
1	-3.36418439	-0.59834266	-1.31889140
6	-2.51072490	-2.21688784	-0.18534977
1	-3.38480309	-2.16035332	0.49226570
1	-2.32496086	-3.30110474	-0.33677048
6	-1.09657491	-1.72007164	1.72955992
6	-0.56244698	-2.95858556	2.18238187
6	-0.28575717	-3.14273493	3.54455708
6	-0.51476841	-2.14185357	4.49474815
6	-1.03186707	-0.92314113	4.03939437
6	-1.33024913	-0.69668415	2.68953070
7	-1.19608974	1.50095778	-2.86273997
6	-2.07556127	-0.65941680	-3.62536997
1	-2.94104070	-1.13638019	-4.12668459
1	-1.20503915	-0.76709825	-4.28840119
6	-2.36712265	0.82683812	-3.44517189
1	-2.62303719	1.23750724	-4.44034665
1	-3.24422678	0.98784570	-2.80434815
6	-1.17939431	2.92646793	-2.83814706
6	-2.06982801	3.64453570	-2.00988495
6	-2.00908645	5.04483203	-2.00132238
6	-1.08105980	5.75778030	-2.76492666
6	-0.18859200	5.02391042	-3.55636053
6	-0.22020641	3.62731141	-3.61011975
6	-0.24933541	-4.06880997	1.21244438
1	0.12783208	-4.10235261	3.86865930
6	-0.24763364	-2.37723359	5.96292456
1	-1.22964399	-0.12524977	4.76074618
6	-1.93226594	0.62793012	2.28412187
6	-3.04908152	2.94407349	-1.10081585
1	-2.70101280	5.59070050	-1.35490774

6	-1.01189688	7.26500918	-2.71022080
1	0.55356378	5.55404117	-4.15869119
6	0.76757833	2.88757194	-4.48165031
1	0.45135074	-4.78774171	1.65653119
1	0.20282522	-3.66338187	0.29637101
1	-1.15298581	-4.62690097	0.92024820
1	-1.20484929	1.26516876	1.75845592
1	-2.28478364	1.17735907	3.16751887
1	-2.77486161	0.48363713	1.59402983
1	-1.16388507	-2.68341433	6.49253352
1	0.12102073	-1.46697992	6.45687987
1	0.49430419	-3.17400757	6.11275210
1	-3.32528976	3.59539332	-0.26159044
1	-2.61617179	2.02007457	-0.69102139
1	-3.98221230	2.67259872	-1.62040603
1	0.26731264	2.21981230	-5.20044030
1	1.45612195	2.26344748	-3.89022652
1	1.37738048	3.59656743	-5.05520347
1	-0.17926311	7.60228752	-2.07289236
1	-1.93601884	7.69294650	-2.29981044
1	-0.84874083	7.69581400	-3.70835186
1	-0.34623376	1.12498499	-3.29876151

Energy = -7584.958089 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 46

Atomic N.	X	Y	Z
8	0.44005972	-1.80309643	-0.51367659
8	1.30679602	-0.59665197	-3.40832733
6	2.09929812	-1.72180547	-3.74567542
1	2.51563672	-1.60461037	-4.76205973
1	1.54445554	-2.68165963	-3.72419581
1	2.95387285	-1.82072310	-3.04952380
8	1.87601590	-2.76373699	0.84389852
6	1.55346395	-1.75305961	0.00202090
6	2.53972402	-0.63476879	-0.24203137
1	3.51352716	-1.05804292	-0.53916433
1	2.15254502	-0.07250515	-1.10126187
6	2.72919953	0.27898602	0.98932023
1	1.74657518	0.50193631	1.43271528
1	3.13389633	1.23740996	0.63260777
6	3.67195829	-0.29396081	2.05250863
1	4.68104165	-0.39435930	1.61579986
1	3.76480329	0.42814547	2.87836506
6	3.24364324	-1.65223980	2.61947549
1	2.28103616	-1.57502147	3.15044681
1	3.98468718	-1.97955205	3.36698191
6	3.13351495	-2.76388727	1.58128386
1	3.97468220	-2.74389445	0.86965104
1	3.12347317	-3.74585026	2.06904754
50	-0.67765269	-0.87506637	-2.91834974
7	-3.27862914	-0.16265433	-1.23596992
6	-4.21772632	-1.27127884	-1.41785485
1	-5.27524816	-0.93034159	-1.44229994
1	-4.11282237	-2.00398089	-0.60813440
1	-3.99238370	-1.78511547	-2.36258908
7	-1.86440307	-0.73476231	1.40144227

6	-3.50844098	0.53981495	0.03736331
1	-4.55501598	0.92149325	0.07920861
1	-2.83792067	1.40823396	0.06748399
6	-3.25894954	-0.28700760	1.29765028
1	-3.48375197	0.36415408	2.15435489
1	-3.97733727	-1.12896000	1.36243695
6	-1.48333364	-1.33224903	2.63761879
6	-1.21367960	-0.50477635	3.75279398
6	-0.79712721	-1.09024797	4.95599744
6	-0.62353417	-2.47141573	5.09041937
6	-0.89149445	-3.27391464	3.97409894
6	-1.32405404	-2.73522964	2.75699971
7	-0.95449896	1.21058118	-2.76278394
6	-3.40198925	0.77312707	-2.36788815
1	-4.36353544	1.33061760	-2.31231062
1	-3.44133298	0.16823007	-3.28957482
6	-2.27170582	1.79387865	-2.50489620
1	-2.55961983	2.45749647	-3.34458853
1	-2.25128290	2.44938267	-1.61438475
6	0.07533703	2.19044109	-2.90465308
6	0.58922060	2.87498618	-1.77601850
6	1.58906611	3.84280986	-1.95064547
6	2.09794011	4.16544809	-3.21109842
6	1.57386228	3.48714290	-4.31803357
6	0.58233639	2.50864510	-4.18992462
6	-1.33287233	0.99567954	3.65342058
1	-0.58605988	-0.43903764	5.80840283
6	-0.13551606	-3.07749683	6.38492217
1	-0.77652714	-4.35816012	4.05512051
6	-1.62840651	-3.65188614	1.59597852
6	0.08863821	2.58440731	-0.38246314
1	1.98041470	4.35747228	-1.06844542
6	3.19210620	5.19310994	-3.37663086
1	1.94949032	3.72504496	-5.31687952
6	0.07998585	1.80113180	-5.42297776
1	-0.69929624	1.48622125	4.40437992
1	-2.36450736	1.34335558	3.82505999
1	-1.04052712	1.34175739	2.65197590
1	-2.64516586	-3.48752578	1.20693352
1	-1.55578091	-4.70147614	1.90811436
1	-0.93042755	-3.50021734	0.75859522
1	0.94999513	-3.26445044	6.35556227
1	-0.62309641	-4.04196272	6.58511699
1	-0.33044040	-2.41274563	7.23714414
1	0.86674186	2.80030047	0.36211777
1	-0.22747064	1.53777972	-0.27567260
1	-0.77956546	3.21289468	-0.12369226
1	-1.01256389	1.68425913	-5.41188539
1	0.51451996	0.79153184	-5.48344806
1	0.36680524	2.35083820	-6.32934536
1	4.16804815	4.71210335	-3.54877021
1	3.28711250	5.82380092	-2.48253227
1	3.00013565	5.84805633	-4.23867435
1	-1.62996853	-1.34132026	0.61449595

Energy = -7584.961660 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 47

Atomic N.	X	Y	Z
8	3.20931937	0.41651152	3.17641942
8	0.11846921	-0.49628935	-1.18177398
6	0.66625466	-1.72051440	-1.63842687
1	0.04247298	-2.22826844	-2.40385371
1	0.79496664	-2.43550701	-0.80365595
1	1.65916504	-1.55065709	-2.09720286
8	3.65816055	-1.50988574	2.18087034
6	3.38495871	-0.16618158	2.12312578
6	3.32214715	0.51515179	0.76917929
1	2.55351271	0.03765721	0.13770994
1	2.97218307	1.53323164	0.97249181
6	4.67053410	0.56347765	0.02126920
1	5.46925098	0.85271600	0.72405519
1	4.60773510	1.36971557	-0.72471258
6	5.04356818	-0.73729908	-0.69680211
1	4.28856922	-0.93655038	-1.47662282
1	6.00203902	-0.59984654	-1.22201150
6	5.13893676	-1.96417638	0.21608198
1	5.95169138	-1.84649182	0.95171672
1	5.39555839	-2.84651794	-0.39314893
6	3.85154053	-2.28914013	0.96949395
1	2.96849842	-2.18976261	0.31894854
1	3.88125951	-3.32048224	1.34371818
50	-1.79564782	-0.00955822	-1.86720443
7	-4.12069162	1.00992890	-0.90708612
6	-5.30375513	0.38077049	-1.49946052
1	-6.22696331	0.95379766	-1.28329741
1	-5.42940060	-0.63954054	-1.11701029
1	-5.17368315	0.31493045	-2.58807501
7	-2.37897187	-0.78737032	0.63034331
6	-4.13305845	0.95808091	0.56074439
1	-5.12756013	1.23012301	0.96939301
1	-3.41832915	1.70451282	0.93378018
6	-3.73532548	-0.41776982	1.09735600
1	-3.78698296	-0.39623844	2.20071318
1	-4.44043660	-1.18763405	0.76196811
6	-1.88476014	-2.06595911	1.08143635
6	-2.42473860	-3.26872906	0.58093459
6	-1.89058280	-4.48296966	1.03379214
6	-0.83588556	-4.54184219	1.94975176
6	-0.29910689	-3.33267142	2.40724336
6	-0.80615371	-2.09611773	1.99447220
7	-1.45927924	2.02485162	-1.23799085
6	-3.91290797	2.36017919	-1.45704568
1	-4.72688261	3.05277647	-1.15759258
1	-3.95470178	2.25557564	-2.55305999
6	-2.56483851	2.96147152	-1.06095335
1	-2.42822105	3.86320827	-1.68871844
1	-2.62968586	3.34540485	-0.02146585
6	-0.17657285	2.64034295	-1.15723602
6	0.30285331	3.18540424	0.06350741
6	1.54424597	3.83395847	0.10086020
6	2.35290836	3.96000447	-1.03235820
6	1.88451544	3.39717712	-2.22421626
6	0.64631160	2.74881374	-2.30896685
6	-3.52799049	-3.29623365	-0.44974282

1	-2.30601226	-5.41241841	0.63645047
6	-0.30002213	-5.86600396	2.43753329
1	0.54205494	-3.34516363	3.10403462
6	-0.17980446	-0.81878891	2.49908952
6	-0.47166460	3.04982040	1.35098539
1	1.89602395	4.23359640	1.05620488
6	3.67089601	4.69492817	-0.97446366
1	2.49710232	3.47385530	-3.12664136
6	0.21516981	2.18089183	-3.63793092
1	-3.48814156	-4.23092536	-1.02385206
1	-3.44211933	-2.46029309	-1.15980066
1	-4.52782685	-3.24528046	0.01168541
1	0.24946795	-0.23213560	1.67076162
1	0.63140226	-1.03001948	3.20513291
1	-0.90696048	-0.17634391	3.02189887
1	-0.83373684	-6.19960700	3.34146277
1	0.76497531	-5.79615459	2.69647942
1	-0.42077585	-6.65133294	1.67904821
1	0.21064492	2.99881982	2.20983460
1	-1.08438826	2.13771702	1.33966705
1	-1.15201573	3.89972771	1.52202906
1	-0.84309382	2.39184780	-3.84707222
1	0.33726237	1.08529173	-3.66297033
1	0.82410447	2.59443900	-4.45303138
1	3.52855624	5.78135415	-1.08976532
1	4.34779117	4.36748975	-1.77543126
1	4.17684730	4.53610349	-0.01159369
1	-1.72424893	-0.07098448	0.95857016

Energy = -7584.966296 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 48

Atomic N.	X	Y	Z
8	0.61123619	-3.04268718	-1.21508302
8	0.26684400	0.27746933	-1.07503121
6	1.22242585	0.51584455	-2.10933637
1	0.90244136	1.32862204	-2.78587931
1	1.41213548	-0.37926042	-2.73242597
1	2.18306215	0.81572391	-1.65561171
8	2.49297412	-4.17379909	-1.34055566
6	1.79186412	-3.09962046	-0.89252293
6	2.47781565	-2.06255279	-0.03083522
1	3.34483704	-1.65126910	-0.57573335
1	1.74895824	-1.24996960	0.08554396
6	2.93453969	-2.59243523	1.34553585
1	2.13004889	-3.19831036	1.78934720
1	3.06031208	-1.72302259	2.00798786
6	4.24679586	-3.38138605	1.31502206
1	5.05817601	-2.71560009	0.97193435
1	4.51025020	-3.68415988	2.34042037
6	4.21869910	-4.62140087	0.41588408
1	3.48537010	-5.35720424	0.78374734
1	5.20268844	-5.11709422	0.45044786
6	3.91093164	-4.32829952	-1.04875643
1	4.45867948	-3.44196298	-1.40759911
1	4.19434718	-5.18001357	-1.67910398
50	-1.30090050	-1.04579641	-1.56025141

7	-3.21688657	0.64700951	-1.16298788
6	-4.35017311	-0.15444059	-1.67266046
1	-5.31729236	0.30052132	-1.39004914
1	-4.30808357	-1.17646561	-1.27768586
1	-4.28725275	-0.20930188	-2.76705917
7	-1.89626241	-1.29360975	0.49434759
6	-3.26199691	0.75212909	0.31357906
1	-4.21243445	1.21819393	0.64297125
1	-2.43047554	1.39815650	0.62265289
6	-3.08455123	-0.60572112	0.98429490
1	-3.00742320	-0.41414802	2.07010156
1	-4.01171461	-1.21024046	0.86668389
6	-1.40397416	-2.28576351	1.38795879
6	-1.65687711	-3.66595586	1.18480071
6	-1.17522568	-4.60265065	2.10913754
6	-0.45279821	-4.22397716	3.24613717
6	-0.19643058	-2.86055971	3.42950785
6	-0.64960710	-1.89154181	2.52485401
7	-0.96482240	2.90202572	-1.57313855
6	-3.28156365	1.97514987	-1.84377674
1	-4.32726477	2.33761364	-1.77772630
1	-3.05514927	1.79911255	-2.90633719
6	-2.39081762	3.10232474	-1.32666624
1	-2.71444601	3.99841481	-1.87660726
1	-2.62204008	3.31510889	-0.26266940
6	-0.13305089	4.04303182	-1.38550251
6	0.71750894	4.15530904	-0.25805454
6	1.55664096	5.26965269	-0.14079458
6	1.57083173	6.29513608	-1.09372591
6	0.72803020	6.16498880	-2.20217522
6	-0.11380774	5.05846729	-2.37166885
6	-2.43346737	-4.14933134	-0.01521533
1	-1.38401592	-5.66222982	1.93860287
6	0.01358125	-5.24952011	4.25236797
1	0.38777581	-2.53854692	4.29642783
6	-0.30614616	-0.44017096	2.74970662
6	0.72086395	3.09962830	0.82233938
1	2.21051092	5.34252476	0.73238331
6	2.45175122	7.50926147	-0.91994949
1	0.74115546	6.93587021	-2.97733678
6	-0.94392817	4.93844727	-3.62555607
1	-2.79545019	-5.17375585	0.14495267
1	-1.80575630	-4.15689808	-0.91984174
1	-3.29544242	-3.50200406	-0.22706840
1	-0.07926010	0.05365479	1.79463445
1	0.55329099	-0.34342884	3.42704211
1	-1.14124442	0.11581858	3.20708179
1	-0.75690972	-5.43810638	5.01693252
1	0.91737454	-4.91233018	4.77882986
1	0.23473065	-6.21261106	3.77167246
1	1.41743591	3.37571053	1.62440245
1	1.00570699	2.10698907	0.44161864
1	-0.27764814	2.98342787	1.27250222
1	-1.97340792	5.30657008	-3.48340843
1	-1.01598690	3.88754051	-3.93983086
1	-0.50252640	5.52806562	-4.43989920
1	3.38767033	7.25618898	-0.40289897
1	1.94815447	8.28441751	-0.32020282

1 2.70624165 7.96112571 -1.88849329
 1 -0.60017623 2.06390698 -1.09668242
 Energy = -7584.967224 Hartree
 Number of imaginary frequencies = 0.

Compound I2b isomer 49

Atomic N.	X	Y	Z
8	3.65849945	2.65487658	-0.57308608
8	-0.05573848	-1.28269467	-0.05861058
6	0.73205551	-2.29092772	0.54982726
1	0.13568157	-3.12902930	0.96781442
1	1.33327364	-1.87864491	1.38237699
1	1.42966595	-2.73209631	-0.18773192
8	4.43230129	0.84420027	0.44008353
6	3.70721850	1.43942324	-0.56146742
6	3.01794653	0.56449187	-1.59153379
1	2.31277649	-0.12457421	-1.09614898
1	2.41415338	1.24955248	-2.19689511
6	3.98399610	-0.22501692	-2.49893491
1	4.80314068	0.43668132	-2.82556193
1	3.43150684	-0.50551497	-3.40802329
6	4.55338824	-1.49672834	-1.86231237
1	3.71962810	-2.18962899	-1.65630759
1	5.20600111	-2.00554524	-2.58937222
6	5.32991595	-1.26539486	-0.56186058
1	6.23083589	-0.65632874	-0.74342657
1	5.68273892	-2.23616322	-0.17628095
6	4.51678747	-0.60270947	0.54729129
1	3.50396929	-1.02993507	0.61402504
1	5.00946997	-0.74817376	1.51718432
50	-2.12947665	-1.47003070	0.12922521
7	-4.29210785	0.08808860	0.64014678
6	-5.29634294	-0.58785777	1.46535259
1	-6.26051232	-0.04219864	1.47050364
1	-4.94412301	-0.68268945	2.49977749
1	-5.46416560	-1.60115928	1.07624697
7	-1.67399429	0.47592923	1.91354999
6	-3.87076690	1.37455468	1.21003505
1	-4.73896535	1.96710333	1.56377943
1	-3.38794645	1.95777629	0.41387419
6	-2.88293278	1.20328373	2.36503428
1	-2.62492353	2.20163092	2.76157237
1	-3.33846785	0.64258052	3.18991432
6	-0.65805693	0.26010150	2.91549604
6	-0.86199103	-0.65508224	3.96842480
6	0.16794073	-0.84498332	4.90056528
6	1.39008338	-0.17216642	4.81351859
6	1.57694351	0.70812140	3.74085510
6	0.57510914	0.94070179	2.79325341
7	-2.36159988	-0.04902906	-1.47550326
6	-4.73321984	0.16984861	-0.76252154
1	-5.61830866	0.83014821	-0.87450229
1	-5.04268302	-0.84849541	-1.04740879
6	-3.62710322	0.64108609	-1.70604767
1	-3.99678287	0.46363332	-2.73451596
1	-3.52669852	1.74364320	-1.62590398
6	-1.40717023	0.15512263	-2.51379291

6	-0.82565525	1.43118971	-2.73854187
6	0.06792519	1.61590135	-3.80185965
6	0.42751142	0.57432091	-4.66182872
6	-0.12960887	-0.68521260	-4.41674492
6	-1.03337014	-0.91253846	-3.37171623
6	-2.12970733	-1.46362575	4.10743171
1	0.00894768	-1.56171357	5.71007109
6	2.47096482	-0.37927051	5.84660830
1	2.53029461	1.22989496	3.63066496
6	0.83177684	1.88238272	1.64174706
6	-1.10893656	2.60282954	-1.83142518
1	0.51098883	2.60543480	-3.94569971
6	1.36241030	0.80764269	-5.82466234
1	0.13707952	-1.52188844	-5.06819176
6	-1.59331874	-2.30069391	-3.18728019
1	-1.92992198	-2.39126200	4.65917667
1	-2.54694804	-1.73752848	3.12700896
1	-2.90932538	-0.91973183	4.66561659
1	0.77421087	1.35424611	0.67614767
1	1.83077815	2.32755849	1.71248686
1	0.10734378	2.71255732	1.61267967
1	2.41946794	0.39078402	6.63244217
1	3.47164042	-0.31647032	5.39778652
1	2.37340117	-1.35642640	6.33833950
1	-0.23997051	3.27220394	-1.78037629
1	-1.34147898	2.25749301	-0.81450748
1	-1.96581850	3.20308974	-2.17772118
1	-2.67157967	-2.28046036	-2.97481270
1	-1.10742512	-2.81864943	-2.34379150
1	-1.42308745	-2.91047346	-4.08471993
1	1.87134277	-0.11935448	-6.12249207
1	2.12887821	1.55629980	-5.57933748
1	0.81702117	1.17936055	-6.70684389
1	-1.24678058	1.01232956	1.15236764

Energy = -7584.966299 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 50

Atomic N.	X	Y	Z
8	1.28129429	-2.47707972	1.82828392
8	-0.15744831	-0.87413333	-0.70725729
6	0.33550975	-1.80632456	-1.67043024
1	-0.41406704	-2.02498786	-2.45214432
1	0.63501634	-2.77151650	-1.21884289
1	1.22437575	-1.38068266	-2.16790922
8	3.33725127	-3.25519698	1.89089010
6	2.44576722	-2.31349430	1.48454647
6	2.92147371	-1.13560597	0.66333086
1	3.41337674	-1.50439013	-0.25307622
1	2.01081426	-0.60589707	0.35511110
6	3.87901977	-0.19048492	1.42065464
1	3.48673861	-0.00641263	2.43228588
1	3.85785224	0.78183471	0.90633646
6	5.32833217	-0.68099425	1.48662444
1	5.73082783	-0.74963545	0.46064824
1	5.94111841	0.07099198	2.00775081
6	5.50602402	-2.03884180	2.17340914

1	5.20494519	-1.98622364	3.23228889
1	6.57384550	-2.31245478	2.16569297
6	4.74145060	-3.18175101	1.51378837
1	4.82581075	-3.14410365	0.41568355
1	5.13155847	-4.14992036	1.85076295
50	-1.23794870	-1.70295605	0.90041334
7	-3.43945898	-0.41373911	0.45393858
6	-4.31731973	-1.09919528	1.42667451
1	-5.26455476	-0.54598441	1.56418451
1	-3.81684344	-1.19490192	2.39760512
1	-4.54223926	-2.10836547	1.05850923
7	-1.11676875	0.10094193	2.07265535
6	-3.11485883	0.95808225	0.90808038
1	-4.04092973	1.55099867	1.04954220
1	-2.51351057	1.43157115	0.12166999
6	-2.29540313	0.95081072	2.19390153
1	-2.00488970	1.99872822	2.38962670
1	-2.94282075	0.66907585	3.05412558
6	-0.07599439	0.43242492	2.98425750
6	0.15810569	-0.32717488	4.15957754
6	1.17214765	0.06051552	5.04501008
6	1.97121759	1.18686761	4.81663994
6	1.73551072	1.92584874	3.65263185
6	0.73989144	1.56764592	2.73380928
7	-2.31245294	-0.06972724	-2.53569666
6	-4.14551421	-0.43837210	-0.86212955
1	-5.18782898	-0.10050784	-0.69221346
1	-4.18281294	-1.49047880	-1.18283399
6	-3.58685271	0.40724055	-2.00424445
1	-4.34021841	0.34360835	-2.80320110
1	-3.56274776	1.47736110	-1.71274806
6	-1.91279106	0.47655041	-3.78875967
6	-0.86989088	1.43184175	-3.87524169
6	-0.47186261	1.89979621	-5.13296823
6	-1.08582758	1.47113679	-6.31608225
6	-2.11163473	0.52649134	-6.21142472
6	-2.52921913	0.01454139	-4.97625531
6	-0.67512972	-1.54283483	4.48317712
1	1.33014790	-0.53003869	5.95156791
6	3.07128067	1.56936255	5.77864449
1	2.35378636	2.80325121	3.44220610
6	0.56267062	2.37712825	1.47343973
6	-0.19475275	1.96101834	-2.63182526
1	0.33668519	2.63380620	-5.18611977
6	-0.66663581	2.02514226	-7.65685472
1	-2.58815463	0.15161362	-7.12118380
6	-3.58686677	-1.06037444	-4.93425974
1	-0.57751455	-1.80714611	5.54466527
1	-0.35479567	-2.41587156	3.89369932
1	-1.73771973	-1.37578111	4.25940442
1	0.31930174	1.72030050	0.62676207
1	1.47361233	2.94700855	1.24509294
1	-0.25966033	3.10640050	1.56121925
1	2.78197613	1.36844878	6.81971149
1	3.32603946	2.63444337	5.69366054
1	3.99165929	0.99518747	5.58339004
1	0.55745440	2.71514291	-2.89681717
1	0.29860174	1.16826302	-2.04909954

1	-0.92055610	2.43683748	-1.95364861
1	-4.59395961	-0.65134021	-4.74989739
1	-3.37522062	-1.77628440	-4.12733320
1	-3.62986779	-1.59852299	-5.89039021
1	0.41271968	2.22914387	-7.68814108
1	-1.18258599	2.97383924	-7.87569783
1	-0.90740903	1.32752509	-8.47059653
1	-1.55967237	-0.03904029	-1.83225855

Energy = -7584.967225 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 51

Atomic N.	X	Y	Z
8	1.13056836	0.02623434	0.79223721
8	0.99581697	2.22895198	-1.45300852
6	1.23422000	3.60987511	-1.25185453
1	0.55477097	4.07665919	-0.50721461
1	1.12146067	4.17635766	-2.19598022
1	2.26812414	3.77914496	-0.89486863
8	2.69155321	-0.42333693	-0.69754218
6	2.25133882	0.28809677	0.35810547
6	3.15278152	1.32487793	0.99096757
1	3.31632422	2.13236203	0.25833489
1	2.57540155	1.75386598	1.81806616
6	4.50794833	0.78587208	1.49474060
1	4.35436984	-0.17216743	2.01694708
1	4.88647647	1.48956272	2.25111787
6	5.56615066	0.63033148	0.39721049
1	5.75631530	1.62096278	-0.05087291
1	6.51602218	0.31011395	0.85280100
6	5.18550026	-0.34963365	-0.71711990
1	5.11467279	-1.37758998	-0.32558684
1	5.98398964	-0.36133693	-1.47690380
6	3.88291117	-0.01742036	-1.43523152
1	3.79521815	1.04975438	-1.68613553
1	3.79830458	-0.58878908	-2.36725216
50	-0.82559456	1.45962488	-0.76779551
7	-2.59751319	-0.84121396	-0.03442122
6	-3.88696077	-0.15591425	-0.17771910
1	-4.72603320	-0.86708041	-0.32225410
1	-3.86714836	0.52995347	-1.03576241
1	-4.08176482	0.43966630	0.72344267
7	-0.98770932	0.16464431	-2.42766095
6	-2.27764041	-1.63975488	-1.22860905
1	-3.08493189	-2.38187819	-1.42080139
1	-1.35480154	-2.19824839	-1.01757495
6	-2.06676732	-0.82691487	-2.50631726
1	-1.84206716	-1.55287442	-3.30402334
1	-3.02328270	-0.35610062	-2.81018963
6	-0.22209872	0.29709626	-3.62584399
6	-0.36009545	1.43701461	-4.45576161
6	0.40087607	1.53618812	-5.62715841
6	1.30209749	0.53969982	-6.01627108
6	1.42731096	-0.58100037	-5.18923529
6	0.68503599	-0.72344651	-4.00967258
7	-0.72750706	-1.27923777	2.79645638
6	-2.63585612	-1.71381294	1.16103647

1	-3.23048576	-2.62322253	0.92415833
1	-3.18275531	-1.18142356	1.95256743
6	-1.26161878	-2.13074734	1.72638888
1	-1.33833467	-3.16769387	2.07880567
1	-0.50462770	-2.12534343	0.93047520
6	-1.48779013	-0.96378051	3.94001608
6	-2.02419404	-1.97341600	4.77990701
6	-2.75609221	-1.60311229	5.91612934
6	-2.95483528	-0.26955703	6.28405670
6	-2.36890137	0.71274128	5.47657378
6	-1.65057938	0.39627044	4.32012674
6	-1.31541460	2.55374142	-4.11112082
1	0.27910450	2.42088513	-6.25781950
6	2.08606853	0.65549338	-7.30173579
1	2.13038966	-1.37222531	-5.46475712
6	0.88319685	-1.95233489	-3.15780078
6	-1.75941153	-3.43886071	4.53495284
1	-3.15863353	-2.39662229	6.55162541
6	-3.77163743	0.09930081	7.49911239
1	-2.48261741	1.76603394	5.74671816
6	-1.04958532	1.50189130	3.48821090
1	-1.54765805	3.15230882	-5.00214853
1	-0.88120619	3.23646715	-3.36365050
1	-2.25683206	2.17088230	-3.69352557
1	0.89595592	-1.69281977	-2.09130687
1	1.82793263	-2.45148340	-3.41271368
1	0.07969714	-2.69196785	-3.30691510
1	1.50459426	0.27811203	-8.15816137
1	3.01618936	0.07240261	-7.25746671
1	2.34581114	1.70032330	-7.52158604
1	-1.92397956	-4.01201618	5.45685578
1	-0.72251661	-3.60137979	4.20586578
1	-2.41734429	-3.87018041	3.76286086
1	-1.40817122	1.47986472	2.44600126
1	0.05012131	1.43702202	3.44037886
1	-1.30337548	2.48304856	3.90918000
1	-3.34733095	0.96892428	8.02069219
1	-3.82443709	-0.73404342	8.21305794
1	-4.80608914	0.36070140	7.22339748
1	-0.25039392	-0.47334349	2.39777272

Energy = -7584.957345 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 52

Atomic N.	X	Y	Z
8	0.85173952	2.52194170	-2.72150726
8	0.47825854	2.50286445	1.65769788
6	0.17098714	2.92723635	2.97286700
1	1.00750084	2.77777412	3.68148513
1	-0.71320165	2.41103738	3.39736934
1	-0.05796157	4.00819316	2.95905606
8	0.04736757	4.23237461	-1.57078835
6	1.08491539	3.42935389	-1.93967585
6	2.46752370	3.70699664	-1.37891549
1	2.43406431	3.60395271	-0.28096338
1	3.10210263	2.89932330	-1.76149739
6	3.05240392	5.08225192	-1.76328862

1	2.85504074	5.28249882	-2.82898531
1	4.14628633	5.02211543	-1.65999886
6	2.54233739	6.24151357	-0.90119983
1	2.84100482	6.05929480	0.14543548
1	3.04501868	7.17160842	-1.20958553
6	1.02497483	6.44721285	-0.94956744
1	0.70281117	6.74617085	-1.96061300
1	0.75362765	7.27897181	-0.27877928
6	0.20693586	5.23299930	-0.52164808
1	0.60847125	4.74218894	0.37895965
1	-0.82851453	5.53042139	-0.31296157
50	1.26489751	0.63282918	1.12606495
7	-0.95564799	0.15508266	0.23182394
6	-1.53803028	1.29920539	-0.51369993
1	-2.60822167	1.11692333	-0.71089939
1	-1.01443350	1.45030319	-1.46328665
1	-1.41367827	2.20334710	0.09326838
7	-0.20452654	-2.30682961	-2.61886855
6	-1.01177987	-1.09104606	-0.58280215
1	-2.03959805	-1.21158942	-0.97266600
1	-0.80912144	-1.93630585	0.09009038
6	-0.01309709	-1.13504648	-1.75427632
1	-0.08494729	-0.22699520	-2.36195038
1	1.01609402	-1.16595789	-1.36427227
6	-1.37982704	-2.39111973	-3.41411333
6	-2.29429715	-3.45667554	-3.22216962
6	-3.42110331	-3.55473410	-4.04542206
6	-3.68483593	-2.62187063	-5.05480704
6	-2.75137723	-1.59868678	-5.25083471
6	-1.59623022	-1.47095697	-4.46880520
7	0.39721899	-0.65988303	2.59123271
6	-1.70921055	-0.01388998	1.51197112
1	-2.73610545	-0.36040132	1.29432958
1	-1.77090804	0.98874328	1.95739221
6	-1.02503412	-0.96325769	2.49245243
1	-1.55801187	-0.84950723	3.45679072
1	-1.19083082	-2.01928727	2.18961250
6	1.14173336	-1.43744919	3.52379890
6	2.04518432	-2.43983864	3.08206336
6	2.78604944	-3.17251120	4.01922255
6	2.66321085	-2.96163618	5.39560551
6	1.75768188	-1.98479244	5.82231006
6	1.00152803	-1.22464859	4.92224191
6	-2.06059663	-4.49685491	-2.15130059
1	-4.11632044	-4.38290602	-3.88571352
6	-4.93308254	-2.71501461	-5.89895565
1	-2.90539495	-0.88548194	-6.06482076
6	-0.58077368	-0.41080733	-4.81927345
6	2.22146639	-2.75811965	1.61588127
1	3.47301861	-3.94241279	3.65777817
6	3.49627279	-3.74035489	6.38505592
1	1.64179025	-1.79483459	6.89300070
6	0.06584103	-0.17233948	5.46198982
1	-2.88090232	-5.22524408	-2.13915310
1	-1.99772075	-4.05267007	-1.14460480
1	-1.12863806	-5.06400387	-2.31369596
1	-0.69686737	0.51365786	-4.23233066
1	-0.67773655	-0.13108496	-5.87653245

1	0.44161661	-0.77447322	-4.64510022
1	-5.24975734	-3.75831626	-6.03466406
1	-4.77800854	-2.27206911	-6.89226398
1	-5.77313416	-2.17793458	-5.42999819
1	2.67241473	-3.75160496	1.49052908
1	2.87936681	-2.03286551	1.11097185
1	1.26086911	-2.73930809	1.08244802
1	-0.95612096	-0.56286072	5.59604881
1	-0.00116639	0.68218155	4.77620647
1	0.40589054	0.18298407	6.44386959
1	4.38957113	-3.17077577	6.68716697
1	3.84333819	-4.68988202	5.95561528
1	2.92996839	-3.96369196	7.29992149
1	-0.07164313	-3.16272560	-2.08236895

Energy = -7584.965945 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 53

Atomic N.	X	Y	Z
8	3.96350106	3.13828837	-2.84998824
8	0.73680559	0.30271273	0.77889231
6	1.29192676	-0.99945778	0.74559404
1	0.54410884	-1.78705997	0.54216696
1	1.76527695	-1.25465146	1.71087700
1	2.06869337	-1.06099551	-0.03990469
8	2.68003073	3.96139939	-1.24255216
6	3.45240209	2.95704740	-1.75958124
6	3.63988147	1.69246047	-0.94348245
1	2.65923180	1.26971821	-0.66729743
1	4.13936468	0.98401498	-1.61454074
6	4.48570875	1.90302064	0.33254706
1	5.35474009	2.53906505	0.09605153
1	4.89139335	0.92478672	0.63196584
6	3.69764485	2.48425930	1.51165812
1	2.90773842	1.76717117	1.79039581
1	4.36683610	2.57998723	2.38146966
6	3.03834233	3.83890772	1.22864209
1	3.79334734	4.61912180	1.03539489
1	2.48069844	4.15738364	2.12469509
6	2.05116354	3.81915374	0.06420548
1	1.43209524	2.90854022	0.08660132
1	1.38539264	4.69020983	0.11141544
50	-1.23668979	0.94764808	0.81184712
7	-3.77106080	0.59876829	-0.12473581
6	-4.39836674	1.87942979	-0.46266861
1	-5.49190708	1.77642968	-0.60710872
1	-3.96209140	2.29117869	-1.38086320
1	-4.21289761	2.59963181	0.34550058
7	-1.38366022	-0.16033567	-1.71621393
6	-3.81071486	-0.35142551	-1.24358676
1	-4.80666772	-0.36139254	-1.73185499
1	-3.64276152	-1.36124840	-0.84234526
6	-2.74379477	-0.05656330	-2.29694413
1	-2.87366015	-0.76047370	-3.13903753
1	-2.86539158	0.95328514	-2.70790292
6	-0.30639280	0.05350802	-2.65717477
6	0.00501793	1.35422403	-3.10993239

6	1.08759594	1.52123727	-3.98106135
6	1.87419656	0.44736988	-4.41457618
6	1.53489958	-0.83135884	-3.96293846
6	0.45375039	-1.05055220	-3.09973026
7	-2.07208618	-0.83359590	1.73693215
6	-4.31508336	0.06358808	1.13469211
1	-5.37727868	-0.24007024	1.02308583
1	-4.28205495	0.88964333	1.86260520
6	-3.50668743	-1.11240050	1.67784631
1	-3.90356709	-1.32398484	2.68838524
1	-3.74446114	-2.01811743	1.08246454
6	-1.35398862	-1.70301426	2.60616294
6	-1.25605681	-3.09627731	2.34245133
6	-0.56717725	-3.93156662	3.23152987
6	0.04874450	-3.44363737	4.38663771
6	-0.04558370	-2.07019845	4.63508754
6	-0.72752544	-1.19829880	3.77804290
6	-0.77126232	2.57497609	-2.67802312
1	1.34901176	2.53247405	-4.29952045
6	3.05778685	0.68004659	-5.31979207
1	2.12787087	-1.68919892	-4.28881107
6	0.12745158	-2.46052111	-2.66155698
6	-1.82967081	-3.70581148	1.08676591
1	-0.49814554	-4.99799909	2.99955672
6	0.81659394	-4.35451492	5.31401739
1	0.41961265	-1.65905924	5.53505566
6	-0.78204462	0.26652911	4.13543724
1	-0.13768866	3.46894488	-2.74055532
1	-1.13636803	2.48820034	-1.64377878
1	-1.64520443	2.75292158	-3.32636602
1	0.30683252	-2.61850113	-1.58559464
1	0.75830766	-3.17963486	-3.19828367
1	-0.92090126	-2.73013927	-2.86618906
1	2.74355829	1.10988918	-6.28277841
1	3.59380133	-0.25589911	-5.52417311
1	3.75843619	1.39275348	-4.85988592
1	-1.27469071	-4.61190762	0.80911944
1	-1.77766514	-2.99369607	0.24970011
1	-2.88682018	-3.99349289	1.20286769
1	-1.77572527	0.69587611	3.94435124
1	-0.05613989	0.85127027	3.54611453
1	-0.53307843	0.41535415	5.19468665
1	1.89651603	-4.32366795	5.09828193
1	0.49092900	-5.39832591	5.21089296
1	0.68867181	-4.05762066	6.36453390
1	-1.28289681	-1.10575971	-1.33589455

Energy = -7584.964967 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 54

Atomic N.	X	Y	Z
8	0.13789150	0.89343343	1.48929848
8	0.45756817	3.26683022	-0.63563052
6	0.56436975	4.66532081	-0.45330303
1	-0.34888596	5.12967671	-0.02167877
1	0.76886212	5.17801500	-1.41249957
1	1.40096051	4.91174917	0.22978393

8	2.12022003	0.73095979	0.53648526
6	1.27833045	1.34279890	1.39499856
6	1.78184851	2.48767916	2.24596549
1	2.04395850	3.32647488	1.58189884
1	0.92317965	2.80816188	2.84722398
6	2.98127222	2.13509706	3.15087709
1	2.81937661	1.14978816	3.61748657
1	3.00360012	2.86413592	3.97469484
6	4.33440361	2.16773209	2.43167821
1	4.50174303	3.18839191	2.04639027
1	5.13764237	1.97705222	3.16040132
6	4.46143016	1.17618895	1.27053752
1	4.43188329	0.13773443	1.63922310
1	5.44480330	1.30669721	0.78991279
6	3.40211010	1.33110929	0.18550643
1	3.23342987	2.37962158	-0.10009195
1	3.69087105	0.77928253	-0.71711529
50	-1.47604589	2.44933419	-0.53714944
7	-3.26456831	0.19893710	-0.42317882
6	-4.44650045	0.84150308	-1.01282189
1	-5.21132744	0.10241752	-1.32572561
1	-4.16248989	1.43357734	-1.89302597
1	-4.89416838	1.52558855	-0.27974683
7	-1.07027532	1.18408696	-2.18142658
6	-2.58168611	-0.66358835	-1.40444446
1	-3.28382634	-1.42644666	-1.80625893
1	-1.78432387	-1.19880048	-0.87448062
6	-1.98714540	0.11055915	-2.57983743
1	-1.45420797	-0.62472111	-3.20410415
1	-2.79844332	0.50031386	-3.22790589
6	-0.01139851	1.41688040	-3.11160390
6	-0.00973066	2.56579167	-3.93963379
6	1.03997312	2.76494506	-4.84539901
6	2.09926917	1.86003770	-4.96690805
6	2.08474281	0.72911324	-4.14398816
6	1.05476932	0.48802371	-3.22603502
7	-1.56116948	-1.85478079	1.45605908
6	-3.68178928	-0.55639816	0.78034992
1	-4.20428400	-1.48186684	0.46914356
1	-4.42407481	0.06949583	1.30078487
6	-2.60461578	-0.87452834	1.82696173
1	-2.11340899	0.06965996	2.10903341
1	-3.13113464	-1.23588214	2.72270783
6	-1.33504878	-2.98774339	2.27618716
6	-2.35084182	-3.95176460	2.49913267
6	-2.07416389	-5.06807265	3.29922914
6	-0.81769724	-5.29488719	3.86783652
6	0.18797239	-4.36218016	3.59219236
6	-0.04389775	-3.22044496	2.81867604
6	-1.11986273	3.58718206	-3.87559111
1	1.02367410	3.65522813	-5.47969330
6	3.20237564	2.07876223	-5.97482230
1	2.90537245	0.00909686	-4.21098007
6	1.11187133	-0.74519231	-2.35976212
6	-3.69792164	-3.86166902	1.82531466
1	-2.86998664	-5.80117458	3.45577394
6	-0.55890802	-6.49200944	4.75052015
1	1.18952458	-4.51855604	4.00166445

6	1.08548999	-2.24879485	2.57484547
1	-1.13094725	4.20241381	-4.78535198
1	-0.99146286	4.27297557	-3.02268384
1	-2.10470543	3.11306089	-3.76392437
1	0.76905970	-0.52565041	-1.34082554
1	2.13663276	-1.13752729	-2.31155620
1	0.47627949	-1.55544839	-2.75231630
1	2.96348606	1.59889205	-6.93745754
1	4.15349029	1.65210934	-5.62710454
1	3.35820429	3.14792337	-6.17371740
1	-4.21733585	-4.82686364	1.88580411
1	-3.58261747	-3.59670714	0.76381044
1	-4.35969878	-3.10619088	2.27508422
1	0.84161124	-1.24280770	2.94845761
1	1.32759114	-2.14155590	1.50506508
1	1.99616330	-2.58959356	3.08375798
1	0.48156670	-6.83539044	4.66684397
1	-1.21778287	-7.33165354	4.48921605
1	-0.73904754	-6.25430153	5.81138160
1	-0.69144744	-1.34864845	1.29158361

Energy = -7584.956091 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 55

Atomic N.	X	Y	Z
8	0.98702894	-0.77306332	-0.23223849
8	0.91961851	2.29342860	-1.78458095
6	1.30780577	3.55404644	-1.26988773
1	0.78418572	3.83363346	-0.33083553
1	1.10879942	4.35514873	-2.00498197
1	2.39385650	3.56692155	-1.05791924
8	2.44820157	-1.81900477	1.03728721
6	2.04795059	-0.70358667	0.38170062
6	2.89351373	0.54792390	0.44141496
1	3.93207792	0.30792070	0.15989100
1	2.48485287	1.21497182	-0.32942649
6	2.87201850	1.22337747	1.83084340
1	1.83838706	1.24260185	2.21104001
1	3.17197313	2.27341222	1.69910068
6	3.80226827	0.56531516	2.85517660
1	4.84485313	0.67863792	2.50951828
1	3.73268083	1.11087310	3.80862134
6	3.52642577	-0.92137228	3.10832443
1	2.52843808	-1.06851718	3.55184296
1	4.25206143	-1.29801313	3.84767072
6	3.64367977	-1.80946656	1.87337127
1	4.51882499	-1.54459347	1.25846691
1	3.73920282	-2.86251588	2.16412739
50	-0.68749902	1.29407241	-0.93849496
7	-3.12667458	-0.60278784	-0.62336675
6	-4.26572717	0.14063537	-1.16544101
1	-5.06775314	-0.52603053	-1.54772232
1	-3.93810190	0.79378719	-1.98380415
1	-4.69081617	0.77593442	-0.37688301
7	-1.09279639	0.30281703	-2.74754542
6	-2.50598121	-1.47835730	-1.63127721
1	-3.20976886	-2.29028266	-1.92521894

8	0.74914162	2.40131436	2.26607798
8	0.32243167	0.60685805	-0.76839312
6	1.34984922	1.39326592	-1.36286339
1	1.36064903	2.43976767	-1.00075449
1	1.24335355	1.43397750	-2.46308779
1	2.33695820	0.95670610	-1.13057918
8	2.52697006	1.16460365	1.81558536
6	1.89913502	2.09940776	2.56146284
6	2.62282712	2.73840502	3.73155676
1	3.56530776	3.19260673	3.38154617
1	1.97007832	3.55164323	4.06867124
6	2.91066842	1.76492718	4.89451554
1	2.01315623	1.15703202	5.08761258
1	3.08229784	2.36665371	5.79975212
6	4.12675143	0.86165850	4.66589599
1	5.03074241	1.49193872	4.59357136
1	4.26953401	0.22108867	5.54996871
6	4.03955172	-0.02046371	3.41563910
1	3.20208982	-0.73229360	3.49163484
1	4.95919703	-0.62303928	3.33675243
6	3.89224822	0.74954305	2.10793980
1	4.55795745	1.62740031	2.07163319
1	4.13287553	0.10573525	1.25350069
50	-1.15194919	1.66142716	0.28804899
7	-3.19133326	0.51801550	-0.80000345
6	-3.96008783	1.46078300	-1.62776109
1	-4.94570048	1.04788437	-1.91314501
1	-3.39052263	1.70771881	-2.53078269
1	-4.11693556	2.38520479	-1.05633709
7	-1.30244600	0.01363561	-3.17255522
6	-2.95568117	-0.78338912	-1.47859205
1	-3.88248961	-1.38982366	-1.42411518
1	-2.18149509	-1.30807535	-0.90074229
6	-2.54380798	-0.73115287	-2.94785581
1	-2.45814773	-1.79022667	-3.26805999
1	-3.35661021	-0.30038519	-3.55539167
6	-0.66049566	-0.22521725	-4.42252527
6	-1.13271070	0.41997451	-5.58835411
6	-0.48392106	0.19419820	-6.80945575
6	0.63133823	-0.64300226	-6.91400879
6	1.09259226	-1.26464271	-5.74708583
6	0.46335730	-1.08354868	-4.51000246
7	-1.68887672	0.00530452	1.55646912
6	-3.88796669	0.28918768	0.48975840
1	-4.85828455	-0.21706601	0.31687183
1	-4.09428866	1.28208134	0.92103330
6	-3.04403718	-0.51886358	1.47309109
1	-3.57424054	-0.48140439	2.44677482
1	-3.05572880	-1.59180244	1.18044526
6	-0.93515457	-0.52876084	2.63892176
6	-0.06578475	-1.63179531	2.43777704
6	0.62843394	-2.17466740	3.52696152
6	0.49465457	-1.66322144	4.82416221
6	-0.35122885	-0.56421197	5.00717954
6	-1.06130056	0.01162705	3.94320547
6	-2.29049159	1.38343046	-5.52186229
1	-0.85164864	0.70909331	-7.70096245
6	1.30305334	-0.88831079	-8.24416637

1	1.96209072	-1.92522235	-5.80094615
6	0.97467393	-1.81904700	-3.29342851
6	0.11000973	-2.22705573	1.06343465
1	1.28621936	-3.03176682	3.35505174
6	1.22927846	-2.28959451	5.98642871
1	-0.46636714	-0.13944651	6.00850044
6	-1.93327605	1.21654656	4.19625246
1	-2.30570692	2.03611279	-6.40448419
1	-2.21792098	2.00562403	-4.61824111
1	-3.26224504	0.86489608	-5.48244004
1	1.32688680	-1.13852957	-2.50436433
1	1.80644166	-2.48033658	-3.56828985
1	0.18698126	-2.43892316	-2.83805562
1	0.94826463	-1.82514923	-8.70289243
1	2.39319892	-0.97421190	-8.13460652
1	1.09294895	-0.07639432	-8.95353693
1	0.88566242	-3.00496548	1.07528808
1	0.38086364	-1.45219696	0.33140620
1	-0.82308860	-2.69441635	0.71044914
1	-2.98334252	1.03237403	3.92443911
1	-1.59729695	2.07634826	3.59886272
1	-1.90455772	1.49939431	5.25707959
1	2.29403800	-2.44579216	5.75581106
1	0.81076452	-3.27603114	6.24029838
1	1.16386260	-1.66163523	6.88519175
1	-0.66221874	-0.08931622	-2.37178256

Energy = -7584.966012 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 57

Atomic N.	X	Y	Z
8	1.31465026	-0.36983195	3.19794309
8	1.69170389	2.08957802	-0.04355275
6	2.96561931	1.92976784	-0.63151745
1	3.09177809	2.57351392	-1.52370539
1	3.17468185	0.88814850	-0.96190716
1	3.76010186	2.21327426	0.08680715
8	2.86521163	-1.37992346	1.99259232
6	2.46937987	-0.36029911	2.79808462
6	3.46750023	0.71308919	3.18513934
1	3.84826418	1.20514157	2.27537209
1	2.89066521	1.46120389	3.74067736
6	4.64323634	0.19961436	4.04386468
1	4.25907262	-0.47991459	4.82180791
1	5.07188788	1.06260996	4.57493343
6	5.75575974	-0.48442105	3.24253061
1	6.19339184	0.25231752	2.54703280
1	6.56493786	-0.78023782	3.92803805
6	5.30260186	-1.70759874	2.43849964
1	4.95700179	-2.51274424	3.10724714
1	6.16487506	-2.11329811	1.88486366
6	4.20474240	-1.42064630	1.41980670
1	4.39315944	-0.48801747	0.86580360
1	4.13035260	-2.23672795	0.69125501
50	0.21641545	0.65281696	-0.54494237
7	-1.16919546	1.76471864	1.21315649
6	-0.40273868	2.91596579	1.75501047

1	-1.04752554	3.51651355	2.42133951
1	-0.01923336	3.53559206	0.94078218
1	0.45939521	2.53946887	2.31469280
7	-1.12520150	1.94624391	-1.63398916
6	-2.34018112	2.25805748	0.43167336
1	-2.91929832	2.96819459	1.05238275
1	-2.97408066	1.39249197	0.20057994
6	-1.91470745	2.90581281	-0.88235731
1	-2.83918473	3.16847840	-1.43179648
1	-1.40630576	3.86911502	-0.67241434
6	-0.85453533	2.21844774	-3.00206455
6	-0.15435148	3.37767195	-3.43390222
6	0.07642399	3.57690335	-4.80214266
6	-0.33946201	2.66096413	-5.77284991
6	-1.00136320	1.50836851	-5.33437551
6	-1.27019612	1.27539448	-3.98104899
7	-1.45429977	-1.34265423	1.45520130
6	-1.61090722	0.95181097	2.38857462
1	-2.28121059	1.58023404	3.00583434
1	-0.71120285	0.74703182	2.98473326
6	-2.32998623	-0.36588528	2.11330953
1	-2.68774347	-0.72899963	3.09830721
1	-3.22854204	-0.20923810	1.50336094
6	-1.97286589	-2.65191247	1.24210713
6	-3.03136541	-2.87075759	0.32986194
6	-3.50098564	-4.17553213	0.12881147
6	-2.94701421	-5.27989803	0.78183433
6	-1.87552046	-5.04671107	1.65200012
6	-1.38251737	-3.76141499	1.89845843
6	0.40629476	4.37363782	-2.44766509
1	0.62387468	4.47127680	-5.11337458
6	-0.09941661	2.91312737	-7.24220939
1	-1.33307163	0.77004000	-6.06953148
6	-2.01764088	0.02885532	-3.57683169
6	-3.62722898	-1.74613567	-0.47925358
1	-4.31369733	-4.32983036	-0.58579870
6	-3.48956368	-6.67218063	0.56620031
1	-1.40822432	-5.89164430	2.16441510
6	-0.22079595	-3.57622093	2.84541537
1	1.22537702	4.94404721	-2.90620147
1	0.78880822	3.86418577	-1.54990659
1	-0.35079481	5.10408668	-2.11868488
1	-1.38024631	-0.67256667	-3.01546862
1	-2.39592557	-0.49905318	-4.46251055
1	-2.86324133	0.27327743	-2.91899630
1	-0.97680824	3.38235918	-7.71587490
1	0.09884179	1.97756498	-7.78382804
1	0.75440174	3.58685521	-7.39784768
1	-4.05537329	-2.13155509	-1.41380976
1	-2.86487089	-0.99676453	-0.73351789
1	-4.44015931	-1.22830585	0.05619429
1	-0.44669321	-2.85755397	3.64789012
1	0.67715660	-3.19926947	2.33112496
1	0.04298750	-4.53221490	3.31525442
1	-2.68715763	-7.42300679	0.57893526
1	-4.01699462	-6.75100462	-0.39407317
1	-4.20511647	-6.94860711	1.35711793
1	-0.56580986	-1.38529145	1.96109157

Energy = -7584.967178 Hartree
 Number of imaginary frequencies = 0.

Compound I2b isomer 58

Atomic N.	X	Y	Z
8	1.96262164	-1.63413853	0.41478488
8	1.15888850	1.33530248	1.97945568
6	2.30435644	2.16180502	1.84245436
1	2.11235578	3.17235022	2.25019197
1	2.63429274	2.29160382	0.79198735
1	3.16066992	1.74228760	2.40454757
8	3.79480000	-2.82626192	0.65441408
6	2.88789204	-1.94674438	1.15440117
6	3.05189378	-1.41868763	2.56276391
1	4.04030005	-0.93755875	2.65933609
1	2.28998133	-0.63475657	2.67497040
6	2.89280706	-2.49766845	3.65611229
1	2.02043266	-3.12731145	3.42184305
1	2.65534185	-1.98084084	4.59791323
6	4.13565666	-3.36638037	3.87240637
1	4.96610845	-2.72429725	4.21509407
1	3.94083025	-4.07903404	4.68892902
6	4.59371450	-4.13720275	2.63017936
1	3.82664127	-4.86160313	2.31195085
1	5.49311767	-4.72390115	2.87913908
6	4.94487446	-3.25503583	1.43658716
1	5.53110160	-2.37365264	1.74330068
1	5.53698862	-3.81756019	0.70442265
50	0.27161170	0.54152457	0.25569932
7	-1.62740167	2.16147287	0.70872688
6	-1.15924591	3.53721516	0.95655013
1	-1.98542532	4.19721073	1.27915887
1	-0.69850405	3.94243636	0.04767352
1	-0.40152684	3.49825971	1.74826514
7	-1.21333362	2.74070876	-2.27088368
6	-2.67677826	2.08373322	-0.34322192
1	-3.65393847	2.36218624	0.09760393
1	-2.75152256	1.03000335	-0.65360698
6	-2.48534038	2.97044075	-1.57385136
1	-3.35129452	2.76697223	-2.23287652
1	-2.56771525	4.02638585	-1.27679297
6	-1.12123593	3.06893692	-3.64758133
6	-1.28145703	4.40339592	-4.08850397
6	-1.16735756	4.68898910	-5.45560855
6	-0.87275325	3.70560648	-6.40424280
6	-0.67419499	2.39895196	-5.94180542
6	-0.79700355	2.06085668	-4.59071146
7	-1.16805321	-0.61082141	1.35593565
6	-2.12321884	1.56604216	1.97892412
1	-3.05278351	2.07754854	2.29746657
1	-1.33923326	1.74518966	2.72863211
6	-2.35597343	0.06572259	1.86442451
1	-2.63011970	-0.28600763	2.87471505
1	-3.24920585	-0.13736296	1.23432980
6	-1.09346184	-2.00019108	1.62776208
6	-1.15436884	-2.95589781	0.57832149
6	-1.08560098	-4.32187730	0.87416889

6	-0.96009468	-4.79555602	2.18559588
6	-0.88148736	-3.84807352	3.21057498
6	-0.93736599	-2.46961629	2.96040739
6	-1.49511033	5.53688684	-3.11513497
1	-1.28711452	5.72584190	-5.78065194
6	-0.78093634	4.03619515	-7.87454537
1	-0.42336397	1.61059072	-6.65610068
6	-0.57689949	0.63244228	-4.15244721
6	-1.29007333	-2.52198569	-0.85981771
1	-1.14107584	-5.03934024	0.05089377
6	-0.92470852	-6.27672031	2.47915665
1	-0.75396808	-4.18852935	4.24252210
6	-0.76807801	-1.50832654	4.11182293
1	-1.22218377	6.49398328	-3.57835743
1	-0.87797675	5.39964639	-2.21476140
1	-2.54253605	5.62202478	-2.78497628
1	0.27930747	0.53205246	-3.46552705
1	-0.37844992	-0.00910163	-5.02000402
1	-1.45436488	0.22132387	-3.62763660
1	-1.73017923	3.82359362	-8.39203959
1	-0.00113345	3.44301278	-8.37225633
1	-0.55428807	5.09952210	-8.03159444
1	-1.62204361	-3.35946058	-1.48806888
1	-0.32914276	-2.16602742	-1.26404255
1	-2.00598727	-1.69433657	-0.96216756
1	-1.73288983	-1.20641682	4.55176737
1	-0.25864694	-0.59133199	3.78146860
1	-0.18554427	-1.97338469	4.91909556
1	-0.25960893	-6.81002981	1.78443906
1	-1.92397798	-6.72914546	2.37825174
1	-0.57699711	-6.47211163	3.50273238
1	-0.87231057	1.79403354	-2.09445479

Energy = -7584.967094 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 59

Atomic N.	X	Y	Z
8	1.76237487	0.12440535	3.03383728
8	2.29315171	1.01082563	-0.91282013
6	3.22429717	0.15558058	-1.54264995
1	3.36035679	0.40830054	-2.61220848
1	2.93591638	-0.91844866	-1.50671277
1	4.21763826	0.24565185	-1.06034144
8	2.46906858	-1.77802107	2.16329707
6	2.69667769	-0.49479885	2.54660311
6	4.08295687	0.09647818	2.38381550
1	4.36611494	0.07489408	1.31886720
1	3.98601901	1.14970730	2.67084426
6	5.16870272	-0.59166631	3.23866675
1	4.77959341	-0.76567618	4.25498874
1	6.00554773	0.11432090	3.34741722
6	5.70456478	-1.89805145	2.64382663
1	6.18219009	-1.67425016	1.67438179
1	6.49934814	-2.29250224	3.29574824
6	4.64354894	-2.98223693	2.42829343
1	4.21621358	-3.31179287	3.38942341
1	5.12131568	-3.86909514	1.98120932

6	3.50090811	-2.57053532	1.50634969
1	3.86460496	-2.03070192	0.61846239
1	2.94538850	-3.45097557	1.16199916
50	0.30475822	0.29108497	-0.74761727
7	-0.12175448	2.36992706	0.57036945
6	1.12465291	3.17803393	0.58955433
1	0.92193009	4.17117012	1.02875508
1	1.52404193	3.28613528	-0.42178238
1	1.87937772	2.65640860	1.18663634
7	-0.64358554	1.64224377	-2.13903908
6	-1.15958331	3.05915170	-0.25053980
1	-1.27215775	4.10097224	0.10555718
1	-2.10890732	2.52958653	-0.09906180
6	-0.82315017	3.02638905	-1.73802349
1	-1.67599858	3.48303012	-2.27627051
1	0.04511262	3.68794810	-1.93523148
6	-0.59891235	1.34174562	-3.52701398
6	0.37566108	1.89121887	-4.40369254
6	0.35768535	1.54575721	-5.76214964
6	-0.57797992	0.65474143	-6.29572593
6	-1.51461788	0.09660084	-5.41812043
6	-1.54663635	0.42512563	-4.05834744
7	-1.48031527	-0.07389295	1.98009948
6	-0.56731950	2.23330588	1.99196495
1	-0.80245364	3.24489471	2.37462353
1	0.29725942	1.86054847	2.55802135
6	-1.76692976	1.33431507	2.27800145
1	-2.01498402	1.48834218	3.34793314
1	-2.65026559	1.65640406	1.71236194
6	-2.48193001	-1.03218290	2.30716900
6	-3.71415949	-1.05577629	1.61322093
6	-4.66718715	-2.02740647	1.94652797
6	-4.43875295	-2.99436941	2.92923440
6	-3.19856441	-2.97708972	3.57829161
6	-2.22198769	-2.01760152	3.29289762
6	1.47314079	2.79492409	-3.89601768
1	1.12079100	1.97350357	-6.41878785
6	-0.59014752	0.31934301	-7.76799578
1	-2.25556952	-0.60843743	-5.80480938
6	-2.60306178	-0.18640133	-3.17183518
6	-4.00616252	-0.10312114	0.48111859
1	-5.61109316	-2.03863224	1.39525687
6	-5.49293160	-4.01438777	3.28642462
1	-2.98201421	-3.73126920	4.33932643
6	-0.90197064	-2.05494819	4.02553315
1	2.32620179	2.78483533	-4.58788525
1	1.81945695	2.47244422	-2.90218128
1	1.14064165	3.84214517	-3.80871778
1	-2.17387877	-0.89215230	-2.44301669
1	-3.34146551	-0.73441016	-3.77238742
1	-3.12121090	0.58609073	-2.58678307
1	-1.31296994	0.94610282	-8.31483719
1	-0.87553320	-0.72807100	-7.93972496
1	0.39570056	0.48508989	-8.22374303
1	-4.73456503	-0.54375752	-0.21208309
1	-3.09264701	0.13065315	-0.08305154
1	-4.43485253	0.84970797	0.83332874
1	-0.66739019	-1.09629821	4.51275458

1	-0.05997840	-2.27779430	3.35155333
1	-0.91957685	-2.83049900	4.80169179
1	-5.04451553	-4.98767607	3.53014324
1	-6.20250024	-4.16136979	2.46094523
1	-6.07480621	-3.69593450	4.16620003
1	-0.58593663	-0.32785367	2.40767815

Energy = -7584.967160 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 60

Atomic N.	X	Y	Z
8	1.26031915	-2.10447076	0.82680479
8	1.98610412	1.24453741	1.24575517
6	3.29446568	1.41517837	0.72326423
1	3.57340506	2.48570499	0.69394426
1	3.41622175	1.01900973	-0.30509159
1	4.03933110	0.90332510	1.36197784
8	2.53359589	-3.82495788	1.33130062
6	2.14861654	-2.54024421	1.54916753
6	2.80730363	-1.73539533	2.64808388
1	3.89760803	-1.71123011	2.47948054
1	2.43165599	-0.70965044	2.52874497
6	2.51528459	-2.26430758	4.06930073
1	1.44445894	-2.50604421	4.15479587
1	2.70191198	-1.43968988	4.77331258
6	3.36890454	-3.46670328	4.48368813
1	4.43083026	-3.16424229	4.49729039
1	3.11659607	-3.75003762	5.51742234
6	3.22083958	-4.69172099	3.57561457
1	2.19157442	-5.08398480	3.60925497
1	3.87464915	-5.49825816	3.94595477
6	3.59162053	-4.44215054	2.11737788
1	4.51238286	-3.84275175	2.03081992
1	3.75579419	-5.39250460	1.59490948
50	0.50271283	0.42416482	0.01457811
7	-0.50482980	2.75161715	-0.00947613
6	0.48319880	3.79884626	-0.32651673
1	0.05724097	4.81169017	-0.20431421
1	0.84170349	3.67247107	-1.35514016
1	1.33095335	3.68136960	0.35902982
7	-0.59672382	2.16716541	-3.01531560
6	-1.71818655	2.81663342	-0.86823556
1	-2.39341907	3.60554468	-0.48300981
1	-2.24789355	1.85755053	-0.75951515
6	-1.49743649	3.11775428	-2.35076708
1	-2.50276767	3.11535904	-2.81431289
1	-1.11239765	4.14244110	-2.45970553
6	-0.70756683	1.98961770	-4.41808005
6	-0.45800843	3.06053773	-5.30769585
6	-0.56257827	2.84013761	-6.68765460
6	-0.87928386	1.58913330	-7.22447822
6	-1.07927351	0.53190215	-6.32828340
6	-1.00564371	0.70643981	-4.94311205
7	-0.97199557	0.38841606	1.57486142
6	-0.88276752	2.83957886	1.42706701
1	-1.45710112	3.76912322	1.60943913
1	0.06026144	2.88292957	1.99061505

6	-1.67520848	1.62600561	1.89341048
1	-1.82286473	1.74806973	2.98098674
1	-2.69805224	1.64445022	1.45801032
6	-1.35637303	-0.74503936	2.33469903
6	-2.00382201	-1.85139047	1.72360870
6	-2.37932615	-2.95503910	2.49871629
6	-2.14231110	-3.01381545	3.87663043
6	-1.48498341	-1.92958232	4.46688668
6	-1.08327456	-0.80784896	3.72899407
6	-0.00701318	4.41215742	-4.81012234
1	-0.36058962	3.67556966	-7.36315900
6	-1.01062705	1.38486120	-8.71464434
1	-1.30981293	-0.46325725	-6.71710764
6	-1.23712996	-0.47077030	-4.02578120
6	-2.29301382	-1.86172354	0.24333310
1	-2.88234769	-3.79265979	2.00793585
6	-2.59860168	-4.19615885	4.69813880
1	-1.25831175	-1.96164864	5.53683826
6	-0.31058313	0.28779061	4.42257413
1	0.48824545	4.96946407	-5.61587344
1	0.70303033	4.30403299	-3.97675974
1	-0.84257481	5.03334574	-4.45050026
1	-0.34604676	-0.71526909	-3.42476344
1	-1.49668834	-1.36478824	-4.60629573
1	-2.05816482	-0.28515911	-3.31458314
1	-2.06444577	1.43163398	-9.03281444
1	-0.62330865	0.40333567	-9.02194214
1	-0.46556016	2.15775847	-9.27330568
1	-3.05118789	-2.61865843	0.00135682
1	-1.38979531	-2.10044622	-0.34040698
1	-2.64666171	-0.88018584	-0.10219389
1	0.41335423	0.74877564	3.73487194
1	0.22451036	-0.11152250	5.29522501
1	-0.96638029	1.09224618	4.79444534
1	-2.01663501	-4.28723362	5.62578813
1	-2.50151911	-5.13703320	4.13826177
1	-3.65784062	-4.09881477	4.98552210
1	-0.59975611	1.26871309	-2.52913200

Energy = -7584.967097 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 61

Atomic N.	X	Y	Z
8	1.92507909	-2.87170211	1.17257934
8	2.22711355	-0.14617527	-2.14398516
6	1.86750664	-0.16817328	-3.51455471
1	1.14261557	0.62113641	-3.78194615
1	1.42417938	-1.14449935	-3.79535919
1	2.76424666	-0.02234197	-4.14370094
8	2.67675445	-3.47654520	-0.81879341
6	2.81942386	-2.78544145	0.34611117
6	4.07693623	-1.96624643	0.56889998
1	4.14459591	-1.19320756	-0.21495227
1	3.92068884	-1.44986635	1.52298501
6	5.37841763	-2.79477554	0.61031990
1	5.21555127	-3.70748241	1.20632443
1	6.13412606	-2.20590427	1.15158440

6	5.93478478	-3.15405931	-0.77122551
1	6.18288881	-2.21998136	-1.30386335
1	6.88186174	-3.70277480	-0.64956125
6	4.98190899	-3.97720717	-1.64419888
1	4.80220179	-4.96981899	-1.19946301
1	5.45656520	-4.15679363	-2.62285510
6	3.63359209	-3.31428713	-1.90784899
1	3.72471425	-2.24253412	-2.14375582
1	3.12851042	-3.80723204	-2.74815357
50	1.38975572	0.97446627	-0.60822435
7	-0.71241804	-0.32773337	-0.73892300
6	-0.47362920	-1.76545947	-1.01696360
1	-1.42511153	-2.26930141	-1.26035411
1	-0.01366058	-2.25620446	-0.15303294
1	0.21988960	-1.85503609	-1.86007171
7	-1.82264589	-0.43752560	2.94062578
6	-1.57619936	-0.16675075	0.46565746
1	-2.47073059	-0.80628615	0.34486231
1	-1.91842019	0.87762637	0.49072229
6	-0.89229025	-0.49802911	1.80506017
1	-0.42843713	-1.48917649	1.77389032
1	-0.07797401	0.21769679	1.99643929
6	-2.85276956	-1.41108962	3.04500012
6	-2.53075944	-2.77198978	3.26934051
6	-3.57167726	-3.70099931	3.39501138
6	-4.92039174	-3.33378217	3.34423416
6	-5.21586493	-1.97550334	3.18165919
6	-4.21288975	-1.01263707	3.02719430
7	0.06357413	2.27318294	-1.69040533
6	-1.36302021	0.30065880	-1.92909723
1	-2.41003964	-0.04649992	-2.00596034
1	-0.81831914	-0.06234952	-2.81088726
6	-1.30836532	1.82512284	-1.89982791
1	-1.69595472	2.17605382	-2.87693279
1	-2.02194259	2.21331182	-1.14490225
6	0.27092500	3.68309946	-1.62075336
6	-0.26497783	4.48777372	-0.57966754
6	-0.02179101	5.86883696	-0.57214401
6	0.75313540	6.49503596	-1.55094288
6	1.29856933	5.69026222	-2.55807763
6	1.07444987	4.31045455	-2.61043093
6	-1.10507283	-3.23149570	3.45342936
1	-3.31082922	-4.74774315	3.57193978
6	-6.01742675	-4.36480468	3.45758953
1	-6.25975614	-1.65172837	3.16709407
6	-4.59382741	0.44003431	2.85962060
6	-1.05226653	3.89457899	0.56287150
1	-0.44006310	6.46860963	0.24089386
6	1.02812341	7.97884744	-1.50515563
1	1.91246785	6.15127945	-3.33650602
6	1.68391782	3.50583782	-3.73126335
1	-1.08041806	-4.15205021	4.05137227
1	-0.50893281	-2.46388134	3.96642804
1	-0.59331438	-3.45243848	2.50390288
1	-4.21388354	1.07055926	3.68104756
1	-5.68521210	0.55126503	2.84856283
1	-4.20789037	0.86657068	1.91950748
1	-6.33232591	-4.72400549	2.46465084

1	-6.90809244	-3.95177333	3.95096864
1	-5.68443046	-5.24141661	4.02988874
1	-0.99079395	4.54093531	1.44817803
1	-0.66178565	2.90217542	0.83426837
1	-2.12031407	3.77408988	0.31995337
1	0.92414616	2.90664640	-4.25144171
1	2.44093165	2.79709259	-3.36310858
1	2.16867164	4.16799711	-4.46082045
1	2.03148976	8.18513443	-1.09997367
1	0.30148416	8.50114452	-0.86875392
1	0.98801633	8.42517017	-2.50897331
1	-2.20689541	0.50205337	3.02714390

Energy = -7584.967112 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 62

Atomic N.	X	Y	Z
8	2.72829622	-3.45643834	-0.19578678
8	1.82813444	0.22549545	-1.96911418
6	1.89985070	0.46690752	-3.36105046
1	1.02909473	1.02600844	-3.74940861
1	1.97244819	-0.48213786	-3.92974803
1	2.80157501	1.06119016	-3.60118405
8	3.97031914	-2.68435339	-1.85783953
6	3.50053529	-2.59518506	-0.57883010
6	3.97858123	-1.45292598	0.29897099
1	3.71157264	-0.49637644	-0.18028742
1	3.39300680	-1.53054488	1.22254103
6	5.48753911	-1.49256750	0.62183679
1	5.78459422	-2.52565099	0.86596091
1	5.65238539	-0.90168975	1.53547337
6	6.38121409	-0.93241515	-0.48967435
1	6.13588637	0.13388483	-0.63361863
1	7.43240360	-0.96740967	-0.16280024
6	6.24456805	-1.65061050	-1.83638218
1	6.58785554	-2.69549911	-1.76148710
1	6.90082622	-1.15931265	-2.57348031
6	4.82964198	-1.64660418	-2.40860946
1	4.33743643	-0.66935710	-2.28819030
1	4.85219365	-1.89005600	-3.47843981
50	0.28028026	0.63274269	-0.61911420
7	-0.98596503	-1.29072991	-1.61286427
6	-0.08463319	-2.43922145	-1.86486179
1	-0.58724181	-3.19783045	-2.49110292
1	0.23218429	-2.90030749	-0.92438132
1	0.81659242	-2.07710661	-2.37130245
7	-1.62891293	-1.21539391	1.45806338
6	-2.21602734	-1.72805895	-0.89823024
1	-2.70718572	-2.51449806	-1.50349652
1	-2.90461969	-0.87078721	-0.87351519
6	-2.04313998	-2.26798968	0.52005639
1	-3.01583793	-2.71689629	0.80580058
1	-1.31050742	-3.08379604	0.54067362
6	-1.57404789	-1.54569643	2.84383916
6	-0.60779268	-2.45393510	3.33363643
6	-0.57553827	-2.73127340	4.70653287
6	-1.44621952	-2.12441144	5.61701299

6	-2.36497200	-1.19516013	5.11571148
6	-2.44904167	-0.89966872	3.75132168
7	-1.18152005	1.55510719	-1.91237081
6	-1.37098074	-0.67161832	-2.91639714
1	-2.05575580	-1.34729117	-3.46343754
1	-0.44833315	-0.58100324	-3.50217376
6	-2.01059153	0.70754688	-2.75913880
1	-2.10532872	1.12905549	-3.78009345
1	-3.05086729	0.59743755	-2.39250662
6	-1.62640399	2.88464751	-1.67287644
6	-2.85603097	3.17829521	-1.02356373
6	-3.23815873	4.51178273	-0.81615529
6	-2.43763279	5.58686759	-1.20509343
6	-1.21161257	5.28973907	-1.81299316
6	-0.79667804	3.97654437	-2.05458664
6	0.42362538	-3.07772601	2.42866535
1	0.17968176	-3.43026281	5.07507480
6	-1.40440844	-2.46618855	7.08687663
1	-3.04374243	-0.68660003	5.80498748
6	-3.45628350	0.11844181	3.26783032
6	-3.74599852	2.09044256	-0.47747587
1	-4.18681521	4.70990318	-0.30944782
6	-2.86270916	7.01566965	-0.96643994
1	-0.55787861	6.10916469	-2.12394224
6	0.52192600	3.74476339	-2.75027050
1	1.31479625	-3.36571119	3.00045742
1	0.73553741	-2.38242092	1.63816291
1	0.05846433	-3.99181606	1.93416466
1	-2.97155803	1.01047341	2.83695508
1	-4.08154040	0.46389731	4.10041979
1	-4.13028882	-0.29271001	2.49906364
1	-2.10854102	-3.27898443	7.32654659
1	-1.68050072	-1.60317722	7.70822636
1	-0.40370716	-2.80179556	7.39117653
1	-4.34519998	2.46706626	0.36211802
1	-3.13936444	1.24463106	-0.12157764
1	-4.44894087	1.69585846	-1.22873082
1	0.38780618	3.15072846	-3.66484860
1	1.24044160	3.19369998	-2.12447470
1	0.98388693	4.70284578	-3.02262169
1	-2.15021088	7.54262380	-0.31369403
1	-3.85191902	7.06303081	-0.49244564
1	-2.91281422	7.58147839	-1.90914047
1	-2.24118295	-0.40877033	1.33313996

Energy = -7584.964663 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 63

Atomic N.	X	Y	Z
8	1.78743642	-3.55110633	-2.56503452
8	2.85520702	1.31675936	0.50053017
6	3.90456811	2.24178438	0.27300549
1	3.55400998	3.28988521	0.17963555
1	4.45954561	1.99814619	-0.65415045
1	4.62348687	2.21010201	1.11035402
8	3.68541332	-3.08903701	-1.52190013
6	2.56196060	-3.85055971	-1.67461061

6	2.34345544	-5.03502256	-0.74878889
1	2.33292971	-4.69376847	0.29981240
1	1.33847564	-5.40364192	-0.98436093
6	3.38103434	-6.16527379	-0.91876322
1	3.55395601	-6.34150469	-1.99270064
1	2.93884530	-7.09146433	-0.52239452
6	4.70966903	-5.90920413	-0.19984090
1	4.51788246	-5.84837424	0.88542498
1	5.37229227	-6.77623791	-0.34655970
6	5.43998415	-4.63617258	-0.64065086
1	5.74662671	-4.70444469	-1.69717876
1	6.36745850	-4.53372742	-0.05418536
6	4.64060764	-3.35028559	-0.45462048
1	4.12370499	-3.32751940	0.51803459
1	5.30197410	-2.47668688	-0.50130411
50	0.86978796	1.90243930	0.28926679
7	0.63354575	0.43989736	-1.71721535
6	2.01020559	0.04565974	-2.12109473
1	1.97504557	-0.77188991	-2.85848027
1	2.58456337	-0.26434087	-1.24325538
1	2.51550815	0.91770068	-2.55667654
7	0.15690031	0.05753185	1.08681780
6	-0.10852966	-0.74236515	-1.18748059
1	0.01589456	-1.59765639	-1.87536163
1	-1.16815787	-0.46850550	-1.12654046
6	0.36096757	-1.09907571	0.22243299
1	-0.25343324	-1.94874806	0.57090711
1	1.40501909	-1.46621595	0.17905880
6	0.00989323	-0.13491946	2.48231034
6	0.92569479	-0.89341502	3.26160413
6	0.69108128	-1.06662255	4.63222678
6	-0.40420361	-0.49205062	5.28399626
6	-1.27345628	0.29100206	4.51626477
6	-1.09305340	0.47596241	3.14112516
7	-1.80646690	2.33682220	-1.76785615
6	-0.02011314	1.03391094	-2.92179629
1	0.10240755	0.33315016	-3.76890223
1	0.55646131	1.93918960	-3.17179302
6	-1.50432037	1.38288229	-2.84131893
1	-1.77476120	1.78307987	-3.83918427
1	-2.10127193	0.47143831	-2.70906271
6	-3.07429563	2.98119346	-1.77129495
6	-4.26945671	2.24573440	-1.59966071
6	-5.49244776	2.92985290	-1.58716487
6	-5.57709696	4.31949584	-1.71088979
6	-4.37868937	5.03270381	-1.83539905
6	-3.13591839	4.39383374	-1.87251828
6	2.19998749	-1.44274065	2.66604476
1	1.41239709	-1.64765383	5.21427517
6	-0.64755575	-0.71868650	6.75692154
1	-2.13376076	0.76330993	4.99837943
6	-2.07978594	1.31688756	2.37088692
6	-4.25994182	0.75559816	-1.36269657
1	-6.40843964	2.35009908	-1.44731430
6	-6.91071581	5.02688273	-1.71778218
1	-4.40913905	6.12252176	-1.91190544
6	-1.87482764	5.21601970	-2.00488337
1	2.92227031	-1.66800047	3.46238964

1	2.65095444	-0.71513904	1.97368396
1	2.03050778	-2.37647247	2.10415354
1	-1.67062888	2.31019018	2.12075484
1	-2.99443806	1.47838463	2.95654340
1	-2.33715643	0.84538885	1.41305259
1	-1.30701148	-1.58546263	6.92544139
1	-1.13032465	0.15140254	7.22324634
1	0.29191324	-0.91610688	7.29177465
1	-5.18300997	0.44426645	-0.85702483
1	-3.40764927	0.46455556	-0.73187219
1	-4.19370010	0.17864342	-2.29906143
1	-1.28375155	4.93050875	-2.89034434
1	-1.21585139	5.11258151	-1.12688053
1	-2.11988160	6.28079302	-2.10279189
1	-6.85534559	5.99458888	-1.20001562
1	-7.68637388	4.42151941	-1.22974149
1	-7.25023174	5.22813966	-2.74639397
1	-1.06633719	3.03765944	-1.72165788

Energy = -7584.964792 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 64

Atomic N.	X	Y	Z
8	2.18662393	-0.27896717	-0.98919009
8	0.93821725	2.30622831	0.30264210
6	1.09011256	2.92705247	1.56392639
1	0.73748528	2.30312143	2.41351468
1	0.52870426	3.87919272	1.60481253
1	2.15375483	3.16583573	1.75952589
8	3.64375267	0.92138975	-2.12222760
6	3.15039518	0.47986583	-0.94120932
6	3.82108603	0.89253202	0.34967524
1	3.77589815	1.98910016	0.44399581
1	3.19772171	0.47921383	1.15004504
6	5.27748585	0.39935381	0.48939539
1	5.34525971	-0.65033621	0.16060679
1	5.52809376	0.40116773	1.56061137
6	6.30515119	1.25719604	-0.25602466
1	6.28406159	2.27746642	0.16442069
1	7.31523347	0.86449674	-0.06172272
6	6.08073563	1.34504371	-1.76891135
1	6.20667605	0.35803287	-2.24314815
1	6.84840017	2.00134231	-2.21031288
6	4.72060983	1.90247697	-2.17367138
1	4.43884581	2.78069268	-1.57272725
1	4.72531880	2.20016010	-3.22914087
50	-0.20578501	0.56603409	0.18159355
7	-0.78755628	-1.77007395	-1.35260223
6	0.20837251	-2.84736691	-1.40890939
1	-0.08982746	-3.65728461	-2.10524540
1	0.35756534	-3.26809915	-0.40701961
1	1.16046760	-2.42275838	-1.74643995
7	-1.49319051	-2.79261080	1.44132881
6	-2.12134326	-2.24099122	-0.92487270
1	-2.64563121	-2.71607962	-1.78126838
1	-2.71696089	-1.35731835	-0.64072356
6	-2.15633500	-3.25893709	0.21564427

1	-3.22528744	-3.48136557	0.39741395
1	-1.70110417	-4.20008249	-0.12666220
6	-1.88752177	-3.35319392	2.68084417
6	-1.70607062	-4.73284864	2.94068393
6	-2.09560941	-5.25267561	4.18204045
6	-2.63617099	-4.45299998	5.19319034
6	-2.76764383	-3.08366492	4.93319975
6	-2.41229427	-2.52162487	3.70296274
7	-0.99783585	1.19962749	-1.66997824
6	-0.87279613	-1.08212192	-2.65421415
1	-1.36000483	-1.73750689	-3.40837430
1	0.15826413	-0.88677685	-2.98076516
6	-1.61704875	0.25072617	-2.59522416
1	-1.61472656	0.66286895	-3.61759137
1	-2.68676485	0.07991694	-2.35482549
6	-1.07455880	2.56814775	-2.06347215
6	-1.92482486	3.47068462	-1.37841869
6	-1.99818212	4.80619227	-1.79355612
6	-1.24925078	5.29164327	-2.87034026
6	-0.40999307	4.39206001	-3.53545224
6	-0.30437409	3.04901983	-3.15344766
6	-1.03141616	-5.64097648	1.94191065
1	-1.94235421	-6.31890314	4.36891319
6	-3.07354524	-5.04400603	6.51194847
1	-3.17100634	-2.42790639	5.70920010
6	-2.58772514	-1.03872028	3.48081035
6	-2.76128614	3.02322912	-0.20391571
1	-2.66780637	5.48620768	-1.26005566
6	-1.31790090	6.74416034	-3.27782228
1	0.19685911	4.74726170	-4.37315173
6	0.65400931	2.14612445	-3.88857184
1	-0.64057895	-6.53606460	2.44327923
1	-0.19442698	-5.12444045	1.44916904
1	-1.71558075	-5.98359769	1.14960175
1	-1.62704652	-0.52559236	3.31097260
1	-3.06070073	-0.57215050	4.35410390
1	-3.21818640	-0.82438049	2.60293702
1	-4.15195147	-5.27033707	6.51043191
1	-2.88940870	-4.35073201	7.34451283
1	-2.54357967	-5.98248736	6.72475034
1	-3.56826117	3.74187161	-0.00700617
1	-2.15954706	2.95256468	0.71726669
1	-3.20571470	2.03284025	-0.37310354
1	0.14536245	1.52977836	-4.64811859
1	1.15488521	1.45616366	-3.19688976
1	1.41486969	2.73882097	-4.41413243
1	-0.54378549	7.33795989	-2.76565742
1	-2.29027150	7.18663095	-3.02108634
1	-1.15972521	6.86658070	-4.35831086
1	-1.46978044	-1.77209746	1.47363004

Energy = -7584.957819 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 65

Atomic N.	X	Y	Z
8	2.74981946	-1.58026390	-0.09156083
8	1.11644074	-2.49819345	-2.69052168

6	2.36083145	-2.45997608	-3.36889891
1	2.67430606	-1.43545078	-3.65599923
1	2.29481081	-3.05517317	-4.29742098
1	3.16684563	-2.88765983	-2.74574854
8	4.50742025	-1.71348295	1.22740953
6	3.47950541	-1.00014591	0.69939263
6	3.28951979	0.44732576	1.11037757
1	4.21332560	1.01293488	0.90123741
1	2.50807835	0.84032398	0.44797474
6	2.88203065	0.63462514	2.58773316
1	2.10214258	-0.09893158	2.84401516
1	2.41817129	1.62776256	2.68334984
6	4.04808321	0.53820202	3.57600130
1	4.76138708	1.35603933	3.37148795
1	3.66924799	0.70830568	4.59563480
6	4.80436458	-0.79370733	3.53550878
1	4.14582214	-1.62883539	3.82367654
1	5.62004083	-0.76836934	4.27644826
6	5.43092106	-1.12075718	2.18367410
1	5.91012928	-0.23561099	1.73421688
1	6.19515827	-1.89976672	2.29306249
50	0.48422741	-0.84647622	-1.61757815
7	-1.81771021	-1.23267793	-2.87151710
6	-1.49901242	-2.09287647	-4.03451994
1	-2.42837165	-2.43061197	-4.52978327
1	-0.89911929	-2.95006051	-3.71427774
1	-0.89602151	-1.52326916	-4.75336644
7	-0.74094519	-2.00739803	-0.30064513
6	-2.59134653	-2.00971434	-1.86617480
1	-3.35853112	-2.62333179	-2.37925366
1	-3.09487832	-1.30090168	-1.19826936
6	-1.67361446	-2.88216805	-1.00534177
1	-2.30848190	-3.42237002	-0.28216282
1	-1.18935949	-3.65214884	-1.63711114
6	-0.33756837	-2.35811578	1.00862573
6	0.21968759	-3.62625005	1.32972119
6	0.56233196	-3.91426854	2.65701404
6	0.40217814	-2.98503072	3.69102096
6	-0.10729725	-1.72522930	3.35560277
6	-0.47950957	-1.39754101	2.04521584
7	-1.93063653	1.73002648	-1.76668560
6	-2.57904890	-0.06313745	-3.39270071
1	-3.48722081	-0.43521230	-3.90894594
1	-1.94622576	0.40506551	-4.16333798
6	-3.03741809	1.00993455	-2.40675148
1	-3.66333612	1.70522073	-2.99607452
1	-3.70429614	0.56651908	-1.65175094
6	-2.05985963	3.10504294	-1.47029471
6	-3.11497952	3.58384197	-0.65673300
6	-3.19497588	4.95539302	-0.38177514
6	-2.25254737	5.87350070	-0.85436205
6	-1.18957522	5.37269070	-1.61569238
6	-1.07689486	4.01646713	-1.93543948
6	0.51770938	-4.63966586	0.25264081
1	0.99608295	-4.89284039	2.88210721
6	0.75025148	-3.33733887	5.11814060
1	-0.24350260	-0.97716360	4.14208920
6	-1.04974516	-0.03298972	1.75026140

6	-4.10512770	2.64514125	-0.01001954
1	-4.01283271	5.30880841	0.25171443
6	-2.38116410	7.34983461	-0.56544051
1	-0.42469049	6.06073409	-1.98518561
6	0.08695313	3.53701445	-2.76978558
1	1.24771243	-5.37596662	0.61396017
1	0.92321573	-4.14876085	-0.64442841
1	-0.38120194	-5.19545395	-0.05898773
1	-0.37647078	0.57924110	1.12863108
1	-1.24114097	0.51927302	2.68029175
1	-1.98433776	-0.11280809	1.17801380
1	-0.05977077	-3.90775210	5.60037644
1	0.92019487	-2.43638700	5.72390093
1	1.65524093	-3.96010977	5.16895798
1	-4.61417917	3.14554020	0.82381385
1	-3.59792736	1.75178374	0.38317312
1	-4.88402376	2.29796076	-0.70652968
1	-0.24551681	3.04165216	-3.69705577
1	0.71830340	2.81057124	-2.23188537
1	0.72698506	4.38052350	-3.05734699
1	-1.39693666	7.82418425	-0.44719953
1	-2.95924496	7.52891793	0.35144395
1	-2.89796451	7.87451473	-1.38512104
1	-1.04491665	1.52743397	-2.22823718

Energy = -7584.962464 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 66

Atomic N.	X	Y	Z
8	0.65560993	-0.04822846	0.55545541
8	2.91450179	0.27369694	-1.57195152
6	3.33444769	1.44602199	-0.88778915
1	3.60955714	2.25251207	-1.58899504
1	4.23046042	1.20606428	-0.28580106
1	2.56427281	1.84347354	-0.20518164
8	1.58571497	-0.18359831	2.54277215
6	1.25102972	-0.75590928	1.36407446
6	1.62389020	-2.19674815	1.09786412
1	1.22758332	-2.83337053	1.90617553
1	1.09893160	-2.47331664	0.17547793
6	3.14407105	-2.42023145	0.93833182
1	3.55522019	-1.63363010	0.28587985
1	3.28344450	-3.36886716	0.39882384
6	3.90121594	-2.49441699	2.26806758
1	3.54700957	-3.37559608	2.83128912
1	4.96941719	-2.66747743	2.06565696
6	3.75417354	-1.25670045	3.16062010
1	4.18981632	-0.36773386	2.67641136
1	4.32345427	-1.41467176	4.09113301
6	2.31854634	-0.92996346	3.55978875
1	1.74994534	-1.83337002	3.83075834
1	2.30168498	-0.24631786	4.41680677
50	1.07330200	-0.39607070	-2.19156358
7	-1.95500505	-0.82291633	-2.53808884
6	-2.11255770	-2.18298219	-3.05090602
1	-3.03769460	-2.30703596	-3.65411845
1	-2.13423979	-2.90147046	-2.22279053

1	-1.24797759	-2.43123346	-3.68173553
7	-2.13950070	-1.38327943	0.41763035
6	-3.07605456	-0.42849651	-1.67552307
1	-4.02613903	-0.40299856	-2.25797675
1	-2.88895412	0.60001105	-1.33163087
6	-3.32054125	-1.31244326	-0.45115556
1	-4.19878812	-0.88613170	0.07436426
1	-3.61390632	-2.32623294	-0.76216278
6	-2.31234140	-1.88262470	1.73607216
6	-2.47628204	-3.27226409	1.94931688
6	-2.59106403	-3.75628673	3.25833889
6	-2.53368150	-2.91204768	4.37295376
6	-2.35526099	-1.54245715	4.14373401
6	-2.25744963	-1.01002316	2.85213946
7	0.13003184	1.43796755	-2.70210619
6	-1.79089898	0.12529773	-3.65220273
1	-2.75616348	0.28607920	-4.18282624
1	-1.10010130	-0.33931499	-4.37471933
6	-1.22304721	1.48937194	-3.26214839
1	-1.21731643	2.09372944	-4.19010068
1	-1.92762563	2.00995646	-2.58366327
6	0.72649173	2.73009899	-2.58478187
6	0.33981278	3.62661059	-1.55733678
6	0.92879147	4.89618577	-1.49144262
6	1.89260984	5.31721272	-2.41276520
6	2.26481743	4.42172672	-3.42173617
6	1.70711275	3.14129389	-3.52224897
6	-2.47604145	-4.23732461	0.79099975
1	-2.70901415	-4.83276009	3.40854510
6	-2.69101898	-3.45600765	5.77292347
1	-2.31258346	-0.85892952	4.99587892
6	-2.11201953	0.48235038	2.66553404
6	-0.67482842	3.23071807	-0.51293487
1	0.62865765	5.57193061	-0.68586877
6	2.53813507	6.67795374	-2.30265296
1	3.01681573	4.72598792	-4.15466202
6	2.17959417	2.21229486	-4.61353313
1	-2.22782345	-5.25192852	1.12910655
1	-1.74574080	-3.92439800	0.03036108
1	-3.45813877	-4.29090620	0.29429823
1	-1.12988053	0.76341252	2.25430785
1	-2.22644907	1.00016637	3.62619932
1	-2.87424280	0.87896492	1.97723607
1	-3.74920951	-3.46474197	6.07951710
1	-2.14581957	-2.84551189	6.50575650
1	-2.32413863	-4.48920227	5.84552301
1	-0.52631361	3.80880016	0.40882266
1	-0.59227924	2.16244890	-0.27361673
1	-1.70624969	3.41982895	-0.85264921
1	1.34231725	1.69237678	-5.09895613
1	2.84583716	1.43491482	-4.20588565
1	2.74170059	2.76669042	-5.37674400
1	3.47816843	6.62612814	-1.73036637
1	1.88130475	7.39312974	-1.78912248
1	2.78361983	7.08651132	-3.29285543
1	-1.65873617	-0.48375079	0.43035008

Energy = -7584.957766 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 67

Atomic N.	X	Y	Z
8	1.16631547	-3.28390000	0.05882838
8	0.86185029	-0.63311506	-2.01246100
6	2.16822418	-1.05555851	-2.38076338
1	2.56670840	-0.41738744	-3.18975737
1	2.19726173	-2.10119112	-2.74759980
1	2.86130802	-0.99293494	-1.52201011
8	1.95915566	-1.47675568	1.05564178
6	1.67792086	-2.79687061	1.06198167
6	2.03339730	-3.63449986	2.27314570
1	1.51271466	-3.23273577	3.15773123
1	1.61768636	-4.62868049	2.07520363
6	3.54996345	-3.72800625	2.54598668
1	4.08303280	-3.90111237	1.59709901
1	3.72491248	-4.62130441	3.16401723
6	4.13312084	-2.50941934	3.26932434
1	3.65457927	-2.42599805	4.26044578
1	5.20470229	-2.67890262	3.45754402
6	3.95508129	-1.18152892	2.52555350
1	4.51303527	-1.18560718	1.57491542
1	4.38339022	-0.36814098	3.13350191
6	2.50535138	-0.81127862	2.23053144
1	1.84622738	-0.99737873	3.09268143
1	2.42479907	0.24944737	1.96427957
50	-0.55093957	-2.18562187	-1.86140928
7	-2.18235546	-0.55416173	-2.87889990
6	-3.08485873	-1.43236890	-3.65194037
1	-3.90655410	-0.85204907	-4.10963682
1	-3.51429446	-2.20201194	-2.99782380
1	-2.51717522	-1.93981198	-4.44312749
7	-1.76730073	-1.50927577	-0.20944343
6	-2.89191416	0.06304724	-1.72874358
1	-3.87731063	0.45815923	-2.04260083
1	-2.26148923	0.88496788	-1.36915538
6	-3.05579500	-0.93135781	-0.58174701
1	-3.49041973	-0.37294361	0.26659610
1	-3.81919555	-1.70084436	-0.84097921
6	-1.65696231	-1.86879376	1.15893865
6	-1.84195739	-3.20259342	1.60575572
6	-1.73879844	-3.49905334	2.97237491
6	-1.45928225	-2.51620291	3.92870980
6	-1.26389344	-1.20531640	3.47664115
6	-1.35761287	-0.86570643	2.12019526
7	-0.44933836	2.01761850	-2.19411355
6	-1.52302907	0.41827771	-3.81776279
1	-2.13427815	0.47952847	-4.73446074
1	-0.54683442	-0.00896456	-4.09508431
6	-1.33448744	1.86388080	-3.35105992
1	-0.94373384	2.40617427	-4.23578673
1	-2.32151785	2.30328558	-3.13987564
6	0.04854732	3.30738739	-1.89501918
6	-0.82900241	4.36716556	-1.55197007
6	-0.30063820	5.63134439	-1.25752651
6	1.07252930	5.88981025	-1.25765593
6	1.92749026	4.82125650	-1.55197064

6	1.44765379	3.54807311	-1.87474430
6	-2.14545509	-4.31412810	0.63144008
1	-1.89691216	-4.53080616	3.29908138
6	-1.40496311	-2.85176454	5.40074101
1	-1.03297141	-0.41896429	4.20147773
6	-1.11790867	0.55635189	1.68154945
6	-2.31699087	4.15534088	-1.41210148
1	-0.99416884	6.43305910	-0.98940693
6	1.61332603	7.26853163	-0.96395068
1	3.00877140	4.98324646	-1.54473017
6	2.42307211	2.44459173	-2.19598087
1	-2.56237888	-5.18577889	1.15398767
1	-1.23562924	-4.64367645	0.10548742
1	-2.85761671	-3.99238105	-0.14031593
1	-0.51604852	0.58300126	0.76287673
1	-0.61593631	1.13178976	2.47132861
1	-2.06146028	1.07727035	1.45113759
1	-2.40164293	-2.77620277	5.86405738
1	-0.74270743	-2.16441526	5.94569889
1	-1.04819206	-3.87779283	5.56768086
1	-2.75176169	4.92852020	-0.76499096
1	-2.53273159	3.17260353	-0.96878112
1	-2.84822769	4.20451141	-2.37623377
1	2.23229851	2.01100007	-3.18984002
1	2.35689493	1.61304911	-1.47830103
1	3.45264219	2.82472564	-2.18375184
1	2.55913216	7.21999750	-0.40610704
1	0.89925825	7.86090800	-0.37551705
1	1.81368101	7.82620652	-1.89307297
1	0.24863656	1.26116588	-2.15595812

Energy = -7584.962923 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 68

Atomic N.	X	Y	Z
8	0.56844085	-0.57285623	0.29837996
8	2.76830477	0.11378737	-1.80719045
6	3.62265563	0.47288124	-0.73010312
1	4.20524535	1.38247655	-0.95603712
1	4.34098139	-0.34947887	-0.55484894
1	3.07475917	0.65046487	0.21081235
8	1.39652977	-2.09635306	1.64988104
6	0.84167425	-1.75912243	0.46355122
6	0.59816128	-2.82545282	-0.58037181
1	-0.00362103	-3.63814594	-0.14086128
1	-0.01292792	-2.34726566	-1.35543930
6	1.89629461	-3.39446673	-1.19490268
1	2.57430143	-2.56010844	-1.43524561
1	1.63012076	-3.85963053	-2.15573839
6	2.58897558	-4.44123055	-0.31667165
1	1.92376730	-5.31638481	-0.21275964
1	3.49356034	-4.80131887	-0.83049391
6	2.96992425	-3.95220700	1.08543531
1	3.71267788	-3.13986173	1.03123079
1	3.45093458	-4.77733275	1.63561345
6	1.79428828	-3.47166603	1.93043034
1	0.91884738	-4.13269211	1.83202842

1	2.07204419	-3.42873549	2.99021717
50	0.81484900	0.57398133	-2.25070503
7	-2.12274940	1.46301969	-2.06943731
6	-2.81927923	0.77887008	-3.15775801
1	-3.71627524	1.33481049	-3.50619030
1	-3.12888022	-0.22392935	-2.83998647
1	-2.13086450	0.65954313	-4.00562493
7	-2.52445709	-0.56995663	0.11974054
6	-2.98671366	1.64929708	-0.89656740
1	-3.84308211	2.31793335	-1.14567517
1	-2.39710182	2.16599751	-0.12426930
6	-3.57214369	0.37363101	-0.28815832
1	-4.20066163	0.69317107	0.56748576
1	-4.25351490	-0.11391628	-1.00138311
6	-2.88926420	-1.63334258	0.98810108
6	-3.60386992	-2.74497135	0.48157915
6	-3.90964480	-3.81118503	1.33660297
6	-3.51800743	-3.82514461	2.67987197
6	-2.79854037	-2.72396372	3.15978307
6	-2.48903597	-1.62554974	2.34828906
7	0.69833380	2.56357701	-1.51492315
6	-1.58877788	2.75243554	-2.53816215
1	-2.40630486	3.49585472	-2.67275179
1	-1.14553736	2.57794899	-3.53224578
6	-0.51698139	3.37217005	-1.64238395
1	-0.26574072	4.34931179	-2.09887014
1	-0.95045300	3.61913580	-0.65302297
6	1.76919984	3.27332864	-0.89158197
6	1.78077235	3.50489962	0.50690732
6	2.83564192	4.22895647	1.07761310
6	3.88796863	4.73887179	0.31076228
6	3.86361811	4.50247757	-1.06812694
6	2.83258538	3.77914957	-1.68047644
6	-3.99142200	-2.81672876	-0.97363313
1	-4.45472986	-4.66709675	0.92975091
6	-3.88588483	-4.97360214	3.58884637
1	-2.48473959	-2.70556560	4.20682298
6	-1.75106189	-0.44454325	2.93461727
6	0.69284184	2.96153003	1.40027226
1	2.83638799	4.38913152	2.15930148
6	5.03170476	5.48709192	0.95301269
1	4.67450244	4.89023330	-1.69047740
6	2.88661048	3.53022267	-3.16785651
1	-4.17789042	-3.85536845	-1.27661234
1	-3.19426012	-2.39691335	-1.60455931
1	-4.90890133	-2.24545194	-1.18813733
1	-0.73749634	-0.33038275	2.51950062
1	-1.65061297	-0.55836050	4.02137189
1	-2.28440910	0.49941006	2.74351281
1	-4.83949222	-4.78173458	4.10621272
1	-3.12369150	-5.13414400	4.36378908
1	-4.00498847	-5.90898092	3.02492100
1	1.06320606	2.83377303	2.42610948
1	0.33500108	1.99046185	1.03365975
1	-0.17333594	3.64142086	1.44960759
1	1.90984356	3.68899408	-3.64497900
1	3.18162858	2.49007813	-3.38106056
1	3.62403526	4.19015639	-3.64378332

1	5.84757261	4.80118017	1.23196667
1	4.71069795	6.00198440	1.86882893
1	5.45573684	6.23492514	0.26870436
1	-1.71788057	-0.06343353	0.48493819

Energy = -7584.957760 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 69

Atomic N.	X	Y	Z
8	-0.23887435	-2.43471656	1.87434791
8	0.47545666	0.70131282	1.64910393
6	0.17166161	0.73955939	3.03001844
1	-0.63908570	1.45738002	3.27172809
1	1.06837682	1.06751193	3.58767339
1	-0.13638119	-0.24241083	3.43292081
8	1.06112393	-3.26399669	3.44805747
6	0.87774403	-2.83667924	2.17289872
6	2.04484821	-2.86030152	1.20570153
1	2.47941902	-3.87315209	1.16861912
1	1.61314167	-2.64661300	0.22017823
6	3.14137386	-1.82452477	1.53856013
1	2.66089145	-0.86099998	1.77307310
1	3.73054088	-1.65891599	0.62393319
6	4.08961115	-2.26131730	2.65967817
1	4.64823501	-3.15409471	2.32740397
1	4.84057430	-1.47312200	2.82360556
6	3.40340928	-2.58609960	3.99139871
1	2.91502016	-1.69201784	4.41154535
1	4.16742757	-2.89648325	4.72272836
6	2.36837982	-3.70476689	3.91404179
1	2.72080561	-4.54301752	3.29143134
1	2.14783804	-4.09538468	4.91472378
50	-0.59771152	-0.27659165	0.14232794
7	-1.46000598	1.99984879	-0.43578934
6	-2.20727985	1.94939213	-1.71299722
1	-2.83548562	2.85097234	-1.82910588
1	-2.85154433	1.06227526	-1.73110847
1	-1.50068268	1.90545555	-2.54804391
7	-2.59755000	-0.25242306	0.91622400
6	-2.39609155	2.19457465	0.70555115
1	-2.98683971	3.11984851	0.56141490
1	-1.77377261	2.31259704	1.60315445
6	-3.33417537	1.00685978	0.89483836
1	-3.87859732	1.19085676	1.84070179
1	-4.11390118	1.01037955	0.10324437
6	-3.37128602	-1.39853316	1.25178151
6	-3.68287019	-2.38847002	0.28331547
6	-4.44144640	-3.50870628	0.64813048
6	-4.91982257	-3.69401783	1.94826289
6	-4.60366174	-2.71736302	2.89755896
6	-3.84360957	-1.58586225	2.57968335
7	0.89634388	2.19917070	-2.43820265
6	-0.43916429	3.08642672	-0.46391841
1	-0.25329821	3.38494820	0.57705629
1	-0.86014396	3.95723108	-0.99968182
6	0.92388603	2.70242357	-1.04838308
1	1.55168949	3.60206233	-1.01393670

1	1.39345738	1.96840500	-0.37014978
6	2.00703706	2.49996212	-3.27274828
6	2.84137446	1.46147699	-3.75409060
6	3.89793245	1.77292269	-4.61636319
6	4.16912748	3.08706343	-5.01510344
6	3.31863229	4.09478897	-4.54860494
6	2.23727422	3.82963446	-3.69908194
6	-3.21823232	-2.27102710	-1.14832107
1	-4.67074928	-4.25666142	-0.11593167
6	-5.76679439	-4.89076859	2.30967017
1	-4.94060777	-2.84735333	3.92996908
6	-3.50512193	-0.60674266	3.67525640
6	2.59414041	0.02483585	-3.35674164
1	4.53326493	0.96130101	-4.98028494
6	5.34370693	3.40561817	-5.90873865
1	3.48156975	5.12471882	-4.87684153
6	1.30144120	4.94995188	-3.31547340
1	-3.80450575	-2.93424403	-1.79873272
1	-2.15860999	-2.55121398	-1.26261765
1	-3.31186065	-1.24209204	-1.52274554
1	-2.52751472	-0.14248796	3.49343348
1	-3.48362309	-1.11188074	4.65022534
1	-4.24795925	0.20485212	3.74843852
1	-6.84121298	-4.65817682	2.23300721
1	-5.57941235	-5.21673342	3.34247736
1	-5.56794872	-5.73951180	1.64109212
1	3.38956054	-0.62328214	-3.74571383
1	1.63966933	-0.35966196	-3.75316458
1	2.55826499	-0.10361855	-2.26341049
1	1.51986402	5.36685206	-2.31946175
1	0.26034262	4.59620064	-3.29556195
1	1.37830697	5.77596470	-4.03449349
1	5.54000479	2.59140782	-6.61996406
1	6.26411107	3.55348384	-5.32133733
1	5.17172007	4.32684131	-6.48201385
1	0.74883365	1.18866929	-2.41132682

Energy = -7584.962261 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 70

Atomic N.	X	Y	Z
8	-0.19099267	-2.71450325	0.74190155
8	0.24322268	0.49472787	0.69341370
6	0.02948204	0.36840425	2.08974909
1	-0.76582925	1.04710158	2.45673255
1	0.95926093	0.63606263	2.62359204
1	-0.24597568	-0.65846154	2.38317927
8	1.34136460	-3.76041699	1.93132146
6	0.93334030	-3.19525596	0.76579363
6	1.88172382	-3.16361566	-0.41650409
1	2.23229148	-4.18342708	-0.64615422
1	1.28184104	-2.81736710	-1.26715093
6	3.08950881	-2.22468962	-0.20477805
1	2.73433923	-1.28159423	0.23980657
1	3.48916548	-1.96353054	-1.19569193
6	4.21334037	-2.83592466	0.63750523
1	4.62492260	-3.70869451	0.10087513

1	5.03721923	-2.11056290	0.72064045
6	3.79125568	-3.28099911	2.04217136
1	3.47127423	-2.41821306	2.64862012
1	4.66204052	-3.71770691	2.55778587
6	2.67733471	-4.32347782	2.07009077
1	2.83157931	-5.10445502	1.30809351
1	2.63209350	-4.81185049	3.05092113
50	-0.87862874	-0.45682982	-0.81235401
7	-2.08814316	1.72676096	-1.28392523
6	-3.04308920	1.41848391	-2.36971519
1	-3.76213863	2.24577128	-2.51274941
1	-3.59460676	0.50209770	-2.13551458
1	-2.48771798	1.26460369	-3.30334101
7	-2.76296514	-0.60382396	0.23613986
6	-2.79479687	1.86835930	0.01397061
1	-3.49715383	2.72453950	-0.02468127
1	-2.03109522	2.08349364	0.77342259
6	-3.56454382	0.60534410	0.40297587
1	-3.89514207	0.76253918	1.44666017
1	-4.50061365	0.54726879	-0.19157713
6	-3.40358553	-1.81019260	0.63195439
6	-3.69254164	-2.83613554	-0.31027738
6	-4.33056830	-4.01195458	0.10459624
6	-4.71193179	-4.22907316	1.43142822
6	-4.41327401	-3.22425918	2.35476003
6	-3.76755737	-2.03656297	1.98966759
7	1.03363271	2.61099197	-0.99680017
6	-1.37359602	2.97787251	-1.66700082
1	-2.11893229	3.80000335	-1.67664625
1	-1.02217422	2.83603115	-2.69782853
6	-0.17851720	3.42093910	-0.81847464
1	0.03603878	4.45877653	-1.10940275
1	-0.46107436	3.46307276	0.24841346
6	2.27031537	3.27693925	-1.17670490
6	3.30666535	3.14562644	-0.21578931
6	4.53428991	3.77883624	-0.43345813
6	4.78143310	4.55821603	-1.57052038
6	3.75496346	4.66801199	-2.51268446
6	2.51636360	4.03326298	-2.34917757
6	-3.33303229	-2.70795463	-1.77073952
1	-4.54398255	-4.78049116	-0.64354382
6	-5.43717197	-5.48701187	1.84515581
1	-4.66739065	-3.37502300	3.40791856
6	-3.43004887	-1.04964870	3.07992513
6	3.09115750	2.34892035	1.04795433
1	5.31742864	3.67246674	0.32228544
6	6.12073707	5.22226436	-1.78488121
1	3.92726052	5.24550651	-3.42487321
6	1.50009880	4.10313394	-3.46217910
1	-3.90234579	-3.43077255	-2.37080268
1	-2.26362051	-2.90308094	-1.95196582
1	-3.53575870	-1.69955862	-2.15717044
1	-2.51740803	-0.49178214	2.83734536
1	-3.27839255	-1.57349896	4.03344262
1	-4.23646264	-0.31516392	3.24127558
1	-6.52829385	-5.37291275	1.74013055
1	-5.23650036	-5.73693005	2.89625606
1	-5.13950582	-6.34479350	1.22616591

1	3.98556012	2.38704639	1.68302252
1	2.86162660	1.29209556	0.84175630
1	2.24302527	2.73794489	1.63228371
1	0.66558173	4.78835877	-3.24477735
1	1.06303015	3.10896798	-3.64043342
1	1.97076202	4.45110281	-4.39094830
1	6.87742859	4.49931639	-2.12926934
1	6.50184431	5.66828139	-0.85482338
1	6.05590149	6.01600854	-2.54109590
1	1.05535433	1.88664773	-0.26469450

Energy = -7584.964349 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 71

Atomic N.	X	Y	Z
8	0.79426290	0.23204442	-0.85188072
8	1.63570696	1.13871814	2.02665472
6	2.50513336	0.65204591	3.03028833
1	2.35938068	-0.42443217	3.26223588
1	2.38420020	1.20964385	3.97911811
1	3.55836111	0.77887864	2.71656952
8	2.65314655	-0.95461892	-0.74484812
6	2.00072081	0.17713249	-1.08423921
6	2.76233712	1.33047179	-1.69454086
1	3.31418957	0.99337941	-2.58752537
1	2.00283892	2.04900930	-2.02195877
6	3.73011435	1.98991340	-0.68460425
1	3.22055084	2.07298407	0.28914053
1	3.92751631	3.01500237	-1.03088148
6	5.06468677	1.24939980	-0.54762558
1	5.58683883	1.26921712	-1.52062348
1	5.70861980	1.79682064	0.15768861
6	4.94705425	-0.20766301	-0.08430923
1	4.55029964	-0.26291448	0.94142726
1	5.95298516	-0.65766070	-0.05443622
6	4.08898350	-1.09668586	-0.97603086
1	4.30091304	-0.93686614	-2.04490845
1	4.26364779	-2.15504966	-0.74907311
50	-0.15780048	0.12290221	1.70219732
7	-2.71367056	-0.38979920	0.14130908
6	-3.56132165	-0.83113454	1.25385051
1	-4.64206704	-0.70154352	1.03716648
1	-3.32347769	-0.26765595	2.16618110
1	-3.37016618	-1.89305031	1.45588085
7	-1.18497113	1.94425184	1.40994761
6	-2.93175772	1.03334236	-0.16693830
1	-3.99697664	1.20569748	-0.44299494
1	-2.31624449	1.28234345	-1.04266384
6	-2.57797849	2.00501573	0.95963479
1	-2.79398645	3.01409948	0.57006156
1	-3.28464956	1.86851832	1.80392927
6	-0.64269146	3.20796515	1.79701926
6	-0.48487839	3.54436275	3.16354939
6	0.03946533	4.79473284	3.51205698
6	0.42127265	5.73518466	2.54858659
6	0.26724119	5.38757420	1.20317719
6	-0.25636410	4.14871723	0.81091996

7	-0.82642418	-2.17644942	-1.97623932
6	-3.00073228	-1.21448111	-1.05311579
1	-3.96793686	-0.88967489	-1.49734845
1	-3.14150620	-2.25463541	-0.72386631
6	-1.91199229	-1.20143209	-2.14338307
1	-2.40189748	-1.36999846	-3.11021833
1	-1.44032671	-0.21059401	-2.20009599
6	-1.10723677	-3.56217134	-1.99871563
6	-1.65044708	-4.17805540	-3.15473648
6	-1.89051732	-5.55855363	-3.14785962
6	-1.58327357	-6.37024834	-2.05233481
6	-0.99136118	-5.75544470	-0.94247403
6	-0.75208105	-4.37876719	-0.89212484
6	-0.86439801	2.57605614	4.25771633
1	0.15110660	5.04084189	4.57148898
6	0.95688770	7.08866706	2.95093087
1	0.57301284	6.09762056	0.42963840
6	-0.37900736	3.82473439	-0.65710322
6	-1.89951905	-3.40456278	-4.42688421
1	-2.30655814	-6.01560889	-4.04983898
6	-1.87997610	-7.85059793	-2.06185809
1	-0.71315643	-6.36427044	-0.07807894
6	-0.10770795	-3.77725271	0.33207941
1	-0.97793179	3.09988003	5.21631700
1	-0.08915859	1.80541152	4.39709120
1	-1.80265817	2.05126925	4.03217802
1	-0.14363445	2.76807712	-0.84493720
1	0.29117921	4.46037899	-1.25191684
1	-1.40188828	3.99663184	-1.03126026
1	0.13818257	7.79106122	3.17536077
1	1.55933978	7.53466590	2.14788494
1	1.58208409	7.02186747	3.85230476
1	-1.86910380	-4.07983506	-5.29237256
1	-1.13903551	-2.62260377	-4.56577710
1	-2.88435932	-2.90955909	-4.44002720
1	-0.72208400	-2.97961377	0.77904076
1	0.87186856	-3.32205548	0.10986198
1	0.05457604	-4.54426510	1.10002556
1	-1.08671699	-8.42383756	-1.56142133
1	-1.98117699	-8.23089754	-3.08749640
1	-2.82154768	-8.07411002	-1.53492332
1	-0.24435141	-1.90788187	-1.18401878

Energy = -7584.958500 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 72

Atomic N.	X	Y	Z
8	1.77355795	-2.78080289	1.38757438
8	0.36398235	0.14894489	0.66489395
6	1.32933504	0.80210709	1.49136398
1	0.87510950	1.59004394	2.12009189
1	2.08808346	1.28471548	0.85023918
1	1.85819728	0.10406646	2.16603653
8	3.88825048	-2.19307854	1.61074850
6	2.83532490	-2.55334033	0.82499739
6	3.02409920	-2.63857823	-0.67457746
1	3.85953612	-3.32113046	-0.90546507

1	2.10673821	-3.09078506	-1.06625192
6	3.26604276	-1.26929731	-1.34548141
1	2.54943415	-0.53961746	-0.93717963
1	3.01650052	-1.37737786	-2.41127554
6	4.70482699	-0.75684862	-1.22559183
1	5.37480141	-1.45208258	-1.76177777
1	4.78884903	0.21081587	-1.74451568
6	5.21613988	-0.60211230	0.21108419
1	4.64486357	0.16851110	0.75325291
1	6.26150351	-0.25297303	0.18541678
6	5.18856851	-1.88652864	1.03420861
1	5.54730868	-2.74943962	0.44991272
1	5.82866496	-1.78803984	1.91962247
50	-0.75211246	-1.34757280	1.63535557
7	-3.13230939	-0.41545730	1.31700847
6	-3.73782189	-0.03254607	2.60235039
1	-4.82337545	0.15471090	2.50436527
1	-3.24515784	0.86619412	2.98986481
1	-3.58306220	-0.84650292	3.32275700
7	-1.68682510	2.27900068	1.12055958
6	-3.33034447	0.61137167	0.26204076
1	-4.37819201	0.56055128	-0.09731388
1	-2.67777714	0.33288721	-0.57747874
6	-3.05910331	2.06120703	0.65475918
1	-3.29430368	2.66308342	-0.24718445
1	-3.77330600	2.38808539	1.42759244
6	-1.25175259	3.63696823	1.14498282
6	-1.63844339	4.47943330	2.21240572
6	-1.18691817	5.80504398	2.23814021
6	-0.34925039	6.32405279	1.24523241
6	0.03484500	5.47106678	0.20376147
6	-0.40841435	4.14527588	0.12735762
7	-1.51095539	-2.17301078	-0.19638886
6	-3.68608043	-1.71357870	0.85865321
1	-4.76779709	-1.61449523	0.64165235
1	-3.57168679	-2.42121101	1.69557614
6	-2.95435150	-2.25985980	-0.36685507
1	-3.30103029	-3.30523288	-0.50108518
1	-3.29767390	-1.72229927	-1.27760990
6	-0.77398569	-2.87408023	-1.19195925
6	-0.37429690	-2.21970804	-2.38362320
6	0.31350638	-2.93773321	-3.37231275
6	0.62639124	-4.29347357	-3.22185724
6	0.23349517	-4.92711147	-2.03651419
6	-0.45340369	-4.24544620	-1.02311565
6	-2.48508478	3.95374985	3.34378395
1	-1.48311070	6.44274858	3.07519100
6	0.10563288	7.76351842	1.28251441
1	0.68983351	5.85123393	-0.58461033
6	-0.00085279	3.28405737	-1.04537841
6	-0.67490420	-0.75623251	-2.59111633
1	0.60949323	-2.41973879	-4.28887573
6	1.39007091	-5.04239207	-4.28837922
1	0.46896477	-5.98515653	-1.89307604
6	-0.82095346	-4.97185926	0.24679886
1	-2.40123006	4.60099588	4.22645039
1	-2.16969663	2.93625541	3.61630479
1	-3.55316302	3.90360303	3.07668771

1	0.57707232	2.39858146	-0.74078211
1	0.61021644	3.86227387	-1.75020969
1	-0.87959603	2.90831364	-1.59228118
1	-0.59758264	8.41700551	0.74172510
1	1.09089500	7.88568119	0.81218269
1	0.16901843	8.13688249	2.31385904
1	-0.16173482	-0.37681563	-3.48497378
1	-0.35828660	-0.16940674	-1.71707644
1	-1.75369968	-0.58153983	-2.73120483
1	-1.87463056	-4.82008329	0.51898725
1	-0.21761902	-4.60810373	1.09237505
1	-0.64200455	-6.05018718	0.14210329
1	2.47101334	-5.05273876	-4.07407691
1	1.25740005	-4.57951108	-5.27565573
1	1.06449826	-6.08987211	-4.35382294
1	-1.02818436	1.67195171	0.61411192

Energy = -7584.966616 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 73

Atomic N.	X	Y	Z
8	0.71855916	-0.18579629	-0.93031049
8	2.03188605	1.36886289	1.45229250
6	2.92242986	1.04761852	2.50287714
1	3.93571910	0.86054362	2.10022282
1	2.62599422	0.14459424	3.07782323
1	3.01432659	1.87988125	3.22726317
8	2.34016196	-1.63191760	-0.53884739
6	1.86166468	-0.55372740	-1.19508503
6	2.73892423	0.17379775	-2.18714905
1	3.11282263	-0.52719166	-2.95162530
1	2.08624049	0.89765115	-2.68753319
6	3.92066328	0.89714615	-1.50056696
1	3.55274177	1.37828125	-0.57986746
1	4.25447480	1.70283274	-2.17073673
6	5.10982455	-0.02317968	-1.20520188
1	5.50686122	-0.41223886	-2.15954358
1	5.92023671	0.57003116	-0.75452701
6	4.79272225	-1.20960733	-0.28692798
1	4.51942169	-0.86353479	0.72209166
1	5.69909476	-1.82621276	-0.17031759
6	3.68971908	-2.13234303	-0.79042138
1	3.79774768	-2.35777433	-1.86301559
1	3.69878610	-3.08104849	-0.24081990
50	0.06939100	0.67180170	1.58088970
7	-2.70378175	0.21119677	0.42982950
6	-3.47252349	0.29944086	1.67568467
1	-4.53633026	0.56028750	1.49664700
1	-3.03997615	1.05782265	2.34216507
1	-3.43220918	-0.66648747	2.19573070
7	-0.67205959	2.47905775	0.78061313
6	-2.72370431	1.48750379	-0.30395809
1	-3.77241966	1.76991877	-0.55104513
1	-2.18759623	1.33531564	-1.25113720
6	-2.08132089	2.66772390	0.42609892
1	-2.17642224	3.53309657	-0.25112652
1	-2.69184727	2.93260724	1.31373135

6	0.11358016	3.66923782	0.69684012
6	0.49303353	4.37460716	1.86488118
6	1.25212341	5.54512932	1.75007226
6	1.65798456	6.04897934	0.50896967
6	1.28323872	5.33894286	-0.63542493
6	0.52157750	4.16502147	-0.56567988
7	-1.40144807	-2.46468535	-1.11876643
6	-3.26108381	-0.86669809	-0.41658554
1	-4.20985780	-0.51407567	-0.87894282
1	-3.52591269	-1.71044124	0.23782091
6	-2.32291980	-1.39329269	-1.51977552
1	-2.94531876	-1.74606643	-2.35122233
1	-1.70361299	-0.57700150	-1.91656631
6	-1.90936414	-3.70850739	-0.67754896
6	-1.56103780	-4.20476016	0.60653384
6	-2.03068746	-5.45694523	1.01578911
6	-2.84900602	-6.24960282	0.20270420
6	-3.14919012	-5.76423153	-1.07349738
6	-2.68589218	-4.52637073	-1.53773884
6	0.10071457	3.88481890	3.23777444
1	1.53314400	6.08041930	2.66108916
6	2.45166014	7.33002940	0.41075822
1	1.60066037	5.70184773	-1.61702366
6	0.16693849	3.43283141	-1.83587952
6	-0.67848256	-3.40080898	1.52883943
1	-1.75328802	-5.81773623	2.00979507
6	-3.39091193	-7.57274206	0.68762799
1	-3.74312484	-6.38187535	-1.75273910
6	-2.95781260	-4.14138508	-2.97184157
1	0.19819462	4.68961335	3.97868975
1	0.74898850	3.05708999	3.56764079
1	-0.93245888	3.51234579	3.25944746
1	0.20791935	2.34530783	-1.68467142
1	0.84943124	3.71492172	-2.64927295
1	-0.85467641	3.67101442	-2.17557146
1	1.79527935	8.21218655	0.48068829
1	2.98760078	7.39538402	-0.54584259
1	3.18803930	7.41036849	1.22278148
1	-0.55381928	-3.91512270	2.49024685
1	-1.08969156	-2.39976255	1.73462884
1	0.32853854	-3.23890334	1.10948695
1	-2.10031249	-3.60530476	-3.40357456
1	-3.83962590	-3.48867088	-3.07878204
1	-3.14893416	-5.03909281	-3.57478991
1	-3.59667877	-8.25249783	-0.15076696
1	-4.33563867	-7.44007761	1.23926635
1	-2.68609016	-8.07140498	1.36749790
1	-0.69199208	-2.08798702	-0.49156270

Energy = -7584.958490 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 74

Atomic N.	X	Y	Z
8	1.06809756	0.56210587	-0.47666975
8	1.15368049	1.37755617	2.81469595
6	2.35362963	0.69683501	3.12826825
1	3.14872101	0.93862478	2.39739837

1	2.24725223	-0.40761339	3.14816198
1	2.70733492	1.01099652	4.12589449
8	2.21097907	-1.25732872	0.04232798
6	1.82302571	-0.32595426	-0.85790338
6	2.34544586	-0.39013660	-2.27717409
1	2.08993105	-1.36761060	-2.71856826
1	1.79322361	0.37899815	-2.82884554
6	3.86595915	-0.14304631	-2.38803308
1	4.14524803	0.70714522	-1.74535495
1	4.08029534	0.16790496	-3.42126310
6	4.72324855	-1.36873296	-2.05531341
1	4.49779546	-2.16531840	-2.78504696
1	5.78542864	-1.11413501	-2.19300043
6	4.51695347	-1.92650307	-0.64279899
1	4.82945039	-1.19474063	0.11982209
1	5.16163418	-2.81010356	-0.50811638
6	3.08750735	-2.36105700	-0.33831741
1	2.63337378	-2.91594349	-1.17332315
1	3.06088247	-3.00437802	0.54929880
50	-0.37774030	0.38074283	1.87998757
7	-3.29268858	-0.13340205	0.63350811
6	-4.12526117	-0.19733375	1.83489981
1	-5.16986446	0.13410990	1.65175379
1	-3.69784754	0.42884297	2.62846475
1	-4.15010797	-1.23229497	2.20161092
7	-1.41094535	2.19443946	1.57565838
6	-3.22290192	1.22541366	0.07350515
1	-4.22119816	1.53197229	-0.31686251
1	-2.52418074	1.20441228	-0.77608426
6	-2.76712322	2.32190749	1.03616694
1	-2.84038081	3.26105364	0.45951340
1	-3.51354644	2.43400282	1.84983615
6	-0.87500327	3.46099587	1.98005643
6	-0.89168300	3.85516531	3.33781358
6	-0.39202603	5.11371582	3.69601115
6	0.13623670	5.99909971	2.75123490
6	0.16170187	5.58787846	1.41428630
6	-0.33272951	4.34107312	1.01166625
7	-1.52301058	-1.80357428	-1.06711185
6	-3.78751929	-1.09365021	-0.36299398
1	-4.76797049	-0.76653329	-0.77955072
1	-3.95979166	-2.04800806	0.15886177
6	-2.83652944	-1.34993308	-1.53458126
1	-3.30387696	-2.12466465	-2.16294854
1	-2.75173246	-0.44505637	-2.15937290
6	-0.87287343	-2.90957593	-1.63167349
6	-0.63446682	-2.98189313	-3.02875034
6	0.03935168	-4.09379442	-3.55121170
6	0.51447254	-5.13371836	-2.74472765
6	0.31017347	-5.02130681	-1.36329002
6	-0.37184204	-3.94165675	-0.79324177
6	-1.40386336	2.93200877	4.41518696
1	-0.41177717	5.40596146	4.74934771
6	0.64072412	7.36362879	3.15675156
1	0.58942466	6.25221044	0.65824937
6	-0.25672715	3.94536437	-0.44233624
6	-1.01079448	-1.84477413	-3.94950100
1	0.21705711	-4.13185136	-4.62944899

6	1.20194310	-6.33903510	-3.34042690
1	0.67865613	-5.81080424	-0.70262292
6	-0.57930732	-3.88263390	0.69980031
1	-1.61389806	3.49009144	5.33747877
1	-0.64837746	2.16464094	4.64514854
1	-2.31865163	2.40705663	4.10720519
1	0.09668366	2.91214546	-0.55642994
1	0.41940453	4.61688282	-0.98822035
1	-1.24129976	4.00224168	-0.93534631
1	-0.16024975	8.11822934	3.09865932
1	1.45386133	7.70155573	2.49934608
1	1.01307020	7.36250552	4.19039661
1	-0.46387503	-1.92531253	-4.89816582
1	-0.77110305	-0.87380725	-3.49060580
1	-2.08390172	-1.82346386	-4.19238132
1	-1.64799899	-3.81048091	0.95919364
1	-0.08751316	-3.00822964	1.15774200
1	-0.17726566	-4.78213096	1.18302939
1	1.96976127	-6.74082443	-2.66451174
1	1.68300719	-6.09398805	-4.29752431
1	0.48570978	-7.15309544	-3.53619741
1	-1.44889189	-1.74008580	-0.05238979

Energy = -7584.958600 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 75

Atomic N.	X	Y	Z
8	1.80585278	-2.57497173	1.71113014
8	0.43244615	0.24506741	0.59174102
6	1.48655244	0.99246791	1.20174169
1	2.19377582	1.32474643	0.42133416
1	2.05857274	0.40150248	1.94045084
1	1.11266394	1.89574082	1.71819467
8	3.94709703	-2.04869970	1.64139927
6	2.81644487	-2.49558567	1.02695426
6	2.86253241	-2.85106924	-0.44383814
1	3.65205325	-3.60134231	-0.61974056
1	1.89964542	-3.32247752	-0.66766169
6	3.08163415	-1.63366311	-1.36769722
1	2.42756268	-0.81185835	-1.03675569
1	2.73134942	-1.91622841	-2.37135977
6	4.53972545	-1.17377714	-1.46588108
1	5.13669136	-1.98217584	-1.92395781
1	4.60345104	-0.31756879	-2.15548942
6	5.18614338	-0.79145573	-0.12971044
1	4.69011840	0.08761644	0.31224083
1	6.23442238	-0.50001305	-0.30720970
6	5.19695526	-1.90837047	0.90967010
1	5.47356052	-2.87616868	0.46065892
1	5.91911205	-1.68541133	1.70476794
50	-0.63545699	-0.99847436	1.91170913
7	-3.00699540	-0.02719392	1.63741914
6	-3.47537190	0.60762067	2.87954508
1	-4.55933796	0.82444845	2.84560555
1	-2.92145720	1.53741510	3.05059638
1	-3.27650949	-0.07013743	3.72010865
7	-1.50498816	2.51466186	0.82734377

6	-3.27413172	0.80202787	0.43447149
1	-4.35274921	0.73779102	0.18505497
1	-2.71414991	0.34699229	-0.39470554
6	-2.92138988	2.28407271	0.53024717
1	-3.22142020	2.72551376	-0.44244962
1	-3.54852240	2.77809531	1.28972506
6	-1.02517024	3.83225586	0.56764360
6	-1.28184577	4.86898566	1.49450603
6	-0.78515308	6.15348886	1.24179229
6	-0.02598161	6.44599669	0.10329630
6	0.22977594	5.40434392	-0.79563388
6	-0.26382512	4.10950987	-0.59314740
7	-1.58801525	-2.10192745	0.33500895
6	-3.63888826	-1.35983030	1.47510037
1	-4.73304914	-1.25228836	1.33973856
1	-3.46599937	-1.91027943	2.41392900
6	-3.04304695	-2.15004704	0.31048913
1	-3.43262173	-3.18503938	0.40023420
1	-3.45454200	-1.76867309	-0.64944901
6	-0.97056845	-3.00051360	-0.58000366
6	-0.66570526	-2.58476100	-1.90000006
6	-0.09860340	-3.49705260	-2.80116600
6	0.18504509	-4.81873056	-2.43868417
6	-0.11234884	-5.21523262	-1.12906422
6	-0.67827443	-4.33464732	-0.19743376
6	-2.03652139	4.59478750	2.77065145
1	-0.98010336	6.94287111	1.97254957
6	0.48111963	7.84463671	-0.15575647
1	0.82131129	5.60572353	-1.69258832
6	0.00296511	3.03557203	-1.62208162
6	-0.93902277	-1.16780218	-2.33899465
1	0.12431328	-3.16221644	-3.81814231
6	0.82035356	-5.77811150	-3.41721743
1	0.10277175	-6.24169677	-0.81996408
6	-0.94585005	-4.80871935	1.20934458
1	-1.85000822	5.38386854	3.51067296
1	-1.73043430	3.62788887	3.19545628
1	-3.12584007	4.55011789	2.60929569
1	0.56983098	2.18622299	-1.21208452
1	0.57134138	3.44742409	-2.46581740
1	-0.93540403	2.61965091	-2.02090092
1	-0.28859076	8.46343774	-0.64410196
1	1.36067072	7.83648593	-0.81349514
1	0.75734156	8.35056880	0.77992734
1	-0.50083489	-0.97579773	-3.32763745
1	-0.52324338	-0.45241215	-1.61521224
1	-2.02029501	-0.96962727	-2.41346217
1	-1.96464903	-4.56429691	1.54056564
1	-0.25578243	-4.32906461	1.91997603
1	-0.80855381	-5.89556884	1.28471962
1	1.91737139	-5.78846824	-3.31261258
1	0.59448052	-5.49951972	-4.45549856
1	0.47100138	-6.80704729	-3.25407448
1	-0.91680369	1.79639652	0.38367331

Energy = -7584.966621 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 76

Atomic N.	X	Y	Z
8	2.38481201	-0.30778342	2.52959670
8	1.56509202	2.19380179	-1.28089142
6	2.96233897	1.99807147	-1.23559295
1	3.43243215	2.39878402	-2.15175461
1	3.25283859	0.92803230	-1.16197109
1	3.41647240	2.52158487	-0.36996921
8	4.18773252	0.96640473	2.65529337
6	3.60272289	-0.25292214	2.49730899
6	4.47813051	-1.47166797	2.26926124
1	5.20416203	-1.57282252	3.09312682
1	3.79992927	-2.33124001	2.31985399
6	5.22326398	-1.45755537	0.91680937
1	4.53093014	-1.13139277	0.12445494
1	5.50088024	-2.49425905	0.67524809
6	6.48976393	-0.59569324	0.91161846
1	7.21069346	-1.02203352	1.63099748
1	6.96735712	-0.66392255	-0.07778600
6	6.26341779	0.87965173	1.25881062
1	5.63751232	1.37333868	0.49837315
1	7.23355139	1.40263145	1.24799020
6	5.63630356	1.12186916	2.62779625
1	6.08984924	0.48242964	3.40244086
1	5.77225433	2.16700901	2.93104478
50	0.25410265	0.62925696	-0.82601486
7	-0.54272137	1.94375695	1.17519819
6	0.40462840	3.07422377	1.34171744
1	0.00253313	3.80223070	2.06873718
1	0.59325338	3.55654629	0.37795708
1	1.36052231	2.68534577	1.71349989
7	-1.43686011	1.72555649	-1.55236769
6	-1.87058968	2.44208341	0.72023022
1	-2.19251005	3.28005201	1.36857799
1	-2.58841585	1.61901953	0.82117375
6	-1.84228809	2.86855472	-0.74622589
1	-2.86563444	3.18664215	-1.01807898
1	-1.20372833	3.76742245	-0.85421600
6	-1.73609325	1.71889955	-2.93990615
6	-1.39900385	2.78663125	-3.81691732
6	-1.75566006	2.70673036	-5.17019054
6	-2.40873002	1.59568330	-5.71164168
6	-2.69692240	0.53312261	-4.84829872
6	-2.38346996	0.57606127	-3.48534729
7	-1.14660214	-1.05419204	1.72060629
6	-0.62350622	1.25107398	2.49676308
1	-0.95325850	1.98792290	3.25502771
1	0.40299596	0.95360789	2.75488069
6	-1.54401514	0.03925369	2.61621579
1	-1.50386511	-0.26626719	3.68144157
1	-2.58593969	0.31877573	2.41981617
6	-1.78861558	-2.31431449	1.86421426
6	-3.17888252	-2.46166272	1.64621217
6	-3.75950094	-3.73015137	1.77986323
6	-3.01408612	-4.86918902	2.09517384
6	-1.63296347	-4.71091455	2.25961831
6	-1.00993666	-3.46399376	2.15460939
6	-0.59043194	3.97322340	-3.35027371

1	-1.48177447	3.53634783	-5.82840664
6	-2.80227848	1.55107625	-7.16881533
1	-3.19966734	-0.35463723	-5.24179108
6	-2.75993733	-0.58773119	-2.60324072
6	-4.04586202	-1.30839078	1.20448877
1	-4.83364677	-3.82810348	1.60218246
6	-3.67188202	-6.21804312	2.25945016
1	-1.01622547	-5.58538174	2.48286428
6	0.48620466	-3.35949095	2.33465281
1	-0.14400461	4.48693461	-4.21236974
1	0.21719921	3.65245332	-2.67461723
1	-1.20262875	4.71518426	-2.81259364
1	-1.87930745	-1.13919861	-2.23538085
1	-3.39169049	-1.29976853	-3.15076886
1	-3.29917410	-0.24258544	-1.71035967
1	-3.81667429	1.95365896	-7.32246826
1	-2.79937991	0.52210129	-7.55459589
1	-2.11866063	2.15029208	-7.78643259
1	-4.93155529	-1.68043826	0.67317485
1	-3.49456654	-0.64125200	0.52714651
1	-4.40855517	-0.70293738	2.05094517
1	0.76428762	-2.65287456	3.13189314
1	0.98872533	-3.01455735	1.41609201
1	0.90766477	-4.33945812	2.59254948
1	-3.03032980	-7.02707909	1.88306418
1	-4.62946968	-6.26337524	1.72328577
1	-3.87916286	-6.43475835	3.31970744
1	-0.13389332	-1.17129546	1.77622799

Energy = -7584.967443 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 77

Atomic N.	X	Y	Z
8	1.38233221	1.49672353	3.70648000
8	3.09472875	-0.27550066	-0.24604134
6	4.34056093	-0.17363385	-0.91845591
1	4.38404608	-0.76063742	-1.85776987
1	5.16006199	-0.53628386	-0.27133046
1	4.56362487	0.87792838	-1.18404321
8	2.64551732	3.14645915	2.93887950
6	2.50575693	1.94589899	3.58282562
6	3.75002551	1.22859266	4.07569453
1	4.31840051	1.88162001	4.75926004
1	3.38015007	0.38026831	4.66292079
6	4.66933579	0.73197368	2.93762183
1	4.05587237	0.29428243	2.13342064
1	5.29016476	-0.08345916	3.33823406
6	5.59045125	1.81512817	2.36758777
1	6.26626600	2.16998080	3.16601186
1	6.23517259	1.36980135	1.59424230
6	4.85605086	3.02196175	1.77450108
1	4.24816501	2.71839271	0.90707583
1	5.59664082	3.74810998	1.40089706
6	3.95214037	3.75843624	2.75920350
1	4.44127497	3.88527684	3.73896269
1	3.70367310	4.75646870	2.37692269
50	1.56459716	-1.39303924	-1.14448058

7	0.23765357	0.64023554	-0.88143406
6	0.92213095	1.84045534	-1.40882288
1	0.36308560	2.75574771	-1.14816969
1	1.02221978	1.77823805	-2.49850707
1	1.92482479	1.88166633	-0.96731439
7	-2.58124880	0.03302776	-3.41918849
6	-1.14159008	0.50519641	-1.41933269
1	-1.73179330	1.39621169	-1.13455546
1	-1.58993986	-0.36661870	-0.92387285
6	-1.21779786	0.29596847	-2.94117699
1	-0.82032929	1.16683322	-3.47365159
1	-0.59100038	-0.56478238	-3.22583273
6	-3.57376218	1.04442874	-3.30811518
6	-3.45822786	2.25131140	-4.03861848
6	-4.47262186	3.21161824	-3.93175675
6	-5.61783754	3.01187528	-3.15505796
6	-5.73993465	1.78789799	-2.48674534
6	-4.74443058	0.80756493	-2.54396487
7	0.39121239	-1.72787239	0.58065946
6	0.21203219	0.71271791	0.61479717
1	-0.42937467	1.55000368	0.94016967
1	1.24361987	0.92368654	0.92307035
6	-0.24334890	-0.59689781	1.25177607
1	0.01902044	-0.52449191	2.32184826
1	-1.35038431	-0.68346538	1.21821322
6	0.26389779	-3.00185173	1.20265395
6	-0.60364771	-3.98041240	0.65444935
6	-0.71233149	-5.23484320	1.26673901
6	0.01230644	-5.56164961	2.41864569
6	0.86484947	-4.58898646	2.95048509
6	1.00905857	-3.32355983	2.36642212
6	-2.31082921	2.49917598	-4.98770083
1	-4.37195529	4.13704633	-4.50489139
6	-6.68177845	4.07631561	-3.03774098
1	-6.63574043	1.58899812	-1.89309132
6	-4.93803775	-0.49461357	-1.80247119
6	-1.42268617	-3.68560383	-0.57985982
1	-1.39035114	-5.97558325	0.83424140
6	-0.09641074	-6.93188703	3.04386854
1	1.44972483	-4.82337877	3.84424036
6	1.97272603	-2.33126650	2.96734999
1	-2.61126120	3.21023264	-5.76842297
1	-1.99048763	1.56470560	-5.47001783
1	-1.42925567	2.93014524	-4.48537500
1	-4.95408996	-1.36485235	-2.47983188
1	-5.89386017	-0.49005750	-1.26434506
1	-4.14363621	-0.67497138	-1.06073391
1	-6.51980073	4.70576542	-2.14815213
1	-7.68360072	3.63484927	-2.94450745
1	-6.68047442	4.74097318	-3.91232656
1	-2.13517895	-4.49865782	-0.77238866
1	-0.79011596	-3.57450876	-1.47445317
1	-1.98733372	-2.74804984	-0.47169602
1	1.46321192	-1.60870638	3.62472198
1	2.47202362	-1.74796770	2.18072522
1	2.73090715	-2.84776420	3.57147640
1	0.60684570	-7.63908576	2.57563054
1	-1.10553548	-7.34948434	2.92200135

1 0.13597371 -6.90236962 4.11699151
 1 -2.92031370 -0.84340172 -3.02567346
 Energy = -7584.967454 Hartree
 Number of imaginary frequencies = 0.

Compound I2b isomer 78

Atomic N.	X	Y	Z
8	3.38563603	-3.08426619	2.16229823
8	2.10828141	0.21837292	-0.92839628
6	2.84678616	1.08586366	-1.77225484
1	2.20705133	1.75199662	-2.38664321
1	3.47422004	0.50529494	-2.47381821
1	3.52064320	1.73918041	-1.18348722
8	5.02883824	-1.61504050	2.38322133
6	4.41439052	-2.63018897	1.69930481
6	5.02635808	-3.11168972	0.39529551
1	6.06597908	-3.43978227	0.56409670
1	4.44416888	-3.99660104	0.11362678
6	4.98433617	-2.06079783	-0.73628425
1	4.00290348	-1.55910950	-0.73873329
1	5.06419758	-2.59570053	-1.69463500
6	6.10753145	-1.02211882	-0.65959101
1	7.08033700	-1.53545532	-0.76162379
1	6.02746571	-0.34040347	-1.52027896
6	6.12131298	-0.19940944	0.63282653
1	5.20507760	0.40677588	0.71768285
1	6.96487021	0.50968663	0.60082387
6	6.26994101	-1.02660888	1.90669572
1	7.03348507	-1.81319715	1.78964284
1	6.57381198	-0.38652312	2.74454249
50	0.00315485	0.40280944	-0.93222539
7	0.32215260	0.48727642	1.51962749
6	1.35482804	1.47336629	1.90309894
1	1.63175549	1.35698308	2.96586188
1	0.99299249	2.49402327	1.73508220
1	2.23422639	1.30360708	1.27084939
7	-2.29799395	2.06091942	0.84847710
6	-0.90826163	0.64281672	2.33812037
1	-0.63732054	0.53004311	3.40548180
1	-1.57286774	-0.19564455	2.08404847
6	-1.67650461	1.95278499	2.17675563
1	-2.42825608	1.98617080	2.99103059
1	-1.01988793	2.81769867	2.33553628
6	-3.06814669	3.23652614	0.59557115
6	-2.42208924	4.47095805	0.36168592
6	-3.19941273	5.60542278	0.09561867
6	-4.59543110	5.55618167	0.02940980
6	-5.21329424	4.31582006	0.22785346
6	-4.47942535	3.16018973	0.51564010
7	-0.44755275	-1.55581725	-0.23118262
6	0.88162635	-0.88933865	1.71192628
1	1.04760694	-1.08355597	2.78632908
1	1.85447800	-0.89035431	1.20593374
6	-0.00207786	-1.96880735	1.09516085
1	0.60613817	-2.89001544	1.08287357
1	-0.86688411	-2.19471435	1.75600527
6	-0.99116252	-2.56286980	-1.07403423

6	-2.37073695	-2.54790745	-1.40230857
6	-2.90003863	-3.53369428	-2.24440396
6	-2.10647370	-4.55341712	-2.78019374
6	-0.74585454	-4.55759533	-2.45475118
6	-0.17318687	-3.58625170	-1.62418079
6	-0.91786762	4.57826197	0.33835053
1	-2.68938307	6.55371299	-0.09188064
6	-5.41033480	6.79896851	-0.23590544
1	-6.30191934	4.24350104	0.16419539
6	-5.19976641	1.84701482	0.71822094
6	-3.28424652	-1.48102102	-0.84817925
1	-3.96752214	-3.50853330	-2.47995450
6	-2.68997919	-5.59087510	-3.70947930
1	-0.09972299	-5.33402625	-2.87415945
6	1.31156038	-3.62006462	-1.36019549
1	-0.60337322	5.44323938	-0.25972251
1	-0.47095749	3.67210297	-0.09570718
1	-0.49275597	4.71281240	1.34672590
1	-4.98376739	1.12606451	-0.08740436
1	-6.28560678	2.00298867	0.72637826
1	-4.92706856	1.36413332	1.66952156
1	-5.76083797	7.25244126	0.70489804
1	-6.30066961	6.57465538	-0.83937407
1	-4.81966781	7.55866698	-0.76520663
1	-4.33609912	-1.73800229	-1.03232140
1	-3.09222113	-0.50125894	-1.31510073
1	-3.13717636	-1.35586251	0.23456832
1	1.55307514	-4.14476936	-0.42182931
1	1.71392275	-2.60063798	-1.27368160
1	1.83377922	-4.14559587	-2.17135579
1	-2.57283542	-5.29180645	-4.76348388
1	-3.76430837	-5.73171338	-3.52797122
1	-2.19145281	-6.56281482	-3.59043280
1	-2.87652015	1.23452519	0.69147749

Energy = -7584.967289 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 79

Atomic N.	X	Y	Z
8	1.70179225	1.53822859	0.56259907
8	1.18076962	0.55038771	-2.48489511
6	1.44809313	1.80428834	-3.09601706
1	0.69111676	2.05901523	-3.85681947
1	2.42930962	1.75289783	-3.60400458
1	1.48470829	2.63605417	-2.37021479
8	3.59565659	2.64325136	0.42007018
6	2.92317655	1.47243968	0.43270140
6	3.67906996	0.16733184	0.29662772
1	4.44910825	0.11217362	1.08511768
1	2.94540856	-0.62221744	0.49793986
6	4.32371299	-0.05589269	-1.08942161
1	3.57751999	0.17551196	-1.86530895
1	4.53435328	-1.13184777	-1.18104844
6	5.62642968	0.71890596	-1.30764332
1	6.38802490	0.34982252	-0.59814216
1	6.01141936	0.49485959	-2.31416854
6	5.50610553	2.23779986	-1.14233768

1	4.82252505	2.66534579	-1.89344306
1	6.49123996	2.69872260	-1.32042049
6	5.04360606	2.68518512	0.23992425
1	5.52789934	2.10367619	1.04078103
1	5.27176121	3.74508419	0.40290619
50	-0.01266539	0.05256021	-0.88109969
7	-1.58532396	0.14902057	1.85035978
6	-0.77463863	0.77537036	2.90089156
1	-1.39875663	1.16858109	3.73157229
1	-0.18210314	1.60074051	2.48901650
1	-0.07764699	0.03416442	3.31376834
7	-1.33003761	1.73142728	-0.85205682
6	-2.53212345	1.11829997	1.26809975
1	-3.11897361	1.60404239	2.08148683
1	-3.24240420	0.56730668	0.63501488
6	-1.89000184	2.21533154	0.41745998
1	-2.69057508	2.93977101	0.19394017
1	-1.14946598	2.76205645	1.02925372
6	-1.57910044	2.54628143	-1.98594499
6	-1.26593524	3.93431779	-1.99670331
6	-1.58389239	4.70894300	-3.11916934
6	-2.18649750	4.16597646	-4.25797066
6	-2.44785329	2.79197086	-4.25408959
6	-2.15726031	1.97694617	-3.15341609
7	-1.64765033	-2.97820742	0.95348321
6	-2.32575085	-1.00450326	2.40143435
1	-3.23590293	-0.65033121	2.93430525
1	-1.69266339	-1.49626044	3.15499800
6	-2.72134668	-2.05644566	1.35174662
1	-3.56238117	-2.63820551	1.74742197
1	-3.08855396	-1.56127852	0.43977396
6	-1.18807255	-3.94111153	1.88408750
6	-2.05145867	-4.96907955	2.34311426
6	-1.56262387	-5.92245147	3.24454441
6	-0.23801342	-5.92456185	3.69328947
6	0.61551181	-4.94040133	3.18306171
6	0.16989555	-3.95558071	2.29484450
6	-0.51025843	4.58171893	-0.86081210
1	-1.32476174	5.77139313	-3.10868196
6	-2.55189823	5.03058062	-5.44039016
1	-2.90305057	2.33357253	-5.13601807
6	-2.46682652	0.50259724	-3.24398206
6	-3.45962532	-5.11598944	1.81908156
1	-2.24084939	-6.71083176	3.58214592
6	0.25038145	-6.94644167	4.69151997
1	1.66505463	-4.93131030	3.48903992
6	1.14809617	-2.93635534	1.76381033
1	-0.02403301	5.50337436	-1.20727826
1	0.26201957	3.90591096	-0.46501033
1	-1.16190838	4.85364121	-0.01608613
1	-1.56247626	-0.08918010	-3.46490282
1	-3.18139990	0.30534350	-4.05431473
1	-2.88699437	0.11946409	-2.30287360
1	-3.58229216	5.41141387	-5.35374798
1	-2.49138890	4.46913831	-6.38298938
1	-1.88868289	5.90330003	-5.51800981
1	-3.77851414	-6.16497934	1.88087421
1	-3.52318665	-4.79043490	0.77110199

1	-4.19222172	-4.52437920	2.39198741
1	0.79124421	-1.90336991	1.90240116
1	1.32360368	-3.05973796	0.68200034
1	2.11735221	-3.03482456	2.26993843
1	1.31603266	-7.17195333	4.54714008
1	-0.31222001	-7.88673342	4.60950535
1	0.13087451	-6.58495292	5.72564938
1	-0.88061133	-2.44568863	0.53760075

Energy = -7584.956169 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 80

Atomic N.	X	Y	Z
8	2.88122983	-1.59441265	2.30739363
8	2.07582221	2.41143937	0.05091459
6	1.89400974	3.77472013	-0.27238539
1	1.32731449	3.92369100	-1.20930152
1	2.88034622	4.25601090	-0.40186521
1	1.36146116	4.33575904	0.52498592
8	4.05758132	0.25523306	2.59834001
6	3.90369982	-0.97848870	2.04851361
6	4.98521555	-1.52463045	1.13548492
1	5.95993594	-1.50242670	1.65083345
1	4.72195546	-2.57555018	0.96859678
6	5.09186288	-0.77798462	-0.21262118
1	4.07980580	-0.60064011	-0.61050581
1	5.59516686	-1.44632810	-0.92733360
6	5.86849905	0.54021051	-0.13313001
1	6.91367765	0.31948661	0.14866599
1	5.90800216	0.99131593	-1.13646660
6	5.28679386	1.56183600	0.85023613
1	4.27397254	1.87734499	0.54232319
1	5.91850007	2.46550960	0.83913844
6	5.22458412	1.08131815	2.29497018
1	6.13722434	0.53990328	2.59428599
1	5.09713200	1.93103416	2.97658842
50	0.73193443	0.84246569	-0.26854932
7	-0.16351778	1.08718422	2.05472649
6	0.65771583	2.11632269	2.73779864
1	0.23461554	2.33735175	3.73369135
1	0.69241074	3.03314790	2.14302333
1	1.68277047	1.74468949	2.84930127
7	-1.07741542	1.99392192	-0.54931969
6	-1.54411192	1.58474344	1.82033957
1	-1.94641811	2.02797979	2.75228415
1	-2.16543003	0.72638229	1.54027253
6	-1.59790156	2.59740515	0.67443819
1	-2.65718620	2.87346881	0.54220250
1	-1.07490741	3.52602277	0.97840774
6	-1.75392224	2.25585866	-1.76214513
6	-2.16142011	3.57232179	-2.13272722
6	-2.87640183	3.77430682	-3.32062349
6	-3.19497172	2.73344316	-4.19597817
6	-2.75461554	1.45353594	-3.84702811
6	-2.05394124	1.19243899	-2.66388672
7	-0.67213660	-1.84562839	1.18779975
6	-0.12503833	-0.13561447	2.91787173

1	-0.42603305	0.15625364	3.94232957
1	0.92732490	-0.45424631	2.96423724
6	-0.99889509	-1.32315274	2.52082830
1	-0.84371609	-2.08500587	3.31094621
1	-2.06172495	-1.05556313	2.56154692
6	-1.29102661	-3.05865795	0.77217510
6	-2.69196876	-3.14995309	0.59799078
6	-3.24675805	-4.36219560	0.16450691
6	-2.46692695	-5.48333013	-0.12980962
6	-1.07892349	-5.35712215	0.00314469
6	-0.47880001	-4.17570809	0.44779225
6	-1.77563584	4.79480417	-1.33094155
1	-3.16836216	4.79592859	-3.58023919
6	-3.99431615	2.97667314	-5.45337933
1	-2.97836851	0.61348045	-4.51037781
6	-1.64698230	-0.23159177	-2.38128968
6	-3.60776600	-1.96703234	0.79985632
1	-4.33018431	-4.41590973	0.02970106
6	-3.09474523	-6.78407578	-0.56901405
1	-0.43751370	-6.20758410	-0.24187664
6	1.02563892	-4.09741612	0.55909909
1	-1.86371854	5.69374827	-1.95521567
1	-0.73899449	4.72730471	-0.97425630
1	-2.41006629	4.95174233	-0.44494641
1	-0.59535172	-0.42458638	-2.65431427
1	-2.26062237	-0.93128817	-2.96448989
1	-1.74371354	-0.48508396	-1.31635583
1	-5.07145158	2.81912018	-5.28112287
1	-3.69223134	2.29488520	-6.26068450
1	-3.87020248	4.00773286	-5.81276539
1	-4.53288759	-2.10069990	0.22437432
1	-3.13046012	-1.03562345	0.46373556
1	-3.89998987	-1.83158207	1.85377154
1	1.36245822	-3.81191277	1.56721963
1	1.45122663	-3.35648080	-0.13767737
1	1.47600952	-5.06851921	0.31799421
1	-2.49264271	-7.28030979	-1.34312160
1	-4.10428605	-6.62436143	-0.97104591
1	-3.18388675	-7.48887706	0.27311326
1	0.34259048	-1.93990331	1.11899965

Energy = -7584.966480 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 81

Atomic N.	X	Y	Z
8	2.69081823	-0.65889702	4.23236773
8	2.27386842	0.09534657	-0.38182389
6	3.19943257	0.48517312	-1.38247229
1	2.74957522	0.55736629	-2.39386220
1	4.02874469	-0.24323885	-1.45038244
1	3.64198416	1.47510735	-1.15488497
8	4.15851064	0.97461937	3.94022759
6	3.79830664	-0.34319587	3.84160143
6	4.77896491	-1.32750896	3.22840399
1	5.73270848	-1.30607096	3.78232363
1	4.33067343	-2.31550508	3.38399732
6	5.03932005	-1.08877955	1.72444715

1	4.08712040	-0.86787212	1.21509897
1	5.41241329	-2.03047196	1.29439894
6	6.05929730	0.01809834	1.44007859
1	7.03455687	-0.27165924	1.87036525
1	6.21328398	0.09553765	0.35278637
6	5.67052926	1.39378802	1.99133079
1	4.75101009	1.76107119	1.50787089
1	6.46459418	2.11847614	1.74701191
6	5.46688216	1.43377861	3.50336239
1	6.25418140	0.87037617	4.03080353
1	5.49553669	2.46910467	3.86572426
50	0.25924217	-0.17618278	-0.96022127
7	-0.16443350	1.30358948	0.97781826
6	0.67576198	2.51921642	0.93212443
1	0.63364625	3.06026785	1.89403065
1	0.34312425	3.18698430	0.12943439
1	1.70706057	2.20877113	0.72721123
7	-2.51485563	1.68570361	-1.04779107
6	-1.58628152	1.63604736	1.25328566
1	-1.63972627	2.18786759	2.21142347
1	-2.11752352	0.68436032	1.39936435
6	-2.31552920	2.45438797	0.18978587
1	-3.27687135	2.77826821	0.63713701
1	-1.76579551	3.37449320	-0.04574476
6	-3.20904014	2.34288077	-2.10834393
6	-2.56362010	3.34725720	-2.86466144
6	-3.25868289	3.95949318	-3.91489071
6	-4.56519074	3.59688978	-4.25871350
6	-5.17281100	2.57562730	-3.51966859
6	-4.52466611	1.94844178	-2.44986681
7	-0.31407221	-1.46952456	0.63006466
6	0.35833964	0.40272497	2.05498947
1	0.20493451	0.86811426	3.04470698
1	1.43690535	0.31714445	1.87638046
6	-0.26672303	-0.98774336	2.00633924
1	0.34864998	-1.62171684	2.66822754
1	-1.28010467	-0.97994959	2.46317638
6	-0.54868168	-2.85842929	0.43955725
6	-1.77112932	-3.30289914	-0.12573975
6	-1.99384977	-4.67111005	-0.32321376
6	-1.04041428	-5.63385483	0.02514408
6	0.16440890	-5.18598024	0.57694684
6	0.43211113	-3.82681849	0.78393300
6	-1.12852809	3.72928880	-2.60113683
1	-2.74687365	4.72840310	-4.49923323
6	-5.29861898	4.29150392	-5.38054914
1	-6.18663313	2.25898150	-3.77696447
6	-5.22956638	0.84926240	-1.68882297
6	-2.84526026	-2.31553708	-0.51431137
1	-2.94578552	-4.99382104	-0.75373187
6	-1.28756367	-7.10267108	-0.22357808
1	0.93358349	-5.91695114	0.84190732
6	1.77509459	-3.41147140	1.33069739
1	-0.67627538	4.16792921	-3.49990497
1	-0.53979019	2.84776998	-2.30847987
1	-1.03580231	4.47743730	-1.79661843
1	-4.75605572	-0.13401512	-1.84499589
1	-6.27105198	0.76008112	-2.02168182

1	-5.24332294	1.03577846	-0.60366907
1	-5.85759617	5.16507033	-5.00891832
1	-6.02362890	3.62120180	-5.86177517
1	-4.60276320	4.65346540	-6.14965330
1	-3.78583966	-2.83557027	-0.74058300
1	-2.55894549	-1.73717847	-1.40780600
1	-3.02937307	-1.59108728	0.29248087
1	1.75078509	-3.26606527	2.42265652
1	2.09810269	-2.45956366	0.88543710
1	2.52983460	-4.18165265	1.12077666
1	-0.92139179	-7.40494921	-1.21790934
1	-2.35957369	-7.34053355	-0.18549269
1	-0.77070002	-7.72792645	0.51735119
1	-2.99295562	0.81385453	-0.81649178

Energy = -7584.967301 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 82

Atomic N.	X	Y	Z
8	2.90461201	-3.10823109	2.43289393
8	2.44352121	-0.05935976	-1.17036677
6	3.06330156	-0.41623448	-2.38878689
1	2.38230308	-0.35576847	-3.25784386
1	3.46103958	-1.45114358	-2.34809463
1	3.91899322	0.25313620	-2.59669582
8	3.32359874	-0.95385391	2.72532697
6	3.73883774	-2.21995307	2.44246340
6	5.20750065	-2.46392160	2.13798550
1	5.83213978	-2.08500094	2.96412682
1	5.31953487	-3.55407540	2.11100540
6	5.67814783	-1.84295947	0.80490585
1	4.91981559	-2.03184809	0.02890794
1	6.58836639	-2.37417821	0.48765101
6	5.98307329	-0.34398813	0.88962051
1	6.82568896	-0.19442878	1.58836034
1	6.33243860	0.00678786	-0.09379584
6	4.79956106	0.52018856	1.33780305
1	3.97734792	0.46840610	0.60342589
1	5.12234122	1.57380732	1.37583373
6	4.25048639	0.17145653	2.71667860
1	5.05624090	-0.01396953	3.44666695
1	3.63146102	0.99273239	3.09823949
50	0.47147677	0.50443732	-0.75002941
7	-0.11884718	-1.92674260	-0.91495940
6	0.92022560	-2.75767586	-0.26379470
1	0.79588687	-3.82092933	-0.53609058
1	0.87692005	-2.66076013	0.82545195
1	1.90370856	-2.39965344	-0.58763234
7	-1.95603365	-0.62931522	1.28121162
6	-1.47747449	-2.32896126	-0.46190510
1	-1.60138641	-3.41231582	-0.65411026
1	-2.20635552	-1.80779978	-1.09976777
6	-1.82185049	-2.06650573	1.00280591
1	-2.76127555	-2.61717197	1.21140221
1	-1.06099844	-2.49407281	1.66687068
6	-2.37765464	-0.25424968	2.59138174
6	-1.52088027	-0.43503569	3.70144588

6	-1.96518950	-0.03614472	4.96846560
6	-3.21474662	0.55788747	5.17466555
6	-4.02713748	0.76757657	4.05484243
6	-3.63601134	0.36866820	2.77217249
7	-0.45641777	0.30143417	-2.69085538
6	-0.02145734	-2.09037992	-2.39609928
1	-0.36543542	-3.10201115	-2.68437843
1	1.04321328	-2.01174709	-2.64787724
6	-0.80393963	-1.02974030	-3.16943707
1	-0.53505481	-1.15634946	-4.23750515
1	-1.88869282	-1.25200210	-3.11474299
6	-1.08177482	1.41315488	-3.31837364
6	-2.48975350	1.60983207	-3.30857535
6	-3.04587014	2.72786368	-3.94629117
6	-2.26099969	3.69117803	-4.58285712
6	-0.87332066	3.50747536	-4.56196639
6	-0.27548579	2.39990599	-3.95208381
6	-0.12548650	-0.98236949	3.54255501
1	-1.29293194	-0.17417047	5.81922828
6	-3.67432622	0.94980205	6.55830699
1	-4.99941048	1.25067688	4.18039221
6	-4.55104074	0.62744829	1.59707565
6	-3.41539846	0.68042158	-2.56471106
1	-4.13153493	2.85723266	-3.92005904
6	-2.87734903	4.90567072	-5.23427383
1	-0.23047809	4.24510798	-5.05001361
6	1.22541932	2.25736677	-4.00839168
1	0.51460801	-0.64956096	4.36923315
1	0.32883232	-0.64300925	2.60182384
1	-0.09346081	-2.08328071	3.54393576
1	-4.11558244	1.34562355	0.88224405
1	-5.50286189	1.05254851	1.93896618
1	-4.78348671	-0.29276061	1.03741056
1	-4.18275166	0.11133142	7.06060615
1	-4.38332639	1.78810542	6.52366601
1	-2.82710391	1.24286762	7.19353236
1	-4.32965831	1.20769837	-2.26136185
1	-2.91928908	0.29277991	-1.66265773
1	-3.72441521	-0.18856217	-3.16766761
1	1.51573166	1.29945074	-4.46146597
1	1.69079322	2.28294190	-3.01106874
1	1.66492187	3.07054619	-4.60095356
1	-2.75503251	5.80132184	-4.60472397
1	-3.95314160	4.76556164	-5.40436300
1	-2.40418064	5.12607827	-6.20203878
1	-2.59579754	-0.22431879	0.59707923

Energy = -7584.964018 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 83

Atomic N.	X	Y	Z
8	2.27147503	1.28863001	1.10235276
8	2.19277879	-2.10567772	0.14097692
6	3.51755689	-2.24088014	-0.34314357
1	3.62928737	-3.14689349	-0.97149593
1	4.22245968	-2.34374965	0.50264101
1	3.85661474	-1.37643526	-0.94883464

8	4.31690196	1.47499222	1.90944717
6	3.00755725	1.12737311	2.06463704
6	2.54249527	0.55472467	3.38658834
1	2.79843891	1.24817992	4.20526459
1	1.44970433	0.50352371	3.32280061
6	3.11951522	-0.84589328	3.68541426
1	3.04876741	-1.46374239	2.77599360
1	2.46376216	-1.32011492	4.43015015
6	4.55136450	-0.83274643	4.22995594
1	4.55579334	-0.31333472	5.20455739
1	4.87087085	-1.86704750	4.43233082
6	5.58060998	-0.15829148	3.31633936
1	5.68664007	-0.70923195	2.36761894
1	6.56877476	-0.18546401	3.80434622
6	5.27456046	1.30059267	2.98970546
1	4.93355388	1.85115914	3.88153552
1	6.17026714	1.80317743	2.60413616
50	0.94647361	-0.64342019	-0.67903898
7	-0.36532309	-2.45536233	-1.94773766
6	0.46927306	-3.67569078	-1.88160233
1	-0.10334441	-4.55906263	-2.21808645
1	0.84189897	-3.82459737	-0.86256415
1	1.34138686	-3.54894758	-2.53674405
7	-0.64170690	-1.21703075	0.65897060
6	-1.58597663	-2.59675860	-1.11553619
1	-2.09863079	-3.55186630	-1.34686832
1	-2.25340012	-1.76151419	-1.35821775
6	-1.25159915	-2.51200713	0.37344194
1	-2.20076591	-2.61273388	0.92842322
1	-0.63418842	-3.38570550	0.65804516
6	-0.84792705	-0.64643686	1.93141292
6	-0.69430979	-1.38445891	3.14030981
6	-0.97150849	-0.76946490	4.36980778
6	-1.36443492	0.56858752	4.46899361
6	-1.45955826	1.29927157	3.27835946
6	-1.21722468	0.72655798	2.02521909
7	-1.32534665	0.20718954	-3.15788035
6	-0.65810549	-2.18886460	-3.38368203
1	-1.02249313	-3.12246045	-3.85596318
1	0.30709514	-1.94793679	-3.85816025
6	-1.67632612	-1.10090965	-3.72027390
1	-1.73253513	-1.07333874	-4.82692512
1	-2.67462732	-1.40283371	-3.37432530
6	-1.95215836	1.36529531	-3.69085611
6	-3.34604917	1.56375640	-3.56042519
6	-3.91944757	2.72937695	-4.08573406
6	-3.16005621	3.72255006	-4.71098590
6	-1.77555056	3.52817616	-4.78682650
6	-1.15978099	2.37311839	-4.29559074
6	-0.13698546	-2.78908960	3.14524545
1	-0.84446428	-1.35644901	5.28435968
6	-1.68811539	1.19703745	5.80345191
1	-1.75226700	2.35192276	3.32033728
6	-1.35799414	1.57461720	0.78758958
6	-4.21748333	0.58996685	-2.80588516
1	-4.99705925	2.87343330	-3.97240984
6	-3.80815798	4.95699097	-5.29006626
1	-1.15118798	4.29735684	-5.24841126

6	0.33956578	2.21964560	-4.40036197
1	0.24011242	-3.04223055	4.14548262
1	0.68946013	-2.88170919	2.42469192
1	-0.88694634	-3.55080552	2.88050861
1	-0.37518922	1.89518417	0.40359581
1	-1.93396399	2.48456095	1.00252727
1	-1.84799699	1.01886692	-0.02399053
1	-2.76642977	1.13989110	6.02361738
1	-1.41062074	2.26035701	5.82564480
1	-1.16253713	0.68849239	6.62389988
1	-5.14164203	1.08179944	-2.47601428
1	-3.69503142	0.20699212	-1.91694783
1	-4.51278067	-0.27776213	-3.41725624
1	0.62561335	1.30920612	-4.95172868
1	0.82281495	2.16279523	-3.41103010
1	0.77697834	3.07630783	-4.92789835
1	-3.16450337	5.84021811	-5.17575766
1	-4.76980781	5.16902090	-4.80339476
1	-4.00578794	4.83600460	-6.36723524
1	-0.31109507	0.32205016	-3.15484125

Energy = -7584.965323 Hartree

Number of imaginary frequencies = 0.

Compound I2b isomer 84

Atomic N.	X	Y	Z
8	1.73273654	-0.94325681	-1.51163556
8	1.65455358	1.81116578	-0.68564943
6	1.66897157	3.04707297	0.00713175
1	1.21783010	2.98621877	1.02143990
1	1.12922116	3.83919593	-0.54528578
1	2.71315249	3.38784380	0.14005377
8	3.03013176	-1.03038987	0.27091908
6	2.88056792	-0.91471736	-1.05887917
6	4.08728132	-0.73996921	-1.95001167
1	4.83787841	-1.51865202	-1.73661584
1	3.72622690	-0.88632818	-2.97432593
6	4.71808187	0.66482221	-1.80088020
1	3.90733898	1.40947344	-1.77066145
1	5.31330809	0.86129224	-2.70474824
6	5.61792888	0.80637917	-0.56931939
1	6.47500096	0.11626367	-0.66530381
1	6.04129146	1.82232381	-0.55179615
6	4.91390962	0.53627713	0.76567830
1	4.10038339	1.25908176	0.93290027
1	5.63593456	0.67061047	1.58749447
6	4.33695596	-0.86749461	0.90414488
1	5.02387070	-1.63734755	0.51738308
1	4.11971506	-1.09771315	1.95358805
50	0.03136533	0.52537025	-0.29578987
7	-1.45940343	-1.74908283	-1.19190021
6	-0.77954967	-3.04490916	-1.29941640
1	-1.43432171	-3.83023615	-1.72942894
1	-0.43182858	-3.36519991	-0.30961838
1	0.09691644	-2.92667954	-1.94705991
7	-1.50738030	-2.21470572	1.82712523
6	-2.67625939	-1.80853730	-0.35539462
1	-3.51782063	-2.23349692	-0.94297250

1	-2.95935701	-0.77425672	-0.09864603
6	-2.58760207	-2.63851043	0.92610927
1	-3.57648434	-2.55439673	1.41654247
1	-2.46632977	-3.69948124	0.66161156
6	-1.61431850	-2.51783286	3.20606500
6	-1.64694966	-3.86133480	3.65140258
6	-1.74029871	-4.12628262	5.02407747
6	-1.77562206	-3.10963511	5.98280484
6	-1.69926947	-1.78830471	5.52612600
6	-1.62619290	-1.47306429	4.16564512
7	-1.00797541	1.07233716	-2.07369478
6	-1.77958266	-1.22286074	-2.53294997
1	-2.61281327	-1.80123912	-2.98751235
1	-0.88468567	-1.36052762	-3.15597833
6	-2.13270252	0.26436501	-2.53845586
1	-2.37264548	0.53077325	-3.58335141
1	-3.07097112	0.42935104	-1.96862253
6	-0.94284484	2.39630888	-2.60043305
6	-1.87271169	3.39400478	-2.21267124
6	-1.78023117	4.68053710	-2.76330227
6	-0.78883134	5.02167330	-3.68699555
6	0.12152123	4.02634397	-4.06344042
6	0.06410148	2.72902845	-3.54235563
6	-1.50522394	-5.01500943	2.68889559
1	-1.75826372	-5.16941788	5.35098722
6	-1.90525986	-3.42204496	7.45432823
1	-1.70893375	-0.97013017	6.25102564
6	-1.56045830	-0.02727356	3.73629588
6	-2.95894546	3.10558603	-1.20541784
1	-2.50162102	5.43965129	-2.44842496
6	-0.68137807	6.42313885	-4.23922017
1	0.90079310	4.26454450	-4.79263342
6	1.06536335	1.69648884	-3.99076751
1	-1.17007980	-5.91578853	3.21964451
1	-0.77112431	-4.77974284	1.90408000
1	-2.45174521	-5.26702844	2.18505478
1	-0.61833129	0.21304439	3.21737103
1	-1.63768736	0.63658769	4.60663936
1	-2.37461881	0.23364141	3.04132696
1	-2.95482396	-3.36256602	7.78455918
1	-1.33234979	-2.71326730	8.06853539
1	-1.54901181	-4.43635712	7.68051055
1	-3.30678314	4.03315794	-0.73185210
1	-2.60207292	2.42315228	-0.41974892
1	-3.83442099	2.62696996	-1.67264097
1	0.57181708	0.77175708	-4.32132591
1	1.72276722	1.42363225	-3.15364489
1	1.67888067	2.08505347	-4.81505586
1	0.08037821	7.00676900	-3.69786360
1	-1.63362404	6.96325024	-4.15001673
1	-0.38914298	6.41567026	-5.29894423
1	-1.26529150	-1.23514027	1.66516256

Energy = -7584.958106 Hartree

Number of imaginary frequencies = 0.

Transition state 2a (TS2a)

Compound TS2a isomer 1

Atomic N.	X	Y	Z
8	-0.39866149	-0.06024110	1.20612001
8	0.69071293	-0.68101114	-0.89185905
6	0.60590482	-1.43629527	-2.09251952
1	0.97865146	-0.82546681	-2.93091321
1	-0.42727533	-1.75397253	-2.32874680
1	1.23779738	-2.33887553	-2.02175546
8	1.22876251	-1.51728714	1.50849187
6	0.06332588	-1.21458137	0.88119370
6	-0.88786525	-2.34180593	0.51727742
1	-0.43950084	-3.01073885	-0.23112167
1	-1.75502634	-1.86618197	0.04188611
6	-1.32092035	-3.17019272	1.74541712
1	-1.49332094	-2.50689650	2.60763001
1	-2.29187918	-3.63577938	1.51979291
6	-0.31899828	-4.27654123	2.10314822
1	-0.23216565	-4.95838022	1.23918235
1	-0.72267056	-4.87992811	2.93098092
6	1.08249342	-3.78325582	2.48495889
1	1.05318391	-3.24139142	3.44400525
1	1.74220705	-4.65327024	2.63786411
6	1.74757266	-2.87164211	1.45636451
1	1.66843808	-3.26982093	0.43314454
1	2.81324244	-2.74905300	1.68889546
50	-0.39523229	1.27419746	-0.70694232
7	-0.51806295	2.95223808	1.49238646
6	-0.96121210	4.24695778	0.95410222
1	-0.86059952	5.05819178	1.70135105
1	-2.00975585	4.17926979	0.64137292
1	-0.36689350	4.50709867	0.06963302
6	-1.30720305	2.56035972	2.68081379
1	-1.20671403	3.33653975	3.46820760
1	-0.85547757	1.63704336	3.07082462
6	-2.80170727	2.32701588	2.47206831
1	-3.21567011	2.08175850	3.46595359
1	-3.32010889	3.22903347	2.12335896
6	0.90790337	2.98172879	1.89084947
1	1.13301444	1.99426925	2.31846285
1	1.08127606	3.74823976	2.67392826
6	1.85487974	3.24175930	0.72361404
1	1.78817654	4.28635359	0.37735584
1	2.88290429	3.09564447	1.10211730
1	-2.34755230	0.48508969	1.60528064
7	-3.03136945	1.24909770	1.48666549
16	-4.60935593	0.60187203	1.53240156
8	-4.74813700	-0.42750779	2.59035492
8	-5.51960182	1.76546192	1.52084243
6	-4.66801500	-0.24714442	-0.05805261
6	-4.45662880	0.47212431	-1.23826504
6	-4.54313421	-0.19322681	-2.45826864
6	-4.84062910	-1.56686461	-2.51907301
6	-5.04761267	-2.26042342	-1.31799030
6	-4.96160078	-1.60988092	-0.08395885
1	-4.21802902	1.53373718	-1.19578052
1	-4.36701059	0.36041674	-3.38214636
6	-4.93792963	-2.26756597	-3.85069990
1	-5.27912569	-3.32665968	-1.34600401

1	-5.12040567	-2.14189959	0.85361326
1	-5.78864670	-1.88514078	-4.43431902
1	-4.03415537	-2.09975624	-4.45401764
1	-5.07341909	-3.34924173	-3.72669435
7	1.54401565	2.29925203	-0.34994116
16	2.29717207	2.50624728	-1.78930175
8	1.45618999	1.69417775	-2.73129773
8	2.57260680	3.92624831	-2.11509252
6	3.90785623	1.68623042	-1.65478015
6	5.05874062	2.36003733	-2.06052780
6	6.29294682	1.70972574	-1.97189820
6	6.38839865	0.40056774	-1.48001575
6	5.20864153	-0.25103319	-1.07671523
6	3.96901584	0.38028979	-1.15797901
1	4.97863340	3.37823176	-2.43965554
1	7.19726515	2.23120308	-2.29133534
6	7.72426367	-0.29084605	-1.36386275
1	5.26597404	-1.27185535	-0.69214255
1	3.05143714	-0.12094145	-0.84008735
1	8.50174332	0.24265988	-1.92538679
1	8.04927063	-0.34513238	-0.31323490
1	7.67466259	-1.32263935	-1.73952889

Energy = -8524.632654 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 2

Atomic N.	X	Y	Z
8	-0.06268904	-0.97838688	1.63301265
8	1.83649874	-1.44877970	0.19589338
6	2.67097855	-2.20413566	-0.66726148
1	3.09657550	-1.54955995	-1.44392896
1	2.12184978	-3.02528358	-1.16807091
1	3.50842714	-2.63898134	-0.09478212
8	1.48736906	-2.09492922	2.73125625
6	0.64638758	-2.04247046	1.67292285
6	0.13293076	-3.33761072	1.06912839
1	0.95700604	-3.92012048	0.63238758
1	-0.52631843	-3.04453945	0.24245638
6	-0.62601703	-4.21037865	2.09179950
1	-1.25761890	-3.57681417	2.73464918
1	-1.31466091	-4.86516476	1.53687584
6	0.30356878	-5.08734035	2.94150114
1	0.86011696	-5.76004553	2.26584983
1	-0.30252233	-5.73742008	3.59149623
6	1.30872846	-4.31628752	3.80640411
1	0.78777933	-3.75992608	4.60230112
1	1.97460163	-5.03457212	4.31240320
6	2.18828201	-3.32894778	3.04395485
1	2.60814643	-3.76717257	2.12611651
1	3.02403069	-2.99560976	3.67165351
50	0.47199398	0.17240088	-0.37004143
7	-0.49976408	2.01179051	1.55472600
6	-0.95542115	3.19001245	0.80522579
1	-1.14575922	4.05533934	1.47083580
1	-1.87792301	2.94924736	0.26406950
1	-0.19865564	3.47464275	0.06422373
6	-1.50314212	1.58393526	2.55217624

1	-1.68505609	2.40479636	3.27788448
1	-1.06063628	0.74502623	3.10721064
6	-2.86733341	1.15788591	2.01271367
1	-3.47171092	0.87526107	2.89290476
1	-3.39273524	1.98155940	1.51300657
6	0.76754045	2.26960397	2.27490950
1	1.02455199	1.33722937	2.79839802
1	0.63497508	3.06841016	3.03381896
6	1.91865432	2.65654445	1.34774816
1	1.79361475	3.69804788	0.99627143
1	2.85154891	2.62343001	1.93582392
1	-2.02807879	-0.63888747	1.37408173
7	-2.72792935	0.04686656	1.04725206
16	-4.19454718	-0.76158965	0.72598022
8	-4.54703808	-1.71685922	1.80376410
8	-5.15881634	0.29071370	0.34320772
6	-3.72248936	-1.72771943	-0.72181785
6	-3.32882023	-1.07309353	-1.89264274
6	-2.99577594	-1.83289361	-3.01077199
6	-3.04903483	-3.23823762	-2.97804308
6	-3.45279479	-3.86517119	-1.79054058
6	-3.78836727	-3.11873388	-0.65758020
1	-3.28275824	0.01464074	-1.91962624
1	-2.67977381	-1.32860041	-3.92564583
6	-2.66454649	-4.04461384	-4.19275331
1	-3.50694442	-4.95452309	-1.74954736
1	-4.10572243	-3.59766340	0.26826847
1	-3.18528199	-3.68402624	-5.09104586
1	-1.58515084	-3.96115994	-4.39139175
1	-2.90233135	-5.10760498	-4.06122732
7	1.95193398	1.71753848	0.23403952
16	3.10743952	1.86184859	-0.90764105
8	4.48308325	1.92072678	-0.36479357
8	2.73532748	0.78146982	-1.88384116
6	2.83085799	3.44589543	-1.74935007
6	1.73474419	3.58730125	-2.60595298
6	1.51357710	4.81048393	-3.23544812
6	2.37133145	5.90433264	-3.02038169
6	3.46020269	5.73612547	-2.15356231
6	3.69784451	4.51378202	-1.51822591
1	1.07436764	2.73835373	-2.78793192
1	0.66236603	4.92049885	-3.91037822
6	2.13634491	7.21456051	-3.72969604
1	4.13798952	6.57290268	-1.97435081
1	4.55399609	4.37460899	-0.85888350
1	2.47242904	7.15801144	-4.77673626
1	1.06904316	7.47525883	-3.74719214
1	2.68513012	8.03477097	-3.24951816

Energy = -8524.628982 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 3

Atomic N.	X	Y	Z
8	0.80265611	-1.55691552	-0.06401067
8	2.03702021	-0.65993553	-1.90567362
6	3.15778136	-0.59408492	-2.77902555
1	2.81058931	-0.31815141	-3.78708863

1	3.70080733	-1.55449951	-2.85123897
1	3.86099243	0.18200964	-2.43222666
8	2.22116256	-0.01484871	0.62358236
6	2.04028058	-1.17841077	-0.04369332
6	3.15928340	-2.20686197	-0.05904061
1	4.04539394	-1.80856419	-0.57494837
1	2.78753901	-3.04543519	-0.66373384
6	3.56142259	-2.69982338	1.34686399
1	2.66735625	-2.85217929	1.96853733
1	4.03738928	-3.68530989	1.23061728
6	4.54895878	-1.76302612	2.05427647
1	5.47362852	-1.70058751	1.45299435
1	4.83678055	-2.20703745	3.01931453
6	4.02207899	-0.34423763	2.30068374
1	3.18603110	-0.36492223	3.01691318
1	4.81937790	0.26307335	2.76033878
6	3.55847883	0.38707584	1.04535913
1	4.26246643	0.26507753	0.20904630
1	3.44149017	1.45966339	1.24071145
50	0.31588095	-2.04139638	-2.24218392
7	-2.20388532	-2.53772354	-0.96025133
6	-2.87593126	-3.09755039	-2.14632726
1	-3.97709394	-3.10628223	-2.02611136
1	-2.62426519	-2.52354026	-3.04641724
1	-2.53419209	-4.13041782	-2.29526687
7	-1.12132072	-0.35324758	-2.43751144
6	-2.64460421	-1.15795803	-0.67990649
1	-3.71220970	-1.12448072	-0.37582335
1	-2.04329991	-0.77877039	0.15712060
6	-2.46901512	-0.22056100	-1.87439466
1	-2.64698339	0.80594432	-1.50622427
1	-3.23441625	-0.42250836	-2.64082050
16	-0.87349313	0.31146556	-3.91644597
7	-0.80221409	-2.84181690	1.92204583
6	-2.48269272	-3.46425128	0.17112342
1	-3.55833697	-3.73718047	0.14319949
1	-1.90814030	-4.38583851	-0.00632701
6	-2.22866631	-2.96855044	1.59278500
1	-2.65354848	-3.72367501	2.26863194
1	-2.78686023	-2.03192544	1.77073860
16	-0.46395364	-2.31238484	3.48801517
8	1.00462973	-2.16170096	3.54896140
8	-1.19016063	-3.20243883	4.41462469
6	-1.19563425	-0.66169071	3.65372586
6	-2.27654004	-0.47419986	4.51521730
6	-2.83709598	0.80022174	4.63604212
6	-2.33522177	1.88554084	3.90370750
6	-1.25077915	1.66327572	3.03613520
6	-0.67401600	0.40080968	2.90719509
1	-2.66059947	-1.32021415	5.08422327
1	0.16617563	0.24351555	2.22876024
1	-0.85212749	2.49388051	2.45028329
6	-2.92695308	3.26444483	4.05514526
1	-3.68122911	0.95148194	5.31139231
8	0.35784122	-0.40327135	-4.40028954
8	-2.08037829	0.31375235	-4.77732420
6	-0.42438668	2.04570293	-3.64939666
6	-1.07855928	3.04241133	-4.37240076

6	-0.71625632	4.37668324	-4.16867256
6	0.28834647	4.72320557	-3.25403738
6	0.92253500	3.69460630	-2.53413010
6	0.57571650	2.35802913	-2.72323847
1	-1.86068106	2.76727509	-5.07901525
1	-1.22587609	5.16155386	-4.73079491
6	0.69682139	6.16212988	-3.05849123
1	1.70083678	3.94789553	-1.81108224
1	1.06489980	1.55918610	-2.16085744
1	-3.93010092	3.22421408	4.49845695
1	-2.29921913	3.88830352	4.71025038
1	-2.99537253	3.77953172	3.08716536
1	1.62392080	6.38340950	-3.61006570
1	-0.07602771	6.85181141	-3.42147374
1	0.89025116	6.38448858	-1.99997962
1	-0.23448411	-2.30326390	1.24175620

Energy = -8524.634531 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 4

Atomic N.	X	Y	Z
8	1.82028127	-2.21663880	-0.65398383
8	3.14921641	-1.72360730	1.33153677
6	3.22890449	-1.93105352	2.73466444
1	3.38992691	-0.97139412	3.24913812
1	4.08149719	-2.59495711	2.96404195
1	2.30073071	-2.37197709	3.13679910
8	1.52454436	-3.74986839	0.92768937
6	2.38844609	-3.05346107	0.13462700
6	3.68732166	-3.71604514	-0.29460537
1	4.31294632	-3.95365524	0.57770717
1	4.22052526	-2.95716095	-0.87821835
6	3.45055199	-4.98580408	-1.13859129
1	2.61629796	-4.81434345	-1.83738005
1	4.34250832	-5.15554571	-1.76021779
6	3.19983077	-6.24044514	-0.29195189
1	4.09138632	-6.42336416	0.33298472
1	3.10465813	-7.11548042	-0.95392239
6	1.96876466	-6.16839552	0.61990821
1	1.04304254	-6.13849640	0.02263219
1	1.91756594	-7.08576679	1.22941399
6	1.95066381	-4.97905397	1.57685328
1	2.92403388	-4.83382130	2.06920981
1	1.19569981	-5.12647390	2.35964084
50	2.08925271	-0.14377210	0.22453544
7	-2.09716511	-0.48420757	-1.14110529
6	-3.26921868	0.03810545	-0.43815351
1	-2.97729993	0.46202591	0.53048903
1	-3.71958613	0.84340763	-1.03353333
1	-4.04655743	-0.73805606	-0.25744268
7	-1.02170467	0.33680958	-4.08065128
6	-2.47119045	-0.92972565	-2.49098468
1	-2.95336270	-1.93465388	-2.45429969
1	-3.22153258	-0.23179629	-2.88966036
6	-1.30034804	-0.98432642	-3.48118830
1	-1.54041529	-1.69426048	-4.28754663
1	-0.38732442	-1.34929407	-2.99259949

16	0.54116499	1.00903308	-3.96985245
7	0.01727660	-0.34745753	1.15837646
6	-1.48250484	-1.60910594	-0.41773465
1	-2.19829130	-2.46463227	-0.37260845
1	-0.60786325	-1.95680380	-0.98422521
6	-1.04782939	-1.35715437	1.02669919
1	-0.71139419	-2.32897520	1.42279303
1	-1.92093146	-1.05935955	1.63127613
16	0.24829590	0.25689656	2.65606284
8	1.62608135	0.87490368	2.54025960
8	-0.01966814	-0.70121592	3.75474191
6	-0.89278132	1.63914704	2.91783643
6	-2.05272841	1.43540061	3.66729307
6	-2.94041467	2.49823141	3.85297704
6	-2.67617249	3.76673651	3.31695509
6	-1.49428225	3.94464898	2.57630444
6	-0.60534155	2.89144039	2.36842108
1	-2.24158549	0.45934975	4.11270094
1	0.31425828	3.03607988	1.80147135
1	-1.26475048	4.92902374	2.16240168
6	-3.61512709	4.92251635	3.55656743
1	-3.84994531	2.34012246	4.43556356
8	1.31839967	0.18121982	-3.02210140
8	1.02296543	1.26039815	-5.34624624
6	0.23380893	2.61612129	-3.21127629
6	0.65393841	3.76517725	-3.87937856
6	0.43706495	5.01054907	-3.28431225
6	-0.19528428	5.11615181	-2.03770924
6	-0.61113256	3.93688107	-1.39410079
6	-0.39606893	2.68428421	-1.96528280
1	1.13679981	3.67647219	-4.85165405
1	0.76294452	5.91458750	-3.80193996
6	-0.40593478	6.46054554	-1.38677430
1	-1.11368299	3.99821377	-0.42715591
1	-0.72627854	1.77274001	-1.46081805
1	-4.61850739	4.57332611	3.83213830
1	-3.24953437	5.55964851	4.37692595
1	-3.70250535	5.56013393	2.66618443
1	0.37710014	6.65749836	-0.63768917
1	-0.36961678	7.27388859	-2.12289691
1	-1.37270772	6.50676346	-0.86687821
1	-1.30012500	0.41312763	-5.05915022

Energy = -8524.618900 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 5

Atomic N.	X	Y	Z
8	3.21783805	-2.94983172	-1.51025224
8	3.74050879	-1.76578224	-3.54597783
6	4.18976402	-0.48597220	-3.98166919
1	3.49816799	-0.09604542	-4.74195051
1	5.19341755	-0.57879698	-4.43103313
1	4.22244120	0.23744057	-3.15041208
8	4.78101873	-1.39387822	-1.21263564
6	4.34753036	-2.47753525	-1.92754054
6	5.38544083	-3.44859338	-2.47336793
1	6.05440044	-2.94630408	-3.18722034

1	4.81552649	-4.19528198	-3.03853607
6	6.20912361	-4.12278986	-1.35778475
1	5.54817200	-4.37267017	-0.51259518
1	6.59277964	-5.07960224	-1.74297702
6	7.39813042	-3.27602005	-0.88524741
1	8.07560539	-3.11674452	-1.74235272
1	7.97657156	-3.84232712	-0.13854399
6	7.02372694	-1.91083634	-0.29529265
1	6.47330284	-2.03385615	0.65139580
1	7.94633055	-1.35858297	-0.05131528
6	6.18594646	-1.02451026	-1.21394145
1	6.58120251	-1.01166046	-2.24138141
1	6.17676258	0.00914984	-0.84463590
50	1.67417860	-2.35356021	-3.02982736
7	-0.42843184	0.77004719	0.71157426
6	0.18528731	2.02360797	1.14569867
1	1.03798687	2.27342057	0.50126380
1	-0.54645598	2.83816314	1.06052458
1	0.54519445	1.98331773	2.19820118
7	-3.73957467	-0.87881434	1.51036906
6	-1.64073694	0.47447526	1.48232329
1	-1.41207719	-0.03068235	2.44542289
1	-2.12512922	1.42998505	1.73004174
6	-2.62372231	-0.37949076	0.67326063
1	-2.11678123	-1.27674484	0.29136509
1	-2.98799706	0.19176877	-0.19187090
16	-5.10647297	0.12840880	1.71967483
7	1.10861146	-0.65182436	-1.67825794
6	0.52658629	-0.34112823	0.76379108
1	1.04692161	-0.36719704	1.75085473
1	-0.02786174	-1.28654695	0.67354989
6	1.59455681	-0.31832930	-0.33274344
1	2.34944630	-1.08016026	-0.08548661
1	2.12484622	0.64660341	-0.35194293
16	0.77188498	0.53489763	-2.75239229
8	0.99336332	-0.20804536	-4.06674337
8	1.50630164	1.79820287	-2.51168871
6	-0.99001104	0.94002563	-2.77140999
6	-1.40557718	2.21409559	-2.38539219
6	-2.76547265	2.52393174	-2.42009521
6	-3.71882677	1.57841957	-2.83062029
6	-3.26665521	0.30868679	-3.22825646
6	-1.91085541	-0.01664702	-3.20180798
1	-0.66433507	2.94838834	-2.07366276
1	-1.57053077	-0.99952239	-3.52905703
1	-3.98946762	-0.43619394	-3.56591797
6	-5.18865585	1.90805602	-2.81346488
1	-3.09511948	3.51925230	-2.11685777
8	-5.11578560	1.21535480	0.71407515
8	-6.23996067	-0.81253654	1.84614325
6	-4.82325459	0.89390171	3.32873178
6	-4.81942892	0.09435007	4.47559166
6	-4.64086437	0.69654232	5.71774721
6	-4.47198677	2.08871269	5.83433104
6	-4.48776674	2.86347318	4.66647720
6	-4.66434669	2.27555490	3.41076851
1	-4.95907545	-0.98275185	4.39094734
1	-4.63461542	0.07729792	6.61666679

6	-4.29123688	2.72465467	7.18954515
1	-4.36230326	3.94526434	4.73746204
1	-4.68093061	2.87422323	2.50089717
1	-5.36835480	2.95287299	-3.10098624
1	-5.75492764	1.25734186	-3.49225497
1	-5.59400177	1.77081418	-1.79888475
1	-5.19726706	2.60686088	7.80280828
1	-3.46573234	2.25370073	7.74250269
1	-4.07860184	3.79752898	7.10409451
1	-4.12768364	-1.76099670	1.16818392

Energy = -8524.624369 Hartree
Number of imaginary frequencies = 0.

Compound TS2a isomer 6

Atomic N.	X	Y	Z
8	2.01942492	-2.84379530	-0.45705172
8	3.41517735	-1.75527966	1.19952583
6	4.62085009	-1.19545913	1.69278955
1	4.39285135	-0.27507287	2.25465727
1	5.33641481	-0.94159693	0.88670039
1	5.11036921	-1.90014577	2.38718462
8	2.97003436	-4.31878185	0.87835044
6	3.12693071	-3.28693223	0.01118095
6	4.39639187	-3.21653128	-0.82259959
1	5.27643824	-3.03912091	-0.18766478
1	4.28135443	-2.33706594	-1.46846712
6	4.62458897	-4.48656321	-1.66954052
1	3.66596794	-4.83694029	-2.08442044
1	5.25273561	-4.21505022	-2.53142071
6	5.32283497	-5.61193514	-0.89371282
1	6.30485868	-5.24007702	-0.55293989
1	5.53250790	-6.45044088	-1.57628834
6	4.54687643	-6.13915157	0.31975433
1	3.63814044	-6.67180967	-0.00436164
1	5.16834641	-6.87741613	0.85305935
6	4.12745857	-5.07096624	1.32641304
1	4.95207739	-4.38547611	1.57352448
1	3.78708553	-5.53731728	2.25954747
50	1.83217406	-0.63443440	0.13887946
7	-0.87837398	-1.70123804	-0.51872182
6	-0.84618467	-2.52122521	-1.73736739
1	-1.77896416	-3.11002541	-1.86098433
1	-0.71331525	-1.88572633	-2.62163234
1	0.00860969	-3.20447803	-1.68262446
7	-0.91979855	1.36118877	-1.11622584
6	-2.02006340	-0.77495992	-0.53514302
1	-2.95884919	-1.33093286	-0.75163198
1	-2.13398910	-0.34744757	0.47116500
6	-1.92802238	0.37940091	-1.53631794
1	-2.93510556	0.82782841	-1.62024224
1	-1.64147234	0.02166824	-2.53333664
16	-0.45266902	2.55799127	-2.22219110
7	0.43381935	-0.93705535	1.84557033
6	-0.93824965	-2.57501602	0.67195886
1	-1.90577304	-3.11821628	0.72597021
1	-0.13531497	-3.31470299	0.55713505
6	-0.72366351	-1.81433177	1.98503196

1	-0.57412922	-2.55869579	2.78522229
1	-1.63101578	-1.23964214	2.25333643
16	0.82690912	0.07287463	3.06133747
8	2.08923006	0.71820945	2.56979966
8	0.77831101	-0.55563265	4.40041924
6	-0.43093491	1.38405716	3.07490039
6	-1.55185306	1.26541483	3.89918399
6	-2.53814387	2.25559759	3.86164594
6	-2.41399217	3.37344933	3.02398229
6	-1.26895547	3.47425294	2.21370292
6	-0.28062806	2.48930836	2.23014641
1	-1.63342905	0.41695604	4.57819080
1	0.61138302	2.58307385	1.60939598
1	-1.13865328	4.34689903	1.57017958
6	-3.45741129	4.46295738	3.02265143
1	-3.41498542	2.16208911	4.50547600
8	0.46619746	3.43056917	-1.46801901
8	-0.05454021	1.84648657	-3.45029497
6	-1.92834735	3.52900743	-2.62031102
6	-2.73495317	3.15266490	-3.69679642
6	-3.88021851	3.89866543	-3.98162651
6	-4.22792339	5.01949978	-3.21187353
6	-3.39410901	5.37812424	-2.13913178
6	-2.24828291	4.64247561	-1.83864748
1	-2.45169163	2.29995036	-4.31293964
1	-4.51115942	3.60928154	-4.82400322
6	-5.44473648	5.84312582	-3.55046582
1	-3.64196491	6.25384808	-1.53620577
1	-1.58693504	4.93734694	-1.02437270
1	-4.43585348	4.08290339	3.34429908
1	-3.17599368	5.27364349	3.71289110
1	-3.56898642	4.91104221	2.02585888
1	-5.17578363	6.67648935	-4.21827888
1	-6.20539284	5.24263000	-4.06603575
1	-5.89695692	6.28040743	-2.65050650
1	-1.10858083	1.79530632	-0.20662244

Energy = -8524.624967 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 7

Atomic N.	X	Y	Z
8	0.85347974	-1.51350081	-0.29140797
8	1.92370677	-0.35292917	-2.08851743
6	2.97978187	-0.13639191	-3.01625586
1	3.55229306	-1.05656183	-3.23547125
1	3.67538357	0.62493622	-2.62426805
1	2.55584240	0.23842652	-3.96108198
8	2.25481963	0.00061710	0.48625338
6	2.07400942	-1.08375823	-0.30294970
6	3.22762823	-2.04996920	-0.51404852
1	4.06390715	-1.54958832	-1.02421880
1	2.85077095	-2.82199407	-1.19889867
6	3.73482871	-2.69662642	0.79191029
1	2.88749146	-2.96580052	1.43894446
1	4.23970747	-3.63709760	0.52391261
6	4.72744036	-1.81091464	1.55541801
1	5.61037731	-1.63226330	0.91593456

1	5.09058619	-2.35733223	2.43906426
6	4.16194010	-0.45967859	2.00846815
1	3.37092352	-0.60858512	2.75970030
1	4.96117210	0.12052137	2.49884295
6	3.59715223	0.40421906	0.88514835
1	4.25725555	0.42771050	0.00429990
1	3.45428586	1.43663597	1.22849500
50	0.23779266	-1.76408195	-2.47514415
7	-2.17420316	-2.50520611	-1.09495330
6	-2.90525651	-2.96030045	-2.29081631
1	-3.99506831	-3.02633405	-2.10333991
1	-2.73361158	-2.28286910	-3.13616323
1	-2.54022217	-3.95646381	-2.57399750
7	-1.26898324	-0.12767678	-2.38668871
6	-2.64103484	-1.18298960	-0.63644427
1	-3.68595433	-1.22635126	-0.26263106
1	-1.99718869	-0.87218988	0.19714998
6	-2.57958531	-0.11536988	-1.72842634
1	-2.76910925	0.85665435	-1.23830891
1	-3.38712621	-0.26591855	-2.46273279
16	-1.14824903	0.70109427	-3.79712629
7	-0.57164866	-3.06317973	1.63993633
6	-2.34637833	-3.55851555	-0.05718308
1	-3.41231346	-3.86848044	-0.04631623
1	-1.75621855	-4.43254137	-0.37130901
6	-2.01239681	-3.20966434	1.39136958
1	-2.36569262	-4.04961681	2.00552273
1	-2.58693171	-2.32051253	1.70731580
16	-0.14266427	-2.69632602	3.22969747
8	1.32101882	-2.49468350	3.21045542
8	-0.77292955	-3.71151590	4.09591866
6	-0.91439432	-1.10460579	3.62861562
6	-1.93001425	-1.05571616	4.58354092
6	-2.52174664	0.17392533	4.88492823
6	-2.11559153	1.35136139	4.24080658
6	-1.09578800	1.26865888	3.27582526
6	-0.48883396	0.05246626	2.96658015
1	-2.23952842	-1.97331989	5.08288622
1	0.30051363	0.00411709	2.21449757
1	-0.77251983	2.17306042	2.75656843
6	-2.73945165	2.68033743	4.58599377
1	-3.31491756	0.21669112	5.63365793
8	0.07347018	0.09842206	-4.43405485
8	-2.41066360	0.74044383	-4.57327652
6	-0.74655235	2.41537189	-3.37267613
6	-1.48319447	3.45360351	-3.94184136
6	-1.15585244	4.77326965	-3.61953163
6	-0.10456236	5.06460333	-2.73843384
6	0.61248273	3.99438000	-2.17415547
6	0.30154228	2.67123485	-2.48325419
1	-2.30085373	3.22079992	-4.62299681
1	-1.72999072	5.59024096	-4.06075335
6	0.26565030	6.49154758	-2.41850877
1	1.42791867	4.20353889	-1.47848427
1	0.85537899	1.83942926	-2.04153728
1	-3.70511746	2.55138779	5.09127760
1	-2.08567643	3.25438976	5.26088238
1	-2.89613509	3.29413271	3.68841791

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1  1.11093175  6.82424974 -3.04116225
1  -0.57156414  7.17585182 -2.60756373
1  0.57357103  6.60119867 -1.36970627
1  -0.06933939 -2.43210769  0.98839933
Energy = -8524.634477 Hartree
Number of imaginary frequencies = 0.

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Compound TS2a isomer 8

Atomic N.	X	Y	Z
8	2.22749186	-1.96654320	0.66482162
8	3.54782057	-0.13129650	1.67265391
6	3.96644187	0.49337283	2.87542081
1	5.00664139	0.19346282	3.10113025
1	3.32068348	0.22425988	3.73049116
1	3.94070125	1.58915210	2.77499795
8	2.64758539	-2.40172052	2.79793549
6	3.12119174	-2.12032080	1.55599737
6	4.51631260	-2.57801008	1.17374885
1	5.26948166	-2.10384440	1.81883860
1	4.67791557	-2.20012021	0.15821391
6	4.67251825	-4.11312914	1.22312438
1	3.76979399	-4.59327126	0.81191266
1	5.50113392	-4.39366770	0.55548131
6	4.97549057	-4.64897394	2.62845898
1	5.92887735	-4.20989418	2.97027707
1	5.13939905	-5.73684025	2.57772756
6	3.89609218	-4.35494423	3.67771268
1	2.96821880	-4.90290737	3.44601607
1	4.23817682	-4.72312641	4.65894508
6	3.54586411	-2.87803698	3.83870959
1	4.44348669	-2.24395895	3.88231778
1	2.97280741	-2.71559954	4.76003599
50	1.76084459	0.31198478	0.49885258
7	-0.80754697	-1.31342423	0.20966797
6	-0.65256184	-2.52362776	-0.60612577
1	-1.52854669	-3.19973111	-0.51315671
1	-0.52792418	-2.26131320	-1.66382504
1	0.25008416	-3.05550194	-0.28334159
7	-2.98992872	0.96835965	-1.84356177
6	-1.97743547	-0.52697659	-0.19952831
1	-2.88516545	-1.17058563	-0.24746624
1	-2.16904306	0.24518324	0.55577427
6	-1.77797699	0.18839963	-1.54178023
1	-1.54053223	-0.52303761	-2.34983587
1	-0.93946004	0.89127862	-1.45032358
16	-2.86943340	2.25346494	-2.94868493
7	0.33829930	0.36056834	2.20981026
6	-0.87382925	-1.68736207	1.63510203
1	-1.80400002	-2.25082994	1.86395919
1	-0.02052868	-2.35338926	1.81971884
6	-0.78135037	-0.49435526	2.59218216
1	-0.65523362	-0.89871728	3.61158347
1	-1.72911692	0.07541891	2.59128547
16	0.50588650	1.82811618	2.90129876
8	1.63938618	2.40770531	2.08609056
8	0.62487257	1.80002093	4.37702942
6	-0.97328359	2.80110478	2.52556705

6	-1.89188015	3.08019590	3.53813457
6	-3.04418540	3.80818486	3.22810507
6	-3.28811145	4.26141548	1.92366481
6	-2.34384942	3.96755123	0.92347610
6	-1.19252717	3.24059510	1.21615040
1	-1.69102073	2.74045444	4.55351973
1	-0.46449873	3.02973509	0.43209803
1	-2.50907755	4.30060625	-0.10230412
6	-4.52227163	5.06280947	1.59416616
1	-3.76566434	4.02835226	4.01731491
8	-4.25526237	2.72840858	-3.11875367
8	-1.78957176	3.12518597	-2.44939756
6	-2.32054996	1.55833077	-4.52365685
6	-0.95561427	1.48739982	-4.80911016
6	-0.54569644	0.93139660	-6.02289486
6	-1.47814000	0.44736445	-6.95273256
6	-2.84581161	0.54247016	-6.64109182
6	-3.27411699	1.09243524	-5.43423796
1	-0.23094268	1.88699186	-4.10043478
1	0.51959670	0.88230973	-6.25463963
6	-1.02997315	-0.16755378	-8.25439644
1	-3.58671403	0.19081783	-7.36154127
1	-4.33509636	1.19109929	-5.20537806
1	-5.26525497	5.00679207	2.40005541
1	-4.26959896	6.12371111	1.44344890
1	-4.98782301	4.70995998	0.66361129
1	-1.65781069	0.16796136	-9.09122753
1	0.01317001	0.08671112	-8.48033905
1	-1.10434115	-1.26534343	-8.21391773
1	-3.79796410	0.39685541	-2.10295224

Energy = -8524.629912 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 9

Atomic N.	X	Y	Z
8	2.15898442	-2.43552637	-0.97457099
8	3.59929299	-0.95109957	0.38778493
6	4.16081381	-0.76370317	1.67759717
1	5.23777437	-1.00973475	1.64507639
1	3.66934443	-1.39699996	2.43791914
1	4.05713558	0.28336683	1.99934208
8	3.02654982	-3.56256557	0.72306609
6	3.22507167	-2.80625200	-0.38320228
6	4.52317715	-2.93865919	-1.15528452
1	5.37927341	-2.66105771	-0.52448899
1	4.46160698	-2.19844174	-1.96059000
6	4.72704554	-4.35842657	-1.72720456
1	3.77280664	-4.74103975	-2.12369418
1	5.40895605	-4.28374577	-2.58739424
6	5.32477188	-5.34206867	-0.71303952
1	6.31699133	-4.96727753	-0.40719080
1	5.50116825	-6.31156874	-1.20449746
6	4.47649288	-5.56724167	0.54475367
1	3.53412724	-6.08038378	0.29302949
1	5.02095222	-6.23621416	1.23129022
6	4.13240910	-4.29882336	1.32023823
1	5.00354767	-3.63793349	1.43917000

1	3.75657344	-4.54725122	2.32043576
50	1.65461171	-0.29727912	-0.32861412
7	-0.84396768	-1.79974771	-0.82464755
6	-0.88621628	-2.67697859	-2.00262356
1	-1.79613912	-3.31089067	-2.01693273
1	-0.85022438	-2.07922220	-2.92080164
1	-0.00170354	-3.32453775	-1.98333323
7	-1.12800372	0.49049121	-2.64441371
6	-1.99294758	-0.88210881	-0.75203198
1	-2.91859722	-1.42811728	-0.46697295
1	-1.78703451	-0.15616713	0.04874759
6	-2.31967521	-0.12341946	-2.04140997
1	-3.08465099	0.62837166	-1.77643096
1	-2.77040195	-0.79079551	-2.78804040
16	-1.33471143	1.73005188	-3.76828289
7	0.49729073	-0.83298177	1.49177659
6	-0.75228667	-2.62532711	0.39598408
1	-1.65667057	-3.26018500	0.51190341
1	0.11433105	-3.28636432	0.26254201
6	-0.56944907	-1.81340849	1.68093598
1	-0.33212006	-2.52102971	2.49364972
1	-1.51795506	-1.31517255	1.95432854
16	0.71828532	0.33726028	2.60760355
8	1.73768806	1.22034216	1.93897617
8	0.97794628	-0.17264535	3.97283697
6	-0.82005835	1.29304373	2.71306777
6	-1.67048621	1.11792707	3.80501866
6	-2.86953425	1.83470798	3.85774207
6	-3.22830749	2.72569776	2.83644271
6	-2.35068679	2.88576436	1.74892044
6	-1.15294361	2.17664862	1.68149722
1	-1.38110113	0.43840754	4.60597038
1	-0.46906075	2.31829929	0.84345078
1	-2.60791278	3.57442164	0.94153804
6	-4.51126003	3.51590228	2.90793729
1	-3.53650427	1.69902742	4.71116734
8	0.01895198	2.05442810	-4.24943066
8	-2.41974425	1.28856885	-4.66514492
6	-1.94304466	3.17289305	-2.85823441
6	-3.31033850	3.44980359	-2.82692146
6	-3.76162267	4.56828022	-2.11948895
6	-2.86639786	5.41336155	-1.44840872
6	-1.49287212	5.11290932	-1.50399435
6	-1.02592552	4.00085926	-2.20125842
1	-4.00211573	2.81149244	-3.37558007
1	-4.82945871	4.79361582	-2.10049844
6	-3.35465431	6.61822319	-0.68367922
1	-0.77840900	5.76596165	-0.99914378
1	0.04089162	3.78482199	-2.26284361
1	-5.19746542	3.10039210	3.65677261
1	-4.31124067	4.56280661	3.18429494
1	-5.02580643	3.53071713	1.93698955
1	-2.81965709	7.52799225	-0.99119997
1	-4.42829704	6.78351784	-0.83778465
1	-3.18232989	6.49654627	0.39683822
1	-0.34487405	0.68547106	-2.00733066

Energy = -8524.628075 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 10

Atomic N.	X	Y	Z
8	0.09170699	-0.39282787	0.31961268
8	2.03717685	0.95928949	1.20634234
6	3.27535653	0.51475614	1.74075842
1	3.33783245	0.74454379	2.81995559
1	4.11400557	1.02866089	1.23879302
1	3.40959740	-0.57684493	1.62630510
8	2.02033901	-1.18096900	-0.42671898
6	1.18581581	-0.12099854	-0.28574178
6	1.22666502	1.00410104	-1.30240524
1	2.21377969	1.48514473	-1.30732036
1	0.50978702	1.75062931	-0.94095969
6	0.86697936	0.52173907	-2.72369099
1	0.03318012	-0.19736081	-2.67701769
1	0.49575415	1.38593602	-3.29483390
6	2.06052232	-0.08362246	-3.47451782
1	2.83706212	0.69419849	-3.57648873
1	1.75445366	-0.34721091	-4.49897432
6	2.68641543	-1.31623101	-2.80928326
1	1.98663628	-2.16760945	-2.83187628
1	3.57246900	-1.62609541	-3.38741612
6	3.13172436	-1.11152637	-1.36350477
1	3.67993188	-0.16698568	-1.22895181
1	3.78472519	-1.93238306	-1.04137385
50	0.24309465	0.55446386	2.47645187
7	-2.61871433	0.11151217	2.17061543
6	-3.14909840	-0.39185819	3.44604468
1	-4.25451899	-0.47235727	3.43834591
1	-2.71918845	-1.37500679	3.67124248
1	-2.85647941	0.29564819	4.24955893
7	-1.34622836	-2.50433064	1.56471884
6	-3.01293063	-0.74181271	1.03365123
1	-4.10310125	-0.64083779	0.83965498
1	-2.48659873	-0.37473527	0.14149255
6	-2.74088168	-2.24112201	1.19433868
1	-3.02372050	-2.71620941	0.23556075
1	-3.38039184	-2.67563248	1.97314715
16	-0.89296281	-4.10349226	1.84343815
7	-0.73813009	2.31835246	1.53265262
6	-3.05201697	1.50517786	1.93333554
1	-4.08645678	1.53458905	1.53044868
1	-3.05790639	2.02923799	2.89875627
6	-2.10361838	2.26939726	1.00193143
1	-2.50814247	3.28458047	0.86299527
1	-2.06472063	1.79809546	0.00697065
16	-0.31120574	3.60711551	2.45811820
8	0.74735022	3.02396774	3.35597348
8	-1.46499622	4.32454062	3.05370665
6	0.53173196	4.79051399	1.37818336
6	0.00619970	6.07103682	1.21559680
6	0.67101687	6.97652340	0.38310224
6	1.85208058	6.61789417	-0.28068364
6	2.35550499	5.31675577	-0.09637683
6	1.70610702	4.39954901	0.72665548
1	-0.90563518	6.34830952	1.74329042

1	2.09203887	3.38706017	0.86826587
1	3.27530980	5.02174711	-0.60624045
6	2.58404016	7.60588646	-1.15457332
1	0.26467782	7.98126030	0.25249654
8	0.53283918	-4.05050898	2.21136713
8	-1.92011702	-4.68274164	2.73196650
6	-1.01160491	-4.96260929	0.25293508
6	-2.13591194	-5.73650932	-0.03719546
6	-2.21744227	-6.38100243	-1.27442396
6	-1.19078898	-6.26454067	-2.22260094
6	-0.07026668	-5.47768068	-1.90201020
6	0.02787174	-4.82776403	-0.67301607
1	-2.92252779	-5.84295082	0.70916849
1	-3.09336233	-6.99083710	-1.50348592
6	-1.26716924	-6.99074650	-3.54226947
1	0.74178809	-5.38170671	-2.62581515
1	0.90464628	-4.23143625	-0.41886961
1	1.95646000	8.47458267	-1.39101219
1	3.49085712	7.97651911	-0.65202361
1	2.90533423	7.14446831	-2.09901047
1	-0.67489189	-7.91855383	-3.51171494
1	-2.30031252	-7.26682186	-3.78916168
1	-0.86665082	-6.37805986	-4.36150408
1	-0.65217465	-2.01525426	0.97511834

Energy = -8524.636501 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 11

Atomic N.	X	Y	Z
8	0.24772745	-0.27700379	0.35611671
8	1.91212142	1.62268782	0.47841990
6	3.30370140	1.58698332	0.75833070
1	3.51665592	2.05903506	1.73468471
1	3.86266637	2.14502239	-0.01346356
1	3.69275451	0.55281633	0.79917842
8	2.12815356	-0.79034537	-0.69245476
6	1.09223306	0.07235250	-0.53964823
6	0.63830751	0.91191137	-1.71847701
1	1.44551587	1.57684219	-2.05338264
1	-0.16205709	1.55249202	-1.33006632
6	0.14310393	0.04683180	-2.89685059
1	-0.44859204	-0.80200440	-2.51755691
1	-0.54550737	0.65509319	-3.50239515
6	1.28024828	-0.44868872	-3.80019855
1	1.79189658	0.43079185	-4.22815132
1	0.85712749	-1.00211799	-4.65304661
6	2.32359743	-1.33080363	-3.10254288
1	1.87920046	-2.29294491	-2.79944038
1	3.12781787	-1.57078981	-3.81737518
6	2.97617674	-0.70594156	-1.87203157
1	3.27557850	0.33826575	-2.04730415
1	3.87025762	-1.27163482	-1.58120954
50	0.57321131	1.15299106	2.20559001
7	-2.07579088	0.05001550	2.70381689
6	-2.19361973	-0.24703775	4.13882971
1	-3.21917081	-0.55987078	4.41970158
1	-1.48781013	-1.03774762	4.41933489

1	-1.93596303	0.65286219	4.71134710
7	-0.31315437	-2.30064964	2.27043986
6	-2.45188642	-1.10636032	1.86831880
1	-3.54704833	-1.28611815	1.93567634
1	-2.22621202	-0.85147625	0.82340986
6	-1.77284849	-2.43482733	2.21742773
1	-2.10590291	-3.16739011	1.45757985
1	-2.10965824	-2.80430770	3.19431353
16	0.58937329	-3.65628099	2.70348954
7	-1.00139201	2.39809132	1.23933649
6	-2.89532161	1.22612405	2.34098673
1	-3.96058655	0.94073617	2.21046066
1	-2.84456563	1.94531095	3.16975808
6	-2.38432932	1.93827856	1.08300221
1	-3.05838251	2.78393531	0.87319386
1	-2.42347360	1.26924491	0.20867620
16	-0.74826384	3.92811084	1.78168595
8	0.58329153	3.80922961	2.47408676
8	-1.90520287	4.50453568	2.50954652
6	-0.47673503	4.97616959	0.33072233
6	-1.34306395	6.03823757	0.07563023
6	-1.11938488	6.84178877	-1.04589772
6	-0.04049940	6.59914732	-1.90763724
6	0.81381732	5.51827812	-1.62324059
6	0.60563201	4.70411968	-0.51174098
1	-2.17293048	6.22914171	0.75509256
1	1.26438844	3.86056137	-0.29141405
1	1.65835357	5.31543446	-2.28545260
6	0.21851128	7.49151897	-3.09594226
1	-1.79461122	7.67476988	-1.25081778
8	1.99447262	-3.21273208	2.69522047
8	-0.05545063	-4.22541809	3.90363574
6	0.39321128	-4.86125231	1.36502314
6	-0.51439404	-5.91183233	1.50259507
6	-0.66156530	-6.82543278	0.45517397
6	0.08661444	-6.70397043	-0.72439337
6	0.99346912	-5.63450861	-0.83427000
6	1.15333903	-4.71439075	0.19994719
1	-1.07909775	-6.01662064	2.42847967
1	-1.36704123	-7.65168047	0.56084651
6	-0.05132779	-7.71020126	-1.83942068
1	1.59003258	-5.52905512	-1.74290752
1	1.86898720	-3.89549923	0.12043029
1	-0.68941587	8.02811432	-3.40033221
1	0.98336905	8.24721432	-2.85699368
1	0.58734614	6.91739655	-3.95699024
1	0.79981321	-8.40864468	-1.84295499
1	-0.96749669	-8.30468845	-1.73222327
1	-0.07021099	-7.21954203	-2.82249546
1	0.09789002	-1.82267463	1.45118392

Energy = -8524.636522 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 12

Atomic N.	X	Y	Z
8	3.05211973	0.49737686	1.48322570
8	3.87761474	0.42697352	-0.73917776

6	4.54017878	-0.19499226	-1.83516324
1	4.00270176	0.04962118	-2.76295590
1	4.55945969	-1.29335916	-1.74356270
1	5.57091141	0.18894716	-1.91523719
8	5.13138247	1.22576427	1.33096611
6	4.25221300	0.22379470	1.05736160
6	4.74958181	-1.21209633	1.11968803
1	5.51920462	-1.39539444	0.35571438
1	3.89052176	-1.84231782	0.85830438
6	5.31267595	-1.57819462	2.50813055
1	4.69188547	-1.12016904	3.29483604
1	5.22609186	-2.66743708	2.63879991
6	6.78519201	-1.18185174	2.68457484
1	7.38078213	-1.71415162	1.92252290
1	7.14591455	-1.54107594	3.66113663
6	7.06803322	0.32146394	2.57134104
1	6.62526894	0.86391628	3.42210817
1	8.15649319	0.48903555	2.62491727
6	6.55948114	0.97629637	1.28900409
1	6.82462883	0.39223608	0.39406720
1	6.99228239	1.97852266	1.17597532
50	1.72855949	0.60915488	-0.26859292
7	-0.34832197	-0.24874067	2.19169521
6	0.47016180	-0.01130180	3.38969254
1	0.05701561	-0.52860159	4.28101015
1	1.49888504	-0.34887737	3.22159195
1	0.50903898	1.06590688	3.59436631
7	1.28196669	-1.53911936	0.02872588
6	-0.40163663	-1.68411839	1.86430478
1	-0.65299231	-2.28020263	2.77015424
1	-1.20972204	-1.84238279	1.13715124
6	0.89873666	-2.22888780	1.25856888
1	0.78060400	-3.30999589	1.07704771
1	1.72365618	-2.12937212	1.98206675
16	1.13548350	-2.24878192	-1.43180656
7	-1.94223118	1.59863138	0.26455408
6	-1.70692980	0.28476194	2.41114020
1	-2.29684186	-0.39862207	3.06101561
1	-1.61989892	1.23993444	2.94630909
6	-2.49054098	0.53383261	1.11958086
1	-3.52167416	0.80297089	1.38568628
1	-2.54809999	-0.37935287	0.50763589
16	-2.40447760	3.20352960	0.59439117
8	-1.23730791	4.02855301	0.22439729
8	-3.03246975	3.29343128	1.93253779
6	-3.71220493	3.49858165	-0.61652577
6	-5.04073572	3.54739094	-0.19718844
6	-6.04087257	3.79585743	-1.14136267
6	-5.72811985	4.00178909	-2.49237418
6	-4.37753201	3.95156550	-2.88281178
6	-3.36817265	3.70417547	-1.95568180
1	-5.27858591	3.40610623	0.85645235
1	-2.32145548	3.68045926	-2.25791264
1	-4.11445475	4.11513233	-3.92957282
6	-6.80673075	4.30085945	-3.50307345
1	-7.08277655	3.83687949	-0.81862307
8	1.56348360	-1.13319850	-2.34899759
8	1.80395114	-3.56789541	-1.51311493

6	-0.61608464	-2.55858994	-1.78394914
6	-1.11487746	-3.85949898	-1.70453286
6	-2.47134900	-4.08594608	-1.95242596
6	-3.33398890	-3.03274035	-2.28912950
6	-2.80215883	-1.73326838	-2.36904073
6	-1.45322478	-1.48952782	-2.11800766
1	-0.43859708	-4.67997789	-1.46718371
1	-2.86391091	-5.10262394	-1.88972032
6	-4.78987503	-3.28634119	-2.59025288
1	-3.45536113	-0.89893764	-2.63201499
1	-1.05023170	-0.47874069	-2.18936038
1	-7.80043173	4.03585720	-3.12015724
1	-6.82107973	5.37318468	-3.75242090
1	-6.63926983	3.75429559	-4.44145298
1	-4.96428919	-3.31471801	-3.67711830
1	-5.12411022	-4.24639559	-2.17654419
1	-5.42765045	-2.49054193	-2.18180013
1	-0.91488492	1.58154953	0.19609787

Energy = -8524.626403 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 13

Atomic N.	X	Y	Z
8	1.46362925	0.39303055	1.07699215
8	3.12546086	2.03383517	1.98129821
6	4.28212214	2.12594438	2.79119992
1	5.05327415	2.72733235	2.28077054
1	4.70485830	1.12980855	3.02953362
1	4.05992270	2.61757255	3.75812721
8	3.41957545	-0.59150803	1.41729319
6	2.71669507	0.36587334	0.79152948
6	3.21297693	0.97152328	-0.49830350
1	4.21970177	1.38693631	-0.35095555
1	2.54979110	1.82000828	-0.70205534
6	3.22801805	-0.04505564	-1.65965807
1	2.29989672	-0.63895947	-1.64490473
1	3.21567154	0.52023858	-2.60343552
6	4.45549679	-0.96557981	-1.65005505
1	5.35606623	-0.34257430	-1.78976107
1	4.41298866	-1.64047384	-2.51925206
6	4.62991285	-1.80434036	-0.37690297
1	3.80904698	-2.52939153	-0.25968620
1	5.55774784	-2.39316058	-0.46303532
6	4.72880888	-0.99573636	0.91270995
1	5.37559032	-0.11201147	0.80362827
1	5.12200212	-1.61464715	1.72788024
50	1.25112307	1.59183252	3.00406003
7	-1.33457172	0.48300421	3.28818488
6	-1.41487920	-0.43522379	4.42989969
1	-2.45713115	-0.58876026	4.77359104
1	-0.97364455	-1.40394700	4.16885042
1	-0.83392084	-0.01296843	5.26127291
7	-0.46477255	-1.81491673	1.55995071
6	-2.07402778	0.01545813	2.10338640
1	-3.16771293	0.15238594	2.24874401
1	-1.77881312	0.65243948	1.25725365
6	-1.87887549	-1.45156252	1.72229028

1	-2.45593524	-1.60041761	0.79051709
1	-2.31276059	-2.11824584	2.47984123
16	-0.13224377	-3.33155537	0.90686297
7	-0.27115849	2.84547734	2.01655507
6	-1.79288340	1.82604897	3.68948793
1	-2.86083651	1.80616212	3.99111772
1	-1.21081257	2.11071944	4.58145285
6	-1.62079704	2.89397120	2.60607576
1	-1.82502246	3.87461662	3.06604767
1	-2.38657498	2.75048590	1.82192719
16	-0.07558293	3.88182855	0.73339671
8	1.32979608	3.76290321	0.28950009
8	-0.64630759	5.21481037	1.04582834
6	-1.12747002	3.19204116	-0.58641064
6	-2.20121169	3.93433356	-1.07558846
6	-2.98795676	3.40415192	-2.10372472
6	-2.71843219	2.14016271	-2.64561439
6	-1.62806165	1.41261458	-2.13437223
6	-0.83398771	1.92907476	-1.11177802
1	-2.40153098	4.91970253	-0.65562856
1	0.00791489	1.36096454	-0.71260172
1	-1.39921820	0.42622483	-2.54508662
6	-3.58113480	1.56066787	-3.73964739
1	-3.82615113	3.98674893	-2.49116445
8	1.33195841	-3.38053632	0.73167688
8	-0.86368561	-4.31238461	1.73130345
6	-0.88839084	-3.36961055	-0.74017662
6	-2.16598344	-3.90958405	-0.90293658
6	-2.75003314	-3.90804434	-2.17193961
6	-2.07726049	-3.37466574	-3.28143907
6	-0.78589356	-2.85258079	-3.09136200
6	-0.19011731	-2.84449482	-1.83097172
1	-2.67799997	-4.34710312	-0.04657363
1	-3.74506092	-4.33730173	-2.30280471
6	-2.72530842	-3.34945107	-4.64276457
1	-0.23610836	-2.45468879	-3.94660044
1	0.82015646	-2.46038938	-1.69144833
1	-4.24011755	2.32201648	-4.17601585
1	-2.96869588	1.13239944	-4.54587936
1	-4.21779919	0.75025940	-3.35167670
1	-1.98598230	-3.49299264	-5.44192219
1	-3.49313688	-4.12812710	-4.73593664
1	-3.21579123	-2.37979317	-4.82321787
1	0.16158056	-1.09282637	1.17325079

Energy = -8524.620969 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 14

Atomic N.	X	Y	Z
8	3.29107213	0.43780717	0.69445741
8	3.29169083	0.27373925	-1.78091979
6	3.30435538	1.05371952	-2.96657252
1	2.56169128	0.67957073	-3.68702483
1	4.30318880	0.98807752	-3.43490219
1	3.07028651	2.11448884	-2.76469851
8	4.20790672	2.24952221	-0.18939550
6	4.20623159	0.90115190	-0.06124987

6	5.49570513	0.12979320	-0.26507896
1	5.87538004	0.27223524	-1.28649545
1	5.22368526	-0.92684054	-0.16614088
6	6.58271933	0.51558942	0.76152903
1	6.12882757	0.63388646	1.75859308
1	7.28695107	-0.32580417	0.84303951
6	7.36757326	1.77442098	0.37100416
1	7.87962294	1.58234620	-0.58786058
1	8.16178036	1.95462513	1.11214674
6	6.52036333	3.04491806	0.22828536
1	6.11075115	3.35261226	1.20412803
1	7.16540623	3.87134218	-0.11261903
6	5.36116552	2.93387175	-0.75794071
1	5.66245508	2.44655252	-1.69691455
1	4.96627378	3.92742085	-1.00345051
50	1.56718349	-0.32903433	-0.60536408
7	0.50635189	0.70297867	1.95302486
6	1.25204039	0.38179699	3.17763877
1	0.86707079	0.93764842	4.05674982
1	1.19930792	-0.69402915	3.38127041
1	2.30421209	0.64725810	3.02143550
7	-0.48218158	-2.06503248	1.94246387
6	-0.92743343	0.38445693	2.05563307
1	-1.44868743	1.11248589	2.71478772
1	-1.36313820	0.48971981	1.05080986
6	-1.26168537	-1.00696111	2.60074782
1	-2.34910798	-1.14412034	2.46115923
1	-1.06601512	-1.06543291	3.67972779
16	-1.01448953	-3.66015816	2.06625962
7	0.45701653	1.59147680	-0.75244099
6	0.70594889	2.12747455	1.61971843
1	0.29388297	2.78107619	2.41808581
1	1.79118741	2.28865433	1.57268953
6	0.07923167	2.54625487	0.28734058
1	0.43696055	3.56369352	0.05401957
1	-1.02039957	2.60625267	0.38641626
16	-0.29835045	1.64308274	-2.19861889
8	0.22218551	0.40103596	-2.87076306
8	-0.18802920	2.94792056	-2.88876486
6	-2.06905675	1.37990868	-1.90356517
6	-2.94916630	2.46112847	-1.96242273
6	-4.30550480	2.25197077	-1.69763505
6	-4.79481602	0.97712231	-1.37869310
6	-3.88641572	-0.09527798	-1.32902491
6	-2.53067875	0.09829319	-1.58831632
1	-2.56956053	3.44712067	-2.22845840
1	-1.83412707	-0.74097306	-1.56447780
1	-4.24388456	-1.09711564	-1.08256245
6	-6.26400661	0.75017935	-1.12288833
1	-4.99547482	3.09669924	-1.74248135
8	0.01251977	-4.47100973	1.39023864
8	-1.38716006	-3.85555005	3.48029852
6	-2.53281283	-3.78851676	1.08736062
6	-3.77542353	-3.68480158	1.71387720
6	-4.93676901	-3.78608584	0.94193244
6	-4.87270832	-3.99352717	-0.44334766
6	-3.60583234	-4.10260868	-1.04583669
6	-2.43826413	-4.00018263	-0.29261225

1	-3.82511187	-3.55691910	2.79471111
1	-5.91064739	-3.71485019	1.42968059
6	-6.12645435	-4.09735537	-1.27528346
1	-3.53464556	-4.27826929	-2.12096190
1	-1.45872438	-4.10941553	-0.75852484
1	-6.77426052	1.68435252	-0.85529512
1	-6.75907326	0.34828013	-2.02076197
1	-6.42132425	0.02416510	-0.31346846
1	-6.11032534	-4.99482393	-1.90971816
1	-7.02385807	-4.13858843	-0.64538443
1	-6.22571707	-3.23199987	-1.94875157
1	-0.13886108	-1.85489464	0.99642664

Energy = -8524.628066 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 15

Atomic N.	X	Y	Z
8	2.81949997	-0.22392572	1.15455139
8	3.02248049	1.64490700	-0.44654584
6	3.51221490	2.02893639	-1.71087992
1	3.02450609	2.96487617	-2.05365181
1	3.34999990	1.26285303	-2.49744034
1	4.59679985	2.24683499	-1.68162203
8	4.46006393	1.12522495	1.72319317
6	3.91170025	0.32828245	0.77277589
6	4.82485914	-0.37600893	-0.21388561
1	5.36734676	0.34283072	-0.84435207
1	4.16825438	-0.95757133	-0.87415689
6	5.83498240	-1.30711341	0.49156511
1	5.33917570	-1.82793796	1.32523572
1	6.13599920	-2.08676195	-0.22402655
6	7.09387255	-0.57424003	0.97386485
1	7.59629297	-0.12996411	0.09673931
1	7.80166912	-1.30502188	1.39513659
6	6.84281445	0.52898276	2.00925970
1	6.49639988	0.09510628	2.96100450
1	7.79318619	1.04375589	2.22700000
6	5.82922173	1.58819091	1.58420801
1	6.00587463	1.94723415	0.55895853
1	5.87664557	2.45351243	2.25756383
50	1.23918927	0.02073040	-0.37979239
7	0.29355234	1.99321866	0.94600725
6	1.14845204	2.15540314	2.14785433
1	0.69465381	2.88784051	2.83991766
1	1.27994275	1.19544220	2.65493703
1	2.13751292	2.50487161	1.83306646
7	-0.30360949	-0.69352990	1.11833620
6	-1.07479870	1.57261491	1.33347511
1	-1.52927554	2.31579208	2.01648521
1	-1.68124115	1.51927054	0.42015979
6	-1.07054949	0.18967706	1.98807549
1	-2.12508702	-0.13098405	2.07956481
1	-0.65754336	0.23017675	3.00998616
16	-0.12497353	-2.26297188	1.55052722
7	-0.39352989	2.41294527	-1.99311030
6	0.31202886	3.29209423	0.22168528
1	0.06279960	4.10506010	0.93140221

1	1.35457039	3.44101405	-0.09710138
6	-0.63309121	3.44278526	-0.96836621
1	-0.50897056	4.46404219	-1.36516762
1	-1.68099904	3.35638952	-0.64850479
16	-1.49960136	2.42292929	-3.31543112
8	-0.82708138	1.62551713	-4.35793018
8	-1.97486210	3.79609823	-3.59611726
6	-2.87946534	1.50166893	-2.61403227
6	-4.12569427	2.11903119	-2.51297283
6	-5.19681454	1.39275706	-1.98567212
6	-5.03268814	0.06768700	-1.55690873
6	-3.76181197	-0.52606839	-1.67154109
6	-2.68488884	0.17922018	-2.20248485
1	-4.24420786	3.15009165	-2.84429097
1	-1.70164132	-0.28426775	-2.28887081
1	-3.61033344	-1.55204451	-1.33128142
6	-6.18945026	-0.71695161	-0.99167222
1	-6.17560530	1.86823344	-1.90281916
8	0.94074428	-2.77268052	0.64022893
8	-0.01570785	-2.44229507	3.01837111
6	-1.66014433	-3.10252881	1.05884004
6	-2.70233369	-3.24137497	1.97634828
6	-3.88569808	-3.87208915	1.57874858
6	-4.03679991	-4.38175249	0.28151560
6	-2.96399903	-4.24323130	-0.61804873
6	-1.78364563	-3.60485721	-0.24036659
1	-2.57212043	-2.88268137	2.99719024
1	-4.70053959	-3.98348618	2.29692483
6	-5.30662918	-5.07857037	-0.14138357
1	-3.05483174	-4.64659929	-1.62902570
1	-0.94713438	-3.50998783	-0.93286037
1	-7.05939245	-0.07448386	-0.80677187
1	-6.49917936	-1.51143050	-1.68763161
1	-5.91161823	-1.20716488	-0.04787694
1	-5.11171770	-6.12598085	-0.41579390
1	-6.05304432	-5.07391071	0.66302669
1	-5.75258207	-4.59538937	-1.02364612
1	0.53762686	2.48172688	-2.41969752

Energy = -8524.619415 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 16

Atomic N.	X	Y	Z
8	3.29981136	0.38808542	0.75001228
8	3.30361986	0.32265592	-1.72251761
6	3.31022215	1.10457850	-2.90679169
1	4.32049799	1.07911026	-3.35421777
1	3.02904582	2.15478802	-2.71039009
1	2.59830141	0.70238900	-3.64311099
8	4.09221315	2.29029894	-0.06246153
6	4.18130398	0.94054168	0.01389349
6	5.52001953	0.26648173	-0.21389712
1	5.88584518	0.46572247	-1.23099709
1	5.32129002	-0.80877656	-0.14669526
6	6.58141375	0.69616550	0.82208854
1	6.12327671	0.75517607	1.82250118
1	7.34144258	-0.09733907	0.87890595

6	7.27785969	2.01622105	0.46730614
1	7.79613543	1.88801980	-0.49885592
1	8.06244755	2.22678232	1.21070588
6	6.34662199	3.23074841	0.36704332
1	5.92453146	3.48105812	1.35392272
1	6.93241119	4.10836744	0.04777535
6	5.19022512	3.07119370	-0.61569470
1	5.51701498	2.63598204	-1.57151723
1	4.72547102	4.04213572	-0.82693911
50	1.58449113	-0.34885421	-0.57454151
7	0.50339293	0.54962432	2.03066301
6	1.24886012	0.17327802	3.23961139
1	0.86070561	0.68460679	4.14398766
1	1.20048177	-0.91128182	3.39148498
1	2.30017471	0.45043489	3.09787226
7	-0.46307763	-2.22090006	1.88263297
6	-0.92837882	0.21701032	2.11321163
1	-1.45635235	0.90798461	2.80606389
1	-1.36171651	0.36920935	1.11335778
6	-1.25419462	-1.20206571	2.58761573
1	-2.33948827	-1.34137011	2.43549824
1	-1.06439257	-1.31116176	3.66378808
16	-0.99943858	-3.81910777	1.89754725
7	0.45428041	1.56397581	-0.62759751
6	0.69458163	1.98977029	1.76773250
1	0.27414012	2.60121512	2.59465384
1	1.77869725	2.16063547	1.73375976
6	0.07131829	2.46868110	0.45380965
1	0.42735398	3.49682283	0.26974848
1	-1.02883554	2.52114820	0.55145454
16	-0.28168714	1.68976653	-2.07838249
8	0.23868552	0.47585535	-2.80088782
8	-0.15206113	3.02324033	-2.70815611
6	-2.05774999	1.42900169	-1.81705678
6	-2.93033266	2.51707935	-1.85494220
6	-4.29174662	2.30826664	-1.61696708
6	-4.79302740	1.02732933	-1.34465599
6	-3.89167690	-0.05183702	-1.31504583
6	-2.53127575	0.14104366	-1.54869938
1	-2.54059720	3.50846720	-2.08346272
1	-1.84041536	-0.70319015	-1.54050863
1	-4.25830841	-1.05856168	-1.10459745
6	-6.26678514	0.80145156	-1.11562753
1	-4.97613764	3.15822434	-1.64561439
8	0.04708804	-4.59128904	1.20646966
8	-1.41503501	-4.09563923	3.28585362
6	-2.48736119	-3.88738084	0.86715937
6	-3.74869061	-3.83420610	1.46153116
6	-4.88588333	-3.88876033	0.64966559
6	-4.77903032	-3.99964809	-0.74394131
6	-3.49384928	-4.05878305	-1.31410658
6	-2.35016012	-4.00230217	-0.52076864
1	-3.83118606	-3.78065658	2.54659700
1	-5.87435961	-3.85667562	1.11152196
6	-6.00608540	-4.05514860	-1.61919820
1	-3.38942742	-4.15821648	-2.39622831
1	-1.35646832	-4.07292080	-0.96365649
1	-6.77909517	1.73408151	-0.84678900

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1 -6.74792862    0.40950850   -2.02533984
1 -6.43902779    0.06768944   -0.31625599
1 -5.97505856   -4.92330933  -2.29287314
1 -6.92360783   -4.11849451  -1.02093697
1 -6.07769632   -3.15983748  -2.25579095
1 -0.09764650   -1.95418990   0.95926762
Energy = -8524.628071 Hartree
Number of imaginary frequencies = 0.

```

Compound TS2a isomer 17

Atomic N.	X	Y	Z
8	2.81127882	-0.22189178	1.16647768
8	2.98073888	1.73884177	-0.32202640
6	3.46668124	2.20861030	-1.55870402
1	4.55064297	2.42740870	-1.51762354
1	2.97540903	3.16392827	-1.83662021
1	3.30509782	1.49594331	-2.39420676
8	4.41694784	1.12973118	1.82256472
6	3.89226580	0.37673587	0.82389766
6	4.82736063	-0.25021657	-0.19394568
1	5.35838652	0.51481098	-0.77813882
1	4.18818045	-0.80712587	-0.89151204
6	5.85272264	-1.19806516	0.46572822
1	5.36250877	-1.77587092	1.26448882
1	6.17553997	-1.92924118	-0.29032350
6	7.09204960	-0.46715760	0.99903899
1	7.59079790	0.03680377	0.15261137
1	7.81257486	-1.20550585	1.38397360
6	6.81006813	0.56996435	2.09316611
1	6.46683073	0.07553580	3.01608753
1	7.74750853	1.09181070	2.34712291
6	5.77632570	1.62946236	1.72048783
1	5.95198011	2.04914188	0.71834582
1	5.80034065	2.45637131	2.44165421
50	1.23373866	0.07385271	-0.36064759
7	0.23651741	1.94363213	1.07348287
6	1.08085811	2.05390310	2.28856444
1	0.60605639	2.73286414	3.01997042
1	1.23273098	1.06876957	2.73842716
1	2.06294870	2.44472218	2.00180578
7	-0.29972863	-0.76233095	1.08333528
6	-1.12362492	1.46910846	1.42616224
1	-1.59946573	2.16026545	2.14814520
1	-1.72355568	1.45518434	0.50703460
6	-1.09054101	0.05068539	1.99883115
1	-2.13782477	-0.29856822	2.06536674
1	-0.68306077	0.04074007	3.02371621
16	-0.08333177	-2.34915400	1.42537439
7	-0.43053070	2.52562642	-1.84399164
6	0.22722921	3.28374314	0.42840895
1	-0.04857126	4.04615259	1.18299568
1	1.26806724	3.47800756	0.12898621
6	-0.71098053	3.48178530	-0.76002544
1	-0.61273211	4.52904129	-1.09090304
1	-1.75900817	3.34558082	-0.45843044
16	-1.51601756	2.59334278	-3.18151355
8	-0.80547023	1.88471568	-4.26227808

8	-2.02467799	3.96894979	-3.37944293
6	-2.88012195	1.59068143	-2.56666040
6	-4.14517212	2.16502976	-2.44767523
6	-5.20350409	1.37535501	-1.99015248
6	-5.00846386	0.02935862	-1.64837492
6	-3.71905994	-0.51961297	-1.77836323
6	-2.65434313	0.24947147	-2.24043393
1	-4.28830576	3.21234632	-2.71110725
1	-1.65670466	-0.17953911	-2.33931875
1	-3.54391646	-1.56147897	-1.50417399
6	-6.15154457	-0.82410532	-1.16022623
1	-6.19689035	1.81685781	-1.89399147
8	0.99683183	-2.77912831	0.49107879
8	0.02743874	-2.60999751	2.88077164
6	-1.59606242	-3.19654632	0.88055509
6	-2.64098430	-3.40426421	1.78239059
6	-3.80884981	-4.03593445	1.34400237
6	-3.94157624	-4.48014021	0.02054733
6	-2.86759996	-4.27131271	-0.86319268
6	-1.70198917	-3.63093448	-0.44403604
1	-2.52548933	-3.09538651	2.82107091
1	-4.62659693	-4.19875765	2.04901171
6	-5.18842983	-5.19375515	-0.44080833
1	-2.94577527	-4.61992645	-1.89535630
1	-0.86464471	-3.48023486	-1.12552512
1	-7.04234743	-0.22009465	-0.94694358
1	-6.42690754	-1.57587206	-1.91553211
1	-5.87516546	-1.37166429	-0.24812075
1	-5.00835562	-6.27511406	-0.54212230
1	-6.01342106	-5.06033754	0.27081782
1	-5.51826048	-4.83014584	-1.42441523
1	0.50495052	2.64453840	-2.24963474

Energy = -8524.619376 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 18

Atomic N.	X	Y	Z
8	2.38311648	-1.53895104	0.85978240
8	2.89580727	-0.28925002	-1.04113078
6	3.62256813	0.77479398	-1.66451609
1	3.82237291	1.59729397	-0.95945525
1	3.02143669	1.17210186	-2.49244905
1	4.57456541	0.38799855	-2.06378746
8	3.80788231	0.14531630	1.24479604
6	3.48004103	-0.97058910	0.47212797
6	4.62959671	-1.86775899	0.02126561
1	5.33400917	-1.31514645	-0.61914903
1	4.16922617	-2.63955021	-0.60754973
6	5.38459444	-2.51366401	1.19898593
1	4.66130447	-2.81139827	1.97473872
1	5.85669470	-3.44168043	0.84154922
6	6.47457027	-1.61476350	1.79719651
1	7.22066164	-1.39986444	1.01184487
1	7.00988817	-2.16833186	2.58471727
6	5.97054291	-0.28627232	2.37304306
1	5.33336830	-0.46034151	3.25472307
1	6.83426046	0.30523038	2.71982741

6	5.18210888	0.57497472	1.38739455
1	5.68644333	0.62760454	0.40884459
1	5.09194756	1.60067809	1.76998329
50	0.82278574	0.01139549	-0.11158414
7	0.07490882	-2.36996770	-0.81712091
6	1.09120286	-2.89488506	-1.75842214
1	0.74031585	-3.83104777	-2.23011708
1	1.30877006	-2.15202308	-2.53216386
1	2.01252079	-3.08702111	-1.20017934
7	-0.28904220	-0.00267511	-2.10479212
6	-1.20902729	-2.14307022	-1.52451015
1	-1.59715867	-3.09689760	-1.93108773
1	-1.93289518	-1.75936806	-0.79186696
6	-1.04934502	-1.11802185	-2.65003395
1	-2.06171393	-0.81470013	-2.97357178
1	-0.55663019	-1.57089913	-3.52769375
16	-0.13762689	1.36345327	-2.97904539
7	-0.25702906	-1.80030525	2.18610907
6	-0.07206984	-3.35788703	0.28396171
1	-0.51757240	-4.28785515	-0.11952332
1	0.94522208	-3.59410977	0.62426883
6	-0.89813268	-2.92783642	1.49263179
1	-1.00143015	-3.80713272	2.14922953
1	-1.91558480	-2.62626123	1.20177150
16	-0.89776194	-1.37751794	3.71600699
8	0.21913777	-0.73547250	4.43295813
8	-1.63216233	-2.52800727	4.28726625
6	-2.11843204	-0.12087423	3.28979015
6	-3.47743368	-0.44012669	3.32689333
6	-4.41228390	0.54596514	3.01011896
6	-4.00678062	1.84511685	2.66265702
6	-2.63299561	2.13501239	2.63820243
6	-1.68361700	1.16148210	2.94957519
1	-3.78712869	-1.44358051	3.61685276
1	-0.61906528	1.39220536	2.93695664
1	-2.29966903	3.13976026	2.37261009
6	-5.03017092	2.90587759	2.34248424
1	-5.47633839	0.30400604	3.04116249
8	0.74942571	2.22222972	-2.13502407
8	0.22426651	1.12085593	-4.39794874
6	-1.77724147	2.14493418	-3.00389886
6	-2.41465878	2.37869477	-4.22116566
6	-3.67344236	2.98803568	-4.22731256
6	-4.30139112	3.36727786	-3.03345299
6	-3.63664317	3.11472797	-1.81922019
6	-2.38341761	2.50723505	-1.79683375
1	-1.91796577	2.08772469	-5.14626884
1	-4.17420769	3.17279530	-5.17962837
6	-5.64886999	4.04571342	-3.04269266
1	-4.11023092	3.40265441	-0.87808555
1	-1.87328994	2.31720614	-0.85125959
1	-5.62553406	3.15895557	3.23264337
1	-4.55421400	3.82748318	1.98438871
1	-5.73518991	2.55892968	1.57315087
1	-5.55634880	5.10695553	-2.76504016
1	-6.11347103	3.99977708	-4.03577900
1	-6.33546448	3.58253050	-2.31968427
1	0.76511639	-1.88987756	2.28053451

Energy = -8524.625703 Hartree
 Number of imaginary frequencies = 0.

Compound TS2a isomer 19

Atomic N.	X	Y	Z
8	3.22103834	0.50434750	1.58330667
8	3.27847457	-0.94370043	-0.31854931
6	4.00595236	-0.64323264	-1.51297522
1	3.28994417	-0.44373256	-2.32513857
1	4.63746738	-1.50022578	-1.80000710
1	4.64391661	0.24521305	-1.38773477
8	5.27753401	0.04776457	0.88035691
6	4.03828812	-0.45100442	1.19938385
6	3.97219706	-1.76682591	1.97088552
1	4.35807467	-2.59635520	1.36009252
1	2.90338469	-1.95271695	2.13627720
6	4.71643114	-1.70187294	3.31773996
1	4.54290342	-0.71975517	3.78448296
1	4.27094889	-2.44594812	3.99474359
6	6.21832609	-1.99054968	3.19357109
1	6.34598637	-3.00684857	2.78068471
1	6.67169809	-2.00840497	4.19710684
6	6.99456739	-1.00150418	2.31551337
1	7.02826405	-0.00726105	2.78898311
1	8.03951263	-1.34140289	2.22219396
6	6.43724823	-0.82320511	0.90516174
1	6.20871449	-1.79023027	0.42893398
1	7.16690063	-0.30088067	0.27180761
50	1.57672346	0.53727323	0.20194289
7	0.33048612	-1.78173184	-1.58509529
6	0.95396918	-2.30036592	-2.80829334
1	0.42272970	-3.19183564	-3.20248508
1	0.97459739	-1.52644551	-3.58490539
1	1.98750150	-2.59284258	-2.58416677
7	-0.40279520	0.62512445	-3.01344633
6	-1.08214009	-1.42970049	-1.79045558
1	-1.70690441	-2.33715940	-1.94581580
1	-1.43951166	-0.94232738	-0.87144548
6	-1.34755957	-0.50166124	-2.98060250
1	-2.39548922	-0.16381723	-2.89466906
1	-1.26274109	-1.04363620	-3.93207598
16	-0.82898510	2.01367021	-3.87412763
7	0.37445518	-1.03232133	1.20962930
6	0.48707351	-2.78025079	-0.51123971
1	0.01636566	-3.74651051	-0.79732579
1	1.56716847	-2.95101857	-0.39733642
6	-0.09881920	-2.36356783	0.83831042
1	0.20768134	-3.12307310	1.57873893
1	-1.20322323	-2.38884258	0.79444212
16	-0.24213168	-0.30842581	2.53883958
8	0.35732937	1.07173824	2.42631841
8	-0.07091905	-1.08205223	3.78745961
6	-2.02983761	-0.13403474	2.29228282
6	-2.90856552	-0.93468970	3.02275133
6	-4.28332853	-0.81121343	2.80538011
6	-4.79149818	0.10272253	1.87080085
6	-3.88291097	0.89757347	1.14952648

6	-2.50876927	0.78545409	1.35443401
1	-2.51102448	-1.63239276	3.75901341
1	-1.81273484	1.41840541	0.80226213
1	-4.25543165	1.61516428	0.41569757
6	-6.27759790	0.25446913	1.66301930
1	-4.97301865	-1.43649542	3.37535644
8	0.34438396	2.89995599	-3.78874850
8	-1.38503408	1.54334068	-5.15701151
6	-2.17369485	2.80579996	-2.95682049
6	-3.49541783	2.62551999	-3.36545897
6	-4.52048492	3.24160051	-2.64087343
6	-4.24173641	4.03511763	-1.51902366
6	-2.89881587	4.19995165	-1.13225198
6	-1.86495852	3.59330583	-1.84177232
1	-3.70833874	2.03090167	-4.25323820
1	-5.55547047	3.10965300	-2.96155500
6	-5.34643269	4.71718597	-0.75136995
1	-2.66040087	4.81956339	-0.26565394
1	-0.82429999	3.74290061	-1.55275202
1	-6.82065868	-0.64838934	1.97063601
1	-6.67003775	1.09411383	2.25779939
1	-6.51541853	0.46255147	0.61108238
1	-5.28908348	5.80982018	-0.86803401
1	-6.33576393	4.39363432	-1.09849679
1	-5.27232552	4.50692797	0.32547516
1	0.02607332	0.86969429	-2.11147285

Energy = -8524.623821 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 20

Atomic N.	X	Y	Z
8	2.40700507	-1.51832032	0.86455160
8	2.93873310	-0.18489140	-0.97502500
6	3.66430521	0.91278785	-1.53845799
1	4.63220835	0.55532104	-1.92661524
1	3.83353829	1.71047246	-0.79773808
1	3.07869029	1.33286619	-2.36615705
8	3.79879951	0.16823824	1.34648407
6	3.50298119	-0.91975182	0.52343822
6	4.67416239	-1.78079450	0.05828989
1	5.38339663	-1.19117582	-0.54248184
1	4.23777294	-2.53023839	-0.61321300
6	5.41410160	-2.46803856	1.22187102
1	4.67880726	-2.81096172	1.96712577
1	5.90806627	-3.37208748	0.83389294
6	6.47669649	-1.58137023	1.88404322
1	7.23771286	-1.32297659	1.12662411
1	7.00147581	-2.16133761	2.65956736
6	5.94128036	-0.28535113	2.50409961
1	5.28652620	-0.50510108	3.36239433
1	6.78874826	0.30141488	2.89605618
6	5.16390228	0.60779840	1.53817141
1	5.68863201	0.70823324	0.57416475
1	5.05184793	1.61504066	1.96173739
50	0.84340268	0.04944245	-0.07686502
7	0.14622182	-2.31269145	-0.88778496
6	1.18294871	-2.77904606	-1.83764577

8	3.18224216	0.51866394	1.68019903
8	3.31375051	-0.84508961	-0.27785856
6	4.05798578	-0.47809339	-1.44317961
1	4.70969152	-1.31034887	-1.75664937
1	4.67774343	0.41407156	-1.26465356
1	3.35377789	-0.25331953	-2.25901437
8	5.26304531	0.13713504	1.00346100
6	4.02861404	-0.40176719	1.27327669
6	3.97654223	-1.74976671	1.98872733
1	4.39222622	-2.54496598	1.35234618
1	2.90905237	-1.96488142	2.12468529
6	4.69288778	-1.72527957	3.35192895
1	4.48851395	-0.76746029	3.85525703
1	4.25090456	-2.50634933	3.98836088
6	6.20301819	-1.97640324	3.24705720
1	6.36134195	-2.97146797	2.79491711
1	6.63650608	-2.02692270	4.25824165
6	6.97466373	-0.93510741	2.42730045
1	6.97734737	0.03880460	2.94235921
1	8.02838039	-1.24883664	2.34122968
6	6.44061756	-0.70971179	1.01468694
1	6.24171734	-1.66102862	0.49545810
1	7.17066145	-0.14677717	0.41762847
50	1.56579757	0.57362789	0.26749384
7	0.41594046	-1.69828057	-1.64349127
6	1.07795513	-2.14845681	-2.87340593
1	0.57800657	-3.03492904	-3.31680083
1	1.09529626	-1.34161854	-3.61584234
1	2.11364412	-2.42479396	-2.63903141
7	-0.35224462	0.75089592	-2.98198891
6	-1.00059783	-1.37320602	-1.86485493
1	-1.59820962	-2.28849745	-2.07255173
1	-1.38986480	-0.93514657	-0.93408805
6	-1.26539660	-0.40161189	-3.01971340
1	-2.32410002	-0.09645907	-2.94355822
1	-1.14424014	-0.89866680	-3.99153328
16	-0.79720658	2.16007113	-3.79874229
7	0.38255364	-1.06733131	1.18060207
6	0.57540184	-2.73728800	-0.60928971
1	0.13540357	-3.70181131	-0.94578397
1	1.65684485	-2.88625598	-0.47891065
6	-0.04907744	-2.39270401	0.74337912
1	0.26094511	-3.17535901	1.45778227
1	-1.15132201	-2.44309092	0.67422110
16	-0.28125972	-0.41459793	2.52374101
8	0.28538179	0.98345178	2.48115039
8	-0.11790068	-1.23434162	3.74362993
6	-2.06691718	-0.27388805	2.24318695
6	-2.94064975	-1.12686920	2.91835713
6	-4.31285667	-1.02907598	2.67387152
6	-4.82355976	-0.08899429	1.76688612
6	-3.92009163	0.75866002	1.10156453
6	-2.54840636	0.67260027	1.33397663
1	-2.54167342	-1.84518838	3.63371372
1	-1.85681820	1.34596145	0.82575351
1	-4.29469252	1.49734795	0.39007762
6	-6.30811071	0.03380133	1.53072464
1	-4.99823952	-1.69562805	3.20058155

8	0.34386045	3.07825613	-3.64273763
8	-1.30082250	1.72568262	-5.11554337
6	-2.19293499	2.87158227	-2.89154196
6	-3.49609160	2.66188264	-3.34351730
6	-4.56125546	3.21496344	-2.62594509
6	-4.34079170	3.97470951	-1.46835363
6	-3.01529932	4.17092657	-1.03842700
6	-1.94211316	3.62682343	-1.74022126
1	-3.66418481	2.09456849	-4.25837040
1	-5.58196306	3.06014156	-2.98035836
6	-5.48907423	4.58739185	-0.70620632
1	-2.82209277	4.76582956	-0.14370044
1	-0.91542685	3.80108833	-1.41708946
1	-6.83308220	-0.89712971	1.78075159
1	-6.73694611	0.83228230	2.15630054
1	-6.52760553	0.28730077	0.48480776
1	-5.45440340	5.68584681	-0.75884748
1	-6.45683479	4.26152420	-1.10765266
1	-5.44909191	4.31794834	0.35933182
1	0.04518546	0.97095692	-2.05955219

Energy = -8524.623824 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 22

Atomic N.	X	Y	Z
8	-0.49819198	-0.15317710	0.24400003
8	1.79616714	-0.19816791	-0.73427814
6	3.10265875	-0.51124257	-0.28501740
1	3.42896295	-1.49154472	-0.67912918
1	3.15641642	-0.56430399	0.81931454
1	3.82770848	0.24612743	-0.63398373
8	1.00074041	0.56414402	1.71835232
6	0.41471606	0.70264190	0.50350076
6	0.36059088	2.04644775	-0.20047322
1	-0.38090277	2.65280628	0.35524428
1	-0.09465344	1.82367516	-1.17342794
6	1.65143466	2.84805870	-0.40605232
1	2.40009785	2.18789268	-0.86634827
1	1.43145919	3.63536239	-1.14371300
6	2.22758198	3.50354075	0.85059828
1	1.49146175	4.21676350	1.26172698
1	3.11105824	4.09929228	0.57271332
6	2.61361337	2.50956798	1.94811571
1	3.39246893	1.81464136	1.59750032
1	3.04757357	3.05936599	2.79992819
6	1.44139051	1.71000981	2.50308776
1	0.57110244	2.36322045	2.68096638
1	1.71411729	1.24505353	3.45852923
50	0.42731440	-1.95556545	-0.92764932
7	-2.40677094	-2.39543796	-1.09841597
6	-2.40675759	-3.59386444	-1.95706701
1	-3.40576434	-3.78077006	-2.39830661
1	-1.67913234	-3.49188137	-2.77127171
1	-2.12416434	-4.46415377	-1.35134554
7	-0.48869485	-1.07448268	-2.76725960
6	-2.78220105	-1.18659008	-1.85480917
1	-3.84166431	-1.23750591	-2.18746209

1	-2.67982960	-0.32695183	-1.17976618
6	-1.91375351	-0.95100832	-3.09572077
1	-2.15079165	0.06235293	-3.46796083
1	-2.18774104	-1.65971327	-3.89312649
16	0.53469169	-1.46804571	-3.98730779
7	-2.34646344	-1.37559235	2.01859379
6	-3.34852386	-2.65246391	0.01654825
1	-4.36691999	-2.81086302	-0.40274230
1	-3.04896450	-3.60072207	0.48476610
6	-3.48614836	-1.58966160	1.11558950
1	-4.34437323	-1.89006615	1.73215437
1	-3.72845078	-0.60398769	0.69284630
16	-1.93489170	-2.65853643	3.04682374
8	-0.77719718	-3.41336870	2.51391816
8	-3.20104170	-3.35193825	3.37425184
6	-1.36185884	-1.78234625	4.51907778
6	-2.29638195	-1.32075536	5.44933891
6	-1.84565210	-0.66820705	6.59496450
6	-0.47278595	-0.47305822	6.82770681
6	0.44065157	-0.95092446	5.87648630
6	0.00638196	-1.60888219	4.72281504
1	-3.35931039	-1.48714256	5.27694988
1	0.71335250	-1.99569452	3.98965788
1	1.51094413	-0.81705999	6.04566956
6	0.00160471	0.20564619	8.08846760
1	-2.57116342	-0.30910304	7.32741690
8	1.71950042	-2.02936387	-3.24735594
8	-0.09832717	-2.27562642	-5.05801582
6	1.08663642	0.07350314	-4.75832558
6	0.80344838	0.31786406	-6.10057545
6	1.23631191	1.51611352	-6.67740011
6	1.94726992	2.46486044	-5.93042994
6	2.21730185	2.18731117	-4.57709932
6	1.79241049	1.00070608	-3.98459554
1	0.26033238	-0.42815280	-6.67959404
1	1.01968336	1.71280646	-7.72907639
6	2.42585015	3.75076604	-6.55753565
1	2.77371860	2.91484261	-3.98173022
1	1.99781358	0.77802187	-2.93450356
1	-0.06214012	-0.47902775	8.94834423
1	1.04618919	0.53096873	8.00116444
1	-0.61582369	1.08241010	8.32837582
1	3.52528977	3.79246116	-6.58216763
1	2.06193352	3.85406184	-7.58753300
1	2.08426976	4.62505722	-5.98435307
1	-1.50678968	-1.02141380	1.52741969

Energy = -8524.630111 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 23

Atomic N.	X	Y	Z
8	2.82687926	-2.21443844	-0.51452655
8	3.97121954	-0.33155432	0.64072096
6	4.96211100	0.60982460	0.27699316
1	4.50996304	1.59915495	0.07772589
1	5.50555658	0.30265519	-0.63759482
1	5.69273043	0.73801351	1.09533906

8	5.00672054	-2.26839399	-0.91157240
6	3.99907136	-2.26761985	-0.00472298
6	4.17498732	-2.90717459	1.36486828
1	4.22262859	-3.99976611	1.18951106
1	3.22455215	-2.71624541	1.87857306
6	5.32687426	-2.46051931	2.27384448
1	5.28690910	-1.36586916	2.35792160
1	5.11929321	-2.85661292	3.27988553
6	6.72187185	-2.91973424	1.84707630
1	6.76628733	-4.02349758	1.86153758
1	7.45690966	-2.57303309	2.59020853
6	7.13957882	-2.43402028	0.45734900
1	7.16599846	-1.33435953	0.41202661
1	8.16536713	-2.77917624	0.24497586
6	6.26361275	-2.96197557	-0.67286491
1	6.04712820	-4.03407717	-0.52864689
1	6.77646542	-2.84866405	-1.63613296
50	1.98158813	-0.09920233	-0.26848298
7	-0.34445059	-2.03234720	-0.52066666
6	-0.10030791	-2.94718742	-1.64373934
1	-0.77133393	-3.83109999	-1.60983348
1	-0.25484523	-2.42851496	-2.59785891
1	0.94258767	-3.28304696	-1.61146450
7	-1.44397831	0.76730913	-1.37785196
6	-1.72900045	-1.53973663	-0.53392369
1	-2.43705916	-2.39279771	-0.62814677
1	-1.93924570	-1.06604826	0.43596995
6	-2.06772280	-0.53612107	-1.63949919
1	-3.16951180	-0.46541837	-1.69904435
1	-1.70565319	-0.88247031	-2.61585712
16	-1.47089994	1.93119884	-2.61044812
7	0.95102650	-0.65031338	1.63222134
6	-0.04825392	-2.71063542	0.75573117
1	-0.80514675	-3.49127078	0.98627669
1	0.92117733	-3.20887208	0.62669182
6	0.04370420	-1.75113511	1.94692004
1	0.39801547	-2.33145142	2.81714964
1	-0.96242964	-1.37515211	2.21380806
16	1.04315662	0.61540931	2.66170311
8	1.97276318	1.55501676	1.95556366
8	1.30094957	0.21446440	4.06337738
6	-0.58457750	1.42474914	2.66698456
6	-1.54080975	1.07038438	3.62122965
6	-2.79949951	1.67774522	3.58882737
6	-3.11285472	2.64894485	2.62652564
6	-2.12778234	2.99533081	1.68460977
6	-0.87066072	2.38918781	1.69506311
1	-1.28796530	0.34533229	4.39449978
1	-0.10937969	2.67497540	0.96833831
1	-2.33783054	3.76484752	0.93886846
6	-4.45480967	3.33797264	2.62836313
1	-3.54704094	1.39998984	4.33455229
8	-0.89706200	3.14286637	-1.99561286
8	-0.88879871	1.28380477	-3.79943180
6	-3.20856833	2.27603388	-2.98702765
6	-3.85900211	1.54117751	-3.98052526
6	-5.20401192	1.80336332	-4.24982691
6	-5.90671968	2.79341745	-3.54653859

6	-5.22432375	3.52169514	-2.55678105
6	-3.88267565	3.27087545	-2.27300143
1	-3.30759549	0.79164582	-4.54722166
1	-5.71454382	1.23313951	-5.02801228
6	-7.34837818	3.09705925	-3.86753893
1	-5.75086308	4.30453730	-2.00740957
1	-3.34690571	3.85518742	-1.52542377
1	-5.23177242	2.70365047	3.07481241
1	-4.41381884	4.26920366	3.21480417
1	-4.76881218	3.60946751	1.61139309
1	-7.42212009	3.96446705	-4.54185057
1	-7.83586407	2.24952865	-4.36606026
1	-7.91829967	3.34210372	-2.96114588
1	-1.73449671	1.20382202	-0.49655494

Energy = -8524.621628 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 24

Atomic N.	X	Y	Z
8	0.49231121	0.41445005	0.72773945
8	2.27300882	-0.57345814	-0.73517537
6	3.11729097	-1.70483720	-0.68554682
1	3.23236322	-2.08433747	0.34925187
1	4.11820364	-1.46019924	-1.08354354
1	2.71432805	-2.53810048	-1.29309833
8	2.24417591	-0.11455092	1.96767461
6	1.73632658	0.59543830	0.94044882
6	2.39060736	1.87379897	0.45041758
1	2.21994472	2.62387371	1.24805391
1	1.77834535	2.18576860	-0.40505275
6	3.86639810	1.86488128	0.03338259
1	4.00194645	1.06109893	-0.70274210
1	4.05661917	2.80959630	-0.49819982
6	4.87578964	1.73163521	1.17426038
1	4.78481483	2.59954405	1.85159123
1	5.89426231	1.77289593	0.75785118
6	4.71884489	0.45177722	1.99864471
1	4.85413742	-0.44372442	1.37262797
1	5.50772762	0.41560000	2.76852250
6	3.39196324	0.34959471	2.73996902
1	3.12600160	1.31393754	3.20346642
1	3.45289993	-0.40334496	3.53524923
50	0.17127404	-0.90119684	-1.19951284
7	-2.40058708	0.49922311	-0.62941819
6	-3.17430377	0.04186425	-1.79367566
1	-4.06017447	0.68253165	-1.98071194
1	-2.54850888	0.03735961	-2.69389987
1	-3.51872873	-0.98400158	-1.61078405
7	-0.12570359	1.01383376	-2.28499508
6	-1.91079378	1.87754226	-0.81001675
1	-2.75415730	2.60273504	-0.82192093
1	-1.27009726	2.11709785	0.04816282
6	-1.10778487	2.08334208	-2.10138702
1	-0.62170798	3.07268190	-2.03493762
1	-1.80116796	2.12627292	-2.96080709
16	0.69121528	0.92005730	-3.70085812
7	-1.65066588	-0.17699623	2.47218227

6	-3.27979016	0.38631201	0.55565864
1	-4.16007805	1.05517530	0.42178264
1	-3.66633606	-0.64235705	0.57854325
6	-2.69117451	0.71056813	1.93579578
1	-3.53372216	0.70207494	2.64099050
1	-2.26621103	1.72459090	1.96173847
16	-2.09310174	-1.77688277	2.80616951
8	-1.59886479	-2.68356109	1.74377596
8	-3.52707720	-1.75169075	3.17361379
6	-1.12808096	-2.12985969	4.29149866
6	-1.67139649	-1.84155667	5.54509211
6	-0.92763913	-2.13153315	6.68805981
6	0.35096830	-2.70719886	6.59638405
6	0.86858529	-2.98636222	5.32224035
6	0.13597880	-2.70659089	4.16688871
1	-2.66896701	-1.40898561	5.61483622
1	0.52996987	-2.93939352	3.17820859
1	1.85752916	-3.43983841	5.23188877
6	1.13062477	-3.04843950	7.84176111
1	-1.34908664	-1.91262603	7.67103529
8	1.51868570	2.11446905	-3.98623681
8	1.34061563	-0.43155140	-3.60336328
6	-0.52700639	0.82415962	-5.04268551
6	-1.18296683	-0.38556221	-5.28901863
6	-2.12636447	-0.45385036	-6.31298780
6	-2.43061948	0.67236948	-7.09746790
6	-1.75938475	1.87393343	-6.82713127
6	-0.80716985	1.95713151	-5.80805302
1	-0.93744552	-1.26677036	-4.69551039
1	-2.63366699	-1.39986348	-6.51200438
6	-3.43090940	0.57804096	-8.22229290
1	-1.98033202	2.75899243	-7.42676306
1	-0.26800907	2.88337874	-5.61200523
1	0.98611563	-2.29224014	8.62529087
1	0.79949999	-4.01319218	8.25687885
1	2.20513940	-3.13151646	7.63329506
1	-2.96093202	0.16451716	-9.12826729
1	-4.26733589	-0.08402403	-7.96047592
1	-3.83653569	1.56424975	-8.48245430
1	-0.77992773	-0.15820137	1.91207933

Energy = -8524.625608 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 25

Atomic N.	X	Y	Z
8	2.94421887	-2.04254413	-0.57276678
8	3.94786096	-0.22950105	0.80338204
6	4.91464472	0.77792555	0.57826197
1	5.59822941	0.85793215	1.44212091
1	4.43130541	1.76361489	0.44520062
1	5.51479626	0.57670712	-0.33030429
8	5.14175844	-1.97891712	-0.85422421
6	4.09014797	-2.09732652	-0.00685849
6	4.22317266	-2.84995914	1.30911314
1	4.32579565	-3.91988277	1.04168856
1	3.24062848	-2.74172020	1.78510571
6	5.30736828	-2.44363689	2.31507277

1	5.21704197	-1.36318660	2.49225521
1	5.06567001	-2.93566537	3.26983833
6	6.74039125	-2.81010914	1.92631221
1	6.83056927	-3.90826917	1.84637547
1	7.42140532	-2.50413370	2.73583913
6	7.20725060	-2.18621945	0.60930204
1	7.18932295	-1.08671355	0.66209555
1	8.25620365	-2.47200966	0.42354974
6	6.41304255	-2.64320540	-0.60889816
1	6.23518324	-3.73132610	-0.57112139
1	6.96925688	-2.42484498	-1.52909982
50	1.99723792	0.00881076	-0.18481544
7	-0.22777095	-1.98749578	-0.73080480
6	0.11543126	-2.78866267	-1.91327250
1	-0.51163787	-3.70174289	-1.98938346
1	-0.01982401	-2.19639611	-2.82666492
1	1.17110872	-3.07795405	-1.85593081
7	-1.41451025	0.83809566	-1.37092626
6	-1.63093793	-1.55320513	-0.77959830
1	-2.29189491	-2.42102838	-0.99822080
1	-1.91733909	-1.18714142	0.21706112
6	-1.95223117	-0.45922050	-1.80150282
1	-3.05028677	-0.43246934	-1.92799127
1	-1.51207685	-0.68768495	-2.78051066
16	-1.44134271	2.12238312	-2.47838473
7	0.89725149	-0.75231743	1.60064566
6	0.03299968	-2.76347065	0.49670404
1	-0.69943565	-3.59069371	0.61789531
1	1.02872574	-3.20982075	0.37816915
6	0.02257614	-1.90992951	1.76918554
1	0.35579881	-2.55122018	2.60425758
1	-1.01100814	-1.59703839	2.01176167
16	0.89449710	0.41375375	2.74528861
8	1.81296480	1.44892669	2.16970277
8	1.11233747	-0.10602283	4.11437225
6	-0.76345158	1.15893781	2.75455070
6	-1.73836553	0.68731666	3.63597989
6	-3.01678705	1.25289321	3.61037087
6	-3.33122015	2.29725528	2.72876549
6	-2.32715225	2.76082206	1.85970104
6	-1.05056512	2.19751501	1.86243331
1	-1.48503709	-0.09566610	4.35034657
1	-0.27573845	2.57408118	1.19382679
1	-2.53770828	3.58973932	1.18074942
6	-4.69630527	2.93929744	2.74019527
1	-3.77922940	0.88387233	4.29922247
8	-0.97756255	3.29185581	-1.70839787
8	-0.75388741	1.63734150	-3.68815446
6	-3.17261195	2.40872931	-2.92670584
6	-3.71138239	1.76763129	-4.04420996
6	-5.05201912	1.98232460	-4.37091112
6	-5.86071253	2.83246589	-3.60146117
6	-5.28984165	3.46837568	-2.48556566
6	-3.95382762	3.26357341	-2.14390349
1	-3.07773137	1.12847638	-4.65816307
1	-5.47531509	1.48560703	-5.24584532
6	-7.29709578	3.08910251	-3.98159719
1	-5.90010214	4.14250135	-1.88143611

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1 -3.50563240  3.77854848 -1.29462016
1 -5.45370817  2.26596451  3.16207218
1 -4.69129372  3.85526180  3.35144877
1 -5.01293373  3.22829008  1.72858167
1 -7.38302803  4.01388216 -4.57319260
1 -7.70405388  2.27073312 -4.58925962
1 -7.93155622  3.21201754 -3.09360027
1 -1.78004229  1.16578853 -0.47049826
Energy = -8524.621639 Hartree
Number of imaginary frequencies = 0.

```

Compound TS2a isomer 26

Atomic N.	X	Y	Z
8	3.97425032	-0.04627308	-0.99444610
8	2.90069175	2.05636334	-0.94807827
6	2.52922845	3.14811468	-1.78648746
1	1.50475585	3.00360537	-2.15918660
1	3.19773054	3.18881941	-2.65885758
1	2.59258604	4.09852743	-1.22872448
8	4.62198687	1.43465900	-2.59526610
6	4.40692663	1.14502501	-1.25389528
6	5.36857462	1.74094343	-0.22412992
1	6.25097609	1.07705474	-0.20347989
1	4.86480808	1.59543240	0.74033570
6	5.81059551	3.20168591	-0.37792355
1	4.93654776	3.83562779	-0.59263259
1	6.19754267	3.53918600	0.59654617
6	6.90069103	3.42748594	-1.43206275
1	7.77766514	2.80912733	-1.17112362
1	7.23939943	4.47495699	-1.38832772
6	6.47270966	3.09670353	-2.86430979
1	5.68571663	3.78980017	-3.20376897
1	7.33004570	3.24170661	-3.54337287
6	5.97030449	1.66828167	-3.06064653
1	6.65706921	0.93701166	-2.60139418
1	5.91119242	1.43708944	-4.13265657
50	1.78420115	0.11449090	-0.52372700
7	-0.60757130	2.05323505	1.02795148
6	0.16430503	2.85098815	1.98114729
1	-0.38621423	3.75258565	2.32832956
1	0.41837323	2.24605680	2.86169648
1	1.10670900	3.17028522	1.51657045
7	-1.35208488	-0.90031761	1.62071097
6	-1.82260644	1.52124536	1.64924514
1	-2.30303907	2.28687501	2.29857731
1	-2.55186009	1.29218280	0.85680103
6	-1.61515820	0.25677437	2.48934293
1	-2.51371789	0.11103705	3.11749983
1	-0.75189084	0.36585850	3.15866232
16	-0.96978056	-2.38195848	2.35340428
7	-0.04387447	1.08500385	-1.66744220
6	-0.91272461	2.81933284	-0.18934295
1	-1.76814544	3.51400852	-0.03789003
1	-0.03393160	3.43750763	-0.41874704
6	-1.20184851	1.93208051	-1.40467834
1	-1.42163074	2.59840012	-2.25820112
1	-2.11462402	1.32954669	-1.22801673

16	0.06312998	0.24246617	-3.03327084
8	1.38573658	-0.49331310	-2.77974868
8	-0.06912103	0.99179816	-4.30264854
6	-1.22240174	-1.03698790	-3.06131482
6	-2.19044566	-1.01826930	-4.06586981
6	-3.18747759	-1.99730754	-4.06845045
6	-3.22615623	-2.99677372	-3.08503723
6	-2.24080229	-2.98737884	-2.08185768
6	-1.24274611	-2.01437449	-2.06238937
1	-2.14559436	-0.25088057	-4.83782911
1	-0.48407322	-2.03255129	-1.27779543
1	-2.24072599	-3.75473285	-1.30523050
6	-4.27722836	-4.07807970	-3.12093902
1	-3.94480419	-1.98667979	-4.85474539
8	-0.88894266	-3.34192371	1.23503375
8	0.16062100	-2.11531663	3.25918460
6	-2.38512278	-2.85371208	3.37830544
6	-2.38301587	-2.54697275	4.74011517
6	-3.48809099	-2.90075541	5.51776123
6	-4.59215879	-3.55845857	4.95533943
6	-4.56476974	-3.85635591	3.58152366
6	-3.47064257	-3.51065254	2.79056168
1	-1.51578867	-2.05684876	5.18127394
1	-3.48850298	-2.66679907	6.58384800
6	-5.76762295	-3.96804333	5.80615759
1	-5.41105223	-4.37554979	3.12779093
1	-3.44213772	-3.76510072	1.73102784
1	-5.18570900	-3.73978209	-3.63633561
1	-3.90446210	-4.96403122	-3.65850949
1	-4.55092859	-4.40598679	-2.10910869
1	-5.70302534	-5.03494024	6.07066441
1	-5.80396986	-3.39699697	6.74254608
1	-6.71769524	-3.82386565	5.27394915
1	-2.07915258	-1.06099629	0.91799384

Energy = -8524.608140 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 27

Atomic N.	X	Y	Z
8	2.32300019	0.17996873	1.47505772
8	0.50741553	-0.00964673	-0.12489965
6	-0.38354504	-1.09703922	0.10016250
1	-1.39480019	-0.81164622	-0.23460479
1	-0.42883897	-1.38510466	1.16313124
1	-0.07254695	-1.97618997	-0.48527378
8	2.21659780	-1.80718935	0.45230013
6	2.24389267	-0.43062776	0.33508697
6	2.95735621	0.18615188	-0.86395365
1	4.03710461	0.16031599	-0.63209152
1	2.68318081	1.25149059	-0.85743803
6	2.68682790	-0.39903888	-2.25563145
1	1.60222399	-0.55327511	-2.36694455
1	2.96896243	0.36398217	-2.99581313
6	3.43316674	-1.69883657	-2.56767249
1	4.51851463	-1.52629268	-2.46152353
1	3.26793694	-1.96987987	-3.62267685
6	3.02894735	-2.87367725	-1.67524254

1	1.97378361	-3.14562964	-1.84287238
1	3.62722301	-3.76171660	-1.94025087
6	3.23272943	-2.62047529	-0.18512180
1	4.22690773	-2.18439889	0.00947390
1	3.17097926	-3.56715083	0.36815318
50	0.81600970	1.83089519	1.48612618
7	-1.98298979	2.53602123	1.18206298
6	-2.09688878	3.63527465	2.15349746
1	-3.15383410	3.91582942	2.33415580
1	-1.64453340	3.35204577	3.11200476
1	-1.56234741	4.51272535	1.76772726
7	-0.56404513	0.80843765	2.94024324
6	-2.63935471	1.31684983	1.67503500
1	-3.72466874	1.48520350	1.84843886
1	-2.55329347	0.54934025	0.89553428
6	-2.03156996	0.78214037	2.98010969
1	-2.41018414	-0.24718757	3.11704469
1	-2.39537930	1.37578630	3.83327556
16	0.21112610	1.00916231	4.37611914
7	-0.79829180	2.07022595	-1.66085267
6	-2.53805280	2.97601008	-0.11152230
1	-3.64281058	3.08287430	-0.03810635
1	-2.12602448	3.97098899	-0.32926571
6	-2.22180629	2.07959938	-1.31217480
1	-2.80553889	2.47025776	-2.15897775
1	-2.56613564	1.04699039	-1.15235341
16	-0.28809944	2.80811954	-3.07572675
8	1.17821848	2.64541864	-3.09094906
8	-0.94309419	4.13066912	-3.12087393
6	-0.96429366	1.85584450	-4.46092510
6	-2.12063336	2.30034685	-5.10432243
6	-2.64192843	1.55225742	-6.16328907
6	-2.02260995	0.36938122	-6.59124899
6	-0.85017395	-0.04575363	-5.93492031
6	-0.31836486	0.68674386	-4.87572718
1	-2.58289266	3.23655581	-4.79353285
1	0.60482919	0.37496811	-4.38758993
1	-0.34064201	-0.95189333	-6.26853657
6	-2.59589577	-0.44393405	-7.72437811
1	-3.54089928	1.90269077	-6.67364168
8	1.52334523	1.61086321	3.93589091
8	-0.60259455	1.72092557	5.39089537
6	0.58941662	-0.62283403	5.05294466
6	0.00826236	-1.01578343	6.25770855
6	0.29906642	-2.28476477	6.76677895
6	1.16178000	-3.15643120	6.08826494
6	1.73123109	-2.72756600	4.87516212
6	1.45367265	-1.46818244	4.34877491
1	-0.65120965	-0.32920307	6.78708220
1	-0.15014124	-2.59871459	7.71082354
6	1.49103224	-4.51774216	6.64854193
1	2.40717244	-3.39318967	4.33424950
1	1.90022480	-1.13664782	3.40850067
1	-3.34443450	0.12627533	-8.28876781
1	-1.81008458	-0.76710790	-8.42123604
1	-3.08547068	-1.35425341	-7.34514952
1	2.53892255	-4.56160784	6.98273373
1	0.85440898	-4.76276684	7.50812960

1 1.36286092 -5.30319023 5.88995028
 1 -0.24738684 1.23694122 -1.39509463
 Energy = -8524.622327 Hartree
 Number of imaginary frequencies = 0.

Compound TS2a isomer 28

Atomic N.	X	Y	Z
8	3.99646282	0.07558260	-1.05052769
8	2.89429855	2.15561175	-0.86806417
6	2.48233342	3.28281045	-1.63776386
1	3.12538314	3.38009048	-2.52470088
1	2.54639125	4.20388174	-1.03295887
1	1.45033002	3.14026570	-1.98986363
8	4.57262897	1.64297926	-2.59518576
6	4.40396261	1.28498006	-1.26397312
6	5.38861799	1.84458017	-0.23573063
1	6.28099585	1.19506562	-0.27565682
1	4.91774988	1.64319396	0.73527449
6	5.80356169	3.31833625	-0.32943162
1	4.91360092	3.94755554	-0.48421639
1	6.21643686	3.61289740	0.64831132
6	6.85573769	3.61490893	-1.40432775
1	7.75023460	2.99966407	-1.20213568
1	7.17914438	4.66461802	-1.31864786
6	6.38760328	3.34828877	-2.83738828
1	5.57941246	4.04362440	-3.11720777
1	7.22048473	3.54160142	-3.53458524
6	5.90186024	1.92288232	-3.08942008
1	6.61417246	1.18180513	-2.68855524
1	5.81255341	1.74402905	-4.16930580
50	1.81981790	0.17705546	-0.51301801
7	-0.58824450	1.97978640	1.19105303
6	0.18186353	2.73071504	2.18270636
1	-0.37932399	3.59961724	2.59105444
1	0.45767701	2.07754755	3.02116275
1	1.11230838	3.09523273	1.72741783
7	-1.25224602	-1.00816000	1.63530648
6	-1.79018152	1.39467406	1.78925741
1	-2.28135872	2.11650634	2.47957730
1	-2.51873374	1.19392169	0.98849034
6	-1.55817986	0.09230020	2.56162524
1	-2.46153164	-0.11016416	3.16694832
1	-0.70837182	0.18653315	3.25009871
16	-0.88703799	-2.52840471	2.29230666
7	-0.05407465	1.16998363	-1.56144631
6	-0.91544348	2.81187081	0.02412187
1	-1.77449584	3.48928738	0.22546247
1	-0.04464507	3.45023251	-0.17946292
6	-1.21287978	1.99472809	-1.23752344
1	-1.44393265	2.70848608	-2.04859209
1	-2.12126875	1.37860358	-1.08730364
16	0.03204418	0.39749786	-2.96958899
8	1.37108552	-0.32867700	-2.78500342
8	-0.14526863	1.20696509	-4.19604778
6	-1.23362720	-0.90071702	-3.02945995
6	-2.24205470	-0.83510029	-3.99118280
6	-3.22421479	-1.82911325	-4.01638365

6	-3.20790482	-2.88943172	-3.09862852
6	-2.18224835	-2.92682767	-2.13700986
6	-1.19876885	-1.94005096	-2.09515667
1	-2.23957729	-0.02066128	-4.71472359
1	-0.40748286	-1.99544549	-1.34533072
1	-2.13841510	-3.74222517	-1.41227257
6	-4.24340105	-3.98445940	-3.16071439
1	-4.01288748	-1.78209853	-4.76980448
8	-0.75277728	-3.41970277	1.12350333
8	0.20332015	-2.30990720	3.25823045
6	-2.33942747	-3.06844854	3.22804379
6	-2.39218950	-2.85260367	4.60600376
6	-3.52592349	-3.25839162	5.31438971
6	-4.60446024	-3.87833405	4.66657448
6	-4.52164793	-4.08492041	3.27807975
6	-3.39873219	-3.68634725	2.55578232
1	-1.54485464	-2.39165854	5.11245060
1	-3.56916332	-3.09552526	6.39273977
6	-5.81340027	-4.34204054	5.43918705
1	-5.34741974	-4.57405090	2.75792766
1	-3.32781172	-3.86966825	1.48360157
1	-5.15571213	-3.64747429	-3.66982031
1	-3.85684657	-4.85343838	-3.71582651
1	-4.51448965	-4.33866119	-2.15680408
1	-5.78345060	-5.43194866	5.59205246
1	-5.86375618	-3.86950278	6.42821455
1	-6.74340057	-4.11729670	4.89907789
1	-1.94880903	-1.12934053	0.89471585

Energy = -8524.608122 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 29

Atomic N.	X	Y	Z
8	3.37726021	2.00787187	1.78961754
8	1.69957101	2.21646976	0.01075304
6	1.94195735	3.34918261	-0.83121097
1	2.21033216	3.01347780	-1.84255457
1	2.73909092	4.00024176	-0.42914873
1	1.02136958	3.95294714	-0.90391475
8	2.56703806	0.11756321	0.79186106
6	3.24379015	1.31644690	0.71264356
6	4.32660675	1.44099784	-0.34141928
1	5.27118444	1.18568134	0.17106846
1	4.41662407	2.51041746	-0.57629812
6	4.16198444	0.60198998	-1.61543477
1	3.13057470	0.68463522	-1.99143589
1	4.80834723	1.04119968	-2.39085984
6	4.54963350	-0.87427628	-1.44478536
1	5.57598352	-0.92862624	-1.04062295
1	4.58506966	-1.35198700	-2.43622518
6	3.61166143	-1.68100226	-0.53992772
1	2.62536001	-1.79057884	-1.01925552
1	4.01354456	-2.69945145	-0.40500730
6	3.39684248	-1.07894695	0.84210968
1	4.34583664	-0.85039079	1.35211003
1	2.83913255	-1.76473165	1.49254537
50	1.43486404	2.97854233	2.18080688

7	-1.42508447	2.90914631	1.38428175
6	-1.69341326	4.34344435	1.59327161
1	-2.78126526	4.55551624	1.60288799
1	-1.26509774	4.67874336	2.54641604
1	-1.22725451	4.92867279	0.78964287
7	0.29951969	1.51479983	3.34134007
6	-1.95674431	2.12571931	2.52300906
1	-2.94383883	2.52567840	2.83450294
1	-2.11005116	1.09007990	2.19767690
6	-1.00136340	2.09953284	3.71644115
1	-1.45622587	1.52724969	4.53786564
1	-0.85670614	3.11997795	4.11636114
16	0.78181112	0.18999121	4.22595978
7	-0.52892172	0.87583339	-1.13262570
6	-2.07949972	2.50566125	0.11323507
1	-3.18021250	2.59677911	0.23710611
1	-1.79073298	3.22186303	-0.66776347
6	-1.77762389	1.08403671	-0.38731784
1	-2.61089373	0.77966779	-1.03758156
1	-1.77518988	0.36720285	0.44647685
16	-0.55857015	1.23016989	-2.77796936
8	0.85811573	1.22064996	-3.20701742
8	-1.41961408	2.39787960	-3.08991385
6	-1.38544071	-0.22086182	-3.46999454
6	-2.55737686	-0.05620199	-4.20574427
6	-3.16049099	-1.17794764	-4.78268290
6	-2.60513401	-2.45613217	-4.63558435
6	-1.42063808	-2.59036422	-3.88714576
6	-0.80762088	-1.48392403	-3.30584383
1	-2.98151422	0.94054472	-4.32177258
1	0.11196903	-1.58943558	-2.73061991
1	-0.97300786	-3.57837176	-3.76307011
6	-3.24716163	-3.66317129	-5.27193213
1	-4.07901812	-1.05428195	-5.35900116
8	2.20560789	-0.04391747	3.91348100
8	0.34347022	0.32373887	5.63743687
6	-0.17494591	-1.20185494	3.54684687
6	-0.94534218	-1.98720801	4.40457439
6	-1.66098416	-3.06897378	3.88314152
6	-1.61692810	-3.37813234	2.51610661
6	-0.83779758	-2.56526136	1.67378581
6	-0.11748507	-1.48295569	2.17837119
1	-0.97782797	-1.74271846	5.46579552
1	-2.26606727	-3.68273664	4.55347061
6	-2.36518669	-4.56624269	1.96424389
1	-0.79880720	-2.78175521	0.60376096
1	0.48119366	-0.85319537	1.51862133
1	-4.21836901	-3.41307068	-5.71670675
1	-2.60734272	-4.07418537	-6.06739664
1	-3.40188313	-4.46637344	-4.53723907
1	-1.71126664	-5.45111370	1.91468227
1	-3.22399974	-4.82852268	2.59583306
1	-2.72887731	-4.37369251	0.94580495
1	0.33346993	1.28235042	-0.70292276

Energy = -8524.608167 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 30

Atomic N.	X	Y	Z
8	5.12065554	-1.01099920	-1.70923269
8	4.49458790	1.16615903	-1.00345254
6	3.87115669	2.31586671	-1.57636046
1	3.16334653	2.72818184	-0.84240800
1	3.32927442	2.07808185	-2.50331116
1	4.62905550	3.08598089	-1.78841221
8	5.26549864	0.58766443	-3.29967737
6	5.58706570	0.16113697	-2.02893186
6	6.96384335	0.49595159	-1.45636249
1	7.67741728	-0.18335737	-1.95675921
1	6.91403389	0.15837121	-0.41315895
6	7.47524977	1.94071794	-1.51030385
1	6.69319582	2.61840582	-1.13664496
1	8.30977249	2.02270341	-0.79626077
6	7.97263861	2.39915586	-2.88475060
1	8.81414795	1.75306594	-3.19115114
1	8.38281250	3.41813087	-2.80146933
6	6.90947056	2.36951756	-3.98577213
1	6.09856033	3.08421564	-3.77200627
1	7.36522388	2.69435263	-4.93630505
6	6.29584980	0.99351758	-4.23138618
1	7.07799053	0.21640025	-4.27446461
1	5.76721573	0.98610634	-5.19330072
50	3.39745784	-0.69924170	-0.36855841
7	-0.01697810	0.77592909	2.17464566
6	0.64851856	0.53274256	3.45401382
1	0.66837132	1.43020582	4.11198425
1	0.14918183	-0.28179494	3.99353123
1	1.68319106	0.21793474	3.26600075
7	-2.33587861	-1.07024193	2.55429029
6	-1.39743757	1.22477078	2.35236287
1	-1.43795311	2.20754981	2.88110828
1	-1.83291435	1.39254200	1.35425472
6	-2.31292772	0.28208172	3.13446498
1	-3.31518412	0.74949551	3.14515090
1	-1.98715401	0.18745792	4.17811394
16	-3.45455408	-2.16370726	3.20381403
7	1.32428133	0.49922997	-0.66401714
6	0.72113842	1.75377452	1.36321652
1	0.46119303	2.79528093	1.65845013
1	1.79433072	1.62936080	1.57148457
6	0.51209319	1.60372043	-0.14914986
1	0.78524184	2.55734777	-0.63558942
1	-0.55979961	1.44335544	-0.36170968
16	0.93930775	-0.17838198	-2.06426096
8	2.15026212	-1.12353277	-2.23775864
8	0.63215089	0.70031750	-3.21544814
6	-0.49065536	-1.26771998	-1.85181570
6	-1.45181680	-1.34711480	-2.86094499
6	-2.52590132	-2.22573042	-2.70529985
6	-2.65002418	-3.02550769	-1.55815494
6	-1.67601871	-2.91048217	-0.55015141
6	-0.59894586	-2.03474331	-0.68918622
1	-1.34852004	-0.72623724	-3.75001311
1	0.14152537	-1.93327475	0.10562342
1	-1.77443504	-3.50257778	0.36099622

6	-3.78608298	-4.00690937	-1.41403437
1	-3.27896428	-2.29358268	-3.49292231
8	-3.35247421	-3.37338638	2.36320972
8	-3.20925951	-2.18951845	4.65680075
6	-5.10156918	-1.45750439	2.94871211
6	-5.74186850	-0.80172056	4.00127125
6	-7.00761223	-0.24984728	3.78856564
6	-7.64141607	-0.34492666	2.54105473
6	-6.97135305	-1.01045740	1.49913824
6	-5.70919609	-1.56773806	1.69385850
1	-5.25603771	-0.74481285	4.97472525
1	-7.51302242	0.26066846	4.61026907
6	-9.02094746	0.22397649	2.32536340
1	-7.45086479	-1.09859693	0.52246094
1	-5.20316505	-2.09818602	0.88705903
1	-3.52962661	-4.96569920	-1.89141309
1	-4.00012732	-4.21597242	-0.35772681
1	-4.70018625	-3.63852739	-1.89961421
1	-9.78271770	-0.56854612	2.38907528
1	-9.26639938	0.98009753	3.08181739
1	-9.11406422	0.68297976	1.33176708
1	-2.38225532	-1.09392715	1.53099704

Energy = -8524.609209 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 31

Atomic N.	X	Y	Z
8	3.21754193	1.16304231	-0.36071315
8	3.95749831	-1.12177765	-0.56961870
6	4.33499479	-2.16544127	0.32727513
1	3.63337278	-3.00483012	0.21971345
1	4.30731440	-1.82549679	1.37479508
1	5.35089874	-2.51917958	0.08477146
8	4.80383492	0.62269557	1.11405694
6	4.40196037	0.65578341	-0.19352341
6	5.42229700	0.91759115	-1.29676044
1	5.73136425	1.97342753	-1.18334484
1	4.83826065	0.87672651	-2.22503400
6	6.65015745	0.00806962	-1.42423904
1	6.31507015	-1.03920138	-1.42322123
1	7.08964539	0.18694943	-2.41789532
6	7.73713923	0.22644466	-0.36893478
1	8.12970638	1.25436914	-0.46284950
1	8.58406353	-0.44588917	-0.57754993
6	7.26662874	0.01574088	1.07226443
1	6.93820238	-1.02217543	1.23720896
1	8.11535358	0.18361504	1.75628757
6	6.15813684	0.96609855	1.51299405
1	6.37355280	1.99595201	1.18102801
1	6.08360815	0.97504181	2.60777617
50	1.86131406	-0.49017572	-0.95896822
7	-0.12705532	2.27426457	1.10525823
6	0.89564896	3.32426906	1.06155694
1	0.84735101	3.99485826	1.94651842
1	1.89555538	2.87666416	1.00931334
1	0.75565958	3.92982292	0.15692130
7	1.13666713	-0.51785052	1.13852012

6	0.02956858	1.41876435	2.29012108
1	0.13151111	2.04088044	3.20897889
1	-0.88483334	0.82034081	2.40889382
6	1.22934496	0.46505389	2.22074556
1	1.33001888	-0.05008505	3.19024277
1	2.16205192	1.02838111	2.07106066
16	0.78801054	-2.07673478	1.46065378
7	-2.06470633	1.29579830	-0.82132995
6	-1.47824657	2.84945512	1.03476489
1	-1.82571638	3.22049952	2.02370024
1	-1.44775724	3.71226025	0.35473946
6	-2.49293685	1.84430325	0.47846243
1	-3.46744347	2.33662987	0.36295715
1	-2.63230515	0.99508518	1.16494918
16	-2.57184958	2.10618496	-2.23014951
8	-1.47145486	1.91999793	-3.19837999
8	-3.10118484	3.45130086	-1.90646815
6	-3.97677660	1.10580885	-2.76869082
6	-5.26928186	1.61287522	-2.64805770
6	-6.34601212	0.83656514	-3.08632851
6	-6.14477110	-0.43255046	-3.64670110
6	-4.82757425	-0.91406763	-3.75950050
6	-3.74340701	-0.15424465	-3.32735181
1	-5.42035007	2.60608315	-2.22676086
1	-2.72315884	-0.52372974	-3.42900920
1	-4.65081930	-1.89832568	-4.19740009
6	-7.30598640	-1.25583529	-4.14502668
1	-7.36041403	1.22910869	-2.99527431
8	1.11895299	-2.72605753	0.13226320
8	1.41613781	-2.59546638	2.69738913
6	-0.99888718	-2.27773643	1.68145168
6	-1.49419987	-2.67027116	2.92516184
6	-2.87412024	-2.80950117	3.09519863
6	-3.76368403	-2.56826735	2.03828025
6	-3.23514795	-2.17466545	0.79580092
6	-1.86229563	-2.02698660	0.61124533
1	-0.79906577	-2.86980271	3.73973846
1	-3.26455832	-3.11464477	4.06785822
6	-5.25014305	-2.75026488	2.21717238
1	-3.90934205	-1.97407269	-0.03911624
1	-1.46814227	-1.71545136	-0.35606533
1	-8.26150227	-0.87452775	-3.76315331
1	-7.35493183	-1.23663127	-5.24471712
1	-7.20830822	-2.30866337	-3.84573078
1	-5.57209301	-3.73095870	1.83341873
1	-5.53640652	-2.69983172	3.27560139
1	-5.81563663	-1.98639667	1.66644204
1	-1.03588998	1.25098586	-0.85568738

Energy = -8524.625244 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 32

Atomic N.	X	Y	Z
8	3.75767279	-1.18474936	-0.57821888
8	2.99567866	1.03504777	-0.47597489
6	2.69694090	2.17294741	-1.28865826
1	3.25844789	2.10669255	-2.23072553

1	2.96997261	3.10029626	-0.75760013
1	1.62744832	2.19151258	-1.53994632
8	4.40096855	0.18113084	-2.28682423
6	4.30910540	-0.06013865	-0.92267185
6	5.46416521	0.40070045	-0.03192276
1	6.22578859	-0.39735246	-0.07653539
1	5.06010628	0.36804166	0.98842782
6	6.11252832	1.76336002	-0.30782109
1	5.33418655	2.52636433	-0.46392915
1	6.65530014	2.06634903	0.60127288
6	7.09969711	1.76738513	-1.48130000
1	7.88489532	1.01652360	-1.28399837
1	7.61095858	2.74217129	-1.52429187
6	6.46472979	1.47331870	-2.84319496
1	5.77614069	2.28413463	-3.13192439
1	7.25296831	1.44426906	-3.61438537
6	5.70354986	0.15226819	-2.91574383
1	6.30022430	-0.67894328	-2.50367451
1	5.47522211	-0.09188231	-3.96178770
50	1.67722535	-0.72321403	0.07428162
7	0.29929709	1.57961977	2.00720429
6	1.42000711	2.31901550	2.60179734
1	1.10191846	3.29658484	3.02175450
1	1.87937176	1.73379540	3.40774155
1	2.18916774	2.49267173	1.83833754
7	-0.17193133	-1.16985381	3.45150208
6	-0.72284371	1.26324618	3.02206659
1	-0.98726147	2.18056512	3.59466529
1	-1.63292980	0.93426001	2.50223231
6	-0.30707812	0.17590569	4.01812029
1	-1.04824317	0.12382704	4.82816601
1	0.64590210	0.43684536	4.50363541
16	-1.41427839	-2.29286098	3.64934826
7	-0.20350127	0.47030723	-0.63179445
6	-0.29345977	2.36650157	0.90740812
1	-0.95998567	3.16394424	1.30126226
1	0.53023571	2.86430216	0.37909916
6	-1.07045686	1.52419937	-0.11103291
1	-1.40407240	2.20584726	-0.91273129
1	-1.97650397	1.09424710	0.35176513
16	-0.24608107	-0.00104042	-2.16998386
8	0.97998244	-0.92616969	-2.18073821
8	-0.32147565	1.07350683	-3.18657255
6	-1.66005731	-1.08858001	-2.48415017
6	-2.75879359	-0.59057677	-3.18516517
6	-3.86052537	-1.42255855	-3.40379453
6	-3.87664247	-2.74520922	-2.93792176
6	-2.74912810	-3.22293949	-2.24545646
6	-1.64585078	-2.40485859	-2.01293206
1	-2.73509240	0.42702287	-3.57330632
1	-0.76984924	-2.79051971	-1.49084961
1	-2.73440766	-4.25350952	-1.88604915
6	-5.06947851	-3.63899732	-3.16559315
1	-4.71906137	-1.03739107	-3.95699978
8	-0.98139912	-3.47080636	2.87589049
8	-1.70035744	-2.34590983	5.09590626
6	-2.90820050	-1.63636160	2.86176825
6	-3.90081096	-1.04586351	3.64594936

6	-5.04000330	-0.52836263	3.02440333
6	-5.20255375	-0.59628761	1.63261318
6	-4.18875122	-1.20126402	0.86871696
6	-3.04539633	-1.72105896	1.47352552
1	-3.78263927	-1.01425087	4.72850275
1	-5.81930542	-0.06781742	3.63452554
6	-6.44750404	-0.06185522	0.96983868
1	-4.29275274	-1.26555061	-0.21628407
1	-2.26907659	-2.19695640	0.87508243
1	-5.79084921	-3.17918897	-3.85263705
1	-4.76558685	-4.60907602	-3.58346248
1	-5.59020805	-3.84755468	-2.21844339
1	-7.15911674	-0.87619096	0.76243305
1	-6.96017218	0.66935343	1.60791087
1	-6.21475744	0.41671261	0.00889275
1	0.23862538	-1.21909416	2.51098013

Energy = -8524.611188 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 33

Atomic N.	X	Y	Z
8	3.16747856	1.25149167	-0.29562804
8	3.93163848	-1.01837337	-0.58979136
6	4.33589745	-2.07848120	0.27545983
1	4.32066011	-1.76436114	1.33129430
1	5.35237885	-2.41275001	0.00880192
1	3.64348102	-2.92418528	0.15819854
8	4.79692698	0.69216329	1.12271082
6	4.36227846	0.75683457	-0.17262278
6	5.35118437	1.06147671	-1.29319131
1	5.65014505	2.11774778	-1.15841711
1	4.74477530	1.03864741	-2.20767093
6	6.58640337	0.17151074	-1.47583997
1	6.26386929	-0.87952060	-1.49511039
1	6.99870682	0.38284621	-2.47474647
6	7.69663286	0.37513614	-0.44202030
1	8.07365513	1.41043699	-0.51661849
1	8.54653263	-0.27971995	-0.69033825
6	7.26508856	0.11805661	1.00380087
1	6.95367718	-0.92826152	1.14733517
1	8.12839031	0.27788913	1.67130053
6	6.15635586	1.04126191	1.49827480
1	6.35109091	2.08271694	1.19060135
1	6.10870790	1.01849592	2.59434390
50	1.82340181	-0.40020224	-0.92647493
7	-0.17273745	2.27133346	1.17525339
6	0.83318084	3.33835173	1.16131616
1	0.76005965	3.99582005	2.05431652
1	1.84079790	2.90761185	1.11849177
1	0.69727194	3.95371270	0.26268318
7	1.12860429	-0.49929434	1.17667460
6	-0.01692078	1.40038753	2.34923387
1	0.06656667	2.00996137	3.27818036
1	-0.92403275	0.78761828	2.44880939
6	1.19643807	0.46382967	2.27769303
1	1.29228997	-0.06773048	3.23878360
1	2.12331247	1.04205346	2.14947009

16	0.79665399	-2.06898046	1.45985305
7	-2.08146524	1.29002857	-0.78262633
6	-1.53178120	2.82736731	1.09735143
1	-1.89393473	3.18249249	2.08687234
1	-1.50642550	3.69842291	0.42757431
6	-2.52749610	1.81515872	0.52038676
1	-3.50725985	2.29621029	0.40243146
1	-2.66086507	0.95609689	1.19571316
16	-2.60240149	2.09711695	-2.18811202
8	-1.47858810	1.97961354	-3.14013720
8	-3.20108581	3.40901899	-1.85001147
6	-3.94789767	1.04033780	-2.76908183
6	-5.26562452	1.48001027	-2.65772390
6	-6.29610062	0.66007227	-3.12681603
6	-6.02403164	-0.58610213	-3.70826411
6	-4.68294525	-0.99912155	-3.81104827
6	-3.64414930	-0.19511968	-3.34853172
1	-5.47202778	2.45584655	-2.21965837
1	-2.60542083	-0.51141453	-3.44239140
1	-4.45124245	-1.96449304	-4.26505136
6	-7.13547993	-1.45705736	-4.23814344
1	-7.32995033	1.00009191	-3.04332614
8	1.12931180	-2.67958117	0.11388459
8	1.43400228	-2.61254835	2.68098497
6	-0.98725086	-2.29430151	1.68273592
6	-1.47392201	-2.70554209	2.92391992
6	-2.85163403	-2.86303473	3.09616017
6	-3.74717903	-2.62217331	2.04426885
6	-3.22714758	-2.20989966	0.80426627
6	-1.85673618	-2.04345965	0.61746913
1	-0.77413154	-2.90583301	3.73429346
1	-3.23565388	-3.18291235	4.06664515
6	-5.23079681	-2.82393813	2.22561002
1	-3.90604782	-2.00995994	-0.02700204
1	-1.46901309	-1.71801710	-0.34783691
1	-8.11583996	-1.12053812	-3.87783837
1	-7.15855885	-1.43492115	-5.33856201
1	-6.99822521	-2.50597692	-3.94040513
1	-5.54450703	-3.79852629	1.82019401
1	-5.51234865	-2.80121732	3.28623533
1	-5.80689859	-2.05315852	1.69578767
1	-1.05209053	1.26543081	-0.81462777

Energy = -8524.625234 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 34

Atomic N.	X	Y	Z
8	2.43238902	0.04316343	1.81871367
8	2.86633873	0.06831004	-0.48139280
6	3.56500483	-0.35397071	-1.65110445
1	2.90630698	-0.98430771	-2.26668739
1	4.44236994	-0.94704145	-1.34943676
1	3.88374758	0.50800943	-2.25739479
8	4.40928411	-0.88532329	1.15442693
6	3.52513194	0.20603219	1.16300023
6	4.13595772	1.60961914	1.18407047
1	4.32526827	1.84372830	2.24673724

1	3.31819630	2.27653575	0.87811840
6	5.39353657	1.89580333	0.35367131
1	5.27957439	1.48610520	-0.66083080
1	5.47066355	2.98737693	0.23097958
6	6.69585848	1.39040685	0.98550195
1	6.79966688	1.83995140	1.98881352
1	7.55204439	1.75451970	0.39586198
6	6.78951597	-0.13246977	1.11468124
1	6.83116484	-0.60407060	0.11925234
1	7.73006105	-0.39606738	1.62762249
6	5.64601898	-0.77237010	1.89732516
1	5.46751976	-0.24291694	2.84875393
1	5.89926958	-1.81348836	2.14162397
50	0.74323249	0.33393189	0.06922697
7	0.51591599	-2.12156296	0.86227775
6	1.70599139	-2.86739540	0.38779613
1	1.58512914	-3.94962525	0.57934195
1	1.84574521	-2.70647550	-0.68560308
1	2.59284163	-2.49389315	0.91106242
7	-0.07851594	-1.01928115	-1.55209458
6	-0.70246410	-2.59054637	0.15767714
1	-0.88118738	-3.66251469	0.36858913
1	-1.55589688	-2.01595473	0.54455680
6	-0.59583694	-2.36588860	-1.35457337
1	-1.60641932	-2.49165821	-1.78399169
1	0.04715024	-3.13181520	-1.82131791
16	0.00409480	-0.38571343	-3.05230260
7	-0.30283272	-0.07416397	3.00420141
6	0.42189425	-2.33262587	2.33077073
1	0.21630415	-3.40238571	2.52964902
1	1.41616857	-2.10075569	2.73629594
6	-0.61580324	-1.50883389	3.08737946
1	-0.62262297	-1.86781418	4.12978649
1	-1.62918115	-1.66717398	2.68901658
16	-1.23120666	0.96497226	3.99849057
8	-0.40628225	2.17794943	4.15121174
8	-1.74645329	0.22455622	5.17107630
6	-2.64081717	1.33694232	2.93715501
6	-3.88133097	0.76116318	3.21475673
6	-4.96904802	1.07041240	2.39561248
6	-4.83129120	1.94600534	1.30744982
6	-3.57145309	2.51880050	1.06243873
6	-2.47383332	2.22073126	1.86813605
1	-3.98709536	0.09789576	4.07255507
1	-1.50034106	2.67208624	1.67986631
1	-3.44949746	3.21446609	0.23015365
6	-6.00467587	2.25134254	0.41093409
1	-5.94385624	0.62944287	2.61152840
8	0.64851815	0.94392580	-2.82475996
8	0.58367610	-1.32013619	-4.04970360
6	-1.70324564	-0.07429190	-3.58366728
6	-2.23117685	-0.76928985	-4.67026424
6	-3.54818630	-0.51648843	-5.06795692
6	-4.34127235	0.42284560	-4.39600229
6	-3.78207946	1.10934544	-3.30204415
6	-2.47377706	0.86584902	-2.89182425
1	-1.60571122	-1.48817241	-5.19848967
1	-3.96316838	-1.05771971	-5.92035389

6	-5.75625896	0.70696956	-4.83529854
1	-4.38250113	1.85054970	-2.76988482
1	-2.04337192	1.40704191	-2.04814935
1	-6.95121002	2.22903705	0.96692562
1	-5.90266371	3.23668718	-0.06224083
1	-6.08225060	1.50412536	-0.39477006
1	-5.85639715	1.74042416	-5.19990444
1	-6.06731367	0.03328866	-5.64358139
1	-6.46404171	0.59050530	-4.00146866
1	0.69101733	0.14334811	3.16202140

Energy = -8524.621446 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 35

Atomic N.	X	Y	Z
8	2.91742206	-0.01398756	2.57389688
8	3.17977786	0.06399514	0.22475199
6	3.57713866	0.27569482	-1.11626542
1	2.80884004	-0.11631127	-1.80645347
1	4.51600027	-0.26496479	-1.33812249
1	3.72450495	1.34431350	-1.36176074
8	4.68716669	-1.18800473	1.95525873
6	4.05439997	0.01645507	1.97459078
6	4.85500717	1.31177998	2.02520490
1	5.30707407	1.33431530	3.03597736
1	4.10038805	2.10930133	2.02577019
6	5.92072725	1.62003076	0.96650994
1	5.47666645	1.52770507	-0.03283405
1	6.19299078	2.68077612	1.08187044
6	7.19680882	0.78022081	1.04916060
1	7.70589638	0.98199958	2.00809622
1	7.89138985	1.10397530	0.25832534
6	6.95857763	-0.72684473	0.93372029
1	6.48175240	-0.98355246	-0.02583926
1	7.92966461	-1.24904275	0.94845992
6	6.12869644	-1.30748332	2.07386851
1	6.44171572	-0.87731266	3.04040051
1	6.26963282	-2.39414716	2.13001585
50	1.26782548	0.77560341	1.30941880
7	0.49915409	-1.65287840	0.87056005
6	1.39325929	-2.41487169	-0.02337725
1	1.06237876	-3.46707487	-0.10704581
1	1.41577470	-1.96184707	-1.02025890
1	2.40951657	-2.37667942	0.38253051
7	-0.70171446	0.04733367	-1.31940079
6	-0.91299289	-1.70604348	0.41804272
1	-1.30090106	-2.73542809	0.55028594
1	-1.49838507	-1.04893935	1.07596767
6	-1.16758502	-1.31856930	-1.03923416
1	-2.24979544	-1.43988597	-1.22514617
1	-0.63521105	-1.98891485	-1.72496200
16	-0.50176883	0.50356245	-2.95028138
7	0.02324240	-0.01745602	3.05327988
6	0.59571683	-2.21838069	2.24777603
1	0.28510508	-3.28063965	2.23952913
1	1.65427589	-2.16164422	2.53423715
6	-0.24482325	-1.43702745	3.25776291

1	0.03973657	-1.76849866	4.27009726
1	-1.31778216	-1.68382025	3.13741755
16	-0.94844693	1.05386543	3.81891203
8	-0.31394809	2.38317537	3.63182664
8	-1.33421791	0.56945795	5.16632938
6	-2.48831177	1.09184444	2.84253287
6	-3.56121564	0.26668161	3.18442655
6	-4.70213127	0.24894816	2.37372088
6	-4.79410648	1.05236554	1.22888196
6	-3.70915079	1.89388227	0.91883963
6	-2.56293225	1.91611660	1.71290433
1	-3.50794077	-0.33131185	4.09404850
1	-1.73245418	2.58693361	1.48703718
1	-3.77669835	2.55824924	0.05378373
6	-6.02141428	1.02473259	0.35131428
1	-5.54274178	-0.39224985	2.64698052
8	-0.05444731	1.90500712	-2.89722633
8	0.30410534	-0.56865740	-3.56611204
6	-2.14136314	0.47242469	-3.70888662
6	-2.57656145	-0.67329586	-4.37661123
6	-3.85660696	-0.68622851	-4.93609762
6	-4.70373297	0.42756405	-4.83892107
6	-4.23452616	1.56910765	-4.16450500
6	-2.96094370	1.60098159	-3.60061288
1	-1.91058612	-1.53009045	-4.47320795
1	-4.20001507	-1.57722104	-5.46449995
6	-6.07525349	0.41893306	-5.46484423
1	-4.87483072	2.44999290	-4.08928108
1	-2.58870029	2.49610424	-3.10232711
1	-6.86399364	0.53637028	0.85750538
1	-6.33256102	2.03992128	0.06740478
1	-5.82929564	0.47216314	-0.58195335
1	-6.09620428	1.04867172	-6.36741924
1	-6.37715197	-0.59434372	-5.75764656
1	-6.83104706	0.81999201	-4.77521992
1	-1.23783875	0.77310115	-0.83287871

Energy = -8524.610538 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 36

Atomic N.	X	Y	Z
8	2.39917326	0.00813234	1.80970013
8	2.88442087	0.30019128	-0.45885301
6	3.60215425	-0.11324966	-1.62070847
1	4.43758202	-0.76407272	-1.31975198
1	3.98507500	0.75663382	-2.17649245
1	2.93180394	-0.67912412	-2.28391528
8	4.42143488	-0.77482110	1.12134242
6	3.49952245	0.27902269	1.19143426
6	4.04725170	1.69706488	1.37282813
1	4.26874781	1.80618238	2.44942021
1	3.18575120	2.35142422	1.18225551
6	5.24914360	2.15529799	0.53748137
1	5.10034323	1.87759852	-0.51655549
1	5.26884604	3.25603962	0.55825102
6	6.60383940	1.64092278	1.03627694
1	6.75080633	1.98047245	2.07676244

1	7.40961313	2.10414577	0.44516867
6	6.75790167	0.11864249	0.98977888
1	6.73895121	-0.24315880	-0.05120532
1	7.74379683	-0.15990333	1.39905727
6	5.70160103	-0.64676118	1.78304613
1	5.56315184	-0.20835739	2.78611374
1	6.02160597	-1.68904531	1.91909051
50	0.73231530	0.35417569	0.09875278
7	0.60847878	-2.16424155	0.70752192
6	1.83958232	-2.82181692	0.20806798
1	1.76472366	-3.91926551	0.32051203
1	1.99135661	-2.57965374	-0.84841555
1	2.69842267	-2.44845247	0.77616489
7	0.03393595	-0.92602307	-1.64063001
6	-0.57289475	-2.63339949	-0.05658136
1	-0.70909452	-3.72419381	0.07510551
1	-1.45881939	-2.12418723	0.34849963
6	-0.44286525	-2.29892945	-1.54676068
1	-1.43957365	-2.42682695	-2.00682378
1	0.23422480	-3.00996494	-2.05090809
16	0.05988825	-0.17108060	-3.08657598
7	-0.32030615	-0.30820864	2.97828317
6	0.49631885	-2.48339438	2.15450430
1	0.32968780	-3.57171488	2.27303576
1	1.47343481	-2.24427843	2.59615517
6	-0.58509552	-1.75483286	2.94660330
1	-0.59993130	-2.19098687	3.95902777
1	-1.58405483	-1.91640735	2.51441360
16	-1.28650033	0.61863256	4.04521370
8	-0.50492376	1.84413147	4.29370213
8	-1.77679110	-0.22683293	5.15628624
6	-2.70771098	1.02069485	3.01080465
6	-3.92999458	0.39051864	3.24777293
6	-5.02850628	0.72475499	2.45314622
6	-4.91931343	1.67833197	1.42932105
6	-3.67716289	2.30317712	1.22391868
6	-2.56937051	1.98168409	2.00614524
1	-4.01385784	-0.33452040	4.05659342
1	-1.60998273	2.47337389	1.84908831
1	-3.57769632	3.05873275	0.44241324
6	-6.10348654	2.01197433	0.55741912
1	-5.98945808	0.24137071	2.63811588
8	0.63667893	1.16876125	-2.76294899
8	0.67135930	-0.99348933	-4.16063166
6	-1.67005396	0.08779576	-3.57277441
6	-2.18344593	-0.56547314	-4.69206095
6	-3.51840115	-0.35598952	-5.05280685
6	-4.34425116	0.50010979	-4.31214380
6	-3.79957008	1.14500952	-3.18632388
6	-2.47325587	0.94340128	-2.81213641
1	-1.53318572	-1.21860349	-5.27314901
1	-3.92222357	-0.86548662	-5.92980385
6	-5.77630186	0.74596131	-4.71798134
1	-4.42598629	1.82035899	-2.59937119
1	-2.05491185	1.45248771	-1.94274330
1	-7.04851341	1.90723693	1.10640931
1	-6.03935623	3.03635097	0.16778390
1	-6.15205145	1.33205616	-0.30797726

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1 -5.89987898 1.76055920 -5.12682438
1 -6.10250378 0.03432444 -5.48693275
1 -6.45669365 0.66023993 -3.85865045
1 0.66504860 -0.07122926 3.16064811
Energy = -8524.621445 Hartree
Number of imaginary frequencies = 0.

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Compound TS2a isomer 37

Atomic N.	X	Y	Z
8	2.94492579	-0.01910491	2.57050276
8	3.16764879	0.20398323	0.22506928
6	3.53798056	0.51006532	-1.10546446
1	4.48601961	0.00821205	-1.37498391
1	3.65652204	1.59550464	-1.28426397
1	2.76738238	0.14493938	-1.80780554
8	4.74822235	-1.08563209	1.85949218
6	4.06981611	0.09028898	1.95850515
6	4.82095718	1.41099882	2.07250762
1	5.28361940	1.39613020	3.07861924
1	4.03641891	2.17743802	2.12411165
6	5.86169243	1.81768155	1.02216339
1	5.41058016	1.76131546	0.02332881
1	6.09346867	2.88070297	1.19213498
6	7.17053747	1.02604294	1.04726732
1	7.68103600	1.19367647	2.01201081
1	7.84380722	1.42102289	0.27047890
6	6.98994017	-0.48029432	0.84844506
1	6.51347876	-0.70073497	-0.12028545
1	7.98056746	-0.96413440	0.82583374
6	6.19426489	-1.15611458	1.96017206
1	6.50039959	-0.76964724	2.94716763
1	6.37704563	-2.23798513	1.95327640
50	1.24717617	0.78373396	1.37424898
7	0.57216543	-1.66304016	0.80751657
6	1.49208593	-2.33290792	-0.13257301
1	1.21226764	-3.39478230	-0.26695335
1	1.48020363	-1.82915652	-1.10508204
1	2.51043987	-2.26397753	0.26379827
7	-0.82766289	0.16104272	-1.17929709
6	-0.83922327	-1.77178729	0.36655703
1	-1.15607536	-2.83333063	0.40897420
1	-1.45761228	-1.21843398	1.08633316
6	-1.14491522	-1.26735556	-1.04354811
1	-2.21061754	-1.47961140	-1.24216807
1	-0.55438972	-1.80665028	-1.79434741
16	-0.65536422	0.79028845	-2.75299406
7	0.05176561	-0.16060151	3.08127856
6	0.71420664	-2.29020905	2.15344334
1	0.45309916	-3.36439657	2.09700632
1	1.77291524	-2.19844747	2.42981601
6	-0.14663237	-1.60065937	3.21266699
1	0.16866387	-1.97005773	4.20251608
1	-1.20841098	-1.89187527	3.09557629
16	-0.98352695	0.82159448	3.88302779
8	-0.40228799	2.18484259	3.79714775
8	-1.38584280	0.23662214	5.18487930
6	-2.49646497	0.86107934	2.86442900

6	-3.53562593	-0.03915156	3.10861993
6	-4.64790297	-0.05496580	2.25912905
6	-4.74646235	0.82487011	1.17223167
6	-3.69948173	1.74238980	0.96370918
6	-2.58055806	1.76373529	1.79690528
1	-3.48029351	-0.69809675	3.97503495
1	-1.78049850	2.49067974	1.64869726
1	-3.77614856	2.46780300	0.14994445
6	-5.94094658	0.79699957	0.25054139
1	-5.46185160	-0.75571847	2.45631933
8	-0.40009674	2.22721267	-2.56039333
8	0.29865012	-0.10579883	-3.43531609
6	-2.25753427	0.61257750	-3.56991816
6	-2.52429199	-0.52473456	-4.33476019
6	-3.77675605	-0.65746307	-4.93781376
6	-4.76293898	0.32989380	-4.79045248
6	-4.46282339	1.46575665	-4.01831913
6	-3.21848369	1.61546063	-3.40842628
1	-1.75111759	-1.28023970	-4.47015429
1	-3.98886347	-1.54239404	-5.54036760
6	-6.10114288	0.19623841	-5.47176743
1	-5.21398449	2.24893785	-3.90039659
1	-2.97808361	2.50868917	-2.83191609
1	-6.78773165	0.27027661	0.70911926
1	-6.26797581	1.81301260	-0.01094627
1	-5.70140123	0.28066587	-0.69263065
1	-6.11477757	0.76326507	-6.41553974
1	-6.32655716	-0.85040098	-5.71271229
1	-6.91159725	0.59154040	-4.84481001
1	-1.44501805	0.77267998	-0.63414717

Energy = -8524.610521 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 38

Atomic N.	X	Y	Z
8	1.93042886	-1.83750296	-0.12367533
8	2.60602212	0.25604197	-1.16512990
6	3.67681336	1.01474798	-1.71718049
1	3.30319285	1.65654349	-2.52853346
1	4.47774458	0.37072253	-2.12493634
1	4.10889196	1.66176295	-0.93352753
8	4.13413191	-1.73179245	-0.33023632
6	2.99039698	-1.17468679	0.16114002
6	3.05833006	-0.32936448	1.41279459
1	3.70437074	0.54530871	1.24592447
1	2.04281688	0.03989754	1.59102130
6	3.55582762	-1.12268245	2.64054704
1	3.10345101	-2.12693810	2.64240575
1	3.17309546	-0.61995119	3.53982019
6	5.08325386	-1.22160745	2.72828221
1	5.49720573	-0.20129497	2.81038761
1	5.36211920	-1.74147689	3.65810752
6	5.75068140	-1.92755818	1.54159987
1	5.46995354	-2.99283767	1.51276612
1	6.84534121	-1.89639664	1.66995037
6	5.43378782	-1.31785369	0.17880234
1	5.50493670	-0.22028460	0.19680995

1	6.13072491	-1.69105625	-0.58239514
50	1.57689774	-1.27119303	-2.42036939
7	-0.63423568	-2.85816646	-1.75876582
6	-0.61730641	-3.66777563	-2.98889518
1	-1.52321661	-4.29939795	-3.07041812
1	-0.55683249	-3.02323651	-3.87530637
1	0.26785824	-4.31802368	-2.98679399
7	-0.36366996	-0.16061623	-2.58011937
6	-1.79608643	-1.94689989	-1.72584426
1	-2.74470639	-2.49243355	-1.90663207
1	-1.83232307	-1.49661779	-0.72818160
6	-1.66804183	-0.81970650	-2.74483204
1	-2.49339771	-0.11238211	-2.55557132
1	-1.80750227	-1.18785429	-3.77477193
16	-0.13967758	1.19948673	-3.47951484
7	-0.54008883	-2.01134038	1.16245449
6	-0.56404501	-3.78234076	-0.59318811
1	-1.12906229	-4.70756054	-0.82254446
1	0.49167892	-4.06793547	-0.47009587
6	-1.12543297	-3.28710151	0.74269480
1	-0.94325984	-4.08684397	1.47976506
1	-2.21782756	-3.16649723	0.66904914
16	-0.92792451	-1.42816794	2.68760300
8	0.15925574	-0.48859236	3.04277635
8	-1.30489898	-2.53184533	3.59876299
6	-2.42406917	-0.46350956	2.37492418
6	-3.60423779	-0.78552151	3.04182863
6	-4.74511051	-0.00946819	2.81343961
6	-4.71790791	1.07863867	1.93054056
6	-3.51074934	1.37860763	1.27144027
6	-2.36551881	0.61703557	1.48784411
1	-3.61935854	-1.63089895	3.72882891
1	-1.43668783	0.85487938	0.96900302
1	-3.46767139	2.21866775	0.57495981
6	-5.94767523	1.91793644	1.68978465
1	-5.67280579	-0.25728315	3.33235216
8	1.33848178	1.23439634	-3.72130632
8	-1.06580091	1.28583312	-4.63326883
6	-0.53993535	2.58840036	-2.38504791
6	-1.54261792	3.48434806	-2.75067878
6	-1.85967839	4.53913116	-1.88792610
6	-1.18794966	4.70625401	-0.66953558
6	-0.17967495	3.78457236	-0.32902145
6	0.14940022	2.72813058	-1.17497337
1	-2.06122994	3.35020447	-3.69938707
1	-2.64353919	5.24448204	-2.17073727
6	-1.52470577	5.84755230	0.25776786
1	0.35156193	3.89618158	0.61859965
1	0.92704511	2.00926995	-0.90478492
1	-6.82187414	1.50722408	2.21019530
1	-5.79572821	2.94872713	2.04350471
1	-6.18246031	1.97845185	0.61722732
1	-0.67483163	6.53947639	0.35684863
1	-2.38531685	6.42134476	-0.10876867
1	-1.75956595	5.48355961	1.26869607
1	0.46054056	-1.87532222	0.92164516

Energy = -8524.628937 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 39

Atomic N.	X	Y	Z
8	2.78067780	-2.20177746	-0.13646296
8	3.43451524	-1.05003715	1.94193518
6	4.32702446	-0.20255820	2.64262581
1	3.76136065	0.51355404	3.26311970
1	4.98878145	0.37359172	1.96645772
1	4.95871449	-0.80344087	3.32153654
8	4.91956997	-1.61758614	-0.22687939
6	3.92660666	-2.29958177	0.40464476
6	4.27424717	-3.50849175	1.25064993
1	4.91053295	-3.21149611	2.09646916
1	3.32311082	-3.85024714	1.67331481
6	4.96175671	-4.62933540	0.44222382
1	4.47473955	-4.73380470	-0.54086393
1	4.79823494	-5.58109808	0.96995312
6	6.47206450	-4.41785431	0.27416515
1	6.93448639	-4.40217352	1.27640831
1	6.90647459	-5.28289080	-0.25110117
6	6.86518669	-3.13454318	-0.46806759
1	6.54605770	-3.18040752	-1.52188146
1	7.96417284	-3.04725933	-0.47850484
6	6.30826092	-1.84822989	0.13692911
1	6.42203426	-1.82480562	1.23108768
1	6.82679844	-0.97439313	-0.27724907
50	1.87748325	-0.19568589	0.64769149
7	-0.24742466	-1.73294246	-0.95581436
6	0.33137172	-2.25026917	-2.20192313
1	-0.31442821	-3.02444983	-2.66777039
1	0.47522342	-1.43574941	-2.92248273
1	1.31520319	-2.68166375	-1.98539281
7	-1.03844047	1.27811956	-1.11819756
6	-1.56797636	-1.13622236	-1.19444776
1	-2.21308088	-1.84447503	-1.76094317
1	-2.05823040	-0.97643954	-0.22327104
6	-1.56920362	0.19330333	-1.95377481
1	-2.60740447	0.38938525	-2.27976155
1	-0.94477582	0.13834108	-2.85447860
16	-0.69987541	2.76695538	-1.85342371
7	0.25955933	-1.21545863	1.79747856
6	-0.33753279	-2.81271362	0.04563833
1	-1.10273802	-3.56796169	-0.23728304
1	0.64065301	-3.31082726	0.05876229
6	-0.64825505	-2.30616522	1.45823097
1	-0.53572816	-3.15721178	2.15189195
1	-1.70458019	-1.98281789	1.52806938
16	0.04070692	-0.39377403	3.18620396
8	1.15212357	0.61741060	3.14619136
8	-0.14337061	-1.25602007	4.37463665
6	-1.50058603	0.55219305	3.01098347
6	-2.70201039	0.01971184	3.48327160
6	-3.88774252	0.73798072	3.30295539
6	-3.88937116	1.99053788	2.67204595
6	-2.66378570	2.50847030	2.21649313
6	-1.47296536	1.79909170	2.37725949
1	-2.69815731	-0.93568748	4.00744867

1	-0.52599204	2.21620989	2.03253198
1	-2.63487840	3.49164486	1.74223661
6	-5.16395664	2.78383803	2.52458549
1	-4.82718992	0.32113686	3.67138267
8	-0.31044507	3.65569115	-0.74254704
8	0.18902653	2.47009206	-2.99088788
6	-2.25333166	3.39585876	-2.54011869
6	-2.61129427	3.07132244	-3.85039401
6	-3.82006073	3.54713607	-4.36299324
6	-4.67307281	4.34803867	-3.58871388
6	-4.28368759	4.66389751	-2.27561951
6	-3.08202529	4.19472980	-1.74701130
1	-1.93732810	2.47357273	-4.46312857
1	-4.10119486	3.29823112	-5.38787651
6	-5.95905972	4.88958740	-4.16026115
1	-4.92829847	5.29624367	-1.66198468
1	-2.76717782	4.46331596	-0.73903763
1	-6.04544926	2.12955618	2.51094532
1	-5.28690004	3.48385882	3.36582232
1	-5.16046286	3.38231277	1.60343874
1	-5.82470131	5.92638493	-4.50594234
1	-6.29776096	4.29664612	-5.01941395
1	-6.75939798	4.90030384	-3.40804744
1	-1.56543148	1.44029069	-0.25376335

Energy = -8524.625626 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 40

Atomic N.	X	Y	Z
8	1.94082963	-1.57096732	-0.28437206
8	2.57191229	0.57420707	-1.23922181
6	3.62489843	1.38695586	-1.74578214
1	4.00962591	2.03580689	-0.93917698
1	3.24646735	2.02832580	-2.55570507
1	4.46197271	0.78525406	-2.14559865
8	4.14388895	-1.38031697	-0.43569854
6	2.96921563	-0.87895703	0.04553259
6	2.97861624	-0.08172292	1.33184969
1	3.57410693	0.83481014	1.20621419
1	1.94116950	0.22143769	1.50962758
6	3.50809193	-0.89186966	2.53518534
1	3.11098862	-1.91805351	2.49657369
1	3.08807850	-0.44617170	3.44750237
6	5.03726053	-0.91158080	2.64009619
1	5.39655685	0.12625267	2.75504398
1	5.33122492	-1.44181204	3.55934644
6	5.75377274	-1.54920268	1.44389737
1	5.52856302	-2.62620282	1.38281476
1	6.84407425	-1.46481597	1.58503425
6	5.41717768	-0.91720557	0.09659953
1	5.43266821	0.18145350	0.14817499
1	6.13827372	-1.23142517	-0.66885996
50	1.62217164	-0.94765842	-2.56808925
7	-0.55730468	-2.57306528	-2.01551104
6	-0.60932612	-3.22969007	-3.33278775
1	-1.52592063	-3.84055328	-3.44503284
1	-0.58171529	-2.48362398	-4.13747501

1	0.26641613	-3.88184190	-3.45032072
7	-0.33252573	0.15368927	-2.68329501
6	-1.70778501	-1.67001629	-1.81146622
1	-2.67231202	-2.19778299	-1.95717013
1	-1.65885675	-1.30704439	-0.77824301
6	-1.66264784	-0.46619576	-2.74903774
1	-2.44586110	0.23611066	-2.41291976
1	-1.92165899	-0.75134790	-3.78177500
16	-0.10657544	1.46095920	-3.65168834
7	-0.46959701	-2.12294507	1.03808582
6	-0.41322741	-3.62611890	-0.96970236
1	-0.92091554	-4.54882431	-1.31119442
1	0.65938973	-3.85804844	-0.88422239
6	-0.99407196	-3.34698129	0.41838434
1	-0.77128637	-4.23685789	1.03075910
1	-2.09113979	-3.26551485	0.35569724
16	-0.70742631	-1.94575953	2.69603443
8	0.22266810	-0.87348133	3.11263561
8	-0.70762944	-3.25372100	3.39082050
6	-2.39630842	-1.30827534	2.77578330
6	-3.37428761	-2.03712606	3.44960666
6	-4.66933489	-1.51721787	3.53529263
6	-4.99465704	-0.28220606	2.95809579
6	-3.98512912	0.42987746	2.28381705
6	-2.68989158	-0.07227038	2.19034648
1	-3.11441994	-2.99438357	3.90007973
1	-1.91060555	0.48463023	1.67009330
1	-4.22032595	1.39269936	1.82620263
6	-6.38847971	0.28396577	3.06270909
1	-5.43940592	-2.08390903	4.06165075
8	1.37601888	1.46721911	-3.88923120
8	-1.02011085	1.49251378	-4.81846189
6	-0.49083063	2.92110515	-2.64924026
6	-1.39297342	3.86779070	-3.13210464
6	-1.67532218	4.99509764	-2.35500026
6	-1.06742263	5.18528748	-1.10622692
6	-0.16771629	4.20764446	-0.64335728
6	0.12625484	3.07748961	-1.40372109
1	-1.86299682	3.71389580	-4.10283852
1	-2.38154459	5.73930454	-2.72822738
6	-1.35082233	6.41774368	-0.28370455
1	0.30842808	4.33531952	0.33108503
1	0.82190424	2.31688523	-1.04116833
1	-7.08591652	-0.44435361	3.49497223
1	-6.40031338	1.18149745	3.69947863
1	-6.77092743	0.58464098	2.07682276
1	-0.53366369	7.14937735	-0.38194504
1	-2.27680779	6.91134644	-0.60572833
1	-1.43976295	6.17570496	0.78438514
1	0.50507557	-1.87918019	0.76897091

Energy = -8524.628917 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 41

Atomic N.	X	Y	Z
8	3.18922901	-1.58437288	-0.44051132
8	3.95646143	-0.25384554	1.42722642

6	4.39047480	0.05019528	2.74062014
1	4.05756569	-0.70504946	3.47557735
1	3.97418833	1.01705158	3.06452298
1	5.49257565	0.12074313	2.76840544
8	5.36599398	-1.80246723	-0.18116181
6	4.13288546	-1.90269923	0.36851355
6	3.89878035	-2.91640115	1.47379732
1	4.49770546	-2.66987801	2.36231065
1	2.84679770	-2.80785871	1.76418555
6	4.21390676	-4.36074114	1.02923918
1	3.86334276	-4.52143335	-0.00329586
1	3.63431931	-5.04839659	1.66357541
6	5.70093441	-4.71993876	1.15320146
1	5.99419832	-4.61767006	2.21245861
1	5.84445047	-5.78121185	0.89609629
6	6.64445400	-3.86705494	0.29592830
1	6.48722029	-4.07224369	-0.77537847
1	7.68711901	-4.14827633	0.51809949
6	6.51680660	-2.36029696	0.50611746
1	6.48885822	-2.09096384	1.57279480
1	7.36576891	-1.83754945	0.04777770
50	2.09487915	0.23800398	0.36589080
7	0.14450306	-1.39165378	-1.32348192
6	0.79952091	-1.73095763	-2.59396911
1	0.26615506	-2.54462886	-3.12905979
1	0.83872527	-0.85160220	-3.24866176
1	1.83064973	-2.04437685	-2.39341021
7	-1.04675043	1.50217628	-1.21179366
6	-1.23574758	-0.94065273	-1.54927409
1	-1.77131784	-1.66350472	-2.20407438
1	-1.76544940	-0.94295460	-0.58541667
6	-1.38827729	0.44817325	-2.17569804
1	-2.42910433	0.53775060	-2.53797436
1	-0.72549957	0.56864291	-3.04209852
16	-0.91848254	3.09457803	-1.77969563
7	0.69062793	-1.11859751	1.50304997
6	0.16743056	-2.55641460	-0.41800573
1	-0.53047884	-3.35047245	-0.76157999
1	1.18574286	-2.96353674	-0.45740131
6	-0.16756256	-2.20687819	1.03498459
1	-0.02460300	-3.12064481	1.63878298
1	-1.23758924	-1.93947875	1.12719572
16	0.36005399	-0.44184101	2.95052052
8	1.35886264	0.67386115	3.03512216
8	0.25575683	-1.42956853	4.05003357
6	-1.27114224	0.34898144	2.83131385
6	-2.41220975	-0.33431295	3.25586152
6	-3.66367292	0.27626753	3.12768221
6	-3.79085565	1.56739438	2.59559393
6	-2.62397265	2.23665977	2.18378401
6	-1.36925185	1.63677335	2.29358649
1	-2.31316447	-1.32254100	3.70420313
1	-0.47131118	2.17109561	1.98179543
1	-2.68941116	3.25082541	1.78426862
6	-5.13731384	2.24145269	2.50430894
1	-4.55601454	-0.25767916	3.46020913
8	-0.72489798	3.91143274	-0.56659758
8	0.05479368	3.06079388	-2.88545799

6	-2.52186775	3.54062796	-2.49441838
6	-2.74813485	3.34303212	-3.85821962
6	-3.99375987	3.67388773	-4.39587879
6	-5.01454306	4.20483065	-3.59275818
6	-4.75635910	4.39762354	-2.22469258
6	-3.51934886	4.07055378	-1.67106986
1	-1.94771540	2.95617342	-4.48801517
1	-4.17273378	3.52383327	-5.46210670
6	-6.34426117	4.59516478	-4.18687725
1	-5.53434372	4.82032251	-1.58601522
1	-3.31200886	4.24623680	-0.61584032
1	-5.95550966	1.51033103	2.53266859
1	-5.28373861	2.93563533	3.34642696
1	-5.23009205	2.83096743	1.58161533
1	-6.36072111	5.66899872	-4.43025780
1	-6.54692745	4.04462528	-5.11449623
1	-7.16785336	4.40898609	-3.48461890
1	-1.61773980	1.49596214	-0.36008313

Energy = -8524.624450 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 42

Atomic N.	X	Y	Z
8	5.19057322	1.58815134	0.27854177
8	3.65887523	2.34325933	1.87251198
6	2.70809841	3.35919046	2.17835617
1	1.87852752	2.90701652	2.74081826
1	2.30537701	3.83352256	1.27030241
1	3.17537141	4.12347317	2.82214761
8	4.57098198	3.72199678	0.00067652
6	5.03276682	2.74804878	0.86065066
6	6.08408594	3.14455223	1.89260733
1	5.69310570	3.91451740	2.57598972
1	6.25492001	2.23988318	2.48829651
6	7.39904356	3.62524271	1.25024390
1	7.62976503	2.98919964	0.38114306
1	8.21426678	3.47027898	1.97335744
6	7.37935734	5.10571623	0.84849358
1	7.22314692	5.71333885	1.75749683
1	8.36888218	5.38995552	0.45692223
6	6.30736637	5.47936201	-0.18210135
1	6.51402235	4.99792910	-1.15125287
1	6.34031677	6.56762505	-0.35760066
6	4.87937784	5.11858559	0.22361918
1	4.67303467	5.40940762	1.26677608
1	4.15840769	5.64169455	-0.41820538
50	3.36023617	0.43832290	0.67315918
7	-0.55789965	-1.07623601	2.16023374
6	0.05601747	-2.02433801	3.08879828
1	-0.32299820	-1.92213023	4.13026285
1	-0.12358710	-3.05382347	2.75432491
1	1.14229000	-1.86628652	3.09767413
7	-1.98507977	-3.02337503	0.40095514
6	-2.01219702	-1.21800268	2.11155176
1	-2.47460794	-0.99413103	3.10308599
1	-2.40428352	-0.46365884	1.41038716
6	-2.53699875	-2.59290218	1.69556332

1	-3.64039230	-2.51933813	1.67630744
1	-2.27500916	-3.35900998	2.43623757
16	-2.62415147	-4.44117785	-0.27100697
7	1.03800428	1.06500685	0.51067072
6	-0.20499077	0.31155372	2.48991704
1	-0.88968688	0.72631913	3.26317692
1	0.80186898	0.31150985	2.93390751
6	-0.19050638	1.25859106	1.28320014
1	-0.27096948	2.29713297	1.65143335
1	-1.08562326	1.07752359	0.66128886
16	1.11010051	1.58665502	-1.00297666
8	2.59463358	1.29184520	-1.31119311
8	0.64245558	2.96046424	-1.29799354
6	0.16837549	0.48003623	-2.08238006
6	-0.58544821	1.01425934	-3.12879848
6	-1.27159691	0.14664333	-3.98082972
6	-1.21234465	-1.24464047	-3.80200577
6	-0.46001458	-1.75303268	-2.72823739
6	0.22850972	-0.89878577	-1.86631715
1	-0.62423468	2.09442210	-3.26421571
1	0.79468268	-1.29819930	-1.02364147
1	-0.42698562	-2.83025074	-2.55728984
6	-1.91641295	-2.17964029	-4.75330257
1	-1.85992932	0.55938959	-4.80279350
8	-1.98153150	-4.57089615	-1.59385419
8	-2.50568366	-5.47762203	0.77009380
6	-4.38963795	-4.15167522	-0.54469430
6	-5.31844425	-4.63163614	0.37914759
6	-6.67825127	-4.39000702	0.16405071
6	-7.12060595	-3.67614198	-0.95839012
6	-6.16108894	-3.20785379	-1.87462795
6	-4.80219030	-3.44023585	-1.67667115
1	-4.97505188	-5.20398664	1.24017227
1	-7.40841341	-4.76977634	0.88080376
6	-8.58801365	-3.41884923	-1.19114673
1	-6.48717880	-2.66054201	-2.76116157
1	-4.06504488	-3.09233928	-2.40047359
1	-1.29797506	-2.35737324	-5.64706612
1	-2.10450649	-3.15567517	-4.28748465
1	-2.87012219	-1.75827456	-5.10019159
1	-8.91627121	-3.84512043	-2.15048289
1	-9.20331001	-3.85718608	-0.39574921
1	-8.79876137	-2.33989716	-1.23016047
1	-1.94881344	-2.28757572	-0.31105843

Energy = -8524.614412 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 43

Atomic N.	X	Y	Z
8	3.02437878	0.81207454	2.31710863
8	2.59213734	1.93065655	0.30625492
6	2.59052181	1.89626372	-1.12165272
1	1.69837010	2.43104219	-1.47500741
1	2.55587244	0.86125904	-1.48977029
1	3.48617721	2.41619349	-1.50109541
8	3.90615487	-0.19144034	0.53102303
6	3.74535108	0.97134632	1.23254859

6	4.93317842	1.92412472	1.32880354
1	5.22129536	2.29137897	0.33154410
1	4.56841469	2.78728700	1.89818752
6	6.14967585	1.28784394	2.02831125
1	5.80227900	0.68411845	2.88162231
1	6.76708269	2.09556317	2.45036316
6	7.02477980	0.44572327	1.09032094
1	7.41172552	1.10185134	0.29053986
1	7.90662575	0.08405335	1.64266813
6	6.31355572	-0.74963313	0.44495308
1	6.03976393	-1.49778199	1.20574641
1	7.00721073	-1.24844861	-0.25238293
6	5.04878616	-0.39411846	-0.33380112
1	5.20897388	0.47782603	-0.98866135
1	4.73945665	-1.23741698	-0.96440589
50	1.03082669	1.59073210	1.85313857
7	-2.01200533	0.70489156	3.15128827
6	-1.78054523	1.27312613	4.47529888
1	-2.52816200	0.93160903	5.22375822
1	-0.78235513	0.99214017	4.83852959
1	-1.81604862	2.36996698	4.41987467
7	0.03937606	-0.46491736	1.44306219
6	-1.76972890	-0.74479163	3.12118649
1	-2.03137088	-1.22293603	4.08809471
1	-2.40676999	-1.20850945	2.35589170
6	-0.30678925	-1.04577839	2.76682496
1	-0.13108467	-2.13204694	2.78537750
1	0.36056700	-0.63674945	3.54866266
16	0.57943630	-1.57544971	0.31909242
7	-2.33001709	0.90291262	0.26840490
6	-3.29233789	1.14745378	2.60124326
1	-4.16471910	0.76801372	3.18275499
1	-3.30904007	2.24515152	2.67429519
6	-3.50781775	0.75086164	1.12918460
1	-4.33409023	1.35041523	0.72499359
1	-3.81271124	-0.30381832	1.04786611
16	-1.94879079	2.38857031	-0.38753712
8	-0.47442916	2.56456494	-0.19648053
8	-2.89922214	3.41922736	0.07938315
6	-2.18603301	2.18038774	-2.16297674
6	-3.20104694	2.88880897	-2.80315065
6	-3.37151504	2.72710586	-4.18096638
6	-2.54203463	1.87084627	-4.91847754
6	-1.52791667	1.17002940	-4.24004030
6	-1.33824670	1.31874144	-2.86806893
1	-3.83814621	3.55902839	-2.22737360
1	-0.54882115	0.76965183	-2.35048413
1	-0.87455165	0.49570057	-4.79697180
6	-2.71293879	1.71668279	-6.40887356
1	-4.16340733	3.27957773	-4.68986082
8	0.81170511	-0.79112679	-0.92235798
8	1.64004898	-2.46720076	0.84225219
6	-0.84242201	-2.67330766	0.00400024
6	-0.86504996	-3.93924737	0.59301060
6	-1.94411719	-4.79214764	0.34733123
6	-2.99916434	-4.40441990	-0.49135411
6	-2.94596815	-3.13004756	-1.08189058
6	-1.87795019	-2.26574183	-0.84211755

1	-0.02918832	-4.25220680	1.21798801
1	-1.96103382	-5.78102303	0.80982989
6	-4.14535332	-5.34097672	-0.78259277
1	-3.75256610	-2.81112075	-1.74542987
1	-1.84638381	-1.28229988	-1.30848837
1	-3.67899966	2.11353397	-6.74572182
1	-1.92216659	2.25816274	-6.95073366
1	-2.64621711	0.66250241	-6.71171427
1	-4.00760317	-5.83732653	-1.75589335
1	-4.22499084	-6.12655926	-0.02009870
1	-5.10223722	-4.80286217	-0.82712561
1	-1.46962273	0.44244745	0.65094346

Energy = -8524.615171 Hartree
Number of imaginary frequencies = 0.

Compound TS2a isomer 44

Atomic N.	X	Y	Z
8	5.21673489	1.63542020	0.31963563
8	3.70738220	2.24883080	1.99433768
6	2.74070930	3.21601200	2.39259958
1	3.20750308	3.95188332	3.06907654
1	1.94200385	2.70649934	2.95104527
1	2.29628730	3.73467660	1.52918279
8	4.52741337	3.76135254	0.18239526
6	5.04267168	2.75484490	0.97114825
6	6.10965252	3.12400723	1.99680448
1	5.71402884	3.83871865	2.73530912
1	6.32594633	2.19178224	2.53213978
6	7.38984585	3.68583918	1.34983253
1	7.61600828	3.11062765	0.43817204
1	8.22990227	3.51566577	2.04038930
6	7.31171656	5.18606567	1.03844643
1	7.16137981	5.73319244	1.98604453
1	8.28048420	5.52595043	0.63939786
6	6.20032120	5.58405352	0.06001775
1	6.39528656	5.16804790	-0.94130510
1	6.19367790	6.68129110	-0.05055970
6	4.79647589	5.15227318	0.48007652
1	4.60984516	5.37389565	1.54371095
1	4.04135036	5.68727207	-0.11059214
50	3.42059422	0.42058864	0.67747521
7	-0.52257353	-1.23074675	2.08597779
6	0.06103838	-2.25269198	2.95403767
1	-0.32586637	-2.21113324	3.99685073
1	-0.13770612	-3.25332522	2.55015540
1	1.15029287	-2.11965704	2.98295665
7	-1.98482239	-3.04578781	0.21551806
6	-1.97960544	-1.33445668	2.02090502
1	-2.44302058	-1.15487766	3.02101350
1	-2.34961534	-0.53376323	1.36060929
6	-2.53426862	-2.67187476	1.52810454
1	-3.63550091	-2.57127881	1.50773883
1	-2.29443002	-3.48257041	2.22778392
16	-2.62546134	-4.43068743	-0.51956195
7	1.08779085	1.01731515	0.58223939
6	-0.14003536	0.12152434	2.51471543
1	-0.80563056	0.48619601	3.32935977

1	0.87350482	0.06976759	2.94000864
6	-0.12787162	1.16049409	1.38587713
1	-0.19142792	2.16714287	1.83646536
1	-1.03262210	1.04131770	0.76343435
16	1.12954926	1.62725401	-0.89972031
8	2.61112499	1.36687028	-1.24841714
8	0.64239621	3.01038718	-1.10557187
6	0.18137792	0.57522315	-2.02720189
6	-0.59546536	1.16115439	-3.02799296
6	-1.28620243	0.33708474	-3.91888976
6	-1.20832205	-1.06140840	-3.82398558
6	-0.43242359	-1.62318766	-2.79424214
6	0.26034424	-0.81322145	-1.89403892
1	-0.64844686	2.24688315	-3.09863639
1	0.84375221	-1.25453639	-1.08483803
1	-0.38531289	-2.70815182	-2.68826818
6	-1.91727066	-1.94799650	-4.81699324
1	-1.89294493	0.79046500	-4.70527792
8	-1.99788582	-4.48865461	-1.85481799
8	-2.48907709	-5.51922750	0.46475258
6	-4.39612865	-4.14005995	-0.75679815
6	-5.31039143	-4.67671204	0.15085544
6	-6.67390347	-4.43454313	-0.03433457
6	-7.13542938	-3.66570592	-1.11253679
6	-6.19072962	-3.13763404	-2.01062322
6	-4.82733297	-3.36988926	-1.84178078
1	-4.95181513	-5.28950644	0.97714680
1	-7.39217186	-4.85580730	0.67126006
6	-8.60962200	-3.43180966	-1.32557285
1	-6.53135347	-2.54153085	-2.85932207
1	-4.10163784	-2.97350621	-2.55207801
1	-1.29687083	-2.09355235	-5.71521807
1	-2.11532998	-2.94140458	-4.39373589
1	-2.86580682	-1.50338733	-5.14837360
1	-8.99538803	-4.08229017	-2.12574911
1	-9.18572330	-3.64656854	-0.41671294
1	-8.81100273	-2.39478827	-1.62738204
1	-1.94394493	-2.27993870	-0.46387458

Energy = -8524.614448 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 45

Atomic N.	X	Y	Z
8	2.06374454	0.18059330	2.31980395
8	3.27532482	1.20167899	0.38597551
6	4.28766108	0.95099467	-0.55470091
1	3.99958158	1.29003739	-1.57434630
1	4.54278994	-0.12507898	-0.64670384
1	5.21608639	1.50082445	-0.30176008
8	3.97377038	-0.88949382	1.95171380
6	3.32898521	0.25790325	2.27920842
6	4.05275106	1.32292008	3.07298565
1	4.91198397	1.70294297	2.50182056
1	3.34098697	2.14898729	3.17850041
6	4.51205873	0.82455242	4.46138954
1	3.71718049	0.21151128	4.91455603
1	4.63420963	1.70285153	5.11296415

6	5.83675289	0.05233078	4.42847776
1	6.62545824	0.72501397	4.04837656
1	6.12796640	-0.21241149	5.45682049
6	5.81961870	-1.21908152	3.57151556
1	5.14228344	-1.97281325	4.00370741
1	6.82692909	-1.66689897	3.57064319
6	5.41548777	-0.99960679	2.11676240
1	5.91416931	-0.12233993	1.67807269
1	5.67063904	-1.87639022	1.50882888
50	1.31954503	-0.18576594	0.21786650
7	0.42810851	2.22110939	0.03982749
6	0.80760878	2.89712691	1.30290926
1	0.32262573	3.88815951	1.36920571
1	0.51765496	2.28586745	2.16328120
1	1.89702940	3.01336861	1.31384563
7	-0.80166340	-0.03731044	1.03204966
6	-1.04441476	2.09005356	-0.06105362
1	-1.52736282	3.08539724	-0.01460886
1	-1.27434337	1.63357091	-1.03219855
6	-1.59945655	1.18284249	1.03797317
1	-2.65999055	0.98600817	0.79322535
1	-1.58695042	1.68623137	2.01977396
16	-1.19598985	-1.22592568	2.08891678
7	0.93631369	1.21763337	-2.78860259
6	1.01408482	3.01527166	-1.07239580
1	0.73306209	4.07944345	-0.94576114
1	2.10499382	2.94557524	-0.94582164
6	0.61624801	2.62436247	-2.49408913
1	1.12044978	3.32121181	-3.18405604
1	-0.46379393	2.75838494	-2.64758468
16	0.41626102	0.65733910	-4.33363819
8	1.18988121	-0.57911295	-4.55171013
8	0.43832380	1.75282538	-5.32864141
6	-1.30894220	0.26561505	-3.99392200
6	-2.30581117	0.90466011	-4.73049259
6	-3.64156485	0.57825774	-4.48206711
6	-3.98680377	-0.36970857	-3.50792813
6	-2.95726490	-0.99438083	-2.77969122
6	-1.62009561	-0.68807280	-3.01937246
1	-2.02977252	1.64324009	-5.48229980
1	-0.82583904	-1.17399514	-2.45189357
1	-3.20545983	-1.72509682	-2.00783539
6	-5.42788029	-0.72886783	-3.24788880
1	-4.42800045	1.07376266	-5.05391455
8	-0.05209457	-2.17770934	2.01839399
8	-1.65987241	-0.69630939	3.39479733
6	-2.62452269	-2.08865571	1.36731958
6	-3.92068505	-1.70076299	1.71045375
6	-5.00931311	-2.36048031	1.13159549
6	-4.82197714	-3.41601086	0.22765973
6	-3.50545716	-3.79613304	-0.08936029
6	-2.41005373	-3.13839555	0.46912828
1	-4.06911373	-0.90798247	2.44331026
1	-6.02353144	-2.05763507	1.39984298
6	-5.99794292	-4.15040350	-0.36788723
1	-3.33733416	-4.62303591	-0.78282797
1	-1.38965297	-3.44110680	0.23354103
1	-6.11264086	-0.02241040	-3.73371363

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1 -5.65369606 -1.73476040 -3.63388109
1 -5.64614439 -0.74175966 -2.17085648
1 -6.12174129 -5.13963318 0.09911667
1 -6.93345308 -3.59518051 -0.22160044
1 -5.86143208 -4.31969786 -1.44552839
1 1.94344831 1.01995361 -2.75552249
Energy = -8524.618627 Hartree
Number of imaginary frequencies = 0.

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Compound TS2a isomer 46

Atomic N.	X	Y	Z
8	2.77308464	1.07930577	1.58477783
8	3.56399965	-0.27019092	-0.29868072
6	4.20959759	-1.44024849	-0.77334630
1	5.20879698	-1.17927110	-1.16387701
1	3.63110805	-1.87723768	-1.60446393
1	4.32620430	-2.20892286	0.01432950
8	4.37626076	-0.30212545	2.25023317
6	3.98119068	0.69882417	1.42343581
6	5.01171303	1.65939808	0.86491489
1	5.73279333	1.12108243	0.23346244
1	4.45441484	2.33501101	0.20680413
6	5.75819969	2.44083500	1.96711075
1	5.04953718	2.74640822	2.75374937
1	6.14596987	3.37009025	1.52335739
6	6.93257713	1.66192901	2.57374215
1	7.65948629	1.44743490	1.77116632
1	7.45781136	2.30051351	3.30103493
6	6.54879522	0.34240976	3.25487375
1	5.94073343	0.52994323	4.15450954
1	7.46517134	-0.16508792	3.59838820
6	5.78724051	-0.63894778	2.36809254
1	6.23943424	-0.72871995	1.36896694
1	5.77057743	-1.63609195	2.82530975
50	1.47168314	-0.30065185	0.31787726
7	-0.19675735	1.78382230	1.41172075
6	-0.01872729	2.10628080	2.83538699
1	-0.59913182	3.00227237	3.13378978
1	-0.32479373	1.25582671	3.45562458
1	1.04588866	2.29364252	3.01745844
7	-1.62398815	-0.66527110	2.27145815
6	-1.60235953	1.51439941	1.05468988
1	-2.18438864	2.46016049	1.02032423
1	-1.60992324	1.09312117	0.03789172
6	-2.36397624	0.57446378	1.99223924
1	-3.33595228	0.37409854	1.50728929
1	-2.58053446	1.06479990	2.95091176
16	-2.48747683	-2.01698256	2.79550982
7	0.89788967	1.25252116	-1.13719058
6	0.34645975	2.88310075	0.58583474
1	-0.21919389	3.82248664	0.76058382
1	1.38210511	3.03902626	0.91599482
6	0.33766568	2.58146787	-0.91486365
1	0.93092662	3.36379075	-1.41883647
1	-0.69204003	2.65156174	-1.31240106
16	0.90767598	0.61839491	-2.64319134
8	1.38150477	-0.78618693	-2.39879632

8	1.59124458	1.46461082	-3.64592028
6	-0.82350117	0.50662690	-3.17952752
6	-1.30728042	1.38932538	-4.14557028
6	-2.64942861	1.31425905	-4.52817583
6	-3.51435494	0.36798581	-3.95988202
6	-3.00063014	-0.50929368	-2.98837447
6	-1.66448069	-0.44573241	-2.59622693
1	-0.62865460	2.11331677	-4.59546041
1	-1.26962352	-1.14019346	-1.85316956
1	-3.65598845	-1.25252759	-2.52969980
6	-4.95439482	0.27031156	-4.39845610
1	-3.02964497	2.00419044	-5.28396511
8	-1.47388113	-3.05138016	3.06268024
8	-3.42429376	-1.52802312	3.82497835
6	-3.47930169	-2.58276320	1.38989866
6	-4.82472563	-2.22476959	1.29840636
6	-5.57351017	-2.66880941	0.20413482
6	-4.99789810	-3.46772170	-0.79374039
6	-3.63979888	-3.81590366	-0.67237121
6	-2.87816739	-3.38010049	0.40942132
1	-5.27871561	-1.62920845	2.08977485
1	-6.62817812	-2.39692974	0.13242640
6	-5.81151581	-3.96229434	-1.96354878
1	-3.17513704	-4.44425869	-1.43475652
1	-1.83254004	-3.67121816	0.51231933
1	-5.30652332	1.21429241	-4.83412266
1	-5.07701826	-0.51204842	-5.16382694
1	-5.61178398	0.00866329	-3.55820465
1	-5.90681744	-5.05818748	-1.94202602
1	-6.82250834	-3.53603315	-1.95805848
1	-5.33373594	-3.70271754	-2.91970325
1	-0.90446609	-0.92595518	1.58355105

Energy = -8524.627645 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 47

Atomic N.	X	Y	Z
8	2.05114579	0.20079808	2.32429647
8	3.22979021	1.30641699	0.41635552
6	4.25249195	1.11172283	-0.52638924
1	5.16067553	1.68770337	-0.25857714
1	3.95538163	1.46299767	-1.53931367
1	4.54518747	0.04745425	-0.64115345
8	4.00118303	-0.78903949	1.94178057
6	3.31268311	0.32643646	2.28993201
6	3.99346161	1.40159357	3.10780573
1	4.83898926	1.82570434	2.54732752
1	3.25053144	2.19767118	3.22796464
6	4.46800900	0.89259344	4.48721647
1	3.69598818	0.24051011	4.92514753
1	4.55490828	1.76132202	5.15702724
6	5.82127953	0.17228179	4.44281864
1	6.58460665	0.88212204	4.07880926
1	6.12000275	-0.10200660	5.46649313
6	5.85455751	-1.08118463	3.56027555
1	5.20543909	-1.86874354	3.97509265
1	6.87819099	-1.49025989	3.55340052

6	5.44564819	-0.84772140	2.10903239
1	5.91163445	0.05657023	1.68969846
1	5.73535395	-1.70166349	1.48430216
50	1.32642555	-0.14825550	0.21248733
7	0.34869897	2.22832131	0.08259050
6	0.69867307	2.89002633	1.36165118
1	0.17812026	3.86136246	1.44696915
1	0.42764613	2.25031590	2.20737338
1	1.78311777	3.04518938	1.38001156
7	-0.80224752	-0.09428638	1.01962292
6	-1.11766946	2.04648757	-0.02792673
1	-1.63655245	3.02246189	0.03796869
1	-1.32724905	1.60334432	-1.00980115
6	-1.64358377	1.09595060	1.04875171
1	-2.69547963	0.86647201	0.79524308
1	-1.65268886	1.57783151	2.04132509
16	-1.15390968	-1.31737554	2.05197930
7	0.90354955	1.30327129	-2.76330447
6	0.91077143	3.06642056	-1.00930250
1	0.59101272	4.11694813	-0.86204076
1	2.00284934	3.03324842	-0.87810653
6	0.53407741	2.69172978	-2.44116831
1	1.01702702	3.41988659	-3.11376214
1	-0.54925007	2.79150248	-2.59762692
16	0.40216750	0.75585055	-4.31911230
8	1.21371067	-0.45174539	-4.55962753
8	0.39071357	1.86973989	-5.29358816
6	-1.31008875	0.30490419	-3.98737097
6	-2.32794189	0.93782985	-4.70044422
6	-3.65300274	0.56929547	-4.45446062
6	-3.96733332	-0.41481033	-3.50581169
6	-2.91750646	-1.03227949	-2.80115533
6	-1.59019232	-0.68377417	-3.03886247
1	-2.07626677	1.70490062	-5.43189144
1	-0.78014565	-1.16350877	-2.48875690
1	-3.14160728	-1.79007947	-2.04828310
6	-5.39704180	-0.81997639	-3.25052142
1	-4.45566750	1.06044066	-5.00722647
8	0.02379376	-2.22521162	1.96319187
8	-1.63677311	-0.83140105	3.36793423
6	-2.55003309	-2.21669054	1.31181252
6	-3.85881853	-1.89136016	1.67060626
6	-4.92273951	-2.58319259	1.08270299
6	-4.69733238	-3.60727954	0.15199801
6	-3.36772776	-3.92716765	-0.17793933
6	-2.29748130	-3.23696637	0.38953593
1	-4.03507566	-1.12585497	2.42607498
1	-5.94677687	-2.33291149	1.36716628
6	-5.84566402	-4.35474682	-0.48006952
1	-3.16919494	-4.73449802	-0.88629216
1	-1.26674843	-3.49547434	0.14638174
1	-6.10257578	-0.08303691	-3.65466404
1	-5.61690855	-1.78844106	-3.72598171
1	-5.59085846	-0.93685675	-2.17535067
1	-5.70701170	-5.44229031	-0.39875802
1	-6.80121899	-4.09539557	-0.00678818
1	-5.92810392	-4.12238693	-1.55327368
1	1.91697383	1.14024305	-2.73345184

Energy = -8524.618625 Hartree
 Number of imaginary frequencies = 0.

Compound TS2a isomer 48

Atomic N.	X	Y	Z
8	2.27108455	-0.88679379	1.62500060
8	2.96932983	0.28638190	-0.22305620
6	3.85390806	0.99186444	-1.09417379
1	3.27388597	1.35620308	-1.95180345
1	4.64699459	0.31577358	-1.45139861
1	4.30588007	1.86288083	-0.59198272
8	4.34332085	-1.39734817	0.95510352
6	3.42515230	-0.39586675	1.27917206
6	3.95212626	0.79319692	2.08549619
1	4.72042608	1.35313606	1.53054953
1	3.09045219	1.46337628	2.20606852
6	4.50320625	0.38379067	3.46406841
1	3.86142755	-0.40141991	3.89347816
1	4.42508173	1.24905252	4.13950872
6	5.96791363	-0.07104402	3.42531443
1	6.58506632	0.76773286	3.05773282
1	6.31267595	-0.27784568	4.45077324
6	6.23866367	-1.29996586	2.54948831
1	5.76218176	-2.19543862	2.98020196
1	7.32353592	-1.49816060	2.53196597
6	5.76424646	-1.16966510	1.10249996
1	6.05764437	-0.19953433	0.66937023
1	6.21863604	-1.95742619	0.48589590
50	0.75903726	0.27112001	0.21094429
7	0.59131891	-2.21609688	-0.47813857
6	1.85196602	-2.57880855	-1.17013216
1	1.76641250	-3.58285403	-1.62485301
1	2.07585287	-1.84436691	-1.95001543
1	2.67153668	-2.56873846	-0.44399238
7	0.11141063	0.00852209	-1.96594310
6	-0.54509562	-2.24033427	-1.43053496
1	-0.68043888	-3.25858998	-1.84320712
1	-1.45492268	-1.96917582	-0.87651289
6	-0.33766299	-1.23813927	-2.57010365
1	-1.30328655	-1.12375295	-3.09593177
1	0.38460842	-1.62709701	-3.30804229
16	0.33227491	1.31998336	-2.90583181
7	-0.49180892	-1.62581873	2.31981134
6	0.40228057	-3.18347001	0.63424402
1	0.23876795	-4.19437599	0.21317282
1	1.34988344	-3.19886112	1.18954837
6	-0.73134410	-2.89415550	1.61355340
1	-0.79243946	-3.74669361	2.30970287
1	-1.70338547	-2.82848477	1.10245395
16	-1.56230545	-1.25944686	3.60671425
8	-0.82624173	-0.29649079	4.44668388
8	-2.12895703	-2.50505280	4.16911554
6	-2.89617515	-0.40130961	2.74952126
6	-4.10886240	-1.05703688	2.53492546
6	-5.13869858	-0.37722799	1.88062978
6	-4.97069407	0.94503611	1.44242561
6	-3.74144006	1.58193278	1.68669808

6	-2.70170665	0.91924942	2.33578563
1	-4.24136448	-2.07654762	2.89545465
1	-1.75273252	1.41769588	2.53006601
1	-3.59845591	2.61592412	1.36735821
6	-6.07594061	1.66291308	0.71000683
1	-6.09228420	-0.88172364	1.71531034
8	0.91701639	2.32871008	-1.96913147
8	1.03512681	1.01801848	-4.17858696
6	-1.31914580	1.91573763	-3.36845374
6	-1.72053945	1.88476026	-4.70301294
6	-2.99721169	2.34342241	-5.04331160
6	-3.87465787	2.83640361	-4.06832170
6	-3.44311738	2.85466695	-2.72912335
6	-2.17648268	2.39698362	-2.37405038
1	-1.02894449	1.51403856	-5.45897675
1	-3.31335974	2.32076740	-6.08799124
6	-5.24031305	3.35809588	-4.44088125
1	-4.11120176	3.24026227	-1.95577908
1	-1.84503651	2.41971970	-1.33511269
1	-7.06093979	1.25221610	0.96658379
1	-6.07657623	2.73715472	0.93794531
1	-5.95018959	1.55901873	-0.37941244
1	-5.26910782	4.45728016	-4.38533163
1	-5.51412439	3.06941986	-5.46361589
1	-6.01400471	2.98069048	-3.75721359
1	0.47086233	-1.52797413	2.67361569

Energy = -8524.626748 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 49

Atomic N.	X	Y	Z
8	2.84491873	1.06626296	2.26825023
8	3.50113988	-0.32021272	0.37626153
6	4.31706572	0.37217197	-0.56894571
1	3.86379719	0.29173666	-1.57050788
1	5.32385397	-0.07480147	-0.60943425
1	4.41899776	1.44781458	-0.33528513
8	3.31037450	-1.06455541	2.70981288
6	3.72439456	0.11913456	2.15580082
6	5.19423914	0.49542996	2.30088782
1	5.82464504	-0.13254748	1.65398848
1	5.27911186	1.52789676	1.94127619
6	5.69713974	0.39302045	3.75586009
1	4.91713667	0.75069755	4.44565153
1	6.55034828	1.07865238	3.86987853
6	6.15516901	-1.02106106	4.13901663
1	6.95730162	-1.32663333	3.44433832
1	6.61062765	-0.99661529	5.14139843
6	5.04983234	-2.08382940	4.12261963
1	4.33408403	-1.90489733	4.94063234
1	5.49566460	-3.07575107	4.30517292
6	4.25298023	-2.15774322	2.82290530
1	4.89966393	-2.19491363	1.93181801
1	3.62290668	-3.05776834	2.81922102
50	1.46432650	0.81222725	0.58409280
7	0.97449988	-1.59596658	-1.12380743
6	1.96145689	-1.99469626	-2.13600492

8	2.75444198	1.09217095	2.34860611
8	3.49980426	-0.20700261	0.42792800
6	4.30888605	0.54519027	-0.47654983
1	4.36612368	1.61560011	-0.20644432
1	3.87966061	0.48125154	-1.48981965
1	5.33214378	0.13664913	-0.50940484
8	3.28839850	-1.03374481	2.73172569
6	3.67022276	0.18133405	2.22501493
6	5.12202835	0.60516983	2.41366768
1	5.78790855	0.02160810	1.76074827
1	5.17649937	1.65120411	2.08907008
6	5.59878922	0.47335666	3.87502694
1	4.79256153	0.78032112	4.55907440
1	6.42404461	1.18492150	4.02892590
6	6.10003901	-0.93525606	4.22257996
1	6.92680311	-1.18918741	3.53604341
1	6.53373337	-0.92735887	5.23482895
6	5.03472376	-2.03575873	4.14846325
1	4.29656792	-1.90937126	4.95629740
1	5.51262093	-3.01653051	4.30877399
6	4.26752567	-2.09578466	2.83029199
1	4.93299866	-2.08099008	1.95250046
1	3.67063618	-3.01701212	2.78465962
50	1.41900456	0.84344238	0.62827867
7	1.05800259	-1.52300024	-1.17719877
6	2.08106375	-1.85066545	-2.17886734
1	1.88185322	-2.82338071	-2.67343068
1	2.13076329	-1.06639457	-2.94347882
1	3.05425572	-1.91012049	-1.67633533
7	0.19254194	0.69368213	-2.87436318
6	-0.29656726	-1.47440791	-1.75289869
1	-0.65566981	-2.49381065	-2.01298213
1	-0.97045565	-1.08092904	-0.97741550
6	-0.44035250	-0.62577087	-3.01990747
1	-1.52311015	-0.54940403	-3.22600961
1	0.01761192	-1.12391245	-3.88469577
16	-0.23921780	1.91466880	-3.96071267
7	0.23838344	-0.82356924	1.43630123
6	1.13287866	-2.50730991	-0.07792350
1	0.94574273	-3.53531837	-0.45552015
1	2.16248488	-2.46556687	0.30409899
6	0.15991573	-2.23122883	1.06964242
1	0.43637392	-2.88827157	1.91204691
1	-0.86965513	-2.50421643	0.77126181
16	-0.76373678	-0.21985543	2.57822323
8	-0.38351616	1.23462617	2.57816291
8	-0.77490973	-0.98885596	3.84055352
6	-2.44672608	-0.32954329	1.90774930
6	-3.32564497	-1.29493797	2.39950252
6	-4.60767937	-1.39343560	1.85131860
6	-5.02459860	-0.53811836	0.82148284
6	-4.11901140	0.42725897	0.34605715
6	-2.83674788	0.53585082	0.88109100
1	-3.00479388	-1.94638181	3.21175361
1	-2.14566374	1.29842579	0.51913202
1	-4.42163944	1.10420728	-0.45555171
6	-6.41965294	-0.62694085	0.25457478
1	-5.29673529	-2.14831924	2.23476982

8	0.60330826	3.06908894	-3.60462952
8	-0.22053456	1.29352582	-5.29855108
6	-1.95462155	2.35806561	-3.59116125
6	-2.99257946	1.80692923	-4.34371805
6	-4.31195927	2.15161681	-4.03604269
6	-4.60592270	3.04113889	-2.99274063
6	-3.53820300	3.58396697	-2.25444007
6	-2.21738601	3.24978065	-2.54537034
1	-2.76129961	1.13849151	-5.17246389
1	-5.12666893	1.72746444	-4.62568426
6	-6.02854156	3.43214893	-2.67974687
1	-3.74607635	4.28449011	-1.44331479
1	-1.39137995	3.68984032	-1.98614991
1	-6.86969376	-1.60931087	0.44723931
1	-7.07498360	0.13199067	0.70987099
1	-6.42291498	-0.44997558	-0.82969630
1	-6.22349358	4.47331285	-2.97855520
1	-6.74637794	2.79263139	-3.20864487
1	-6.23354912	3.36513424	-1.60172403
1	0.24092580	1.06039286	-1.91519475

Energy = -8524.620381 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 51

Atomic N.	X	Y	Z
8	0.93838358	-0.97306198	-0.62477362
8	2.19107461	0.74543697	-1.58041298
6	3.18970633	1.67962575	-1.96876907
1	2.72462344	2.45250964	-2.60017610
1	4.01296186	1.21289766	-2.53847504
1	3.60996604	2.16952538	-1.07412255
8	1.98323309	0.22829784	0.92850775
6	2.08426070	-0.54641783	-0.18381061
6	3.29705238	-1.44234931	-0.39356980
1	3.15484715	-2.28047919	0.31430912
1	3.16213632	-1.87759423	-1.39408028
6	4.71820354	-0.87627792	-0.27159423
1	4.81955814	0.02252118	-0.89430577
1	5.39929295	-1.62464869	-0.70569688
6	5.17996502	-0.57208902	1.15533030
1	5.17136431	-1.50393820	1.74596441
1	6.22600317	-0.22865969	1.12983322
6	4.31863642	0.46871635	1.87309039
1	4.33867359	1.43546045	1.34380925
1	4.73513603	0.65517753	2.87698460
6	2.87107801	0.03638975	2.07111073
1	2.80700207	-1.01643729	2.38840723
1	2.39244747	0.65541553	2.84032965
50	0.85760248	-0.50554198	-2.84780240
7	-1.54570556	-2.13299704	-2.46284747
6	-1.96760523	-2.13692570	-3.87360239
1	-3.03233933	-2.42436481	-3.98362589
1	-1.82113147	-1.14925003	-4.32730722
1	-1.35379314	-2.85939288	-4.42754745
7	-0.99696869	0.67710632	-2.49318457
6	-2.35197759	-1.20104218	-1.65264869
1	-3.40716386	-1.54057562	-1.57313871

1	-1.92723262	-1.18340135	-0.64016259
6	-2.36167264	0.22608134	-2.20311308
1	-2.83562517	0.86224812	-1.43383491
1	-2.99382305	0.28952003	-3.10352254
16	-0.83128184	2.05706835	-3.35470033
7	-0.11199586	-3.53129506	-0.01109595
6	-1.64662230	-3.53205252	-1.97512245
1	-2.64803696	-3.93316960	-2.24159431
1	-0.90004671	-4.12494659	-2.52428198
6	-1.48214519	-3.78112292	-0.47737372
1	-1.70226681	-4.84447098	-0.30735794
1	-2.23218369	-3.20202518	0.09058093
16	0.19786990	-3.87313700	1.60929227
8	1.56505930	-3.36494350	1.86045790
8	-0.15098085	-5.28768349	1.84221292
6	-0.95376647	-2.87678456	2.59550142
6	-1.88360178	-3.51996183	3.41266394
6	-2.76281381	-2.75103688	4.17934942
6	-2.72955346	-1.34971738	4.13424683
6	-1.79047668	-0.73007274	3.29092336
6	-0.90012783	-1.48040676	2.52385616
1	-1.90648329	-4.60876274	3.44266415
1	-0.18215136	-0.98247421	1.86975944
1	-1.75765848	0.35964248	3.23146820
6	-3.66307950	-0.52367538	4.98312664
1	-3.48989534	-3.25137091	4.82167721
8	0.58624339	1.95425308	-3.85602045
8	-1.91757262	2.29500651	-4.33414030
6	-0.88268548	3.43077922	-2.17535758
6	-1.68708134	4.53744125	-2.44487691
6	-1.70704937	5.59861803	-1.53605700
6	-0.93518126	5.56518793	-0.36576512
6	-0.14258802	4.43012810	-0.11819855
6	-0.10885906	3.36170506	-1.01268935
1	-2.28813338	4.55562115	-3.35326958
1	-2.33621573	6.46690035	-1.74083662
6	-0.93628615	6.72646999	0.59700161
1	0.45675942	4.38225985	0.79333210
1	0.50311869	2.47905016	-0.81403357
1	-4.54627657	-1.10044086	5.28631401
1	-3.15796709	-0.18513405	5.90119410
1	-4.00084019	0.37488115	4.44928455
1	-0.05964596	7.37191868	0.43050945
1	-1.83200181	7.34897900	0.47438797
1	-0.89180344	6.38355541	1.63977098
1	0.25813550	-2.58626580	-0.23235507

Energy = -8524.628883 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 52

Atomic N.	X	Y	Z
8	2.61268640	-1.29678166	-2.50448370
8	3.96587133	-0.63649815	-0.53358173
6	4.87982082	0.44597787	-0.64970517
1	4.48773289	1.32807612	-0.10970158
1	5.05551434	0.75458050	-1.69895959
1	5.85067177	0.18738179	-0.19389664

8	3.14275527	-2.92864966	-1.12512720
6	3.58390236	-1.93439066	-1.93992722
6	4.86453152	-2.10849905	-2.74984932
1	4.67592001	-2.99455810	-3.38496041
1	4.88818073	-1.24896240	-3.43280172
6	6.22818804	-2.24707031	-2.06160545
1	6.43695116	-1.33608556	-1.48678255
1	6.98705435	-2.28623748	-2.85943866
6	6.40180254	-3.45970178	-1.14766705
1	6.34596825	-4.38937426	-1.74181294
1	7.41489601	-3.43095684	-0.71605819
6	5.36815548	-3.52714920	-0.02019192
1	5.30730438	-2.57566571	0.52857602
1	5.67382622	-4.29689693	0.70753354
6	3.97738600	-3.93171740	-0.48370272
1	4.04220295	-4.79173231	-1.17400682
1	3.36965394	-4.22817564	0.38102859
50	1.85480058	0.16867998	-0.92916036
7	-0.50919604	-1.07365775	-1.97479606
6	-0.46070331	-1.07671428	-3.44470716
1	-1.22231603	-1.75693703	-3.87699652
1	-0.63587242	-0.06530103	-3.83244991
1	0.53680474	-1.39694035	-3.76738381
7	-1.31761193	1.61089766	-0.56380665
6	-1.82417405	-0.61889362	-1.49158204
1	-2.63092780	-1.13987160	-2.04962659
1	-1.92779016	-0.91904521	-0.43901348
6	-2.08270812	0.88642132	-1.58842516
1	-3.17185640	1.04635489	-1.48508406
1	-1.77969551	1.28297520	-2.56609654
16	-1.34004915	3.30936313	-0.60144973
7	0.87734854	-1.29222703	0.41517720
6	-0.20507991	-2.42502832	-1.45665967
1	-1.01819003	-3.14139152	-1.69727147
1	0.70712936	-2.75647736	-1.96715355
6	0.04574220	-2.43660474	0.05651922
1	0.53406978	-3.39361167	0.30751240
1	-0.91306370	-2.41441917	0.61050862
16	1.36664462	-1.11790204	1.96543908
8	2.26356554	0.07489016	1.91856992
8	1.82779312	-2.38725376	2.57832551
6	-0.10776678	-0.61439085	2.89998102
6	-0.87922335	-1.57242095	3.55993938
6	-2.02939057	-1.17145956	4.24608564
6	-2.41277146	0.17659108	4.29456234
6	-1.61222672	1.12155151	3.62846017
6	-0.46629393	0.73776960	2.93134499
1	-0.56332624	-2.61535096	3.55247355
1	0.15954371	1.47988927	2.43359637
1	-1.87929511	2.17968082	3.67174244
6	-3.62757373	0.61073118	5.07674265
1	-2.63278890	-1.92012846	4.76331568
8	-0.59916598	3.72006416	0.60525995
8	-0.92983902	3.69292307	-1.96374464
6	-3.06323338	3.82369208	-0.39355412
6	-3.85585499	4.05428028	-1.51968074
6	-5.18847132	4.43467283	-1.34618008
6	-5.73821497	4.59315586	-0.06519065

6	-4.91464853	4.35870600	1.04977012
6	-3.58322549	3.97637987	0.89516431
1	-3.42221808	3.95708704	-2.51445413
1	-5.81039333	4.61963844	-2.22386408
6	-7.16724968	5.03871298	0.11591618
1	-5.32184792	4.48774529	2.05443120
1	-2.93866062	3.81984806	1.75980067
1	-4.34343147	-0.21276209	5.19747591
1	-3.34202862	0.94972008	6.08486748
1	-4.14190912	1.44935286	4.58771563
1	-7.21436787	6.11953020	0.32104185
1	-7.76488256	4.84720278	-0.78436744
1	-7.64242601	4.52744341	0.96405768
1	-1.50245726	1.29592526	0.39402378

Energy = -8524.615507 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 53

Atomic N.	X	Y	Z
8	1.19168544	-0.96089691	-0.41180122
8	2.62623358	0.79084229	-1.37504542
6	2.76041770	2.18332195	-1.16251957
1	3.82655311	2.45436811	-1.05224133
1	2.22748113	2.49779963	-0.24511504
1	2.34625077	2.74629760	-2.01239204
8	2.00998139	0.29260379	1.21131206
6	2.25644708	-0.50669706	0.15256636
6	3.55071330	-1.29311919	0.04897135
1	3.48049712	-2.07304502	0.83033234
1	3.48328590	-1.82851994	-0.90793943
6	4.89313078	-0.55561012	0.12181312
1	4.87351227	0.27266705	-0.60067272
1	5.66682100	-1.25698113	-0.22700658
6	5.28879261	-0.05100842	1.51099741
1	5.39983749	-0.91153401	2.19312835
1	6.27870846	0.42780328	1.45193791
6	4.28779221	0.93008417	2.12544179
1	4.18947649	1.83856404	1.51045752
1	4.66136646	1.26001155	3.10921001
6	2.90684485	0.33372730	2.36595011
1	2.97522926	-0.68531722	2.77798486
1	2.34079576	0.95341885	3.07230306
50	1.29873657	-0.40271345	-2.65150809
7	-1.03916669	-2.29627228	-2.44045663
6	-1.35161161	-2.29565835	-3.87775517
1	-2.38298464	-2.65162873	-4.07728815
1	-1.23962462	-1.29152322	-4.30463791
1	-0.64939833	-2.96314049	-4.39466333
7	-0.72176367	0.59689844	-2.38673043
6	-1.95737219	-1.43823099	-1.67375541
1	-2.98983526	-1.85209322	-1.66184282
1	-1.60053480	-1.40553844	-0.63543546
6	-2.05145359	-0.00745744	-2.20654941
1	-2.64489794	0.56617367	-1.47170258
1	-2.61292243	0.00844337	-3.15438175
16	-0.64589912	1.86296809	-3.41681361
7	0.28409117	-3.60916519	0.09775785

6	-1.07977319	-3.70711589	-1.98562276
1	-2.02694035	-4.17402220	-2.33408785
1	-0.25296009	-4.23625278	-2.48269606
6	-1.01539898	-3.97246838	-0.48306105
1	-1.15204847	-5.05412865	-0.34426922
1	-1.85758436	-3.47204757	0.02770593
16	0.48668104	-3.93530250	1.73837519
8	1.77168715	-3.30203605	2.10860682
8	0.25356540	-5.37854242	1.93664551
6	-0.83326524	-3.06285262	2.62638307
6	-1.79175270	-3.80094481	3.32038426
6	-2.80146050	-3.12634635	4.01210976
6	-2.86903191	-1.72596586	4.01325607
6	-1.89534032	-1.00906324	3.29488730
6	-0.87696296	-1.66426146	2.60454392
1	-1.73416460	-4.88886499	3.31735682
1	-0.13121836	-1.09361434	2.04868412
1	-1.93687141	0.08184938	3.27570558
6	-3.94699049	-0.99987435	4.77832460
1	-3.55104876	-3.70122099	4.55901575
8	0.83475047	1.94571793	-3.70793867
8	-1.57483041	1.79052496	-4.57035160
6	-1.10389626	3.35334778	-2.49362063
6	-1.75213063	4.39329004	-3.16370392
6	-2.08045793	5.55247641	-2.46061730
6	-1.77565992	5.68627119	-1.09618330
6	-1.13876820	4.61702728	-0.44649166
6	-0.79862088	3.45163918	-1.13506258
1	-2.00274587	4.28069592	-4.21782207
1	-2.58917522	6.36680174	-2.98007035
6	-2.11049676	6.95568132	-0.35375616
1	-0.90778399	4.69690514	0.61746085
1	-0.31541222	2.61756516	-0.62610775
1	-4.76432085	-1.67606580	5.05921698
1	-3.54237890	-0.56325650	5.70448399
1	-4.36834717	-0.17339344	4.18931723
1	-1.33535910	7.72001171	-0.52003485
1	-3.06355262	7.38105917	-0.69600403
1	-2.17619920	6.78314066	0.72830480
1	0.58904731	-2.63620639	-0.09517628

Energy = -8524.629059 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 54

Atomic N.	X	Y	Z
8	2.77203655	-1.51138568	-1.32069528
8	3.62217093	-0.41415682	0.72131145
6	3.92777824	-0.90025401	2.02103138
1	4.98620653	-0.69069749	2.25669146
1	3.75389051	-1.98786247	2.10017657
1	3.30293036	-0.39530113	2.77211356
8	4.32176256	-2.76846504	-0.36195862
6	3.98161578	-1.57214212	-0.89679480
6	5.03064632	-0.68576366	-1.55183554
1	5.33607912	-1.21207976	-2.47697067
1	4.47817850	0.20258535	-1.88343334
6	6.26427174	-0.25107899	-0.75134522

1	5.92074013	0.17627282	0.20114565
1	6.74186230	0.57024813	-1.30776238
6	7.30758667	-1.34377539	-0.50943023
1	7.70863199	-1.68612480	-1.47994006
1	8.15919781	-0.91283715	0.03972005
6	6.77699852	-2.55933046	0.25424480
1	6.42633963	-2.27815056	1.25907624
1	7.59870338	-3.27978802	0.40264931
6	5.66832066	-3.31410718	-0.46897873
1	5.90983677	-3.43275547	-1.53863227
1	5.54633665	-4.31495571	-0.03688191
50	1.61024165	-0.03378517	-0.06744993
7	-0.21945091	-1.69640398	-1.55583203
6	0.10894288	-1.97009838	-2.96293354
1	-0.57266510	-2.72281742	-3.40745950
1	0.05655395	-1.04554367	-3.54934502
1	1.13687706	-2.34731436	-3.01084304
7	-1.03202403	1.01579046	-2.38774991
6	-1.59377503	-1.19396806	-1.37853432
1	-2.33164644	-2.01357007	-1.51538587
1	-1.68846774	-0.84568185	-0.33926514
6	-2.02295327	-0.06780952	-2.32313442
1	-3.00462389	0.28536841	-1.95824730
1	-2.17392063	-0.44383565	-3.34352946
16	-1.49671960	2.49296165	-3.06011605
7	0.54515243	-1.53058326	1.17793691
6	-0.00453371	-2.92172837	-0.75680220
1	-0.68713248	-3.73205113	-1.08907080
1	1.02817190	-3.24187541	-0.94832277
6	-0.19739109	-2.71494007	0.74727410
1	0.15848777	-3.62397218	1.26119137
1	-1.27320790	-2.61333132	0.98129070
16	0.23915759	-0.90698922	2.65983152
8	1.03503811	0.36598176	2.64984441
8	0.42280751	-1.88409710	3.75610280
6	-1.51185250	-0.43073320	2.70118618
6	-2.43857789	-1.24955654	3.34796596
6	-3.78968096	-0.89123368	3.33863521
6	-4.22693205	0.27631623	2.69675803
6	-3.27150297	1.08599448	2.05698252
6	-1.92127275	0.73992109	2.05512881
1	-2.09446001	-2.14542437	3.86383104
1	-1.18170822	1.38052189	1.57251239
1	-3.58792830	2.00068235	1.55150795
6	-5.68163681	0.67523593	2.71446586
1	-4.51600647	-1.53115821	3.84324789
8	-0.28189796	3.32565451	-3.05559349
8	-2.23653698	2.16222239	-4.29280472
6	-2.67354631	3.24833679	-1.90982914
6	-4.04504681	3.08312702	-2.10922933
6	-4.93856573	3.66900706	-1.20773160
6	-4.48098660	4.41959476	-0.11507553
6	-3.09323549	4.57791424	0.05383239
6	-2.18819618	3.99708962	-0.83218491
1	-4.40113926	2.52859783	-2.97683120
1	-6.01203346	3.55003166	-1.36554587
6	-5.44652843	5.04148865	0.86244613
1	-2.71735501	5.17213106	0.88895041

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1 -1.11426187  4.14081907 -0.71235603
1 -6.33095980 -0.18280986  2.93080187
1 -5.86873627  1.43535829  3.48905420
1 -5.98858595  1.10935128  1.75295079
1 -5.18969250  6.09078455  1.06406724
1 -6.47701263  5.00498199  0.48744962
1 -5.42171288  4.51428652  1.82895148
1 -0.45745194  1.15366650 -1.54649663
Energy = -8524.623980 Hartree
Number of imaginary frequencies = 0.

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Compound TS2a isomer 55

Atomic N.	X	Y	Z
8	4.26832151	0.11979998	-0.74348080
8	3.31144547	1.64993405	0.82176769
6	3.75597143	2.86855507	0.20161828
1	2.90689206	3.56077552	0.13315564
1	4.13815355	2.68050385	-0.81377167
1	4.54271793	3.32954025	0.81782585
8	3.69877315	-0.54611695	1.41208506
6	4.39724684	0.37722859	0.49402964
6	5.76433897	0.80175525	1.05067301
1	6.33931208	1.16917384	0.18909977
1	5.64052105	1.64008391	1.74988902
6	6.54428864	-0.31576985	1.77189469
1	6.19951773	-0.37984276	2.81597590
1	7.59768629	0.00287626	1.81604350
6	6.46225595	-1.72232771	1.15026307
1	6.50571299	-1.65844154	0.05080154
1	7.34756470	-2.29663467	1.46557891
6	5.21029949	-2.50006723	1.58575141
1	5.17669249	-2.53156638	2.68793368
1	5.27934504	-3.54588795	1.24051952
6	3.89625001	-1.93626034	1.05576229
1	3.84416032	-2.03734899	-0.03902364
1	3.04058337	-2.47226977	1.49215937
50	1.73912656	0.41302320	-0.38141987
7	0.26866740	1.07373476	2.02455688
6	1.05531883	0.57517570	3.16581464
1	0.68724430	0.99149328	4.12505007
1	0.99558854	-0.51940298	3.21386886
1	2.10854673	0.84322017	3.02498388
7	-1.40485108	-0.84639394	0.20257641
6	-1.13850939	0.64723277	2.14091563
1	-1.47435713	0.73990726	3.19432688
1	-1.76318133	1.33720207	1.55471051
6	-1.42924821	-0.78041989	1.67136621
1	-2.40680170	-1.08620262	2.08716249
1	-0.67156458	-1.48205054	2.04429793
16	-1.54343772	-2.37079096	-0.54161626
7	0.52800065	2.33521938	-0.44911286
6	0.36019051	2.55049348	1.95215452
1	-0.20892356	3.02828360	2.77667093
1	1.42079186	2.80302930	2.08111453
6	-0.11787020	3.10361481	0.60444212
1	0.15453479	4.17221022	0.55963534
1	-1.22160530	3.05418420	0.52816063

16	0.75508398	2.93334198	-1.93857765
8	1.73764169	1.92688501	-2.49809241
8	1.08462191	4.37764740	-1.98481643
6	-0.77957278	2.72092605	-2.87854028
6	-1.49790061	3.84262204	-3.29155016
6	-2.69216752	3.66468883	-3.99613142
6	-3.17355728	2.38262963	-4.29663181
6	-2.42856479	1.26997793	-3.86540556
6	-1.23759174	1.42955458	-3.16002512
1	-1.11131358	4.83722591	-3.07141137
1	-0.66645861	0.55419159	-2.84715557
1	-2.77744865	0.26055917	-4.09244871
6	-4.44075346	2.19605398	-5.09338331
1	-3.25498557	4.54074669	-4.32416773
8	-1.58688664	-2.07293916	-1.98543394
8	-0.50445008	-3.21656394	0.07117352
6	-3.15089250	-3.04975605	-0.06792973
6	-3.23881578	-3.91815829	1.02186823
6	-4.48845768	-4.42322445	1.38712919
6	-5.64839363	-4.07636690	0.67781258
6	-5.52751875	-3.20200849	-0.41643909
6	-4.28878784	-2.68770480	-0.79537022
1	-2.33503461	-4.20646858	1.55754983
1	-4.56187677	-5.10595655	2.23547053
6	-6.98894691	-4.65362549	1.05525351
1	-6.41775990	-2.92791963	-0.98546237
1	-4.19453335	-2.03018975	-1.65957737
1	-5.06679583	3.09735751	-5.06990623
1	-4.20924711	1.98060727	-6.14816999
1	-5.03283596	1.35127699	-4.71521044
1	-7.22378349	-5.52929926	0.43030798
1	-7.00448275	-4.98262501	2.10210657
1	-7.79615164	-3.92384624	0.90722549
1	-2.05709291	-0.20009615	-0.25027207

Energy = -8524.610342 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 56

Atomic N.	X	Y	Z
8	3.29616880	0.19870950	1.32592595
8	3.75837922	-1.36127937	-0.43307731
6	4.56387424	-1.48329401	-1.60062981
1	3.91498351	-1.46359277	-2.49181795
1	5.10534334	-2.44293833	-1.59348524
1	5.29002571	-0.65638936	-1.67810214
8	5.42876959	0.23208244	0.63223445
6	4.36654854	-0.50214064	1.09731793
6	4.60688162	-1.69406199	2.01707697
1	4.91314840	-1.27679336	2.99426365
1	3.60995054	-2.12701988	2.16662097
6	5.57370043	-2.80137944	1.58026707
1	5.31237793	-3.12077236	0.56123084
1	5.38518667	-3.67316222	2.22558355
6	7.05976629	-2.44573259	1.66801643
1	7.31592464	-2.22255874	2.71886206
1	7.65932512	-3.32555556	1.38632238
6	7.47304344	-1.25301766	0.80249828

1	7.31516743	-1.46587276	-0.26660916
1	8.55432320	-1.07395804	0.92602807
6	6.76847363	0.05193910	1.16062438
1	6.74217272	0.19317277	2.25449061
1	7.30825424	0.90362418	0.72721720
50	2.01323676	0.01100813	-0.47938886
7	-0.39650133	0.91226768	2.44184756
6	0.63339561	1.41557622	3.35663915
1	0.34300411	1.29831302	4.42287636
1	1.58207655	0.89036483	3.18966722
1	0.80612195	2.48094821	3.15744233
7	0.69818002	-1.31903768	0.70421696
6	-0.65348494	-0.51958710	2.65188289
1	-0.81988835	-0.73305798	3.73265052
1	-1.57966661	-0.78690094	2.12412953
6	0.47006130	-1.43248677	2.14455080
1	0.23137192	-2.47471786	2.41347814
1	1.41441822	-1.18897283	2.65538597
16	0.31638306	-2.53885698	-0.30655402
7	-1.72424316	2.00099587	0.08240886
6	-1.63320172	1.69928443	2.55663991
1	-2.24382806	1.38888919	3.43272138
1	-1.35634780	2.75194407	2.70836973
6	-2.48361301	1.61224687	1.28474045
1	-3.35856223	2.26740193	1.38887620
1	-2.85771871	0.58958972	1.12306166
16	-1.76860833	3.63901925	-0.38381925
8	-0.45867905	3.89249253	-1.01745176
8	-2.27438712	4.49063969	0.71772194
6	-3.03577089	3.63998079	-1.67157829
6	-4.26669359	4.24534798	-1.42501259
6	-5.23013401	4.25989580	-2.43762493
6	-4.97499084	3.68372822	-3.68990993
6	-3.72120357	3.08419013	-3.90903592
6	-2.75000167	3.06023836	-2.91113925
1	-4.45512342	4.70549583	-0.45571154
1	-1.77456629	2.60761380	-3.08832836
1	-3.50332689	2.63377666	-4.87928295
6	-6.00528669	3.72779584	-4.79038572
1	-6.19565773	4.73329115	-2.25044918
8	0.97371382	-2.06286907	-1.58485913
8	0.62505370	-3.88813162	0.21763192
6	-1.46832168	-2.52027988	-0.62319446
6	-2.24384093	-3.61400509	-0.23822682
6	-3.62083101	-3.58923507	-0.47532690
6	-4.23087740	-2.49007368	-1.09654427
6	-3.42360163	-1.40167332	-1.47339618
6	-2.05008459	-1.40920722	-1.24070013
1	-1.76395023	-4.47100163	0.23280501
1	-4.23054123	-4.44297218	-0.17354760
6	-5.71221733	-2.48180962	-1.37998712
1	-3.87824893	-0.53209025	-1.95211172
1	-1.43873513	-0.55537617	-1.53341126
1	-7.00242472	3.96373439	-4.39753342
1	-5.74939156	4.49863291	-5.53371382
1	-6.06086063	2.76984811	-5.32569790
1	-5.91117573	-2.77414894	-2.42289162
1	-6.24902153	-3.18638754	-0.73176718

1 -6.14147520 -1.48081243 -1.23745418
 1 -0.73171908 1.74913156 0.19543207
 Energy = -8524.623324 Hartree
 Number of imaginary frequencies = 0.

Compound TS2a isomer 57

Atomic N.	X	Y	Z
8	3.47028995	-1.08881879	-0.74114245
8	3.06989884	-0.16296440	1.41634309
6	3.20588779	-0.81831944	2.67826176
1	3.66145396	-0.13624080	3.41606379
1	3.83056259	-1.72038591	2.59456062
1	2.20986199	-1.11897743	3.04054809
8	5.12681818	-1.43871701	0.72007930
6	4.26496744	-0.53477025	0.14556339
6	4.76782656	0.86551386	-0.19828315
1	5.49086046	0.74327612	-1.02396846
1	3.89852524	1.36768162	-0.64336008
6	5.35874748	1.73532712	0.91858780
1	4.67648602	1.71610057	1.78244531
1	5.37118816	2.77611518	0.55878270
6	6.77542782	1.35759926	1.35859358
1	7.46132851	1.47221541	0.50104767
1	7.12026834	2.06910896	2.12553859
6	6.90255117	-0.06972039	1.89622772
1	6.29408216	-0.20672297	2.80465245
1	7.94855165	-0.25166798	2.19470763
6	6.53795242	-1.15208220	0.88335800
1	6.97288895	-0.92332941	-0.10418859
1	6.93940926	-2.12101579	1.20717394
50	1.45394695	-0.95462304	-0.01609567
7	0.04743185	1.16562462	1.89393318
6	0.21880484	1.21255541	3.35079956
1	-0.26427972	2.10559583	3.79959464
1	-0.19903724	0.31098133	3.81446075
1	1.29041934	1.25456297	3.58248878
7	-1.59516144	-1.19864047	2.19512081
6	-1.37048185	1.17962158	1.50406253
1	-1.83814609	2.16690040	1.71480489
1	-1.41704905	1.02191603	0.41678432
6	-2.23845840	0.12414928	2.19740200
1	-3.20995164	0.11501663	1.67235434
1	-2.44114470	0.40127653	3.24065208
16	-2.56306362	-2.56762552	2.39379239
7	1.03880847	1.06986845	-0.82620573
6	0.78529567	2.29102135	1.29072332
1	0.42196131	3.26300192	1.69120908
1	1.83623707	2.17364359	1.59173477
6	0.70648038	2.36356640	-0.23477191
1	1.40718508	3.15110922	-0.56322813
1	-0.30411202	2.68801975	-0.54417336
16	0.84486306	0.85645217	-2.43546081
8	1.08907735	-0.62612414	-2.56818581
8	1.61422253	1.80420661	-3.27005816
6	-0.90289015	1.14482009	-2.82300735
6	-1.27717590	2.30633855	-3.49998951
6	-2.62938166	2.53256202	-3.76865411

6	-3.61193347	1.61278772	-3.37338257
6	-3.20622659	0.45044354	-2.69428706
6	-1.86092746	0.21131659	-2.41745043
1	-0.50977242	3.01053929	-3.81959081
1	-1.55444741	-0.70140356	-1.90466607
1	-3.95365095	-0.27917102	-2.37621021
6	-5.06667280	1.84680688	-3.69549203
1	-2.92484236	3.44066954	-4.29748297
8	-1.62677884	-3.70350742	2.44475007
8	-3.49668884	-2.25018811	3.49110341
6	-3.54178429	-2.74093199	0.88071519
6	-4.86619520	-2.30327868	0.85461420
6	-5.60442638	-2.44218993	-0.32492700
6	-5.03812790	-3.01322770	-1.47344959
6	-3.70055413	-3.44675159	-1.41600347
6	-2.95021391	-3.31622386	-0.24978048
1	-5.31283474	-1.88419402	1.75569761
1	-6.64346409	-2.10838294	-0.34745076
6	-5.84111166	-3.18203855	-2.73892975
1	-3.24326849	-3.89980316	-2.29767728
1	-1.92161763	-3.67489100	-0.20275120
1	-5.28838062	2.91699195	-3.79849243
1	-5.33743620	1.36232400	-4.64672518
1	-5.72086287	1.42841673	-2.91900897
1	-6.01561022	-4.24694395	-2.95405364
1	-6.81892872	-2.69003534	-2.66286755
1	-5.31037092	-2.76396537	-3.60655117
1	-0.89310616	-1.34817171	1.45867050

Energy = -8524.619721 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 58

Atomic N.	X	Y	Z
8	3.15793014	-1.99531245	2.32907772
8	2.36108518	0.08734379	1.58644927
6	2.98843741	1.35084152	1.90437412
1	3.44030213	1.78223610	1.00431550
1	3.74771619	1.24232948	2.69056320
1	2.18989182	2.02029181	2.25652623
8	4.66498566	-0.61442286	1.34327221
6	3.40759945	-1.19995809	1.28835547
6	2.93405056	-1.75281644	-0.05091761
1	3.46723080	-2.70751119	-0.19552927
1	1.89112484	-2.04804325	0.12116595
6	3.06679511	-0.85759544	-1.28913176
1	2.74126959	0.16731440	-1.05422068
1	2.36715245	-1.23593974	-2.05171990
6	4.47238016	-0.83046108	-1.89987385
1	4.76238966	-1.85892010	-2.17856407
1	4.45222139	-0.24951592	-2.83528638
6	5.54323578	-0.24946290	-0.97313493
1	5.34941864	0.81775767	-0.77892458
1	6.52600098	-0.30400774	-1.47132933
6	5.67391539	-0.96797502	0.36688742
1	5.69620323	-2.06262708	0.23614436
1	6.60950279	-0.67429888	0.86136961
50	1.67677271	-1.06258714	3.51653171

7	-0.93615079	0.80332994	3.20403218
6	-0.75844944	1.46964157	4.50215292
1	-1.69665480	1.94813716	4.85246277
1	-0.43470755	0.74647057	5.26186752
1	0.01900085	2.24096894	4.42020464
7	-0.18775602	-2.07577372	2.97462940
6	-1.90430939	-0.30508646	3.32529569
1	-2.75048327	-0.00883431	3.98157811
1	-2.32456017	-0.51854640	2.33505177
6	-1.27285886	-1.59737253	3.85237265
1	-2.04923129	-2.36882925	3.96424246
1	-0.87523317	-1.43555987	4.87062979
16	-0.48170605	-3.50504899	2.16986132
7	-0.07293655	1.30294561	0.07670289
6	-1.39701056	1.80284011	2.21776199
1	-2.43601131	2.11899066	2.46048236
1	-0.76609319	2.69765925	2.30767560
6	-1.37647581	1.33340418	0.75742179
1	-2.03321528	1.99992192	0.17946140
1	-1.81083536	0.32818824	0.65948290
16	0.46421579	2.75306439	-0.60613549
8	1.88414049	2.52447867	-0.95080215
8	0.07593752	3.93007874	0.20675752
6	-0.50354648	2.82673430	-2.12935209
6	-1.36074483	3.90472651	-2.34508824
6	-2.06754208	3.97879744	-3.54841113
6	-1.92335224	2.99422193	-4.53609753
6	-1.05115163	1.91826415	-4.28818893
6	-0.33941954	1.82859671	-3.09457254
1	-1.46433675	4.66995478	-1.57662666
1	0.33938861	0.99661446	-2.90795708
1	-0.92754602	1.14188516	-5.04551601
6	-2.66283679	3.09510541	-5.84620142
1	-2.74229765	4.81898594	-3.72151613
8	0.75930190	-3.83725214	1.44053411
8	-1.10756373	-4.49530411	3.07909632
6	-1.75548851	-3.11459351	0.92940909
6	-3.06900907	-3.54061675	1.13265955
6	-4.04278040	-3.24073577	0.17622501
6	-3.72238207	-2.52768970	-0.98828751
6	-2.39094377	-2.11535382	-1.17154312
6	-1.40981603	-2.40435481	-0.22394921
1	-3.31117916	-4.11485243	2.02639675
1	-5.07000017	-3.57437658	0.33603120
6	-4.76950073	-2.23970008	-2.03513217
1	-2.11923695	-1.55900943	-2.07108426
1	-0.37952638	-2.08537769	-0.38056734
1	-3.52948642	3.76369166	-5.76781797
1	-2.00529265	3.49557328	-6.63341713
1	-3.01202917	2.11093950	-6.18691921
1	-4.76100254	-3.01312137	-2.81909776
1	-5.77764225	-2.22430062	-1.60086942
1	-4.58874750	-1.27529752	-2.52875376
1	0.69948345	0.83611673	0.57702476

Energy = -8524.610578 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 59

Atomic N.	X	Y	Z
8	3.20526505	1.19099927	-0.10056966
8	3.08742309	-0.35033235	-2.02542686
6	2.91818261	-0.14000481	-3.42047501
1	2.00485444	-0.64162648	-3.77219367
1	3.77755976	-0.56664425	-3.96742558
1	2.83908558	0.93424255	-3.66355777
8	4.38613415	1.98703361	-1.79566598
6	4.15770102	0.96998888	-0.93162841
6	5.28150702	0.02975675	-0.52144033
1	5.97140312	0.63490921	0.09821881
1	4.81131887	-0.68372679	0.16719346
6	6.06094885	-0.73630244	-1.59719896
1	5.33583450	-1.24335885	-2.24910069
1	6.62916231	-1.52909803	-1.08643365
6	7.03676701	0.10396121	-2.42350864
1	7.81286669	0.52115381	-1.75750077
1	7.56287193	-0.55150741	-3.13491225
6	6.38058710	1.25590253	-3.18818808
1	5.64390039	0.88371372	-3.91653275
1	7.15105104	1.78835618	-3.77056336
6	5.71841288	2.29866099	-2.29595995
1	6.36331797	2.54251981	-1.43503428
1	5.54251099	3.22335076	-2.85925293
50	1.50547218	-0.23964383	-0.50865936
7	0.56852877	1.93799388	1.13702261
6	1.43720555	2.37426496	2.24059677
1	1.05929446	3.29768896	2.72352886
1	1.51857781	1.58134854	2.99297237
1	2.43798590	2.56661606	1.83723509
7	-0.13501404	-0.41524073	2.77173281
6	-0.81259769	1.66333067	1.57265413
1	-1.35398841	2.61128616	1.78071630
1	-1.33281898	1.17211115	0.73686862
6	-0.95994627	0.80004543	2.82865286
1	-2.03678703	0.56940275	2.92161345
1	-0.67070353	1.35875463	3.72842288
16	-0.46115696	-1.66178954	3.86237121
7	0.20337015	1.19994128	-1.58398223
6	0.58537686	2.96061969	0.06927377
1	0.16999917	3.92158103	0.43936557
1	1.63956070	3.12005687	-0.19331565
6	-0.19011724	2.55092406	-1.18484414
1	0.03359611	3.28722525	-1.97536004
1	-1.27765226	2.60501671	-0.99299085
16	-0.70773864	0.40998575	-2.69038725
8	-0.10593517	-0.96551043	-2.68742013
8	-0.85419941	1.14878643	-3.96437812
6	-2.38184404	0.25235951	-2.00725055
6	-3.39414454	1.10616183	-2.44778347
6	-4.66932583	1.00022268	-1.88526177
6	-4.94851828	0.04975729	-0.89265418
6	-3.91157317	-0.80118763	-0.47055128
6	-2.63409615	-0.70522267	-1.02001774
1	-3.18073273	1.83022594	-3.23346186
1	-1.83769560	-1.37940443	-0.70149636
1	-4.10533524	-1.54968357	0.30045259

6	-6.33370018	-0.08192848	-0.30995813
1	-5.46201420	1.66800845	-2.22791648
8	0.57335585	-2.68054962	3.61517334
8	-0.64978868	-1.01353168	5.17404413
6	-2.05201387	-2.38022399	3.38103294
6	-3.22516799	-1.95381403	4.00510073
6	-4.44507027	-2.51546788	3.61617303
6	-4.50706053	-3.49840760	2.61817622
6	-3.30664706	-3.91504645	2.01365256
6	-2.08272409	-3.36303210	2.38547683
1	-3.17344785	-1.21429312	4.80351305
1	-5.36392117	-2.19077182	4.10774565
6	-5.82376146	-4.10158300	2.19728255
1	-3.33224583	-4.68921280	1.24432135
1	-1.15202975	-3.70398545	1.93171024
1	-6.91694307	0.83756429	-0.44828480
1	-6.88625717	-0.90023649	-0.79768419
1	-6.29534960	-0.31092063	0.76387185
1	-5.79268551	-5.19929075	2.24897528
1	-6.64703751	-3.75212431	2.83271980
1	-6.06379938	-3.83752275	1.15590620
1	0.06259551	-0.78360265	1.83246076

Energy = -8524.623973 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 60

Atomic N.	X	Y	Z
8	2.93050280	0.29874623	0.83670254
8	2.97430856	0.89740805	-1.49419849
6	3.29946456	0.70970325	-2.85087874
1	2.49652060	1.11546135	-3.50201997
1	3.43095278	-0.35401458	-3.13348601
1	4.22134213	1.25645006	-3.12510797
8	4.66535108	1.60258925	0.36205440
6	4.00225530	0.43144470	0.14417086
6	4.76375541	-0.82797429	-0.24702876
1	5.14625548	-1.23831572	0.70704422
1	3.99321544	-1.54242546	-0.57095854
6	5.89380748	-0.77777980	-1.28423650
1	5.54493080	-0.27626720	-2.19623211
1	6.11150009	-1.81800942	-1.57285151
6	7.19302723	-0.12317804	-0.80987682
1	7.57389494	-0.66318209	0.07466195
1	7.95836255	-0.23589138	-1.59370393
6	7.03979595	1.35721021	-0.45860855
1	6.71039944	1.93736814	-1.33586984
1	8.01943492	1.76700653	-0.16077335
6	6.07912509	1.62006345	0.69455084
1	6.26052744	0.91875644	1.52615780
1	6.21964223	2.63815170	1.07919626
50	1.19863436	-0.29700515	-0.39770631
7	0.36810579	2.12357935	-0.32326435
6	1.36852577	2.89781436	0.45256861
1	0.99100384	3.91853059	0.64459951
1	1.58638449	2.39647147	1.39954058
1	2.30036116	2.94428003	-0.12133852
7	-0.13920429	0.02957592	1.40687636

6	-0.92451660	2.06643770	0.40232939
1	-1.30423840	3.08795004	0.59654151
1	-1.64501325	1.53989425	-0.23644155
6	-0.79704297	1.29321364	1.71617466
1	-1.82120676	1.14369621	2.10623065
1	-0.24703985	1.87552263	2.47439250
16	0.13890002	-1.02968842	2.62387692
7	-0.76723800	0.84584162	-2.84769038
6	0.24886723	2.77872863	-1.65327198
1	0.08382705	3.86428240	-1.50757672
1	1.23050410	2.66317233	-2.13589926
6	-0.86351831	2.29027897	-2.57942448
1	-0.81560063	2.89165731	-3.50244879
1	-1.85008886	2.47990407	-2.13388679
16	-2.06335426	0.18417045	-3.77218916
8	-1.54195385	-1.10835427	-4.25457512
8	-2.60462120	1.18686003	-4.71645746
6	-3.30043435	-0.07877844	-2.48949326
6	-4.53353909	0.56410295	-2.59520033
6	-5.49706517	0.34015281	-1.60846740
6	-5.23905797	-0.51011728	-0.52330716
6	-3.98403821	-1.14165860	-0.44454348
6	-3.01422495	-0.93665051	-1.42278033
1	-4.72491701	1.22681894	-3.43835597
1	-2.04228187	-1.42636356	-1.35626461
1	-3.75802451	-1.79593913	0.39933322
6	-6.28408804	-0.75990519	0.53444840
1	-6.46421967	0.84025417	-1.68282402
8	1.08917255	-2.01874167	2.03729472
8	0.44600918	-0.35731188	3.90955948
6	-1.42364062	-1.92022045	2.88771128
6	-2.32647133	-1.47157709	3.85264507
6	-3.53285715	-2.15583041	4.03288182
6	-3.84448434	-3.29184069	3.27236596
6	-2.90834887	-3.73295029	2.31941969
6	-1.70740134	-3.05364776	2.11962114
1	-2.06823209	-0.61382645	4.47337578
1	-4.23710409	-1.80868848	4.79165129
6	-5.14650256	-4.02904543	3.46733198
1	-3.12260002	-4.62668764	1.72931056
1	-0.97528719	-3.40485878	1.39234539
1	-7.08857887	-0.01499639	0.48939410
1	-6.74049441	-1.75316934	0.40263078
1	-5.84338975	-0.73841595	1.54073751
1	-4.97996463	-5.10922547	3.58519162
1	-5.68320690	-3.66672893	4.35332592
1	-5.80932586	-3.90066473	2.59737842
1	0.08575023	0.58637613	-3.35638517

Energy = -8524.610277 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 61

Atomic N.	X	Y	Z
8	2.59671608	0.34745976	0.86496982
8	2.30822643	1.61349720	-1.17220597
6	2.37002523	1.77785434	-2.56701997
1	1.48236076	2.33769536	-2.93172325

1	2.39170509	0.82103204	-3.12792389
1	3.25389250	2.37197055	-2.86793478
8	4.33806816	1.67371243	0.46786858
6	3.54599577	0.64035406	0.05754344
6	4.11706231	-0.46613764	-0.81828681
1	4.59599837	-1.17302538	-0.11437909
1	3.24251175	-1.00709478	-1.20786740
6	5.08188329	-0.13639460	-1.96544832
1	4.65642834	0.65308194	-2.59894755
1	5.14897294	-1.03446773	-2.59944612
6	6.49618313	0.26346833	-1.53843386
1	6.93902836	-0.54687185	-0.93320318
1	7.12813943	0.35977140	-2.43529127
6	6.54865681	1.56607327	-0.73919120
1	6.17031216	2.40952955	-1.33927711
1	7.59671146	1.80241710	-0.48981838
6	5.77789394	1.51466162	0.57410980
1	5.99785725	0.58525235	1.12553485
1	6.06513555	2.35848020	1.21432296
50	0.62025023	0.24018257	-0.13482743
7	0.06786622	2.56378522	0.75759802
6	1.26754835	3.04719156	1.48581768
1	1.03292436	3.98576212	2.01963516
1	1.61216656	2.29043003	2.19584884
1	2.07312410	3.21675652	0.76329673
7	-0.32436942	0.08919217	1.92221028
6	-1.06570303	2.36070243	1.69434182
1	-1.29721819	3.30227699	2.22794896
1	-1.94449916	2.06766992	1.10516669
6	-0.76361811	1.24510164	2.69526317
1	-1.69805680	1.04007593	3.24962870
1	-0.01317141	1.56629762	3.43726267
16	0.07602183	-1.27886970	2.72971400
7	-1.63797898	2.07230732	-1.71074433
6	-0.23425807	3.56736510	-0.29638713
1	-0.26680097	4.57539449	0.16204439
1	0.62389387	3.55221464	-0.98429173
6	-1.54587277	3.39700002	-1.06027802
1	-1.61292839	4.22542024	-1.78613861
1	-2.40879201	3.48683254	-0.38904254
16	-3.23150156	1.72020410	-2.29447620
8	-3.48669062	2.42962701	-3.56825150
8	-4.12052038	1.92540221	-1.13313049
6	-3.07638004	-0.03421935	-2.65002464
6	-3.04983318	-0.95155243	-1.59538239
6	-2.95657975	-2.30837826	-1.89260650
6	-2.88406622	-2.76126044	-3.22196914
6	-2.91907184	-1.81445978	-4.25602083
6	-3.01614261	-0.44892984	-3.98029800
1	-3.10724681	-0.60763527	-0.56318920
1	-3.05946973	0.29035926	-4.77917557
1	-2.87378072	-2.14879691	-5.29371579
6	-2.75234908	-4.23290312	-3.51968145
1	-2.93347182	-3.03266143	-1.07674678
8	0.69931269	-2.14613327	1.68768079
8	0.78680044	-1.01228714	4.00392792
6	-1.49852451	-2.05816183	3.19001986
6	-2.00074219	-1.90388705	4.48193725

6	-3.22807948	-2.48704130	4.81295522
6	-3.95722616	-3.22804424	3.87321283
6	-3.41947328	-3.38132134	2.58227909
6	-2.20153231	-2.80032721	2.23618569
1	-1.42019484	-1.35206491	5.22071818
1	-3.62057135	-2.37025916	5.82501114
6	-5.28612627	-3.84738025	4.22871462
1	-3.96383855	-3.97341581	1.84309368
1	-1.77092707	-2.93565200	1.24368849
1	-1.74492036	-4.59157578	-3.25854060
1	-3.46719968	-4.82456746	-2.93115836
1	-2.91999568	-4.44506265	-4.58291707
1	-5.32499411	-4.90607187	3.93465809
1	-5.48144585	-3.78379394	5.30669816
1	-6.11094734	-3.33782111	3.70740452
1	-1.01256309	2.01466369	-2.52291961

Energy = -8524.608913 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 62

Atomic N.	X	Y	Z
8	2.62398568	0.27915193	0.83459174
8	2.45734612	1.59303483	-1.18991745
6	2.55564112	1.77715726	-2.58133535
1	1.66640561	2.32296171	-2.95945489
1	2.60874955	0.82807896	-3.15307684
1	3.43856140	2.38829898	-2.84939251
8	4.41414301	1.56711847	0.54046604
6	3.61408563	0.56359759	0.07384350
6	4.19412547	-0.53573649	-0.80434600
1	4.63252756	-1.26956702	-0.10147735
1	3.32357098	-1.04706552	-1.24022408
6	5.20757280	-0.19672714	-1.90603318
1	4.82385825	0.62239772	-2.52847431
1	5.27602841	-1.07648267	-2.56502248
6	6.61445719	0.15474559	-1.41652996
1	7.01429863	-0.68268244	-0.81831623
1	7.28194426	0.25896749	-2.28636928
6	6.66825537	1.43368276	-0.58011205
1	6.33517744	2.30212051	-1.17129341
1	7.71102501	1.63627812	-0.28330813
6	5.84388466	1.36826186	0.69963802
1	6.01892705	0.41980498	1.23457239
1	6.12601983	2.18802810	1.37261680
50	0.68469863	0.25338258	-0.26400325
7	0.14438473	2.56992111	0.73925776
6	1.41292788	3.15764706	1.23863602
1	1.21319342	4.12976802	1.72441771
1	1.88526021	2.47726015	1.95306573
1	2.10367980	3.28206548	0.39774443
7	-0.27533960	0.01173829	1.76861524
6	-0.78594652	2.34084622	1.87717785
1	-0.84547986	3.24985004	2.50525850
1	-1.78261552	2.12569428	1.47351943
6	-0.36051897	1.12867757	2.70441303
1	-1.13557524	0.96169821	3.47305811
1	0.58915447	1.30456557	3.23698606

16	-0.23108020	-1.50948636	2.36538306
7	-1.78649116	1.85168002	-1.53226812
6	-0.40940296	3.50947117	-0.27040203
1	-0.49784407	4.51914802	0.17805471
1	0.34270511	3.58206229	-1.07058445
6	-1.77924463	3.16931121	-0.86029445
1	-2.05636233	3.98584086	-1.54756103
1	-2.54642036	3.14036641	-0.07647800
16	-3.38554910	1.20573549	-1.73332307
8	-4.13778509	1.97499125	-2.75001429
8	-3.91891838	1.08494642	-0.35972871
6	-3.00499448	-0.41400338	-2.40895944
6	-2.42892305	-1.39059266	-1.59087329
6	-2.16204382	-2.64715608	-2.12774675
6	-2.46433707	-2.94092472	-3.46895142
6	-3.04818599	-1.94120783	-4.26278752
6	-3.32026509	-0.67398011	-3.74367533
1	-2.19245285	-1.18358570	-0.54874842
1	-3.78297830	0.10266446	-4.35148022
1	-3.29661643	-2.15646160	-5.30333358
6	-2.14680540	-4.29850984	-4.04181308
1	-1.69986553	-3.40214660	-1.49000710
8	0.00633826	-2.36754517	1.16408174
8	0.65486198	-1.67833066	3.54326119
6	-1.91451207	-1.85477257	2.96960280
6	-2.06750147	-2.74470544	4.03644632
6	-3.35003937	-3.06114591	4.48426578
6	-4.48916547	-2.49424102	3.88880354
6	-4.30680535	-1.58840988	2.83321518
6	-3.02911936	-1.26725110	2.36862128
1	-1.18276124	-3.16698487	4.51194789
1	-3.46914815	-3.75524116	5.31888248
6	-5.87236828	-2.86144240	4.36658885
1	-5.17458476	-1.11799541	2.36700134
1	-2.90704161	-0.54591636	1.55993505
1	-1.06296254	-4.40662184	-4.20189995
1	-2.45040800	-5.10071510	-3.35545193
1	-2.64661108	-4.45649911	-5.00573365
1	-6.19373839	-3.82194564	3.93412947
1	-5.90330020	-2.97231470	5.45927137
1	-6.61124346	-2.10433593	4.07372849
1	-1.37444266	1.90971135	-2.47029630

Energy = -8524.608281 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 63

Atomic N.	X	Y	Z
8	3.18093228	1.25591111	-0.04479104
8	3.14973164	-0.29789466	-1.96472383
6	2.99362564	-0.12888557	-3.36675620
1	3.87672544	-0.53518909	-3.89098883
1	2.87697530	0.93547100	-3.63740706
1	2.10504913	-0.67250562	-3.71965122
8	4.30540228	2.11507893	-1.74789333
6	4.14426661	1.09252214	-0.87528712
6	5.32455349	0.22691818	-0.46134493
1	5.97219944	0.87719184	0.15847489

1	4.89871740	-0.51303869	0.22800046
6	6.15613174	-0.49075490	-1.53114235
1	5.46856213	-1.05058467	-2.18073130
1	6.77533770	-1.24009240	-1.01409948
6	7.07429790	0.40699828	-2.36273623
1	7.81924868	0.88122815	-1.69930315
1	7.64476013	-0.21730138	-3.06796288
6	6.34239149	1.50506318	-3.13756299
1	5.63126469	1.07765543	-3.86090136
1	7.07499695	2.08222175	-3.72614169
6	5.61369705	2.50948405	-2.25333214
1	6.24207735	2.80252457	-1.39550841
1	5.37640333	3.41574621	-2.82398558
50	1.53758323	-0.23222770	-0.47860545
7	0.50196511	1.93307018	1.14595187
6	1.33857965	2.39908504	2.26173568
1	0.92775297	3.31490564	2.73236990
1	1.42789865	1.61310744	3.02050805
1	2.34097695	2.61587143	1.87503576
7	-0.16888209	-0.43385774	2.77377343
6	-0.87845922	1.62434793	1.55916190
1	-1.44775891	2.55848742	1.75529075
1	-1.37195134	1.11736000	0.71667624
6	-1.02406025	0.76082730	2.81521297
1	-2.09623528	0.50391150	2.89227366
1	-0.76234853	1.32849181	3.71782160
16	-0.47876519	-1.68443751	3.86448765
7	0.21093363	1.16767573	-1.57877743
6	0.51065123	2.94826794	0.07153049
1	0.06101933	3.89975595	0.42608717
1	1.56470382	3.13608146	-0.17190862
6	-0.22810394	2.50906396	-1.19490516
1	-0.01024016	3.24731207	-1.98528337
1	-1.32026100	2.53302026	-1.02444422
16	-0.65759385	0.34479412	-2.69461703
8	-0.01753514	-1.01359189	-2.66875243
8	-0.80165470	1.06764913	-3.97803068
6	-2.33899450	0.14608581	-2.04067755
6	-3.36619163	0.96682745	-2.50825930
6	-4.64813042	0.83109707	-1.96759999
6	-4.91894674	-0.11645233	-0.97013038
6	-3.86679912	-0.93443084	-0.52084017
6	-2.58278728	-0.80846721	-1.04822433
1	-3.15853238	1.68866909	-3.29750180
1	-1.77404845	-1.45729208	-0.70878488
1	-4.05375099	-1.68059981	0.25411677
6	-6.30958652	-0.27934152	-0.40868518
1	-5.45258713	1.47305369	-2.33147168
8	0.57797438	-2.68269682	3.62794018
8	-0.69078273	-1.03780425	5.17334414
6	-2.05154133	-2.43496180	3.37267542
6	-3.23786926	-2.02761722	3.98468184
6	-4.44371510	-2.61309385	3.58757496
6	-4.47893000	-3.60127616	2.59332967
6	-3.26569295	-3.99952722	2.00238681
6	-2.05533361	-3.42319608	2.38218331
1	-3.20670056	-1.28412473	4.78046894
1	-5.37265253	-2.30322838	4.06970119

6	-5.78160810	-4.22561693	2.16000700
1	-3.27014947	-4.77831078	1.23731601
1	-1.11442041	-3.74965310	1.93891132
1	-6.92905378	0.60458314	-0.60741949
1	-6.81484365	-1.14673471	-0.86147457
1	-6.28472567	-0.44882208	0.67669910
1	-5.71880579	-5.32295561	2.16564035
1	-6.60847092	-3.92550611	2.81574702
1	-6.03956556	-3.92532754	1.13259685
1	0.05167780	-0.80001825	1.83893061

Energy = -8524.624039 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 64

Atomic N.	X	Y	Z
8	2.92627862	0.30028621	0.85432201
8	2.95589709	1.06327164	-1.42539917
6	3.28610172	0.99599149	-2.79215867
1	4.19524087	1.58468270	-3.01791432
1	2.47423586	1.43611948	-3.40886379
1	3.44201098	-0.03721678	-3.16176765
8	4.62848684	1.67587608	0.47657772
6	3.99390856	0.50811539	0.17287140
6	4.78573112	-0.70313684	-0.30235233
1	5.18525957	-1.16293574	0.62175881
1	4.03148709	-1.41527433	-0.66696117
6	5.90665159	-0.55919243	-1.34066388
1	5.53716145	-0.01483553	-2.21926941
1	6.15107024	-1.57391513	-1.69192455
6	7.19066638	0.10244693	-0.83601102
1	7.59673768	-0.48137188	0.00857832
1	7.95077602	0.06356798	-1.63197582
6	6.99751947	1.55162318	-0.38764032
1	6.63866355	2.17720622	-1.22103392
1	7.96841105	1.97132906	-0.07537743
6	6.04563287	1.70886109	0.79193367
1	6.25693043	0.95743906	1.57112682
1	6.16442706	2.70160722	1.24420783
50	1.20687720	-0.24520081	-0.41855569
7	0.32194658	2.14750654	-0.17110988
6	1.30933575	2.88832666	0.65244015
1	0.91026681	3.88430077	0.91704067
1	1.54415899	2.32717326	1.56099089
1	2.23653760	2.99563742	0.07918564
7	-0.13289093	-0.07688596	1.40649359
6	-0.96443558	2.01032850	0.55485689
1	-1.36481129	3.00688849	0.82325268
1	-1.67758668	1.51498235	-0.11633714
6	-0.81225010	1.14828670	1.80940912
1	-1.83047163	0.95107990	2.19377006
1	-0.26796911	1.68582208	2.60398178
16	0.17198247	-1.21675558	2.54132872
7	-0.78999244	1.02196273	-2.77656473
6	0.17864591	2.89239825	-1.45042040
1	-0.01569177	3.95977354	-1.22692467
1	1.16072951	2.83929918	-1.94295770
6	-0.92372616	2.44066046	-2.40683575

1	-0.89520810	3.10684949	-3.28512647
1	-1.91338005	2.57176004	-1.94722252
16	-2.06806765	0.39395887	-3.74853938
8	-1.51389486	-0.84907613	-4.31673032
8	-2.63210798	1.44516814	-4.62433900
6	-3.30045300	0.01318721	-2.49126660
6	-4.55071583	0.62717800	-2.56013158
6	-5.51108361	0.31043097	-1.59590877
6	-5.23306966	-0.60344347	-0.56899880
6	-3.96097593	-1.20365261	-0.52613155
6	-2.99396233	-0.90640190	-1.48312940
1	-4.75778009	1.33946680	-3.35794396
1	-2.00902720	-1.37263838	-1.44478612
1	-3.71991964	-1.90705485	0.27287349
6	-6.27364643	-0.95255730	0.46474409
1	-6.49181237	0.78694461	-1.64190853
8	1.13230190	-2.14526277	1.87682346
8	0.48023200	-0.63591450	3.87045035
6	-1.37433084	-2.14883402	2.75134842
6	-2.28190845	-1.77691267	3.74405882
6	-3.47876414	-2.48772884	3.87935587
6	-3.77489923	-3.57677411	3.04753174
6	-2.83538409	-3.94005028	2.06551835
6	-1.64412241	-3.23268400	1.90998975
1	-2.03690526	-0.95588496	4.41746958
1	-4.18861327	-2.19815554	4.65683912
6	-5.05519564	-4.35853863	3.21042363
1	-3.04043754	-4.79337386	1.41531350
1	-0.91024318	-3.52225648	1.15776811
1	-7.11126352	-0.24390760	0.44797028
1	-6.68192509	-1.95834422	0.28114463
1	-5.84197075	-0.95983334	1.47522552
1	-4.85226400	-5.38047541	3.56475901
1	-5.72741252	-3.88014762	3.93410533
1	-5.59102932	-4.45269734	2.25443417
1	0.06929885	0.82152712	-3.30109154

Energy = -8524.610252 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 65

Atomic N.	X	Y	Z
8	2.92342199	0.30527357	0.85924841
8	2.94799197	1.05574103	-1.42512671
6	3.27484638	0.97763839	-2.79206894
1	4.18848086	1.55703972	-3.02352811
1	2.46573025	1.42158964	-3.40984627
1	3.42093250	-0.05910914	-3.15586680
8	4.62560660	1.67701181	0.46819103
6	3.98898643	0.50813336	0.17301161
6	4.77836494	-0.70666388	-0.29754250
1	5.17984348	-1.16167644	0.62806260
1	4.02232098	-1.42001615	-0.65611824
6	5.89648049	-0.57019575	-1.33986755
1	5.52491435	-0.03137430	-2.22096184
1	6.13911459	-1.58737469	-1.68525359
6	7.18257860	0.09383023	-0.84362661
1	7.59160006	-0.48541855	0.00267463

1	7.93965207	0.05007965	-1.64223549
6	6.99160797	1.54565489	-0.40292485
1	6.62998045	2.16649416	-1.23868154
1	7.96378325	1.96695052	-0.09679339
6	6.04374527	1.71009760	0.77894228
1	6.25680104	0.96255135	1.56135635
1	6.16511092	2.70513411	1.22542259
50	1.20141686	-0.24919303	-0.40555992
7	0.31907653	2.14015664	-0.17204459
6	1.29091918	2.87827718	0.67198834
1	0.88703225	3.87354162	0.93178056
1	1.50793129	2.31417251	1.58322609
1	2.22865130	2.98782745	0.11655820
7	-0.14603715	-0.07027448	1.41303015
6	-0.98122528	2.00205507	0.52745780
1	-1.39079791	2.99815170	0.78329777
1	-1.67813723	1.50186633	-0.15696344
6	-0.85564633	1.14603817	1.78914485
1	-1.88473373	0.93734962	2.13772026
1	-0.34533317	1.69398093	2.59918692
16	0.14973535	-1.19800514	2.56176545
7	-0.77110952	1.01776412	-2.78206347
6	0.20093732	2.88557555	-1.45364159
1	0.01121351	3.95445070	-1.23368346
1	1.18982908	2.82366393	-1.93105122
6	-0.89229711	2.44067704	-2.42392225
1	-0.84368231	3.10039849	-3.30606264
1	-1.88670582	2.58681548	-1.97944877
16	-2.05981641	0.39078415	-3.74083451
8	-1.51781730	-0.86007011	-4.30353759
8	-2.62290963	1.43988798	-4.61958924
6	-3.28533257	0.02630721	-2.47202547
6	-4.52188260	0.66960814	-2.51777443
6	-5.47453071	0.36888279	-1.54081756
6	-5.20252215	-0.55859712	-0.52445483
6	-3.94457380	-1.18913806	-0.50548831
6	-2.98539127	-0.90748404	-1.47502423
1	-4.72459977	1.39118156	-3.30847508
1	-2.01118847	-1.39680085	-1.45508044
1	-3.70807256	-1.90353778	0.28504504
6	-6.23547028	-0.89077651	0.52239427
1	-6.44435532	0.86858667	-1.56843274
8	1.13336787	-2.12011352	1.92362402
8	0.42507987	-0.60255514	3.89178354
6	-1.38915820	-2.14700608	2.74930062
6	-2.32050177	-1.77869613	3.72104472
6	-3.51023219	-2.50445613	3.83977245
6	-3.77599712	-3.60439713	3.01198181
6	-2.81327371	-3.96302139	2.05089662
6	-1.62869101	-3.24119949	1.91212964
1	-2.09922756	-0.94885670	4.39188008
1	-4.23836346	-2.21822458	4.60143784
6	-5.04878444	-4.40179931	3.15683759
1	-2.99438204	-4.82441665	1.40423696
1	-0.87684726	-3.52730254	1.17655168
1	-7.04623592	-0.15146978	0.53665364
1	-6.68488491	-1.87641604	0.32579335
1	-5.78526603	-0.93597778	1.52368058

1	-4.83732503	-5.42442986	3.50389031
1	-5.73277838	-3.93722773	3.87844062
1	-5.57514208	-4.49334515	2.19529965
1	0.08417363	0.80539607	-3.30832268

Energy = -8524.610257 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 66

Atomic N.	X	Y	Z
8	3.35215735	-1.10636365	-0.40507045
8	3.85119915	1.17460966	-1.08637953
6	3.93626952	1.10398936	-2.51467657
1	3.20913863	1.80130732	-2.95432186
1	3.71222615	0.09085493	-2.89111018
1	4.94289589	1.39831138	-2.84952116
8	4.31610012	0.18058896	1.11331558
6	4.38407993	-0.36731100	-0.14961968
6	5.72900772	-0.79997659	-0.71701002
1	6.09983444	-1.58439505	-0.03209991
1	5.48998308	-1.31164289	-1.65865850
6	6.82601547	0.24508837	-0.97000974
1	6.42949343	1.03156888	-1.62529016
1	7.62572098	-0.25632760	-1.53753126
6	7.43532562	0.90177315	0.26881787
1	7.95366096	0.14178988	0.87978315
1	8.20843792	1.61503243	-0.05724213
6	6.40876961	1.62305129	1.14526844
1	5.82763433	2.35193372	0.55913997
1	6.93580580	2.18871546	1.93112278
6	5.45584965	0.67459160	1.86072314
1	6.00728750	-0.19805507	2.25282741
1	4.97825193	1.17865407	2.71034861
50	1.79157913	0.54282284	-0.27527753
7	0.06976902	-2.59270906	-0.16151705
6	1.17174423	-3.50909400	0.15977792
1	0.93063700	-4.55905342	-0.11112006
1	2.08525252	-3.20558357	-0.36358151
1	1.37840438	-3.46423674	1.23666275
7	0.94238144	-0.41370651	-2.07191157
6	-0.20893662	-2.58404422	-1.60673177
1	-0.28286552	-3.62478161	-1.99564898
1	-1.18730044	-2.11021566	-1.76720929
6	0.83457738	-1.82418919	-2.43806124
1	0.58192319	-1.92446828	-3.50664520
1	1.82999861	-2.27663016	-2.31142974
16	0.31772348	0.76795846	-3.00426602
7	-1.57187498	-0.64853317	1.47214437
6	-1.13267410	-2.96426010	0.60449195
1	-1.65247607	-3.83325338	0.14405718
1	-0.81718427	-3.27345467	1.61056912
6	-2.12550855	-1.80890357	0.75344503
1	-3.01007509	-2.16906762	1.29564846
1	-2.47180986	-1.45187509	-0.22844955
16	-1.72002017	-0.61784256	3.16747117
8	-0.53044838	0.11495859	3.64631605
8	-2.06779885	-1.95982182	3.68864870
6	-3.17063046	0.43084151	3.41294885

6	-4.36240387	-0.13641234	3.86093807
6	-5.47093534	0.68956929	4.06739902
6	-5.39921999	2.07078242	3.83798337
6	-4.18094540	2.61337900	3.39000463
6	-3.06684351	1.80496740	3.17828202
1	-4.40944815	-1.20766616	4.05316257
1	-2.12077999	2.22990108	2.84344769
1	-4.10528612	3.68724585	3.20908380
6	-6.58769083	2.96358252	4.09262037
1	-6.40660954	0.25091189	4.41882038
8	0.77605689	1.99481201	-2.25031400
8	0.63982838	0.62299687	-4.44173861
6	-1.49193525	0.75615793	-2.89759040
6	-2.23926449	0.31781989	-3.99147201
6	-3.63314533	0.29034752	-3.89698076
6	-4.29038715	0.70341945	-2.72901392
6	-3.51142550	1.14515090	-1.64460099
6	-2.12044430	1.17277575	-1.72040367
1	-1.72779882	0.01804094	-4.90538597
1	-4.21998262	-0.05324155	-4.75090170
6	-5.79611778	0.70318949	-2.64272237
1	-4.00158310	1.46971118	-0.72461659
1	-1.52816629	1.51911235	-0.87307250
1	-7.52089500	2.38770795	4.13560677
1	-6.47924995	3.49238491	5.05230284
1	-6.68783998	3.73014545	3.31199169
1	-6.19588947	1.71820581	-2.79221916
1	-6.24196959	0.05563302	-3.40850759
1	-6.14012766	0.36311266	-1.65632725
1	-0.57903105	-0.49238944	1.25108624

Energy = -8524.618740 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 67

Atomic N.	X	Y	Z
8	3.38641334	-1.09991801	-0.73997557
8	3.58019066	0.97775328	0.57217890
6	4.09268284	2.14640522	-0.05883375
1	3.27456379	2.87229824	-0.21692325
1	4.54816675	1.93917382	-1.04609632
1	4.84590578	2.63316107	0.58229327
8	3.79593277	-1.36717844	1.40433562
6	4.20086336	-0.82093281	0.23085272
6	5.68184948	-0.73771691	-0.12017198
1	6.02742386	-1.78844655	-0.11166421
1	5.71022511	-0.42116761	-1.17126822
6	6.64500475	0.12991627	0.69890034
1	6.34094763	1.18161035	0.62008303
1	7.63083506	0.06009911	0.21215440
6	6.78951359	-0.23351797	2.17636013
1	7.23328733	-1.24026501	2.27499771
1	7.50489092	0.46459287	2.63866735
6	5.46665907	-0.19296578	2.94640183
1	4.92858362	0.75080746	2.77357006
1	5.67347193	-0.24676064	4.02803135
6	4.54256010	-1.36392093	2.65478611
1	5.10730028	-2.31209230	2.69169474

1	3.74463654	-1.40326059	3.40750527
50	1.67803335	0.32559788	-0.50026464
7	0.47106680	-2.08982301	-0.94840533
6	1.03581452	-2.88125014	-2.05496383
1	0.58914876	-3.89307547	-2.10522032
1	0.87285870	-2.36527967	-3.00797462
1	2.11628079	-2.97389364	-1.89490390
7	-0.83291966	-0.39170811	-3.02522993
6	-0.99279112	-1.91274476	-1.05390275
1	-1.51376295	-2.84746647	-0.76020974
1	-1.28192592	-1.13919401	-0.32545391
6	-1.53458059	-1.54004955	-2.43575764
1	-2.61600351	-1.35042524	-2.30230308
1	-1.43670952	-2.37894964	-3.13686895
16	-1.46469760	0.27396899	-4.44996500
7	0.72203052	-0.49092683	1.30097878
6	0.82087487	-2.72828102	0.34197286
1	0.35740316	-3.73300338	0.41740623
1	1.91159022	-2.84659195	0.34349859
6	0.40559420	-1.89344823	1.55667424
1	0.94964737	-2.28352451	2.43380857
1	-0.67458099	-2.01868725	1.76028872
16	0.56318653	0.59421045	2.51917601
8	0.94585794	1.89122391	1.88972962
8	1.21454203	0.15197933	3.77677417
6	-1.21459150	0.67463279	2.87903857
6	-1.72567546	0.05309170	4.01769781
6	-3.09962440	0.11367042	4.27064848
6	-3.96846461	0.78879529	3.40241790
6	-3.42431879	1.41469240	2.26603484
6	-2.05815649	1.35934567	1.99843788
1	-1.04525340	-0.45154595	4.70283222
1	-1.63582504	1.86374462	1.12887609
1	-4.08237314	1.96121335	1.58719337
6	-5.45197248	0.84266287	3.67083144
1	-3.50106311	-0.36677516	5.16496229
8	-0.55812258	1.38122261	-4.79666805
8	-1.71558976	-0.86712700	-5.35043859
6	-3.06938481	0.99188066	-4.02215338
6	-4.23788881	0.25784695	-4.23327017
6	-5.46694946	0.82244229	-3.88263011
6	-5.54370785	2.10916328	-3.32956719
6	-4.34989214	2.82557225	-3.13193035
6	-3.11518025	2.27827716	-3.47499490
1	-4.17911816	-0.73112726	-4.68663788
1	-6.38376045	0.25421482	-4.04990530
6	-6.87511873	2.72849965	-2.98649168
1	-4.39061642	3.83240867	-2.71202826
1	-2.19357657	2.84549093	-3.34384346
1	-5.68816423	0.49826309	4.68560219
1	-5.84179401	1.86376131	3.55431867
1	-6.00372219	0.20411578	2.96375299
1	-7.19707394	3.42171717	-3.77904892
1	-7.65674734	1.96600711	-2.87688828
1	-6.81988811	3.30727649	-2.05445552
1	-0.56425130	0.35023367	-2.36845541

Energy = -8524.616760 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 68

Atomic N.	X	Y	Z
8	2.97092652	-0.79121059	0.76725352
8	2.84796619	0.13233519	-1.48015571
6	3.25970435	1.14620268	-2.40326142
1	3.32885456	2.13284516	-1.92072034
1	2.53902793	1.20521545	-3.23100400
1	4.24568367	0.87591016	-2.81585741
8	3.88502216	1.30358136	0.44938961
6	3.79300618	-0.06744582	0.12825815
6	5.12513828	-0.65139794	-0.33245829
1	5.01596403	-1.74417830	-0.30013284
1	5.32720327	-0.36988023	-1.37445199
6	6.30826902	-0.19629261	0.55290353
1	6.70297289	0.75485921	0.16399644
1	7.11321211	-0.93721074	0.42904484
6	6.01060104	-0.01545025	2.05627489
1	5.37071705	-0.83472842	2.42341328
1	6.96018887	-0.09663186	2.60760283
6	5.38246202	1.34695077	2.40346742
1	6.03472519	2.14427781	2.01022053
1	5.35080099	1.47412765	3.49868846
6	3.96489048	1.55480647	1.87837386
1	3.24363136	0.91118497	2.40198636
1	3.65013885	2.59964037	2.00100183
50	0.90382588	0.26984027	-0.42086700
7	0.72489268	-2.32055259	-0.70959228
6	1.75452816	-2.73784566	-1.69026673
1	1.60199845	-3.79186583	-1.98726141
1	1.71710980	-2.09560657	-2.57501674
1	2.74251342	-2.62248683	-1.23411596
7	-0.38360974	-0.29173705	-2.17995024
6	-0.63177818	-2.50267315	-1.28518808
1	-0.79866272	-3.56732011	-1.53889573
1	-1.36297381	-2.21145058	-0.51825315
6	-0.84330571	-1.62882900	-2.52353072
1	-1.92118561	-1.64809442	-2.76651263
1	-0.31027070	-2.04244423	-3.39647961
16	-0.62627417	0.95540828	-3.20084000
7	0.49680388	-1.43481982	2.22307539
6	0.90706241	-3.15457892	0.50978506
1	0.66897112	-4.20775414	0.26469418
1	1.97465336	-3.10295224	0.76238114
6	0.09930891	-2.76645398	1.74531293
1	0.27553734	-3.54388237	2.50710535
1	-0.98185503	-2.75922036	1.53941786
16	-0.03600949	-0.97038215	3.77446890
8	0.91540623	0.07523097	4.19939709
8	-0.29857874	-2.16379309	4.60879707
6	-1.63026655	-0.20666417	3.41691065
6	-2.80496788	-0.86444622	3.78329825
6	-4.03290892	-0.25517082	3.51638865
6	-4.09925461	0.99885529	2.89020586
6	-2.89739847	1.64035404	2.54381275
6	-1.66276884	1.04737341	2.80152059
1	-2.74706721	-1.82963145	4.28522682

1	-0.73323715	1.55103564	2.53809619
1	-2.92914224	2.62329865	2.07005954
6	-5.43011904	1.63625252	2.57953286
1	-4.95535564	-0.76080912	3.80746794
8	0.09901905	2.07807922	-2.52383518
8	-0.31833401	0.63330519	-4.61516809
6	-2.39687896	1.34439862	-3.14006257
6	-3.17713571	1.20056665	-4.28645945
6	-4.54120016	1.50132167	-4.22540569
6	-5.13320541	1.94745457	-3.03590226
6	-4.32165194	2.08061337	-1.89437628
6	-2.96191835	1.78170323	-1.93816578
1	-2.70899367	0.86567581	-5.21154547
1	-5.15443468	1.38982821	-5.12162161
6	-6.59812069	2.30296493	-2.98192787
1	-4.76466608	2.42918277	-0.95890355
1	-2.33744192	1.89283085	-1.05077839
1	-6.19418955	1.34856451	3.31354785
1	-5.35708952	2.73156548	2.56475019
1	-5.79244947	1.31640363	1.58956456
1	-6.73700333	3.39476228	-3.01594210
1	-7.14652491	1.87313116	-3.82982969
1	-7.06380749	1.94710517	-2.05240297
1	1.50930071	-1.25315297	2.16044497

Energy = -8524.622363 Hartree

Number of imaginary frequencies = 0.

Compound TS2a isomer 69

Atomic N.	X	Y	Z
8	2.78366017	1.58932710	1.88971353
8	3.38124561	0.18107696	0.06349078
6	4.06307888	0.55895829	-1.13343537
1	4.58804560	1.51797271	-1.00820220
1	3.33112502	0.66877556	-1.94949055
1	4.79677820	-0.21498382	-1.41598260
8	4.91634464	1.79001796	1.24794853
6	3.88908792	0.94488645	1.59459198
6	4.18692589	-0.28601420	2.44773340
1	4.46878529	0.08860775	3.44760466
1	3.21031260	-0.76992792	2.58186889
6	5.21175194	-1.30878329	1.94100749
1	4.98305559	-1.55132067	0.89173096
1	5.06353045	-2.23906302	2.51152349
6	6.67673922	-0.88583094	2.07600522
1	6.91169214	-0.73765945	3.14456701
1	7.32565928	-1.70556462	1.72917259
6	7.02893829	0.39620891	1.31792259
1	6.88537598	0.26737893	0.23301637
1	8.09904099	0.61979312	1.46352291
6	6.25386620	1.62695110	1.78139210
1	6.20647764	1.66502380	2.88277864
1	6.75733185	2.54006696	1.43846798
50	1.29872692	1.08773625	0.42255235
7	0.88571751	-1.53658664	-1.33318555
6	1.68837082	-1.87816596	-2.51349187
1	1.45943856	-2.89549470	-2.89420152
1	1.51716769	-1.15076077	-3.31595063

1	2.75107527	-1.84858716	-2.24223948
7	-0.45175108	0.51592171	-2.86943889
6	-0.55717278	-1.62097704	-1.60390151
1	-0.88015789	-2.67523646	-1.75245035
1	-1.08376110	-1.24138033	-0.71612465
6	-1.02772152	-0.83680636	-2.83364344
1	-2.13140774	-0.81872624	-2.79769802
1	-0.74578714	-1.35034478	-3.76265597
16	-1.22044539	1.69876587	-3.79661918
7	0.56580520	-0.74625498	1.43619418
6	1.27906621	-2.41765165	-0.21801996
1	1.13210130	-3.48688912	-0.48691711
1	2.35423255	-2.25541782	-0.05504597
6	0.53081036	-2.16550326	1.09163857
1	1.01261580	-2.78301549	1.86984491
1	-0.51203918	-2.52186561	1.00358307
16	-0.32650602	-0.21171011	2.69747448
8	-0.16314849	1.28177488	2.56327748
8	-0.01491177	-0.87139702	3.98371482
6	-2.06398153	-0.59095657	2.34313321
6	-2.70222449	-1.61740875	3.04067755
6	-4.03217745	-1.92133975	2.73957062
6	-4.73375225	-1.21214831	1.75348139
6	-4.06629133	-0.18245921	1.06708574
6	-2.73903441	0.13203675	1.35545945
1	-2.15932107	-2.15529895	3.81712556
1	-2.23468995	0.94357908	0.82917386
1	-4.59187126	0.38210124	0.29426798
6	-6.17926025	-1.52357054	1.45647871
1	-4.53364897	-2.72396135	3.28357053
8	-0.36094397	2.89080548	-3.69717264
8	-1.55326366	1.05678821	-5.08248949
6	-2.78014326	2.08577228	-2.96295929
6	-3.97130680	1.51852977	-3.41629767
6	-5.16518021	1.82786095	-2.75694132
6	-5.18325996	2.69537830	-1.65569270
6	-3.96619821	3.25432110	-1.22335672
6	-2.76765275	2.95717955	-1.86770368
1	-3.95961547	0.86662728	-4.28920269
1	-6.10083342	1.39358950	-3.11389780
6	-6.47266150	3.03863978	-0.95255941
1	-3.96028328	3.93915939	-0.37323454
1	-1.83051276	3.41131282	-1.54465401
1	-6.42574692	-2.56358218	1.70679617
1	-6.84613228	-0.87666792	2.04780054
1	-6.41615152	-1.35447931	0.39755568
1	-6.67727709	4.11792517	-1.00834489
1	-7.32512903	2.50896454	-1.39589536
1	-6.42444324	2.77813816	0.11527066
1	-0.15617990	0.89583826	-1.96068990

Energy = -8524.619739 Hartree

Number of imaginary frequencies = 0.

Transition state 2b (TS2b)

Compound TS2b isomer 1

Atomic N. X Y Z

8	-0.17980824	-1.00735784	-0.22878501
8	0.06811032	-0.23812197	2.11850190
6	1.07489479	-0.08265512	3.10024643
1	0.89109117	0.84224808	3.67630005
1	2.09756374	-0.02049766	2.67869353
1	1.05139124	-0.91886944	3.82216120
8	-1.22515750	-2.28553557	1.23661506
6	-0.05706797	-1.71059644	0.83700436
6	1.23953855	-2.45618582	1.11942911
1	1.46959674	-2.45211911	2.19416738
1	2.03157616	-1.88260567	0.62165302
6	1.21468198	-3.91771102	0.62295419
1	0.69273478	-3.98143935	-0.34514597
1	2.25219822	-4.23518419	0.43707275
6	0.58473331	-4.88440657	1.63608217
1	1.15984178	-4.82266808	2.57634687
1	0.69880468	-5.91816711	1.27361679
6	-0.89573646	-4.62459755	1.94147396
1	-1.51583087	-4.86411381	1.06239092
1	-1.22343743	-5.30011702	2.74895787
6	-1.22312689	-3.19478631	2.36477876
1	-0.54736632	-2.82145452	3.14833236
1	-2.24819946	-3.13858986	2.75367713
50	-0.00025157	1.23565602	0.39111322
7	-1.44209456	1.45922196	-1.78972983
6	-1.21144247	2.82650709	-2.28340507
1	-1.84635186	3.05297685	-3.16103721
1	-0.15783457	2.95235658	-2.55625844
1	-1.44210839	3.54769826	-1.49023223
7	1.22983623	0.20133410	-2.71667576
6	-1.24814010	0.45208505	-2.86141276
1	-2.04333854	0.57838535	-3.62479711
1	-1.38928914	-0.53334272	-2.39402318
6	0.08919366	0.47755346	-3.59871984
1	0.00234631	-0.27094099	-4.41334963
1	0.24004374	1.44627762	-4.09645319
6	2.49094272	0.03468788	-3.35910058
6	3.20102215	1.16666424	-3.82107162
6	4.44292784	0.98849374	-4.44375134
6	5.02232933	-0.27429929	-4.60458374
6	4.31485653	-1.38130021	-4.12132406
6	3.06282020	-1.25174916	-3.50995755
7	-2.00075603	1.68416595	1.03595138
6	-2.81528354	1.31226456	-1.24719024
1	-2.96515560	0.24010623	-1.05481267
1	-3.55921793	1.64372373	-1.99969649
6	-3.00941730	2.06838489	0.06234337
1	-3.02750492	3.16466188	-0.12834537
1	-4.02454853	1.82735157	0.42284703
6	-2.37833858	1.79178262	2.40032411
6	-3.32166028	0.88745636	2.96254158
6	-3.67048025	0.99656165	4.31307459
6	-3.11738825	1.97276676	5.15013933
6	-2.18596554	2.85194230	4.59129047
6	-1.81212747	2.78370404	3.24152517
6	2.66703010	2.55992675	-3.60463309
1	4.98317957	1.87254763	-4.79222012
6	6.38256121	-0.43597707	-5.24000645

1	4.74338150	-2.38072777	-4.23380804
6	2.33775330	-2.48223519	-3.01897645
6	-3.91735125	-0.22312184	2.13499641
1	-4.38589907	0.28090718	4.72869158
6	-3.53374577	2.08566928	6.59740353
1	-1.74116516	3.62788033	5.22058105
6	-0.81609225	3.78989530	2.71292949
1	3.47762132	3.29807925	-3.66024375
1	2.18608689	2.63374257	-2.61852765
1	1.91782308	2.84416008	-4.36166334
1	2.25898147	-2.50175905	-1.92073953
1	2.87103319	-3.39116812	-3.32507825
1	1.31149650	-2.54282761	-3.41180062
1	6.59786081	0.38252345	-5.94005680
1	6.45843315	-1.38524401	-5.78836203
1	7.17981243	-0.43499333	-4.47962666
1	-4.30524445	-1.02063358	2.78363347
1	-3.16479516	-0.64584649	1.45572197
1	-4.76162815	0.12481978	1.51720428
1	-1.06265700	4.10026121	1.68853056
1	0.20936553	3.38611078	2.68016362
1	-0.78952193	4.68051434	3.35574484
1	-3.68149900	1.09517694	7.05117178
1	-4.48535299	2.63180494	6.69865561
1	-2.78178048	2.62457657	7.18955088
1	1.00566339	-0.59166890	-2.11098313

Energy = -7584.952132 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 2

Atomic N.	X	Y	Z
8	0.50533301	-0.29961848	0.30359727
8	1.53379798	0.93390870	2.09358716
6	2.53165841	1.09986162	3.08464599
1	2.61844182	2.16818953	3.34727788
1	3.52945304	0.74347347	2.76290274
1	2.25049949	0.56427962	4.00758171
8	-0.21793514	-0.98457640	2.27174067
6	0.85137093	-0.73574203	1.46688724
6	2.08495307	-1.61748219	1.60833299
1	2.55582666	-1.49089909	2.59408283
1	2.80095363	-1.25288641	0.85985047
6	1.77695537	-3.11148310	1.37748575
1	1.06581187	-3.22364140	0.54418904
1	2.70508265	-3.60687804	1.05485404
6	1.25823486	-3.82301927	2.63474298
1	2.03349376	-3.75343418	3.41796637
1	1.13474059	-4.89617729	2.42081308
6	-0.05843094	-3.27194595	3.19661689
1	-0.89188415	-3.48346877	2.50746322
1	-0.29345334	-3.79138374	4.14044523
6	-0.05629333	-1.77150941	3.47970033
1	0.84589577	-1.45708370	4.02584457
1	-0.92851782	-1.49540150	4.08587646
50	1.76729798	1.57699156	-0.05619313
7	0.52506942	1.95944941	-2.44353461
6	1.45629549	1.73832238	-3.55702376

1	1.08319485	2.16872644	-4.50690460
1	1.63028646	0.66421801	-3.68580627
1	2.41656184	2.21227312	-3.31260395
7	-0.15730731	-1.04906034	-2.54138303
6	-0.81239682	1.36557364	-2.68033218
1	-1.39844704	2.03641915	-3.34339309
1	-1.33226883	1.33328474	-1.71160877
6	-0.85253483	-0.02022074	-3.32356286
1	-1.92839086	-0.25607491	-3.45695114
1	-0.42607623	0.02179555	-4.33800220
6	-0.44847217	-2.39863300	-2.89706445
6	0.17069153	-2.97844911	-4.02774334
6	-0.10544606	-4.31310034	-4.35252476
6	-0.96547204	-5.10315752	-3.58321381
6	-1.55806112	-4.51647472	-2.45823193
6	-1.32785678	-3.18089724	-2.10851860
7	0.22541574	3.00868344	0.24850363
6	0.39404777	3.40911341	-2.17853165
1	-0.11222526	3.91306996	-3.02752090
1	1.41620719	3.81560588	-2.10877633
6	-0.34930396	3.72339630	-0.88227153
1	-0.28678516	4.82144594	-0.74247694
1	-1.43096232	3.50722218	-1.00840211
6	-0.28184998	3.40610433	1.51988912
6	-1.50912607	2.89769244	2.01134825
6	-1.98167574	3.32300949	3.25952768
6	-1.27710521	4.23765659	4.04988956
6	-0.06871818	4.73603058	3.55102777
6	0.43781570	4.33790541	2.30701256
6	1.16052759	-2.19668365	-4.85346317
1	0.38838136	-4.75222254	-5.22331905
6	-1.26461589	-6.53343916	-3.96427035
1	-2.23536825	-5.11124897	-1.83951843
6	-2.03086376	-2.58602095	-0.91080016
6	-2.30628967	1.89482951	1.21609497
1	-2.92874002	2.91829777	3.62729383
6	-1.79013729	4.65143108	5.40881634
1	0.49575898	5.46111012	4.14381218
6	1.74535573	4.91505480	1.81840742
1	1.78395176	-2.87082124	-5.45509815
1	1.81089425	-1.59562659	-4.20194197
1	0.66572142	-1.50094497	-5.55022144
1	-1.33194232	-2.26196527	-0.12517172
1	-2.71812296	-3.31805849	-0.46752533
1	-2.61814952	-1.69649029	-1.18585527
1	-2.20567203	-6.60565710	-4.53257132
1	-1.37304783	-7.17210627	-3.07656455
1	-0.46898341	-6.95410967	-4.59394264
1	-3.05938411	1.40810502	1.84962940
1	-1.65027452	1.12233448	0.79316187
1	-2.84189773	2.37412190	0.38015553
1	1.66929901	5.28387356	0.78608412
1	2.55187297	4.16438532	1.81794703
1	2.06657386	5.74440956	2.46273541
1	-1.44990444	3.95485520	6.19186449
1	-2.88855290	4.66053200	5.43762732
1	-1.43104815	5.65236473	5.68508244
1	-0.29373214	-0.89131469	-1.53955650

Energy = -7584.949449 Hartree
 Number of imaginary frequencies = 0.

Compound TS2b isomer 3

Atomic N.	X	Y	Z
8	1.94981384	-1.93702650	-0.34400553
8	0.17605473	-0.85577708	0.75524503
6	-0.38077480	-0.21388665	1.89695489
1	0.38447100	0.23329684	2.55527139
1	-0.98248029	-0.92885053	2.48217845
1	-1.04376328	0.59454727	1.55313957
8	0.64319754	-3.32791066	0.78136945
6	1.38501644	-2.17661119	0.80643362
6	2.18997073	-1.88021111	2.07026768
1	1.53684795	-1.71283400	2.93958020
1	2.71517134	-0.93590254	1.87344587
6	3.19802332	-2.99974942	2.39661574
1	3.64103627	-3.37775373	1.46186328
1	4.02467394	-2.56451058	2.97871828
6	2.58275628	-4.14662838	3.21082878
1	2.20682120	-3.73356462	4.16353703
1	3.37188745	-4.86649132	3.47988486
6	1.44086075	-4.89574766	2.51280332
1	1.82284045	-5.46387672	1.64957249
1	1.01271033	-5.63372707	3.21163249
6	0.30355540	-4.00681829	2.01214242
1	-0.02279161	-3.28920341	2.78202033
1	-0.56468815	-4.62121010	1.73978674
50	1.33909845	0.10062443	-0.95173389
7	0.29260236	2.45614934	-2.66555667
6	1.38240588	2.61742139	-3.63016987
1	1.05616212	3.13695049	-4.55584002
1	1.79265070	1.63911819	-3.91119742
1	2.19220543	3.19916391	-3.16978192
7	0.02079535	-0.60108167	-2.45006847
6	-0.81303018	1.65759480	-3.21260977
1	-1.23179173	2.14370179	-4.12364769
1	-1.60786319	1.62174845	-2.45429754
6	-0.44524935	0.21757805	-3.57288384
1	-1.36529005	-0.23248337	-3.98412228
1	0.27331713	0.21572705	-4.41896486
6	-0.35800931	-1.97781265	-2.57028842
6	0.51594919	-2.92777705	-3.14794540
6	0.09591065	-4.25765705	-3.27945018
6	-1.16458464	-4.68406439	-2.84917879
6	-2.01444173	-3.73463941	-2.27176619
6	-1.63639605	-2.39425039	-2.12695456
7	-0.40956795	3.12653089	0.16428074
6	-0.16618527	3.77954769	-2.21463203
1	-0.70207775	4.31292772	-3.03176785
1	0.73159856	4.37424564	-1.98186719
6	-1.07093334	3.76855946	-0.98256457
1	-1.31387186	4.82048750	-0.75305414
1	-2.02511477	3.27085590	-1.21561563
6	-0.55997568	3.65982628	1.46268785
6	-1.84357321	3.82370949	2.03818202
6	-1.94751263	4.33587027	3.33762264

6	-0.82712448	4.66657066	4.10685015
6	0.43345273	4.45207214	3.53703332
6	0.58936226	3.96292710	2.23624897
6	1.90224040	-2.54433155	-3.60353851
1	0.78001225	-4.98234797	-3.72904205
6	-1.60629129	-6.11684513	-3.03187442
1	-3.00103092	-4.04472160	-1.91642272
6	-2.58873034	-1.41419017	-1.48963928
6	-3.09341168	3.38165808	1.31525660
1	-2.94485402	4.45229197	3.76990199
6	-0.97214466	5.24486828	5.49395943
1	1.32989347	4.68329000	4.11819172
6	1.97448373	3.76432824	1.66891551
1	2.30159187	-3.29337502	-4.30034351
1	2.58499241	-2.48757029	-2.74203253
1	1.91747117	-1.56444919	-4.09961081
1	-2.07754374	-0.82346511	-0.71779495
1	-3.43859506	-1.93987286	-1.03438091
1	-2.99650335	-0.70147020	-2.22475815
1	-2.07539129	-6.26639032	-4.01766396
1	-2.34492731	-6.40824366	-2.27240229
1	-0.75605339	-6.80992746	-2.96825600
1	-3.92887163	3.28828979	2.02095652
1	-2.94073606	2.40607095	0.82934177
1	-3.40525341	4.08642244	0.52933383
1	2.13429451	4.35917282	0.75456893
1	2.17365837	2.71293569	1.40141678
1	2.73627949	4.06722879	2.39803433
1	-0.11626041	4.98150921	6.13047981
1	-1.88694119	4.88455105	5.98460960
1	-1.03058577	6.34483004	5.46478844
1	0.56507981	2.93005943	-0.05822818

Energy = -7584.943302 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 4

Atomic N.	X	Y	Z
8	0.31355259	-0.55969578	-0.50727451
8	1.43800354	0.24447709	-2.56502843
6	2.51161838	1.04829633	-3.00785327
1	2.19862533	1.70438778	-3.83784890
1	3.33128357	0.41002291	-3.39103985
1	2.90902424	1.69453311	-2.20516920
8	2.46401620	-0.22635941	-0.11567446
6	1.50766182	-0.82970977	-0.86753672
6	1.82831812	-2.14933014	-1.55203533
1	2.64607215	-2.02681375	-2.27565813
1	0.93015581	-2.40907907	-2.12467194
6	2.17384362	-3.26924872	-0.54752195
1	1.49899304	-3.21649575	0.32148612
1	1.97086489	-4.23602533	-1.03219295
6	3.64021683	-3.24822688	-0.09675707
1	4.28010607	-3.39573383	-0.98431748
1	3.83139205	-4.10704041	0.56554401
6	4.07894802	-1.96216297	0.61445749
1	3.56790853	-1.86027265	1.58549762
1	5.15758848	-2.02254558	0.83483166

6	3.84396195	-0.67992061	-0.17997606
1	4.16062355	-0.78237575	-1.22880208
1	4.40345383	0.15410300	0.26223421
50	-0.75154799	0.45710444	-2.33092952
7	-3.02656817	0.81852269	-0.75182056
6	-4.11431646	-0.04609632	-1.22062814
1	-5.10765839	0.29569823	-0.86682671
1	-3.94191289	-1.07455194	-0.88380295
1	-4.11666965	-0.04517089	-2.31920934
7	-2.11366677	-1.43573320	1.13128901
6	-2.94062567	0.89246160	0.72259420
1	-3.72228432	1.58367181	1.10594928
1	-1.96635783	1.33728635	0.97350401
6	-3.10771894	-0.41761208	1.49136508
1	-3.05139041	-0.14482889	2.56516433
1	-4.12078094	-0.82028478	1.33597159
6	-1.97931254	-2.52281928	2.04258776
6	-2.92751598	-3.57167864	2.03310204
6	-2.76963496	-4.64704514	2.91669583
6	-1.69121826	-4.72947598	3.80373287
6	-0.75451320	-3.68919969	3.78899312
6	-0.88400751	-2.58487320	2.93842196
7	-0.72714442	2.45253015	-1.57658362
6	-3.17815733	2.17247343	-1.32025445
1	-4.07722044	2.67287421	-0.90255809
1	-3.33986712	2.05042148	-2.40393066
6	-1.96171069	3.06992269	-1.10305727
1	-2.17043614	4.01541662	-1.64352071
1	-1.89320087	3.35693336	-0.03330103
6	0.39456874	3.33190274	-1.54886985
6	1.15393221	3.51637983	-0.36741823
6	2.24750304	4.39342213	-0.38133898
6	2.61444688	5.10806370	-1.52623868
6	1.84391522	4.93091345	-2.68152738
6	0.74863666	4.05971384	-2.71276617
6	-4.07138777	-3.57156944	1.05114233
1	-3.50359821	-5.45679951	2.89064741
6	-1.55527461	-5.88838148	4.76232052
1	0.09777490	-3.72776389	4.47268295
6	0.13154373	-1.46787572	2.99802876
6	0.80353713	2.78565955	0.90451014
1	2.83027506	4.51909733	0.53536439
6	3.81671548	6.02196836	-1.52611649
1	2.10237718	5.48697186	-3.58681560
6	-0.03659662	3.89843869	-3.99246812
1	-4.48716164	-4.58119249	0.93770880
1	-3.73190832	-3.21266937	0.06892814
1	-4.89515209	-2.91304231	1.37073159
1	0.68466395	-1.34814048	2.05432963
1	0.86297530	-1.65691662	3.79424477
1	-0.34500894	-0.49660319	3.20165730
1	-2.04309559	-5.66824007	5.72536182
1	-0.50090271	-6.11178017	4.97551489
1	-2.02382708	-6.79725742	4.36051750
1	1.65100324	2.79239154	1.60253978
1	0.52666146	1.74421942	0.69710875
1	-0.04700052	3.26276231	1.41877913
1	-1.11967742	3.96415567	-3.82086229

1	0.14335428	2.91655087	-4.45891619
1	0.24980609	4.66818905	-4.72137785
1	4.70564699	5.50998688	-1.92804027
1	4.06363964	6.35898447	-0.51031691
1	3.64568853	6.91011858	-2.15045404
1	-1.20886791	-1.00238860	0.93376809

Energy = -7584.947671 Hartree
Number of imaginary frequencies = 0.

Compound TS2b isomer 5

Atomic N.	X	Y	Z
8	0.19077258	-2.58165383	-0.18420228
8	0.54442585	-0.53626221	-1.35530066
6	0.87617344	-0.03566423	-2.65259004
1	0.28567144	0.87594289	-2.83028483
1	0.65752590	-0.75969595	-3.45667148
1	1.94306159	0.23768590	-2.69808555
8	2.14621758	-1.64126992	0.24090998
6	1.26313651	-2.07261920	-0.71792603
6	1.84525764	-2.76258636	-1.94893610
1	2.45262671	-2.07699752	-2.55695772
1	0.98409182	-3.06281662	-2.56093264
6	2.69128227	-3.99584174	-1.57224846
1	2.21950507	-4.52255392	-0.72824579
1	2.67885041	-4.69530773	-2.42186069
6	4.15169859	-3.64713359	-1.25227273
1	4.59755373	-3.16962624	-2.14253592
1	4.71967459	-4.57587242	-1.08580387
6	4.34543848	-2.72172141	-0.04486090
1	4.07832670	-3.24442244	0.88745433
1	5.41175604	-2.45330977	0.03866039
6	3.53794098	-1.42644310	-0.09453784
1	3.63161945	-0.91741401	-1.06688130
1	3.89033270	-0.73120338	0.67915910
50	-1.54103923	-1.56937408	-1.06805098
7	-3.18567801	0.87992549	-0.98267072
6	-4.23764896	0.35818580	-1.86990213
1	-5.16801023	0.95696163	-1.79322755
1	-4.47426891	-0.68384856	-1.62161875
1	-3.88355112	0.38142428	-2.90894818
7	-2.29575038	-1.25551188	0.91028011
6	-3.60521364	0.79049462	0.42896432
1	-4.60999298	1.24831569	0.56043714
1	-2.88986254	1.36230278	1.03333902
6	-3.62424517	-0.64223468	0.96846229
1	-3.95412612	-0.58227158	2.01904702
1	-4.41234875	-1.22293615	0.44545594
6	-1.97238755	-2.11115837	2.00777555
6	-2.66600275	-3.32608175	2.23632503
6	-2.32790613	-4.12086058	3.34097624
6	-1.31559491	-3.75844598	4.23314571
6	-0.63215208	-2.56107378	3.99016309
6	-0.93962729	-1.73640358	2.90282583
7	-0.44581723	2.53744984	-1.09891164
6	-2.92785764	2.28412867	-1.38092697
1	-3.85333538	2.87924385	-1.21458745
1	-2.73084354	2.28208828	-2.46324277

6	-1.77390850	3.01715899	-0.69619071
1	-1.86018193	4.07041788	-0.99227351
1	-1.89652073	3.01078939	0.40298322
6	0.62327093	3.47502160	-1.09940016
6	1.69884598	3.34837914	-0.18587229
6	2.76397491	4.25282764	-0.25021929
6	2.79901600	5.29771423	-1.18185580
6	1.73730052	5.39562559	-2.08628845
6	0.65955544	4.50045919	-2.07471299
6	-3.75155520	-3.80316663	1.30239451
1	-2.86671400	-5.05959129	3.49674964
6	-0.98306036	-4.61547852	5.43131351
1	0.16561246	-2.25342679	4.67160034
6	-0.17675683	-0.45437992	2.70081353
6	1.70197022	2.25290251	0.85254121
1	3.58613276	4.14303446	0.46191430
6	3.93772602	6.28907394	-1.19952822
1	1.75612724	6.17851830	-2.84899163
6	-0.40259030	4.60666656	-3.14163089
1	-3.90819812	-4.88437176	1.41065931
1	-3.49976254	-3.59510422	0.25112268
1	-4.71586084	-3.30931020	1.50231421
1	0.44871938	-0.50817651	1.79936421
1	0.47744310	-0.25440109	3.56032419
1	-0.85784686	0.39889857	2.57082462
1	-1.43161893	-4.20703363	6.35104656
1	0.10217136	-4.66937923	5.59818745
1	-1.36149454	-5.63914680	5.30730629
1	2.58821034	2.33494997	1.49464488
1	1.70433927	1.24709928	0.40351433
1	0.81470233	2.30538511	1.50192690
1	-1.29876149	5.14873266	-2.79919291
1	-0.73303914	3.60711455	-3.45970297
1	-0.01566726	5.14651775	-4.01578712
1	4.89881229	5.80192661	-0.98278201
1	3.79474950	7.07462025	-0.44042084
1	4.01871443	6.78728247	-2.17509174
1	-0.19353820	1.68831611	-0.59176421

Energy = -7584.942249 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 6

Atomic N.	X	Y	Z
8	1.66119587	0.63922691	-1.46143925
8	1.34102714	2.11961102	0.38640538
6	1.95871210	2.48109698	1.61159086
1	1.21456456	2.42585564	2.42411947
1	2.33250165	3.51914501	1.56565416
1	2.79431915	1.80837476	1.87009919
8	3.55458903	1.13955021	-0.38666061
6	2.39908934	1.59794211	-0.99416155
6	2.47611332	2.88487363	-1.80331826
1	2.76082516	3.73372769	-1.16280055
1	1.45273602	3.06578946	-2.15118623
6	3.43725491	2.77712917	-3.00313520
1	3.32634020	1.78598428	-3.47019386
1	3.12472010	3.51134014	-3.76102495

6	4.90366554	3.04334283	-2.64015889
1	4.98645353	4.07240009	-2.24780488
1	5.51832390	3.01359963	-3.55380011
6	5.49639702	2.07636499	-1.60819650
1	5.56509018	1.05814886	-2.02366900
1	6.52664423	2.38951683	-1.36959946
6	4.72149277	1.99348629	-0.29410759
1	4.44875431	2.99506044	0.07556735
1	5.33445024	1.50742841	0.47717026
50	0.21841975	0.10560460	0.12943934
7	-2.00722003	0.59977144	1.83660460
6	-2.05703402	2.04060626	2.10991216
1	-3.06618190	2.36513233	2.43659616
1	-1.76821220	2.60536838	1.21700025
1	-1.34678662	2.27943587	2.91375327
7	-1.37394011	0.94326568	-1.00356770
6	-2.95667958	0.19403683	0.78686029
1	-4.00786924	0.34785289	1.11274827
1	-2.80696464	-0.88257951	0.61393327
6	-2.75751281	0.94072443	-0.53304189
1	-3.42280459	0.44703943	-1.26866448
1	-3.15210199	1.97173882	-0.43024832
6	-1.22544301	1.50648677	-2.30707288
6	-1.27244556	2.90916467	-2.51050353
6	-1.15269387	3.42485380	-3.80862761
6	-0.98421204	2.59883690	-4.92439508
6	-0.91975713	1.21827507	-4.70713377
6	-1.03440368	0.66055024	-3.42801356
7	-1.34253085	-2.35438180	2.36945915
6	-2.21042466	-0.12385861	3.11120701
1	-3.09568357	0.29412934	3.63723421
1	-1.33306766	0.08814259	3.74472785
6	-2.43400145	-1.63302040	3.03405666
1	-2.55660295	-1.97664845	4.07786465
1	-3.39391589	-1.83244562	2.53224945
6	-1.02010214	-3.66662312	2.78721809
6	-1.98091269	-4.70349932	2.72348022
6	-1.62286139	-5.99292326	3.13847756
6	-0.33671531	-6.30538750	3.58820891
6	0.61237496	-5.27588367	3.59921312
6	0.29780352	-3.96890044	3.21509600
6	-1.38984847	3.86589241	-1.34940660
1	-1.18054163	4.50939941	-3.94628310
6	-0.89574146	3.17451549	-6.31765032
1	-0.77444935	0.54991031	-5.55993080
6	-0.92647767	-0.83480829	-3.26309299
6	-3.35299087	-4.46984148	2.13937140
1	-2.37409854	-6.78473663	3.07722139
6	0.01532779	-7.69796228	4.05346346
1	1.63257742	-5.49194670	3.92683125
6	1.36214745	-2.89868760	3.25665951
1	-1.12679172	4.88527346	-1.66183782
1	-0.71747935	3.56385231	-0.53324771
1	-2.41245079	3.90522361	-0.94103760
1	0.06840781	-1.11483288	-2.88145947
1	-1.06281197	-1.34227216	-4.22734308
1	-1.66630375	-1.22277629	-2.55026650
1	-1.88231468	3.18320847	-6.80802488

1	-0.22271705	2.58377552	-6.95449829
1	-0.53110510	4.21076202	-6.30033875
1	-3.81427312	-5.42474413	1.85595715
1	-3.29016280	-3.83557272	1.24236560
1	-4.03818560	-3.97174358	2.84300184
1	1.06664670	-2.04858851	3.89321303
1	1.58008087	-2.48703051	2.25762343
1	2.29939032	-3.30479527	3.65730119
1	1.04473281	-7.96627474	3.77757716
1	-0.66094482	-8.44687748	3.61929274
1	-0.06006930	-7.78463840	5.14935207
1	-0.51433039	-1.76754177	2.27176595

Energy = -7584.945971 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 7

Atomic N.	X	Y	Z
8	0.59880579	-0.06104051	-0.20734297
8	1.48036814	2.13196111	0.42099115
6	2.45303440	2.67179608	1.29402292
1	1.97145569	3.29060197	2.07526803
1	3.15880299	3.31622863	0.73955739
1	3.02581573	1.88357937	1.81806076
8	2.72646666	-0.16891262	0.44390252
6	1.78641832	0.38992575	-0.38318846
6	2.20693851	0.85051978	-1.76687562
1	2.98130012	1.62792087	-1.69629443
1	1.31867421	1.32394922	-2.19999957
6	2.70012045	-0.31121838	-2.65356588
1	2.05885077	-1.19335628	-2.49690199
1	2.57066703	-0.01836535	-3.70666814
6	4.17380953	-0.66959345	-2.42323470
1	4.78991270	0.21151753	-2.67499828
1	4.47283983	-1.46423137	-3.12504268
6	4.51270723	-1.11225402	-0.99444699
1	4.02420044	-2.07082677	-0.75679165
1	5.59904814	-1.28699172	-0.92014271
6	4.13321447	-0.10919657	0.09357265
1	4.42052031	0.91755819	-0.18250100
1	4.64019346	-0.36020690	1.03466821
50	-0.36981434	1.21802795	1.38341093
7	-3.16342616	0.50472862	2.06575871
6	-3.57773876	1.48561978	3.07161713
1	-4.67620945	1.48799467	3.23125148
1	-3.27221966	2.49435043	2.76716685
1	-3.08371997	1.26062202	4.02641344
7	-1.70075142	2.06278300	-0.05773371
6	-3.72447228	0.80905229	0.74246705
1	-4.83291578	0.90011030	0.79607260
1	-3.48602939	-0.03069814	0.07501769
6	-3.15371561	2.08295178	0.11763684
1	-3.64332914	2.19096875	-0.86555362
1	-3.49216747	2.96588111	0.70039982
6	-1.26022267	2.72398019	-1.24371850
6	-0.74144620	4.04032564	-1.19298673
6	-0.31872100	4.66456604	-2.37436581
6	-0.39404395	4.03033781	-3.61833739

6	-0.91261989	2.73088551	-3.65668178
6	-1.34951127	2.07121515	-2.50076866
7	-1.32010233	-1.87863159	1.99106050
6	-3.50757551	-0.85395283	2.51490521
1	-4.60112429	-1.03566670	2.42871046
1	-3.26641178	-0.91315496	3.58906221
6	-2.77467370	-1.98431909	1.79419959
1	-3.17146087	-2.93781495	2.19233680
1	-3.01100993	-1.97198021	0.72146940
6	-0.51173997	-3.03289986	1.82860088
6	-0.44362444	-3.71427703	0.59139949
6	0.37982422	-4.84246969	0.48209131
6	1.16484571	-5.30690813	1.54164302
6	1.12295389	-4.58655500	2.74122810
6	0.30256054	-3.46661615	2.90490270
6	-0.63311559	4.78676939	0.11341586
1	0.07794199	5.68185616	-2.31775069
6	0.03781480	4.73474693	-4.88265657
1	-0.97335696	2.20751095	-4.61500931
6	-1.88303423	0.66454673	-2.60353279
6	-1.16929638	-3.20807815	-0.63010406
1	0.42570451	-5.35721588	-0.48124501
6	2.01935601	-6.54390192	1.40234745
1	1.74330807	-4.90782404	3.58193731
6	0.30435896	-2.72448468	4.22102833
1	-0.54902530	5.86742735	-0.06371476
1	0.25976348	4.46798801	0.67183840
1	-1.50023150	4.60040617	0.76072574
1	-1.43605506	0.02881581	-1.82766950
1	-1.66134048	0.23588011	-3.58993196
1	-2.97614360	0.62924266	-2.46863556
1	-0.81036592	5.24979210	-5.36143017
1	0.44285485	4.02579784	-5.61827374
1	0.80576307	5.49294281	-4.67717075
1	-0.72316074	-3.63194823	-1.53922141
1	-1.09761906	-2.11284971	-0.68946135
1	-2.23650169	-3.48105884	-0.63375491
1	-0.69669884	-2.69117403	4.68206024
1	0.64829421	-1.68288231	4.10826349
1	0.97747594	-3.21354175	4.93613148
1	2.95903206	-6.44949532	1.96454000
1	2.26836777	-6.74119425	0.35074612
1	1.49894428	-7.43514490	1.78834224
1	-1.13658702	-1.45075202	2.89746118

Energy = -7584.946605 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 8

Atomic N.	X	Y	Z
8	2.08147120	-0.94519418	1.86371505
8	1.26208282	0.12896381	-0.11976964
6	1.48396540	1.31610644	-0.87053227
1	0.52986330	1.84819078	-1.01004624
1	1.88850021	1.06669915	-1.86724174
1	2.18229222	2.00096416	-0.35980037
8	3.58019280	0.42031449	0.93219262
6	2.69226694	-0.62545222	0.77121216

6	3.05875969	-1.73564684	-0.20226780
1	3.16219592	-1.33884251	-1.22364259
1	2.19856310	-2.41401649	-0.20616215
6	4.34081459	-2.48672128	0.20694523
1	4.34995985	-2.62723088	1.29945183
1	4.30407715	-3.49523640	-0.23253813
6	5.62935495	-1.79668665	-0.25891942
1	5.62013674	-1.74725258	-1.36214185
1	6.49768496	-2.41778803	0.01297142
6	5.83614874	-0.38074067	0.29259846
1	5.99693441	-0.40744531	1.38243866
1	6.75055361	0.04877940	-0.14994323
6	4.68763161	0.58764273	0.01304905
1	4.34575176	0.51662540	-1.03176332
1	5.01288319	1.62198913	0.18916982
50	0.16234373	0.21547174	1.89266813
7	-2.74805522	0.65900397	2.43108892
6	-2.89258647	1.65107715	3.49525070
1	-3.87207437	1.57312214	4.01363277
1	-2.79387069	2.66664004	3.09303474
1	-2.09157014	1.51070750	4.23400688
7	-2.24170160	1.94768167	-0.32408920
6	-3.72547531	0.86395353	1.35793304
1	-4.75551367	0.94887763	1.77243459
1	-3.72061563	-0.03113426	0.71790081
6	-3.47067475	2.08832026	0.47791180
1	-4.36379719	2.22681427	-0.16395661
1	-3.39043832	2.99534726	1.09041643
6	-1.95202696	3.01965332	-1.21923769
6	-1.48064041	4.25407267	-0.71405971
6	-1.17101204	5.28275537	-1.61247396
6	-1.29119897	5.12844610	-2.99762583
6	-1.72651064	3.88819885	-3.47836971
6	-2.06465912	2.83690453	-2.61892700
7	-0.93135381	-1.58782363	1.59052992
6	-2.81294942	-0.70043892	2.98797774
1	-3.84649825	-0.95921010	3.30941629
1	-2.18155456	-0.70608860	3.89136267
6	-2.30535483	-1.78850925	2.04547906
1	-2.39016008	-2.74086213	2.60482812
1	-3.00475860	-1.90485013	1.18974972
6	-0.40395921	-2.75050259	0.94757968
6	-0.57188773	-2.94573641	-0.44413123
6	-0.06573225	-4.10531950	-1.04747927
6	0.60764450	-5.08754253	-0.31340700
6	0.75991327	-4.88463068	1.06316674
6	0.27003571	-3.73998857	1.70520794
6	-1.25081837	4.46158886	0.76227838
1	-0.79897684	6.22902155	-1.21122563
6	-0.97792453	6.26513767	-3.94057131
1	-1.81470692	3.73281169	-4.55661297
6	-2.52680063	1.51863587	-3.19546676
6	-1.26016974	-1.90573692	-1.29281664
1	-0.20053154	-4.24052858	-2.12401938
6	1.17724538	-6.31331968	-0.98729575
1	1.27911699	-5.63945103	1.65979791
6	0.49197072	-3.56403923	3.18612218
1	-0.48607305	5.23178911	0.92738456

1	-0.92131740	3.52954721	1.24402869
1	-2.16308880	4.79838610	1.28144443
1	-1.79673111	0.71090126	-3.02238798
1	-2.66347218	1.60199988	-4.28085804
1	-3.48484087	1.18894124	-2.76425600
1	-1.87717640	6.86594009	-4.15064478
1	-0.60095161	5.89588928	-4.90410137
1	-0.22587217	6.94308233	-3.51443076
1	-1.31911385	-2.23626184	-2.33836579
1	-0.70081764	-0.95932716	-1.25378168
1	-2.28406453	-1.70277131	-0.94394845
1	-0.43018797	-3.28024888	3.71212721
1	1.22650528	-2.76597190	3.36746168
1	0.87251282	-4.49229193	3.63253212
1	2.23668385	-6.16564465	-1.25194526
1	0.63846773	-6.54754496	-1.91546416
1	1.12782884	-7.19235516	-0.32979006
1	-2.29208779	1.06938875	-0.84198898

Energy = -7584.948623 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 9

Atomic N.	X	Y	Z
8	2.07794976	-0.62431306	1.98480463
8	1.25314915	0.16350181	-0.12711819
6	1.43636084	1.25894403	-1.01488996
1	0.46177587	1.72121012	-1.23718858
1	1.87666917	0.90976906	-1.96544611
1	2.08835316	2.03598905	-0.58044320
8	3.53007889	0.69461894	0.92132622
6	2.69793224	-0.40691358	0.87275195
6	3.13960457	-1.60528421	0.04618039
1	3.24702954	-1.32876205	-1.01370060
1	2.31343412	-2.32193851	0.10931330
6	4.44676781	-2.23598385	0.56473094
1	4.43736982	-2.24395490	1.66627133
1	4.46908092	-3.29042006	0.24924822
6	5.71075439	-1.54205370	0.04095549
1	5.72452879	-1.62578928	-1.06013072
1	6.60163641	-2.08111882	0.40070668
6	5.83611822	-0.06158178	0.42077282
1	5.97338295	0.05067004	1.50837553
1	6.73842192	0.35773081	-0.05515026
6	4.64875603	0.80699468	0.00748663
1	4.33458567	0.59485418	-1.02684462
1	4.91993475	1.87000966	0.06359569
50	0.10696338	0.43912211	1.84201658
7	-2.82584786	0.80062622	2.30956054
6	-3.02913141	1.89138031	3.26173759
1	-4.01279211	1.82553267	3.77386165
1	-2.96660304	2.86278296	2.75635600
1	-2.23508048	1.86405253	4.02053976
7	-2.32433486	1.79628694	-0.56674671
6	-3.79220438	0.85090733	1.20818567
1	-4.83138418	0.94056994	1.59794903
1	-3.74389219	-0.10697049	0.66863567
6	-3.56569552	1.98356438	0.20594558

1	-4.45544815	2.02810001	-0.45326215
1	-3.51880932	2.94961286	0.72466660
6	-2.05910349	2.76868701	-1.57591879
6	-1.63543534	4.06830168	-1.21207297
6	-1.34561479	4.99623537	-2.22028375
6	-1.44071639	4.67921782	-3.57941031
6	-1.83032203	3.37820721	-3.91801596
6	-2.14698601	2.42247605	-2.94631529
7	-0.89731389	-1.43740034	1.73666930
6	-2.84224439	-0.49472404	3.00522971
1	-3.86938214	-0.76489145	3.33772397
1	-2.22782850	-0.37764460	3.91267276
6	-2.27013516	-1.65093720	2.18951654
1	-2.32415700	-2.54251933	2.84452653
1	-2.94759846	-1.88715863	1.34075308
6	-0.30434558	-2.63888860	1.23828542
6	-0.43500614	-2.99872518	-0.12410276
6	0.13593920	-4.19388914	-0.58326107
6	0.83822155	-5.05320406	0.26820606
6	0.95312464	-4.68822908	1.61481738
6	0.39851752	-3.50291228	2.11425829
6	-1.43614113	4.45334101	0.23272128
1	-1.01008320	5.99443817	-1.92734027
6	-1.14924645	5.70876694	-4.64449644
1	-1.89876068	3.09683728	-4.97189856
6	-2.56042743	1.03233790	-3.37110209
6	-1.15421557	-2.09680104	-1.09613991
1	0.02914217	-4.45686722	-1.63910890
6	1.47556150	-6.31995964	-0.25164679
1	1.49381089	-5.34488201	2.30168796
6	0.58111221	-3.14985800	3.56867123
1	-0.70188594	5.26523161	0.31615335
1	-1.08145106	3.59621835	0.82337672
1	-2.36808109	4.81383944	0.69826436
1	-1.80764437	0.27382657	-3.10013247
1	-2.68654585	0.98604167	-4.45999146
1	-3.51292181	0.72346717	-2.91300201
1	-2.06664109	6.23907137	-4.94603157
1	-0.72990626	5.24514198	-5.54792070
1	-0.43864951	6.46561909	-4.28544617
1	-1.17545652	-2.54580092	-2.09806418
1	-0.64157099	-1.12544870	-1.15654933
1	-2.19373608	-1.90708125	-0.78840536
1	-0.36473566	-2.85717654	4.04552460
1	1.27079034	-2.29925036	3.66892219
1	0.99841982	-4.00083399	4.12314224
1	2.54252481	-6.16452789	-0.47877458
1	0.99057084	-6.66236639	-1.17576718
1	1.41789889	-7.13114548	0.48755544
1	-2.34076047	0.86407208	-0.98253220

Energy = -7584.948627 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 10

Atomic N.	X	Y	Z
8	0.48153958	0.15520923	-0.54095501
8	0.35156780	2.63420200	-0.49110493

6	1.20647514	3.71570516	-0.17733349
1	0.84589148	4.25932789	0.71671802
1	1.24113309	4.43454695	-1.01496959
1	2.23679972	3.38063955	0.04898871
8	2.45618582	1.07970941	-0.97066474
6	1.13224554	0.97293812	-1.28031504
6	0.68578911	1.21904588	-2.70739985
1	0.94740242	2.23858476	-3.02307510
1	-0.40756932	1.16600442	-2.68640661
6	1.27381802	0.18810049	-3.69403434
1	1.25680029	-0.81509739	-3.23893476
1	0.61296862	0.13943529	-4.57261896
6	2.68970203	0.54199344	-4.16698742
1	2.64802790	1.50765824	-4.70045567
1	3.02622199	-0.20254409	-4.90532017
6	3.73620439	0.64393681	-3.05028987
1	3.91187572	-0.34109360	-2.58870912
1	4.69805479	0.96016490	-3.48665929
6	3.39240360	1.63164437	-1.93790948
1	3.01088190	2.58350348	-2.33749533
1	4.28074408	1.84979796	-1.33131206
50	-0.41390187	1.37797248	1.19541562
7	-1.64816439	-0.97548264	2.00925636
6	-1.92976236	-0.63457221	3.41391706
1	-2.63601804	-1.35279691	3.87368441
1	-2.36156869	0.37213960	3.48612857
1	-0.99209762	-0.64184844	3.98415399
7	-2.38632011	1.40191984	0.38814867
6	-2.87956166	-0.90474969	1.19516432
1	-3.67922688	-1.51766133	1.66292024
1	-2.65186071	-1.33896160	0.21257915
6	-3.39006042	0.52193326	0.98407578
1	-4.27174568	0.45248049	0.32595572
1	-3.78100300	0.92317331	1.94313490
6	-2.87138033	2.32582736	-0.57708776
6	-2.94868469	3.71182084	-0.28979003
6	-3.41797709	4.59996414	-1.26583564
6	-3.82604861	4.16666603	-2.53156042
6	-3.74701524	2.79706097	-2.80520964
6	-3.28277969	1.87451327	-1.85950446
7	1.09659326	-2.54661632	0.62309611
6	-1.07159317	-2.34391379	1.95585263
1	-1.88265789	-3.07243705	2.16651535
1	-0.34712717	-2.43619847	2.77785969
6	-0.35956657	-2.72237849	0.63784796
1	-0.60732508	-3.76587129	0.40567890
1	-0.74862295	-2.11545944	-0.19077094
6	1.91340530	-3.18935728	1.57820737
6	1.93790638	-4.60342550	1.69235218
6	2.77873898	-5.20138168	2.63990617
6	3.63076925	-4.46055841	3.46433973
6	3.63840389	-3.07108927	3.29634905
6	2.80194020	-2.42472005	2.38067627
6	-2.54402304	4.25302839	1.05976129
1	-3.47345352	5.66473532	-1.02352619
6	-4.36179447	5.13838673	-3.55585694
1	-4.04390478	2.43225765	-3.79260683
6	-3.19301558	0.41563326	-2.23458672

6	1.14855158	-5.49083614	0.76101178
1	2.78595185	-6.29263210	2.70889068
6	4.50286007	-5.13145971	4.49818563
1	4.31200838	-2.46221495	3.90521836
6	2.85901761	-0.92306125	2.25081420
1	-2.97912979	5.24795389	1.22461212
1	-1.45081794	4.36153793	1.14718509
1	-2.86391187	3.58896399	1.87431824
1	-2.28278661	-0.03802889	-1.81718481
1	-3.18759751	0.29456055	-3.32618570
1	-4.04637527	-0.16627853	-1.84961271
1	-4.15767145	4.79457521	-4.57939816
1	-3.91780353	6.13591290	-3.43401051
1	-5.45367718	5.25397539	-3.46339679
1	1.59809875	-6.49182463	0.72070223
1	1.13176620	-5.07459402	-0.25685707
1	0.10075201	-5.62055016	1.07822835
1	1.88414562	-0.45039123	2.45705509
1	3.15092182	-0.59679568	1.23965967
1	3.58701563	-0.50325567	2.95666695
1	5.44171858	-4.58111572	4.65049124
1	4.75336313	-6.16010475	4.20389748
1	3.99591255	-5.18643761	5.47516918
1	1.32302749	-1.56134498	0.48514202

Energy = -7584.951780 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 11

Atomic N.	X	Y	Z
8	2.98496914	-0.34043169	0.38941967
8	0.96026611	0.34717810	-0.73964536
6	0.30857465	1.50247788	-1.24621069
1	-0.73400104	1.52870154	-0.88800806
1	0.28523806	1.46945655	-2.34950900
1	0.80637252	2.43619442	-0.92796212
8	3.25226355	1.56083333	-0.74086976
6	2.85639644	0.24600868	-0.75110143
6	3.05103087	-0.56654066	-2.01881814
1	2.47462368	-0.13225500	-2.84924078
1	2.61740088	-1.54942942	-1.80460548
6	4.53502846	-0.69807428	-2.41658878
1	5.14574099	-0.85861927	-1.51389098
1	4.64632368	-1.60640776	-3.02801085
6	5.06147003	0.49976954	-3.21743846
1	4.47954035	0.57752973	-4.15264988
1	6.10369587	0.31016222	-3.51945138
6	4.99166441	1.84493971	-2.48394990
1	5.67727995	1.85403037	-1.62127256
1	5.33167458	2.64428401	-3.16335869
6	3.60092854	2.22814393	-1.98154557
1	2.83005452	2.05201960	-2.74782491
1	3.57303953	3.29283714	-1.71447575
50	1.04312718	-0.07280579	1.46897244
7	-1.41567862	-0.78635651	3.22225404
6	-1.50937629	-0.10888625	4.51571083
1	-2.11831331	-0.68004590	5.24875641
1	-1.95648003	0.88680631	4.40468884

1	-0.50007612	0.02167770	4.92932940
7	-2.50295877	1.24394417	1.38458097
6	-2.72237635	-0.92129308	2.56549358
1	-3.42903781	-1.50660396	3.19695187
1	-2.56832337	-1.47767484	1.63155842
6	-3.38466406	0.41259068	2.21843410
1	-4.30321884	0.18466926	1.66239142
1	-3.70374322	0.94422108	3.13641095
6	-3.02388978	2.47533011	0.90024269
6	-2.48645329	3.70806694	1.34673560
6	-2.97810888	4.90502119	0.81534386
6	-3.99937010	4.92921209	-0.14208242
6	-4.49920559	3.70168304	-0.58792353
6	-4.02534771	2.47731566	-0.09941670
7	0.52039456	-2.11081529	1.23446012
6	-0.75115806	-2.08735156	3.40522242
1	-1.37905586	-2.76455140	4.02686405
1	0.17518499	-1.89552271	3.97202086
6	-0.38619259	-2.83295035	2.12437654
1	0.08002543	-3.78246617	2.45492172
1	-1.30973089	-3.14030576	1.59318089
6	0.97310370	-2.91484094	0.14280443
6	0.19629984	-3.05214500	-1.03374696
6	0.67166632	-3.85136676	-2.08329749
6	1.89197290	-4.52977085	-2.00673556
6	2.64042139	-4.39756393	-0.83085889
6	2.20726299	-3.60549736	0.23988815
6	-1.38390791	3.74465537	2.37907004
1	-2.55287576	5.84800625	1.16846991
6	-4.54712152	6.23496866	-0.66592777
1	-5.26822519	3.68892813	-1.36476088
6	-4.54294777	1.19127345	-0.69533455
6	-1.13626468	-2.36086702	-1.17933381
1	0.06676901	-3.94064665	-2.98969221
6	2.40036440	-5.35738564	-3.16337419
1	3.59346843	-4.92573738	-0.74141574
6	3.06773329	-3.48858166	1.47318804
1	-1.12610912	4.78148937	2.62877250
1	-0.46125576	3.25380015	2.02745032
1	-1.67660606	3.24108601	3.31387329
1	-3.74583268	0.43557268	-0.74483567
1	-4.92602539	1.36661172	-1.70923984
1	-5.36984491	0.75811869	-0.10968865
1	-5.32355165	6.63873959	0.00341050
1	-5.00403500	6.10791826	-1.65673375
1	-3.76041532	6.99796772	-0.74643523
1	-1.41672134	-2.27765870	-2.23769307
1	-1.10933709	-1.35564220	-0.74102747
1	-1.93817532	-2.92279863	-0.67302036
1	2.47974920	-3.59172297	2.39534497
1	3.55433559	-2.50289083	1.50984335
1	3.85088778	-4.25837851	1.47095633
1	3.10568333	-4.78249598	-3.78484440
1	1.57845700	-5.68182707	-3.81570458
1	2.93432784	-6.25171804	-2.81281996
1	-1.62879753	1.39468181	1.89097834

Energy = -7584.949875 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 12

Atomic N.	X	Y	Z
8	2.89240050	-0.09432401	0.63465250
8	0.94596142	0.64825231	-0.55563450
6	0.37818980	1.86043489	-1.03623581
1	-0.64354038	1.97112441	-0.64049762
1	0.32154730	1.84469450	-2.13881969
1	0.96164590	2.74118781	-0.71802741
8	3.22980595	1.80562246	-0.48563614
6	2.78419137	0.49852189	-0.50847423
6	3.01980519	-0.31881830	-1.76980722
1	2.50230479	0.13432315	-2.62898993
1	2.54362869	-1.28732014	-1.58157861
6	4.51633596	-0.50236779	-2.08902383
1	5.07129049	-0.67854238	-1.15394294
1	4.63030577	-1.41666961	-2.69121075
6	5.12494707	0.67323238	-2.86433148
1	4.59590912	0.76682258	-3.82920694
1	6.17454529	0.44681743	-3.11082053
6	5.06255531	2.02302694	-2.13905096
1	5.70241785	2.01239538	-1.24195719
1	5.46349621	2.80781174	-2.80223560
6	3.66082525	2.45269036	-1.70832074
1	2.92630911	2.29870391	-2.51475573
1	3.65470457	3.52015162	-1.44917095
50	0.93473536	0.17657055	1.69037116
7	-1.40205586	-0.62073559	3.38391042
6	-1.40354240	0.18609397	4.60328531
1	-1.95735562	-0.30423155	5.43218184
1	-1.85643506	1.16741359	4.41719198
1	-0.36748111	0.35803756	4.92593098
7	-2.66916299	0.88215613	1.00899768
6	-2.75409031	-0.79896200	2.84583092
1	-3.44680333	-1.17136514	3.63429999
1	-2.71184826	-1.58183134	2.07373643
6	-3.37658525	0.45443457	2.22935486
1	-4.44248295	0.22785917	2.02574325
1	-3.37227726	1.28295457	2.94894123
6	-3.21436429	2.01220274	0.33125231
6	-3.05713129	3.30743885	0.87767094
6	-3.57233262	4.40719604	0.18006326
6	-4.22070646	4.27510118	-1.05228996
6	-4.33427954	2.98889637	-1.59269476
6	-3.85128975	1.85852087	-0.92426580
7	0.51978660	-1.89906788	1.45227396
6	-0.72949350	-1.90631068	3.62463260
1	-1.34920788	-2.57574487	4.26202488
1	0.19164839	-1.68439114	4.18777990
6	-0.34172741	-2.65952516	2.35480261
1	0.17164800	-3.58162642	2.69163156
1	-1.25477910	-3.02259922	1.83596599
6	1.07120275	-2.71870160	0.41919363
6	0.37594420	-2.91167545	-0.79864377
6	0.92561322	-3.73966646	-1.78696656
6	2.15226746	-4.38886452	-1.60991824
6	2.82538748	-4.19399548	-0.39840010

6	2.31144857	-3.37456346	0.61510402
6	-2.29640555	3.53056216	2.16101503
1	-3.43713617	5.40401125	0.60774118
6	-4.79162502	5.47551298	-1.76807940
1	-4.82095623	2.85643172	-2.56236029
6	-3.99766922	0.49482903	-1.55857325
6	-0.93349057	-2.20984912	-1.06040359
1	0.37785172	-3.87682652	-2.72323012
6	2.74523878	-5.24878502	-2.70081544
1	3.78371215	-4.69382286	-0.23397465
6	3.09830356	-3.18047428	1.88653123
1	-1.87707627	4.54482985	2.18767333
1	-1.47434998	2.80709863	2.26100683
1	-2.94029427	3.42578244	3.04965138
1	-3.02472639	0.06787641	-1.85260952
1	-4.60917330	0.55849183	-2.46725941
1	-4.47977781	-0.22945265	-0.88367528
1	-5.85075045	5.62781858	-1.50578368
1	-4.74125719	5.35484266	-2.85892177
1	-4.25389099	6.39480257	-1.49902940
1	-1.33300984	-2.48988056	-2.04419446
1	-0.78626305	-1.11993706	-1.03709376
1	-1.69252002	-2.46009088	-0.30373210
1	2.47520542	-3.30846334	2.78252530
1	3.51363373	-2.16284037	1.92414868
1	3.93030262	-3.89518404	1.93878818
1	3.41736245	-4.66273546	-3.34819388
1	1.96409440	-5.67632771	-3.34411359
1	3.33707547	-6.07482100	-2.28297353
1	-2.61624122	0.08781075	0.37001887

Energy = -7584.948622 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 13

Atomic N.	X	Y	Z
8	1.39549029	0.62418067	1.39632726
8	2.23111796	0.52298099	-0.76442069
6	3.11728311	0.02280619	-1.76208746
1	2.60877538	0.08793971	-2.73536658
1	3.39280748	-1.03216851	-1.59533930
1	4.03445148	0.63318628	-1.81066811
8	3.34638119	1.67320645	1.11256909
6	2.59163427	0.50554323	0.90977746
6	3.31983161	-0.82050103	1.15367591
1	4.15007639	-0.97432375	0.44832113
1	2.57382751	-1.60068023	0.94705713
6	3.85081720	-0.94831175	2.59375668
1	3.12889361	-0.49573848	3.29191256
1	3.90814424	-2.01666260	2.85329223
6	5.24298668	-0.32964438	2.78253961
1	5.94746399	-0.84638470	2.10704589
1	5.59709597	-0.53191298	3.80600643
6	5.32103872	1.17846870	2.51593280
1	4.76216412	1.73490751	3.28573298
1	6.37236786	1.50394440	2.59151244
6	4.78697824	1.61661839	1.15134752
1	5.18638992	0.98229408	0.34290728

1	5.10094976	2.64923596	0.94301361
50	-0.02415902	-0.08290197	-0.44533697
7	-0.66948992	2.29605699	0.09848684
6	0.47220948	3.19131112	-0.21078417
1	0.16039303	4.24868441	-0.13185433
1	0.83707851	2.99540186	-1.22338796
1	1.28592455	2.98484135	0.49149379
7	-0.81753302	0.86162901	-2.27768922
6	-1.79098129	2.55076551	-0.83826840
1	-2.10199380	3.61173272	-0.77598828
1	-2.63604021	1.91939187	-0.52993727
6	-1.39835346	2.19065142	-2.26977110
1	-2.31941223	2.22748017	-2.88361001
1	-0.73967612	2.98651123	-2.67644978
6	-0.67547929	0.22402510	-3.53641748
6	0.19583453	0.72417140	-4.54333258
6	0.32725856	0.03898196	-5.75858593
6	-0.37483537	-1.13878834	-6.03023767
6	-1.23325729	-1.62287664	-5.03675032
6	-1.40318370	-0.96777558	-3.81131887
7	-1.51702607	0.20543040	2.11379457
6	-1.05973792	2.54478693	1.51211190
1	-1.46560764	3.57076025	1.60077310
1	-0.12978727	2.49772620	2.09547114
6	-2.06647491	1.56805503	2.11093974
1	-2.29296565	1.92506850	3.13464236
1	-3.01595926	1.58327401	1.56036365
6	-2.24240875	-0.81736106	2.78933859
6	-3.49660134	-1.25688756	2.30930448
6	-4.16446304	-2.28175449	2.99309373
6	-3.62435246	-2.90480328	4.12152719
6	-2.36157775	-2.48224711	4.55485296
6	-1.66444206	-1.45216835	3.91657090
6	1.02132297	1.96686256	-4.31667233
1	1.01491320	0.43567351	-6.51113415
6	-0.23708864	-1.84655738	-7.35707045
1	-1.80503559	-2.53574967	-5.22534227
6	-2.38844013	-1.52813423	-2.81312346
6	-4.10545492	-0.69719982	1.04760015
1	-5.13052893	-2.61849713	2.60842896
6	-4.37624931	-3.99033689	4.85311794
1	-1.90373838	-2.96529078	5.42179775
6	-0.30401981	-1.03715813	4.42618418
1	1.90719783	1.96915352	-4.96619797
1	1.35120344	2.03284645	-3.26999307
1	0.45497096	2.88622355	-4.53585386
1	-1.88766658	-2.05874419	-1.98823059
1	-3.06716466	-2.24027395	-3.30166674
1	-2.98208594	-0.72565508	-2.35392070
1	-1.05313301	-1.57011318	-8.04397011
1	-0.27211416	-2.93846321	-7.23642588
1	0.70873582	-1.58697462	-7.85197163
1	-4.80661869	-1.41880190	0.60890412
1	-3.32926464	-0.47546476	0.30096337
1	-4.66974449	0.23197530	1.22886372
1	-0.27483720	0.02746520	4.70739460
1	0.48563087	-1.18853593	3.67307568
1	-0.03298915	-1.62239707	5.31367874

1	-3.69861436	-4.77874565	5.20941973
1	-5.13403797	-4.45535040	4.20843220
1	-4.89768171	-3.58765745	5.73608923
1	-0.54733282	0.23774365	2.43973136

Energy = -7584.946990 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 14

Atomic N.	X	Y	Z
8	0.91687328	-1.76018894	1.36472237
8	1.78896570	0.26913619	0.34955817
6	2.48712587	0.11801046	-0.88608414
1	2.02381945	0.77185869	-1.64270008
1	2.44775057	-0.91527009	-1.27534115
1	3.54380178	0.41224450	-0.77323920
8	1.86511588	-0.27402773	2.72709012
6	1.97393060	-1.03781760	1.58754408
6	3.33109856	-1.68572628	1.31454968
1	4.06594658	-0.94030160	0.97651571
1	3.17015314	-2.38664103	0.48652804
6	3.89546347	-2.42816329	2.54299355
1	3.07872891	-2.93379736	3.08096433
1	4.56942749	-3.22107291	2.18429875
6	4.68488121	-1.51293051	3.49004865
1	5.50600672	-1.04748380	2.91677094
1	5.16462278	-2.12363529	4.27122498
6	3.85708427	-0.40977937	4.16075754
1	3.16442728	-0.84750795	4.89723301
1	4.52983189	0.26142001	4.72055721
6	3.02823329	0.44081458	3.20107603
1	3.61928535	0.81453025	2.34981561
1	2.61879086	1.31288099	3.72980738
50	-0.42254147	-0.51950359	0.11183753
7	-1.01104236	2.09602261	-0.44280636
6	0.10708900	2.97804427	-0.81203592
1	-0.21235603	4.03391933	-0.91178781
1	0.54554367	2.64505720	-1.75984192
1	0.87649685	2.90876508	-0.03396653
7	-0.79090399	0.90003109	-3.24937558
6	-2.09092498	2.09147120	-1.46104825
1	-2.70751715	3.00657225	-1.34947968
1	-2.75018406	1.23563504	-1.24334991
6	-1.65930855	2.04146075	-2.92796731
1	-2.59441829	2.02152228	-3.52100039
1	-1.15234303	2.98162770	-3.18985152
6	-0.69535744	0.49849138	-4.60898924
6	-0.10445234	1.34834719	-5.57353687
6	-0.00789103	0.91230136	-6.90137625
6	-0.45407262	-0.34827954	-7.30952740
6	-0.99994743	-1.18945491	-6.33283091
6	-1.13491940	-0.79137444	-4.99873304
7	-1.47841346	0.21330594	1.81112778
6	-1.55792701	2.49921227	0.87554616
1	-2.20034027	3.39618921	0.76037872
1	-0.70286584	2.76731920	1.51026523
6	-2.32752228	1.37822378	1.57253313
1	-2.70563531	1.77986050	2.52562404

1	-3.23584414	1.12343419	0.98582506
6	-1.62665129	-0.43074232	3.06839418
6	-2.14288020	-1.74943113	3.16091824
6	-2.29920173	-2.35018134	4.41588116
6	-1.95860445	-1.69560409	5.60397959
6	-1.43895233	-0.40178239	5.50249815
6	-1.25832701	0.23465855	4.26835394
6	0.48593473	2.68388844	-5.19305611
1	0.45784980	1.57710540	-7.63363600
6	-0.36311388	-0.78195661	-8.75282574
1	-1.34287429	-2.18755150	-6.61708403
6	-1.74124908	-1.74067998	-3.99274254
6	-2.53547263	-2.52919173	1.93034446
1	-2.70984054	-3.36246014	4.46402407
6	-2.11046743	-2.37789702	6.94264650
1	-1.14300323	0.12757479	6.41263628
6	-0.61935490	1.59990990	4.23650503
1	1.21864498	3.00648999	-5.94417191
1	0.99132770	2.62400270	-4.21787882
1	-0.27506575	3.47698879	-5.11948919
1	-1.03027773	-2.02013898	-3.19846296
1	-2.06563306	-2.66606760	-4.48492289
1	-2.61904716	-1.30367517	-3.49028373
1	-1.28667009	-0.53706259	-9.30150986
1	-0.21265019	-1.86693382	-8.83748627
1	0.46573466	-0.27969691	-9.27026558
1	-3.19877148	-3.36365390	2.19543052
1	-1.65437400	-2.96597958	1.43182683
1	-3.04952216	-1.89585555	1.19311881
1	-1.35274625	2.41309905	4.11008787
1	0.08871359	1.66253674	3.39839983
1	-0.08213949	1.79536724	5.17441320
1	-1.23613691	-3.00867915	7.17020655
1	-2.99412608	-3.03130794	6.96205950
1	-2.20734119	-1.64669979	7.75675535
1	-1.01747704	0.10685334	-2.64498806

Energy = -7584.945017 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 15

Atomic N.	X	Y	Z
8	1.56733251	-0.19548781	1.34002674
8	1.99640000	1.30402660	-0.37576920
6	2.72534084	1.76729167	-1.50909460
1	2.04175448	2.35523009	-2.13927650
1	3.12496066	0.94272536	-2.12323022
1	3.55619121	2.42203355	-1.19733906
8	3.33946872	1.11867785	1.68706536
6	2.65951681	0.25839975	0.80877471
6	3.52667356	-0.73597467	0.02950798
1	4.22370100	-0.23117509	-0.65592450
1	2.82213211	-1.30691659	-0.59141451
6	4.32054663	-1.67943096	0.95239580
1	3.70337653	-1.94197214	1.82623315
1	4.51262951	-2.61933994	0.41231668
6	5.66760206	-1.09532273	1.40041888
1	6.27746677	-0.89845383	0.50101978

1	6.21801376	-1.85102212	1.98330700
6	5.57035112	0.19581644	2.22205663
1	5.11649323	-0.00699886	3.20563984
1	6.58721590	0.57708567	2.41584635
6	4.76284361	1.31549525	1.56356430
1	5.05940533	1.45692301	0.51116252
1	4.94778776	2.26452518	2.08644223
50	-0.09989183	0.22890270	-0.37870684
7	-0.83872986	1.49075353	1.67819595
6	0.14465097	2.56274605	1.96880579
1	-0.23755240	3.22533488	2.76654053
1	0.33228040	3.15227008	1.06652808
1	1.08856630	2.10407615	2.27969456
7	-1.29484725	1.97245049	-1.02127695
6	-2.13095832	2.08043170	1.25090098
1	-2.51640892	2.75696826	2.03828835
1	-2.84681487	1.25769281	1.11492455
6	-1.97818315	2.82953119	-0.07137908
1	-2.99606562	3.08544421	-0.42483708
1	-1.47763431	3.80218387	0.11843756
6	-1.33256233	2.35853910	-2.38529491
6	-0.70995593	3.54951859	-2.85153151
6	-0.74654675	3.87094784	-4.21490335
6	-1.38129175	3.05569243	-5.15644836
6	-1.99469626	1.88757682	-4.69026232
6	-1.99128592	1.53017402	-3.33672547
7	-1.11302793	-1.51879871	1.80630898
6	-0.98341626	0.67298371	2.91222930
1	-1.45567942	1.28881061	3.70148516
1	0.03832901	0.43293706	3.23719501
6	-1.77229571	-0.62424743	2.76741338
1	-1.83797443	-1.07647002	3.77633405
1	-2.80433011	-0.43217492	2.44630337
6	-1.60859442	-2.84706569	1.66629672
6	-2.88143277	-3.09185982	1.10478699
6	-3.32028151	-4.41603470	0.96798074
6	-2.53294182	-5.50806236	1.34233260
6	-1.26184571	-5.24335670	1.86752737
6	-0.78697568	-3.93991709	2.03894281
6	0.03103063	4.46561527	-1.90875316
1	-0.24766278	4.78475952	-4.55048943
6	-1.43151629	3.43603373	-6.61699343
1	-2.50922012	1.23576581	-5.40175486
6	-2.72161770	0.27920911	-2.90922475
6	-3.75618935	-1.97130907	0.59996605
1	-4.30561972	-4.59350348	0.52957398
6	-3.01434231	-6.92589617	1.14866257
1	-0.61935830	-6.07736826	2.16137695
6	0.59138262	-3.71158576	2.61406827
1	0.77930248	5.05923843	-2.45130205
1	0.54016989	3.89037585	-1.12228942
1	-0.64415395	5.17554998	-1.40461516
1	-2.03218317	-0.55464214	-2.70390606
1	-3.41390491	-0.04927001	-3.69620204
1	-3.28812122	0.45163903	-1.98367226
1	-2.37414241	3.95074987	-6.86340380
1	-1.36672032	2.55135226	-7.26584911
1	-0.60981601	4.11565590	-6.88140345

1	-4.45694542	-2.34450078	-0.15794235
1	-3.15040088	-1.17452693	0.14473137
1	-4.35992098	-1.51521766	1.40131629
1	0.56182390	-3.09869146	3.52879953
1	1.25609636	-3.19257069	1.90521455
1	1.06251276	-4.66866302	2.87038040
1	-2.56630969	-7.37929153	0.25035635
1	-4.10506678	-6.96466827	1.02848721
1	-2.74123645	-7.56294584	2.00192642
1	-0.10667929	-1.52540755	1.99312437

Energy = -7584.946956 Hartree
Number of imaginary frequencies = 0.

Compound TS2b isomer 16

Atomic N.	X	Y	Z
8	1.32793581	-1.98747623	-0.27607411
8	1.82473075	0.32195485	0.28491217
6	2.27875042	1.15724802	-0.77983135
1	1.62567139	2.04258704	-0.84412444
1	2.24679041	0.65224445	-1.76188684
1	3.31001282	1.49941421	-0.59226459
8	2.40552425	-1.61797976	1.63930285
6	2.34766889	-1.40334499	0.28013769
6	3.67250752	-1.44176996	-0.48241735
1	4.26539755	-0.53463650	-0.29383922
1	3.40849829	-1.44569492	-1.54691029
6	4.52459574	-2.68007541	-0.13718370
1	3.87246728	-3.55787921	-0.00952775
1	5.17547750	-2.89860916	-0.99754518
6	5.41014004	-2.47684312	1.10070062
1	6.06118107	-1.60316432	0.92075288
1	6.08273029	-3.34184575	1.21358752
6	4.64590645	-2.26746774	2.41371965
1	4.15161562	-3.20315099	2.72020435
1	5.35978079	-2.01083708	3.21436429
6	3.57629538	-1.17901182	2.36371875
1	3.95450282	-0.23455115	1.94102144
1	3.20952058	-0.96578318	3.37756205
50	-0.32562137	-0.51684785	-0.22370043
7	-1.20832670	1.63524759	1.20713675
6	-0.26094624	2.73975110	1.42427599
1	-0.67387176	3.51351380	2.10069394
1	-0.00376906	3.20285869	0.46464267
1	0.65543830	2.33044720	1.86576509
7	-1.48497105	2.64034224	-1.66927826
6	-2.47207952	2.08762002	0.57305270
1	-3.11922717	2.56274271	1.33814204
1	-3.00552106	1.19117081	0.21782839
6	-2.35083151	3.09497833	-0.57216984
1	-3.38432193	3.28576946	-0.92139876
1	-1.98134339	4.05234480	-0.17647800
6	-1.64578617	3.24961972	-2.94263840
6	-1.34042883	4.61761284	-3.13294601
6	-1.49021089	5.18078661	-4.40726471
6	-1.90933883	4.43312502	-5.51142550
6	-2.16962194	3.07210636	-5.31082678
6	-2.05325198	2.46963286	-4.05419827

7	-1.08296442	-1.30519164	1.60573101
6	-1.49959970	0.96035719	2.49546957
1	-2.20886946	1.57127488	3.09057903
1	-0.55184764	0.89743876	3.04689574
6	-2.03591514	-0.45918053	2.31992412
1	-2.23161125	-0.86377209	3.32543969
1	-3.02880216	-0.42910364	1.82224989
6	-0.94885725	-2.63943219	2.07440758
6	-1.35653508	-3.74212289	1.27844095
6	-1.23233843	-5.04432201	1.77576518
6	-0.71093327	-5.31139326	3.04639482
6	-0.30031621	-4.22100592	3.81775975
6	-0.39957082	-2.90191507	3.35715771
6	-0.79140127	5.46719980	-2.01324534
1	-1.24350011	6.23742580	-4.54025793
6	-2.08675694	5.07018852	-6.86866903
1	-2.48377490	2.45668054	-6.15771294
6	-2.35779357	0.99856025	-3.89925480
6	-1.92877436	-3.54645586	-0.10394022
1	-1.56295776	-5.87743807	1.14939570
6	-0.56967318	-6.72865725	3.54850650
1	0.13203792	-4.39929676	4.80645800
6	0.13459946	-1.78636122	4.21956968
1	-0.26001203	6.33799696	-2.41880870
1	-0.08988615	4.89003038	-1.39297676
1	-1.58040023	5.84955025	-1.34627998
1	-1.47592688	0.41902995	-3.58163834
1	-2.70469356	0.57598180	-4.85052681
1	-3.14174271	0.81673717	-3.14670086
1	-3.13811803	5.34911871	-7.04395533
1	-1.79497504	4.38436890	-7.67621326
1	-1.48578823	5.98483562	-6.96248865
1	-2.47580695	-4.44243765	-0.42724657
1	-1.13490856	-3.37029600	-0.84867525
1	-2.61296701	-2.68677711	-0.14441438
1	-0.65785253	-1.25826156	4.77500200
1	0.64958107	-1.04329479	3.59502578
1	0.84036946	-2.17975950	4.96365929
1	0.27882341	-7.24077082	3.06759071
1	-1.46883774	-7.32349443	3.33149052
1	-0.39873627	-6.75282621	4.63311291
1	-1.51563799	1.62064075	-1.74061513

Energy = -7584.945008 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 17

Atomic N.	X	Y	Z
8	1.34472501	-1.72759664	-0.34788418
8	2.77505064	0.19125709	-0.23518533
6	3.46718717	0.29410604	-1.47330379
1	3.22727203	1.26407015	-1.93287456
1	3.17763591	-0.50637931	-2.17728925
1	4.55833578	0.24278092	-1.31843758
8	2.17623973	-1.15893888	1.64310575
6	2.42764854	-1.42060745	0.28522056
6	3.68956280	-2.25092268	0.00082800
1	4.59201384	-1.62437534	0.05848447

1	3.59938622	-2.59501600	-1.03747845
6	3.85630274	-3.45591307	0.94655502
1	2.87435222	-3.91154337	1.14987731
1	4.45145655	-4.22184753	0.42535168
6	4.57066250	-3.10483408	2.26082087
1	5.54670477	-2.65215421	2.01212072
1	4.79510021	-4.03253555	2.81123114
6	3.80018377	-2.15427566	3.18579626
1	2.92672324	-2.67052364	3.61594677
1	4.44517183	-1.86719704	4.03333998
6	3.29512572	-0.88026667	2.51281166
1	4.08751726	-0.35350320	1.95827734
1	2.90010452	-0.18510915	3.26735950
50	0.36655840	0.55753547	-0.16423418
7	-0.20799284	-0.26891515	-2.60016394
6	0.39197594	-1.50536621	-3.14380383
1	-0.00596481	-1.71659005	-4.15448904
1	0.20335135	-2.35711265	-2.48599958
1	1.47753894	-1.38260281	-3.20652390
7	-1.76958621	-1.64378846	-0.45639333
6	-1.68914473	-0.37179106	-2.60943294
1	-2.04937696	-0.42652348	-3.65680408
1	-2.08905506	0.55051810	-2.16525459
6	-2.24520731	-1.57731926	-1.84602618
1	-3.33769798	-1.47888720	-1.84159219
1	-2.02799153	-2.51233029	-2.39398766
6	-2.63956857	-2.22306371	0.51392424
6	-2.29235840	-3.44248390	1.14322853
6	-3.14254999	-3.97212100	2.11978722
6	-4.33545923	-3.34011769	2.49045277
6	-4.64549971	-2.12382030	1.87397301
6	-3.81694579	-1.54483056	0.90444380
7	0.37338772	2.32304525	-1.48930967
6	0.24286348	0.87527078	-3.44074917
1	-0.18001105	0.77907753	-4.46008205
1	1.33601534	0.79431659	-3.51627922
6	-0.11007101	2.23571014	-2.85592484
1	0.37199500	2.99352193	-3.50596905
1	-1.20050287	2.41142058	-2.96252465
6	0.20833981	3.57287359	-0.82901168
6	-1.06739974	4.15122795	-0.57528633
6	-1.15822697	5.38128805	0.09078660
6	-0.03145426	6.07076550	0.54436749
6	1.21836770	5.48596001	0.31235757
6	1.35857403	4.26571417	-0.35752162
6	-1.01706529	-4.16667652	0.78174186
1	-2.86351466	-4.91305685	2.60075307
6	-5.25912905	-3.95540357	3.51387787
1	-5.54849529	-1.58673775	2.17537665
6	-4.15846968	-0.18326914	0.35155430
6	-2.34931946	3.45212388	-0.95311224
1	-2.15084720	5.80034590	0.27835068
6	-0.15628476	7.37534094	1.29386628
1	2.12017488	6.00148010	0.65389657
6	2.74315214	3.71767163	-0.59592485
1	-0.93179733	-5.09864759	1.35453153
1	-0.12195938	-3.55927801	0.98856723
1	-0.98322189	-4.42962790	-0.28755099

1	-3.24759889	0.41895339	0.22393051
1	-4.83482599	0.34834737	1.03313708
1	-4.66058350	-0.23217545	-0.62825829
1	-5.97065496	-4.65075684	3.04040408
1	-5.84971762	-3.18799973	4.03259945
1	-4.69989872	-4.52605915	4.26792192
1	-3.17545962	3.79246831	-0.31502196
1	-2.24947071	2.36317968	-0.83243877
1	-2.64229488	3.64214516	-1.99808311
1	2.89505434	3.48271251	-1.65914166
1	2.92229486	2.78678942	-0.03753209
1	3.50287700	4.44861937	-0.28824955
1	-0.09395175	7.21667957	2.38239837
1	-1.11720562	7.86565685	1.08764279
1	0.64942414	8.07236958	1.02284634
1	-0.84257776	-2.07445049	-0.40871570

Energy = -7584.938422 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 18

Atomic N.	X	Y	Z
8	2.01883483	-1.25081873	-0.52958161
8	2.51222444	1.04739249	-1.07811821
6	2.79597449	1.05605340	-2.46853685
1	2.08834481	1.72620511	-2.97940183
1	2.70300865	0.04823675	-2.91588640
1	3.81943154	1.42435181	-2.65748000
8	2.93619061	0.00963161	1.06647611
6	2.99164104	-0.46294722	-0.24906904
6	4.39169455	-0.80049843	-0.77761894
1	4.93403339	0.11452470	-1.05785620
1	4.23702669	-1.38134384	-1.69562936
6	5.24449158	-1.60532010	0.22284849
1	4.61198902	-2.33696771	0.74984419
1	5.98420191	-2.18808103	-0.34785801
6	5.99981499	-0.72225904	1.22764790
1	6.62297392	-0.00899766	0.65988648
1	6.69911671	-1.34662092	1.80653656
6	5.10960150	0.05873591	2.20236301
1	4.63639212	-0.63152838	2.91931272
1	5.73458242	0.74835241	2.79446077
6	3.99711585	0.86843526	1.54103816
1	4.36578369	1.50394142	0.72083390
1	3.51601195	1.52463949	2.28012824
50	0.27821091	0.49444774	-0.34671113
7	-0.59815443	-1.02093625	-2.27806377
6	0.25159740	-2.16971397	-2.65805817
1	-0.20311990	-2.72082448	-3.50310731
1	0.39308229	-2.84180975	-1.80815697
1	1.24289906	-1.80814052	-2.94504619
7	-1.84260333	-1.78269362	0.47165939
6	-1.97924519	-1.49017358	-1.98889673
1	-2.37688231	-1.99635577	-2.89099860
1	-2.60504174	-0.60199904	-1.82147205
6	-2.13878202	-2.44527411	-0.80671781
1	-3.17818165	-2.82912087	-0.84349030
1	-1.48538005	-3.31855845	-0.91705269

6	-1.96736825	-2.56299210	1.66131365
6	-1.03377497	-3.58241487	1.95637941
6	-1.18082440	-4.30688381	3.14634562
6	-2.19935036	-4.04200315	4.06756687
6	-3.08501172	-2.99884820	3.77495599
6	-2.99152279	-2.26043820	2.59058905
7	-0.64700943	1.81973183	-1.85885918
6	-0.63502485	-0.05619587	-3.41505361
1	-1.16552472	-0.51015013	-4.27490282
1	0.40813679	0.11511363	-3.71284461
6	-1.27381873	1.27986443	-3.05095768
1	-1.13174343	1.94456577	-3.92827034
1	-2.37413287	1.15584147	-2.96187043
6	-1.14471614	3.06840038	-1.38932502
6	-2.46562624	3.22488832	-0.88200599
6	-2.89945817	4.47573090	-0.42130274
6	-2.06961298	5.59877539	-0.42092714
6	-0.76525503	5.43531275	-0.90057725
6	-0.29253006	4.20822191	-1.37878859
6	0.14509214	-3.86424422	1.05892992
1	-0.45033425	-5.08862448	3.36968756
6	-2.34457445	-4.85913897	5.32859278
1	-3.87728262	-2.75209379	4.48611116
6	-3.96892738	-1.13651621	2.33115864
6	-3.41662955	2.05989933	-0.77240872
1	-3.91750741	4.56495190	-0.03167628
6	-2.54480457	6.92886686	0.11224102
1	-0.09055684	6.29574680	-0.91424072
6	1.11801219	4.12485123	-1.90431786
1	0.93400842	-4.37981939	1.62178934
1	0.57001323	-2.93792725	0.64621115
1	-0.12189777	-4.52080584	0.21397755
1	-3.47190571	-0.15235154	2.30575180
1	-4.72365761	-1.09427631	3.12617826
1	-4.50372171	-1.25941753	1.37581015
1	-3.01218891	-5.72095203	5.16913891
1	-2.77191329	-4.26312256	6.14650774
1	-1.37576425	-5.25508118	5.66236830
1	-4.16300201	2.24106956	0.01231925
1	-2.86422944	1.14156938	-0.52325451
1	-3.96459961	1.86940706	-1.70939648
1	1.13346171	3.73120046	-2.93074918
1	1.74482858	3.45384312	-1.29894722
1	1.58447111	5.11912489	-1.90901816
1	-2.16810369	7.10709572	1.13206804
1	-3.64133382	6.97501183	0.15300313
1	-2.19011807	7.76155472	-0.51194519
1	-2.44154525	-0.96030629	0.55441660

Energy = -7584.935642 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 19

Atomic N.	X	Y	Z
8	2.05377531	0.00758524	-1.18215966
8	2.08558846	1.60584307	0.68563700
6	2.35699129	1.75358999	2.06580496
1	1.53731954	2.30490756	2.56133366

1	3.28308058	2.33838511	2.21502090
1	2.46536756	0.78174597	2.58564925
8	3.34889007	-0.71289533	0.47788960
6	3.05573654	0.26160333	-0.43323812
6	4.17448187	1.14326549	-0.95541418
1	4.60797596	1.73980308	-0.13959444
1	3.69239879	1.84265363	-1.64720237
6	5.28247404	0.34252337	-1.67236888
1	4.82714939	-0.44747055	-2.29106903
1	5.79760361	1.02086830	-2.36932015
6	6.32250309	-0.25584838	-0.71658683
1	6.81143999	0.57051492	-0.17167085
1	7.11482191	-0.74892765	-1.30143249
6	5.76055288	-1.25280905	0.30395684
1	5.39649963	-2.16281962	-0.19964346
1	6.57080460	-1.57221401	0.98005080
6	4.62685013	-0.70771068	1.16890883
1	4.85233927	0.29957873	1.55049598
1	4.45277548	-1.36491501	2.03057218
50	0.20662096	0.50689256	0.06832628
7	-0.84113163	-0.46121803	-2.13677955
6	-0.10189172	-1.55792677	-2.78631520
1	-0.57076943	-1.85452771	-3.74392295
1	-0.05963018	-2.42294526	-2.11408615
1	0.92295265	-1.22116792	-2.97451544
7	-1.81344509	-2.57653308	-0.12782206
6	-2.25836706	-0.81508964	-1.85954094
1	-2.85327315	-0.68909246	-2.78600574
1	-2.64661741	-0.08736330	-1.12943506
6	-2.53494883	-2.23349142	-1.35980701
1	-3.63135457	-2.29576612	-1.21721828
1	-2.28865433	-2.95264673	-2.15468216
6	-2.32809615	-3.61072540	0.69383347
6	-2.41762948	-4.93962431	0.21632300
6	-2.91970062	-5.93769360	1.06198645
6	-3.31240606	-5.67701578	2.37792325
6	-3.17379498	-4.36474991	2.84622693
6	-2.69790506	-3.33084750	2.03401089
7	-0.47209486	2.21159554	-1.03884888
6	-0.77723044	0.76131296	-2.97762489
1	-1.36189640	0.61388022	-3.90785432
1	0.27924430	0.90502644	-3.24414515
6	-1.26338792	2.00570488	-2.24281430
1	-1.13580096	2.85853386	-2.93808246
1	-2.35841107	1.93554890	-2.06280971
6	-0.65750796	3.47052145	-0.39205214
6	-1.81151998	3.76176620	0.38111874
6	-1.93885231	5.01654291	0.99473262
6	-0.96187752	6.00760841	0.86744124
6	0.16569746	5.71500921	0.09099534
6	0.33515760	4.47469044	-0.53482264
6	-1.91378927	-5.32179403	-1.15396810
1	-2.97680950	-6.96055698	0.68035251
6	-3.87515831	-6.76585913	3.25958037
1	-3.45446086	-4.13160276	3.87660527
6	-2.57827973	-1.93367743	2.59416699
6	-2.91995311	2.75249720	0.56162989
1	-2.83122253	5.22036123	1.59301639

6	-1.10322893	7.34029245	1.56335020
1	0.93850923	6.47802496	-0.03691037
6	1.57059205	4.21583319	-1.35788822
1	-1.70453846	-6.39865351	-1.19685364
1	-0.98785776	-4.77864265	-1.39421535
1	-2.64089417	-5.09965038	-1.95115662
1	-1.53665125	-1.57352114	2.60163379
1	-2.94603729	-1.90148258	3.62742734
1	-3.16041422	-1.20306587	2.00965524
1	-4.97693396	-6.75991440	3.24766803
1	-3.56213212	-6.63892365	4.30536222
1	-3.55023479	-7.75999641	2.92362785
1	-3.52244520	2.99102807	1.44795132
1	-2.52131557	1.73399210	0.67888045
1	-3.60169315	2.73639727	-0.30389482
1	1.32100856	3.78018570	-2.33522940
1	2.21630502	3.48941207	-0.84382558
1	2.13286161	5.14628601	-1.51542926
1	-0.54950261	7.35249424	2.51576304
1	-2.15404820	7.56377077	1.79198682
1	-0.70406139	8.15843105	0.94733989
1	-1.60651183	-1.73513162	0.41402110

Energy = -7584.950080 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 20

Atomic N.	X	Y	Z
8	1.56578815	-1.24454832	1.15547693
8	2.05619407	-0.93664473	-1.16078079
6	2.92754555	-0.19484732	-1.99988055
1	2.33419204	0.32333514	-2.77204919
1	3.63693857	-0.86746901	-2.51341105
1	3.49508023	0.56735283	-1.43918204
8	3.64280248	-0.51397616	0.77564895
6	2.65384316	-1.43479240	0.47526297
6	3.07209611	-2.87388301	0.20754419
1	3.72764635	-2.93366241	-0.67485923
1	2.14291763	-3.40038037	-0.03827905
6	3.75335026	-3.53223419	1.42295396
1	3.23145008	-3.22509360	2.34277797
1	3.62099195	-4.62183523	1.34301078
6	5.25343847	-3.22826171	1.52456200
1	5.75240231	-3.61883545	0.61998409
1	5.68263912	-3.78233838	2.37439942
6	5.59975624	-1.74177599	1.67192662
1	5.24127674	-1.35278499	2.63850117
1	6.69642544	-1.62453866	1.67218328
6	5.03828573	-0.84462267	0.57006258
1	5.19635868	-1.28624964	-0.42707017
1	5.53871346	0.13324644	0.58608270
50	0.26231438	0.05683770	-0.07092652
7	-1.33897161	0.61347854	-2.34124160
6	-0.82684904	-0.17191480	-3.47030473
1	-1.59159076	-0.30249622	-4.26292372
1	-0.49225077	-1.15622914	-3.12578344
1	0.03359514	0.35008094	-3.91151977
7	-1.06916320	-1.56663489	-0.41146860

6	-2.52234221	-0.00491852	-1.72024715
1	-3.38138318	-0.02804650	-2.42462921
1	-2.80155182	0.62273061	-0.86036670
6	-2.27114916	-1.43249559	-1.23161209
1	-3.17362356	-1.72509301	-0.65953076
1	-2.24532604	-2.11583328	-2.10433626
6	-0.92404133	-2.86253834	0.16902576
6	-0.50054699	-3.97168684	-0.60658413
6	-0.39767033	-5.23573065	-0.00892344
6	-0.69736862	-5.44724894	1.34035349
6	-1.09448183	-4.34066391	2.09887099
6	-1.21059334	-3.06102204	1.54299510
7	-1.73225987	3.09489226	-0.56143850
6	-1.58491719	1.99626052	-2.80927992
1	-2.15599704	1.96752429	-3.76197290
1	-0.60076803	2.43741322	-3.03966904
6	-2.35878849	2.92729473	-1.87774479
1	-2.43225765	3.89537764	-2.40726209
1	-3.39101243	2.55838037	-1.77203190
6	-1.86729360	4.32734108	0.11983832
6	-3.14450026	4.82468319	0.47104406
6	-3.23833799	6.04549837	1.15232646
6	-2.11159635	6.78255415	1.52790248
6	-0.85551983	6.24987173	1.21240687
6	-0.71081978	5.04662275	0.51549321
6	-0.09882181	-3.80972147	-2.05216122
1	-0.05946442	-6.07789469	-0.61916316
6	-0.61447799	-6.82460833	1.95388162
1	-1.32137692	-4.47441816	3.15988803
6	-1.61565614	-1.90762830	2.42650437
6	-4.39928865	4.02956915	0.20339841
1	-4.23155212	6.41376877	1.42242444
6	-2.24140310	8.10772896	2.23971248
1	0.04581728	6.79218721	1.50956702
6	0.67029732	4.52648640	0.19617714
1	0.46804717	-4.68552256	-2.39512205
1	0.52712029	-2.91439533	-2.17887783
1	-0.96898180	-3.70458007	-2.71988797
1	-0.74007744	-1.29591858	2.69702101
1	-2.06109571	-2.27310300	3.36137652
1	-2.33266711	-1.24168229	1.92809677
1	-1.59976721	-7.31754494	1.96032369
1	-0.26814321	-6.78026819	2.99590135
1	0.07128063	-7.47263575	1.39110935
1	-5.22043324	4.38826227	0.83742476
1	-4.23592854	2.96278644	0.41817766
1	-4.73722315	4.10354042	-0.84211016
1	0.81322730	4.37527037	-0.88636744
1	0.87492186	3.55850649	0.68217266
1	1.43571019	5.23465347	0.53742754
1	-1.45015466	8.24021435	2.99087524
1	-3.21185708	8.19527340	2.74688077
1	-2.16278219	8.95031834	1.53412795
1	-0.76833916	2.76190519	-0.56410390

Energy = -7584.946015 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 21

Atomic N.	X	Y	Z
8	-0.05734480	-0.32684493	-0.44645774
8	2.03672767	-0.06818291	-1.75598454
6	2.39219999	-0.32668859	-3.09940934
1	2.35878372	0.60153043	-3.70332336
1	1.69432044	-1.03913522	-3.57834864
1	3.41590643	-0.73784757	-3.16102672
8	0.25959438	-2.03068542	-1.84493732
6	0.73474884	-1.26744270	-0.82082778
6	1.68769717	-1.85768223	0.20521808
1	1.08965278	-2.56885338	0.80767572
1	1.92645586	-1.01793706	0.86604232
6	2.99388695	-2.51369071	-0.25765777
1	3.50864601	-1.81412959	-0.93082178
1	3.63731718	-2.61677718	0.62968743
6	2.84433246	-3.88599825	-0.91624951
1	2.40411735	-4.59392405	-0.19147635
1	3.84286022	-4.27979040	-1.16294301
6	1.97821367	-3.87864327	-2.17765498
1	2.41927910	-3.23880386	-2.95728803
1	1.93925548	-4.89776182	-2.59787107
6	0.53245056	-3.45795441	-1.93845248
1	0.13218622	-3.94795418	-1.03479958
1	-0.09452236	-3.75658274	-2.78807092
50	0.59518552	1.62706065	-1.44998765
7	-1.18524396	2.83466721	0.12500302
6	-2.25640488	3.45199394	-0.66952121
1	-2.83553553	4.19360828	-0.08678570
1	-2.92714429	2.67350483	-1.04895985
1	-1.80277944	3.96260047	-1.52986825
7	-3.05568433	0.35944524	0.07363330
6	-1.67605424	2.07642365	1.30311692
1	-1.79690540	2.76895332	2.16126633
1	-0.89389884	1.35293996	1.57731080
6	-3.01572490	1.35274875	1.15595818
1	-3.21322274	0.88953573	2.14395738
1	-3.81640720	2.09090757	1.00274682
6	-4.15991259	-0.53854996	0.09117368
6	-5.46402264	-0.07814137	-0.21126094
6	-6.53385448	-0.98283070	-0.19179642
6	-6.36159611	-2.33974409	0.09553950
6	-5.06066465	-2.78449059	0.35750383
6	-3.96480989	-1.91511297	0.36841190
7	1.68715572	2.31984925	0.27047083
6	-0.21223377	3.87190652	0.53448951
1	-0.68219072	4.57897186	1.24837899
1	0.05182849	4.43772840	-0.37369850
6	1.05995536	3.30035806	1.15087843
1	1.73667550	4.15805244	1.33151352
1	0.82208192	2.89539576	2.15434122
6	2.99348998	1.90922785	0.63979995
6	3.25231957	1.22360837	1.85728693
6	4.56324577	0.84136415	2.17676973
6	5.64604902	1.10802948	1.33551550
6	5.38283777	1.79170716	0.14267509
6	4.09265184	2.19530034	-0.21579681
6	-5.72189236	1.34986925	-0.62263179

1	-7.53249645	-0.61168295	-0.43688163
6	-7.53525496	-3.28865743	0.13510634
1	-4.89009857	-3.84289694	0.57166284
6	-2.58690929	-2.45818615	0.66047007
6	2.14375234	0.85251093	2.81345510
1	4.73602486	0.30527329	3.11451268
6	7.04389477	0.65553439	1.68391085
1	6.21202755	2.03200197	-0.52844155
6	3.89568019	2.95896268	-1.50155687
1	-6.66285181	1.42308438	-1.18335140
1	-4.90694904	1.72308147	-1.25874889
1	-5.80451632	2.03123760	0.23935927
1	-1.93053269	-2.38264298	-0.21982417
1	-2.64610791	-3.51534390	0.94976103
1	-2.09042907	-1.90901661	1.47513747
1	-7.90431261	-3.42462420	1.16433775
1	-7.26187181	-4.28299475	-0.24476014
1	-8.37414169	-2.91168094	-0.46556517
1	2.42440677	-0.03018258	3.40446424
1	1.21404362	0.62938142	2.27076888
1	1.92075014	1.66157651	3.52744508
1	3.21018529	3.80679679	-1.36430812
1	3.46227121	2.32549596	-2.29230857
1	4.85589790	3.33474493	-1.87986159
1	7.30425262	-0.27846396	1.16043484
1	7.14741468	0.46829614	2.76125789
1	7.79276419	1.40632129	1.39381647
1	-2.16095304	-0.13303521	0.00724980

Energy = -7584.946973 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 22

Atomic N.	X	Y	Z
8	0.21263766	-0.38137466	0.50775015
8	1.79389572	-1.23583114	-1.15916753
6	2.09765840	-2.47550631	-1.76597691
1	1.66562271	-2.52773499	-2.78511047
1	1.67399311	-3.32479000	-1.19775248
1	3.19066429	-2.61790061	-1.85110044
8	0.86853874	-2.47611380	0.93956202
6	1.20524204	-1.16586840	0.72023296
6	2.44917488	-0.57584554	1.36527133
1	2.22213507	-0.47844693	2.44450068
1	2.50367999	0.44542307	0.97060466
6	3.80152273	-1.27058196	1.16857064
1	3.94075203	-1.46564770	0.09574463
1	4.58360291	-0.54926842	1.45257390
6	4.00401258	-2.55238247	1.97981048
1	3.93996930	-2.31343222	3.05644703
1	5.02359915	-2.93333530	1.80970609
6	2.99252295	-3.65705848	1.66543972
1	3.08114815	-3.98679662	0.61850280
1	3.21319771	-4.53990126	2.28910780
6	1.54195511	-3.27551031	1.94634712
1	1.45759857	-2.76423836	2.92050672
1	0.91747212	-4.17723989	1.98711514
50	-0.25340810	-0.39032307	-1.72746491

7	-2.33700919	1.37100446	-2.63419509
6	-3.27401710	0.71564001	-3.54634094
1	-3.90539575	1.44707417	-4.09289789
1	-3.93095160	0.02932223	-2.99989367
1	-2.71079803	0.12200069	-4.27921772
7	-2.72473645	0.29069769	0.14510818
6	-3.02238846	2.08225441	-1.54931593
1	-3.78924823	2.78182864	-1.94944298
1	-2.27555633	2.69787979	-1.02654183
6	-3.69900179	1.16594493	-0.52654129
1	-4.24298143	1.81180549	0.19117700
1	-4.45907879	0.53904599	-1.00992894
6	-3.24594355	-0.62562245	1.10920894
6	-3.97081661	-1.76424420	0.69325829
6	-4.45632744	-2.65269065	1.66167033
6	-4.22909880	-2.46567488	3.02849889
6	-3.47461081	-1.35185277	3.41609812
6	-2.98424602	-0.42909449	2.48647475
7	0.53830892	1.59567547	-1.95768750
6	-1.40952516	2.22973752	-3.38562989
1	-1.92724502	3.12288260	-3.79938102
1	-1.04870474	1.63342035	-4.23869944
6	-0.20402613	2.69260716	-2.57340336
1	0.44603640	3.24774814	-3.27771354
1	-0.52726257	3.44988632	-1.82835543
6	1.78793716	2.02078700	-1.41526079
6	1.86083078	2.75823903	-0.20621911
6	3.10988069	3.16776371	0.28349370
6	4.30191422	2.87737346	-0.38584310
6	4.21541214	2.16495180	-1.58798122
6	2.99066424	1.73648477	-2.11245966
6	-4.18085718	-2.07387877	-0.76798064
1	-5.00874805	-3.53486824	1.32771313
6	-4.78750658	-3.42418694	4.05275249
1	-3.26381660	-1.19017029	4.47639036
6	-2.16665864	0.75044560	2.95849061
6	0.62083101	3.09771848	0.58262569
1	3.14734650	3.72518086	1.22363281
6	5.63950348	3.29663754	0.17621017
1	5.13100481	1.93911219	-2.14134288
6	2.96739316	0.98609239	-3.41985607
1	-4.33928776	-3.15060830	-0.91237766
1	-3.30729628	-1.76683724	-1.36100972
1	-5.06514978	-1.56081176	-1.18110394
1	-1.13354290	0.70411754	2.57763481
1	-2.11665845	0.76815385	4.05444956
1	-2.59643865	1.71072257	2.63138628
1	-5.75491190	-3.07052708	4.44391632
1	-4.11132956	-3.53351855	4.91200972
1	-4.95517969	-4.41952324	3.61930442
1	0.86192560	3.24787331	1.64347398
1	-0.11241077	2.28527021	0.50106353
1	0.14462876	4.02336264	0.22123305
1	2.17928767	1.35976374	-4.08765507
1	2.76140451	-0.08075964	-3.25038981
1	3.93574405	1.07010579	-3.93109012
1	6.12966919	2.46249604	0.70360172
1	5.53171873	4.12113571	0.89376694

1 6.32505846 3.62155151 -0.61924434
 1 -2.00492477 0.86277902 0.58913463
 Energy = -7584.945724 Hartree
 Number of imaginary frequencies = 0.

Compound TS2b isomer 23

Atomic N.	X	Y	Z
8	-0.48781273	-2.89645934	-0.37807596
8	0.51953298	-0.97620010	0.64418250
6	1.78241456	-0.31916022	0.68525046
1	1.69773781	0.66178083	0.18919346
1	2.56034422	-0.90319145	0.16521412
1	2.09764957	-0.15436514	1.72953486
8	1.68504536	-3.17251134	0.11580344
6	0.42036304	-2.83204675	0.54595101
6	-0.02102736	-3.19961905	1.95613325
1	-0.13668971	-4.29929066	1.96670628
1	-1.03419149	-2.78990340	2.04163146
6	0.82177109	-2.74056101	3.15147257
1	1.03388810	-1.66632521	3.04857993
1	0.19452789	-2.83926129	4.05110884
6	2.11856127	-3.52273178	3.37571263
1	1.86949921	-4.57985210	3.57638144
1	2.61895299	-3.14732718	4.28254032
6	3.09613180	-3.46945596	2.19899392
1	3.44307923	-2.43994808	2.01816082
1	3.99396563	-4.05996418	2.44820452
6	2.54041767	-4.04254580	0.89755082
1	2.00951672	-4.99109030	1.08767927
1	3.36243033	-4.25465536	0.20133363
50	-0.67548436	-0.88132954	-1.28434551
7	-1.99739027	1.65998197	-2.52839255
6	-2.75770640	1.09689522	-3.64547706
1	-3.59559321	1.75286210	-3.96376705
1	-3.17213917	0.11839920	-3.37098908
1	-2.08727098	0.94639957	-4.50211334
7	-2.47924113	-0.39784765	-0.27283409
6	-2.83672428	1.86657178	-1.34052157
1	-3.67102599	2.56872106	-1.57131791
1	-2.21204567	2.33165836	-0.56460267
6	-3.44703627	0.59448588	-0.75116462
1	-4.06577492	0.92924029	0.09964675
1	-4.17004395	0.15918835	-1.47213197
6	-2.95060897	-1.13242149	0.85964054
6	-3.59869576	-2.38078761	0.70390910
6	-4.05459118	-3.06585717	1.83938229
6	-3.89191389	-2.55559182	3.13126755
6	-3.24713588	-1.32028699	3.26997185
6	-2.77954221	-0.60062313	2.16339397
7	0.82504851	2.40288520	-1.86350036
6	-1.34589612	2.91073728	-2.94851565
1	-2.09320140	3.72726345	-3.06798434
1	-0.90623176	2.73321891	-3.94276667
6	-0.24069446	3.40629625	-2.01562428
1	0.16202833	4.33376789	-2.45695949
1	-0.66329432	3.68311381	-1.03665924
6	2.17998409	2.80015373	-1.88215411

6	2.66875625	3.74926543	-0.95207268
6	4.02253723	4.10642958	-0.99044776
6	4.92365503	3.53602982	-1.89530373
6	4.43057966	2.56149173	-2.77133870
6	3.08365345	2.18611932	-2.78614020
6	-3.78729224	-3.00293040	-0.65761679
1	-4.55229712	-4.02990150	1.70556581
6	-4.41882801	-3.29737544	4.33677530
1	-3.09737659	-0.90386009	4.26981497
6	-2.07965302	0.71887362	2.36971402
6	1.78222561	4.31475115	0.13151474
1	4.38652754	4.83736563	-0.26357076
6	6.37154198	3.96236014	-1.93356228
1	5.11345816	2.08086061	-3.47662425
6	2.60643888	1.13330138	-3.75745749
1	-4.57381678	-3.76867175	-0.62733090
1	-2.85640931	-3.48663783	-0.99030483
1	-4.05641079	-2.25628686	-1.41639984
1	-1.11944890	0.73447841	1.83615756
1	-1.89948618	0.89938617	3.43768716
1	-2.67662430	1.56135011	1.98615539
1	-5.41062307	-2.92074704	4.63354635
1	-3.75503135	-3.17653584	5.20445347
1	-4.52436972	-4.37119484	4.13160086
1	2.39176273	4.76345873	0.92646509
1	1.15934598	3.52398682	0.57647175
1	1.09792054	5.09437609	-0.23670714
1	1.81018853	1.51293838	-4.41867590
1	2.20000505	0.24466424	-3.24632621
1	3.43281388	0.79503042	-4.39490318
1	7.02625704	3.13486147	-2.23996186
1	6.70952559	4.32016182	-0.95122433
1	6.52790976	4.78400183	-2.65099502
1	0.64867854	1.60618925	-2.47359300

Energy = -7584.943121 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 24

Atomic N.	X	Y	Z
8	0.30074060	-0.65919781	-0.87161577
8	1.75867105	0.41414911	-2.51627111
6	2.41936302	0.03156806	-3.70780921
1	1.83793104	0.34739694	-4.59522104
1	2.53096986	-1.06610787	-3.77402115
1	3.41920209	0.49671111	-3.76697111
8	1.87340653	-2.04010820	-1.66033745
6	1.56177115	-0.85115260	-1.05604827
6	2.52250695	-0.22713849	-0.05532363
1	2.47605276	-0.85536420	0.85445791
1	2.05487013	0.72770792	0.20816004
6	3.97968554	0.02015633	-0.46240699
1	3.98881650	0.54248124	-1.42955744
1	4.40783119	0.72390300	0.26800948
6	4.86566305	-1.22632194	-0.51489806
1	4.90597582	-1.68569088	0.48878348
1	5.89766741	-0.92820519	-0.75839567
6	4.39546776	-2.28396797	-1.51595986

1	4.42059374	-1.89251769	-2.54498100
1	5.08973217	-3.14086103	-1.49242294
6	3.00514913	-2.84192586	-1.22795022
1	2.89077902	-3.06352067	-0.15318552
1	2.85339975	-3.77793813	-1.78079212
50	-0.49571070	0.53142917	-2.60108685
7	-2.81237888	0.66913432	-1.25013340
6	-3.84885192	-0.08331969	-1.97355294
1	-4.86512136	0.16610695	-1.61064637
1	-3.68734479	-1.16137242	-1.86439061
1	-3.78465509	0.15915038	-3.04259515
7	-2.64216328	-1.10383809	2.08838820
6	-2.85347533	0.42072755	0.20410264
1	-3.81241679	0.81185108	0.61418831
1	-2.04069948	0.99249995	0.66908050
6	-2.69067907	-1.04453599	0.61343455
1	-3.52241039	-1.65933561	0.22231852
1	-1.75361907	-1.42959929	0.19262651
6	-2.67240310	-2.38877177	2.69746113
6	-1.57512891	-3.27246785	2.57014990
6	-1.62639463	-4.51563740	3.21322036
6	-2.71360040	-4.91103029	3.99959373
6	-3.77100706	-4.00601959	4.14591503
6	-3.77358103	-2.76156712	3.50699306
7	-0.50500154	2.42150545	-1.58184958
6	-2.95684505	2.11531758	-1.53839886
1	-3.88766456	2.51173854	-1.08425987
1	-3.05232811	2.20998812	-2.63209820
6	-1.76530099	2.95006061	-1.07339668
1	-1.94378436	3.97930741	-1.44345248
1	-1.78319132	3.03090429	0.03188043
6	0.63660347	3.23045707	-1.34224212
6	1.13389409	3.45483136	-0.03111996
6	2.26409340	4.26340151	0.15467621
6	2.93572044	4.86518860	-0.91303140
6	2.43455148	4.64202404	-2.20081639
6	1.30813491	3.84533381	-2.43249488
6	-0.33404386	-2.87686777	1.81095362
1	-0.76936603	-5.18686533	3.11222601
6	-2.75133991	-6.27023411	4.65593910
1	-4.62703323	-4.27747583	4.76901436
6	-4.94481039	-1.82541621	3.69837594
6	0.49816108	2.80873060	1.17608368
1	2.63637781	4.41445160	1.17207313
6	4.17313814	5.70184374	-0.69123673
1	2.93005490	5.11213207	-3.05478954
6	0.80948305	3.66872835	-3.84533978
1	0.52870518	-3.45697308	2.16585732
1	-0.12265162	-1.80598652	1.93962419
1	-0.42733815	-3.05269456	0.72823799
1	-4.65705967	-0.89731449	4.22068596
1	-5.72460127	-2.30495691	4.30304623
1	-5.40211344	-1.53171396	2.73987842
1	-3.23639727	-7.01443720	4.00404787
1	-3.31589222	-6.24620962	5.59818363
1	-1.73904622	-6.63834190	4.87239408
1	1.23356020	2.69046593	1.98363423
1	0.09404477	1.81845438	0.92252249

1	-0.33106700	3.41031313	1.58240891
1	-0.28385198	3.76286864	-3.90098119
1	1.05975664	2.67326856	-4.24663496
1	1.26615047	4.41110420	-4.51365852
1	5.08917093	5.10639763	-0.83467263
1	4.20392466	6.10961914	0.32827750
1	4.22091770	6.54245806	-1.39789426
1	-3.41032219	-0.54286587	2.45803714

Energy = -7584.946159 Hartree
Number of imaginary frequencies = 0.

Compound TS2b isomer 25

Atomic N.	X	Y	Z
8	0.69001049	-3.00433922	-0.52181071
8	1.17192447	-0.75360280	0.03088070
6	1.95180511	0.34671992	-0.44100535
1	1.27115917	1.15203309	-0.75811708
1	2.57926130	0.05530218	-1.29786181
1	2.59685230	0.73173827	0.36529481
8	2.76546764	-2.32221842	-1.08199930
6	1.78927207	-2.44011116	-0.10588126
6	2.20170522	-2.77309489	1.32339656
1	2.52443647	-3.83006668	1.31335020
1	1.26434648	-2.75024509	1.89160573
6	3.25045276	-1.90202963	2.02480888
1	2.98436236	-0.84196979	1.90035236
1	3.17492938	-2.10391092	3.10462189
6	4.69750977	-2.14480829	1.58651483
1	4.96869993	-3.19054317	1.81593168
1	5.37174988	-1.51382136	2.18733191
6	4.95730877	-1.89079762	0.09945903
1	4.79321337	-0.83164668	-0.15537859
1	6.01671505	-2.10268307	-0.12356377
6	4.12350798	-2.75967050	-0.83978689
1	4.11200476	-3.80725646	-0.49300984
1	4.56189919	-2.74838400	-1.84654522
50	-0.67094535	-1.38262260	-1.13152325
7	-3.47503710	0.34274429	-1.38107145
6	-4.24029636	-0.38613823	-2.39381933
1	-5.33081532	-0.18269105	-2.33042836
1	-4.08832407	-1.46748316	-2.28132248
1	-3.88837743	-0.10503828	-3.39546251
7	-1.91496944	-1.52053976	0.58025002
6	-3.87241650	-0.05535833	-0.02155724
1	-4.98229504	-0.03163940	0.07451196
1	-3.46294618	0.67894053	0.68503660
6	-3.37212515	-1.44330955	0.40222907
1	-3.86129761	-1.67503226	1.36218381
1	-3.75407386	-2.19961262	-0.31044194
6	-1.47358811	-2.04284525	1.83205509
6	-1.57147312	-3.42995954	2.11844969
6	-1.12805486	-3.91470337	3.35436702
6	-0.57607305	-3.07239985	4.32749128
6	-0.48573622	-1.70871627	4.03267145
6	-0.92612129	-1.17812896	2.81096506
7	-1.17178655	2.21680903	-1.56998885
6	-3.61230159	1.79497063	-1.57375562

1	-4.57358122	2.16962528	-1.15777957
1	-3.63785553	1.98855257	-2.65752506
6	-2.46116614	2.60215878	-0.97075522
1	-2.66537428	3.66671419	-1.16466606
1	-2.43877578	2.47413421	0.12401175
6	-0.30296251	3.20170760	-2.08539343
6	0.16955028	4.25076151	-1.25890791
6	1.04710519	5.19965553	-1.79810166
6	1.50502253	5.13429976	-3.11828804
6	1.06875718	4.05879545	-3.90128279
6	0.17623676	3.09773636	-3.41607475
6	-2.11984944	-4.39178944	1.09558809
1	-1.20532155	-4.98653316	3.55596614
6	-0.08375451	-3.62576270	5.64373922
1	-0.06746685	-1.02840865	4.77923536
6	-0.83593035	0.30947864	2.57765150
6	-0.18237291	4.31229687	0.20846580
1	1.40665638	6.00152397	-1.14781940
6	2.42737818	6.18895483	-3.68085480
1	1.42605424	3.96615648	-4.93013144
6	-0.26358107	1.96073043	-4.30676651
1	-2.00552702	-5.42841768	1.43789339
1	-1.58844185	-4.28321981	0.13908893
1	-3.18870878	-4.22044420	0.89729762
1	-0.31865710	0.53545153	1.63687873
1	-0.29743564	0.79625386	3.40172052
1	-1.83621883	0.76458269	2.51447964
1	-0.85271966	-4.24049187	6.13435078
1	0.19829156	-2.81998968	6.33422184
1	0.79835463	-4.26947165	5.50166130
1	0.51776749	4.96948004	0.74022079
1	-0.13207202	3.31161046	0.66334295
1	-1.19712651	4.69642115	0.39296952
1	-1.35848415	1.93557656	-4.43261623
1	0.03466814	0.97650152	-3.90837932
1	0.18222594	2.05845809	-5.30442572
1	3.09685779	5.77115059	-4.44537973
1	3.04686260	6.64018822	-2.89348865
1	1.85958910	7.00506496	-4.15610981
1	-1.30753446	1.43866539	-2.21346688

Energy = -7584.942920 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 26

Atomic N.	X	Y	Z
8	0.73218948	-2.79311466	-1.23086691
8	1.16369820	-0.79153824	-0.04320805
6	2.00736427	0.35962301	-0.11518616
1	1.37804985	1.24852061	-0.27699938
1	2.72701669	0.27849570	-0.94476873
1	2.55847931	0.48895216	0.83029372
8	2.86895323	-2.08022785	-1.33580112
6	1.77561867	-2.40671611	-0.55035770
6	1.99918449	-3.12229514	0.77689338
1	2.31137204	-4.15182495	0.52392966
1	0.99719661	-3.21072388	1.21297705
6	2.95709753	-2.51242042	1.80690706

1	2.71800590	-1.44684052	1.93899834
1	2.74258256	-2.98889875	2.77610278
6	4.44611168	-2.69181490	1.49766922
1	4.67700386	-3.77148795	1.47118092
1	5.04360914	-2.27010894	2.32161832
6	4.89548016	-2.06658125	0.17457162
1	4.77423000	-0.97177613	0.19306135
1	5.97286654	-2.25660300	0.03278624
6	4.18135262	-2.62220001	-1.05572414
1	4.11683846	-3.72262931	-1.00398779
1	4.74508619	-2.36521411	-1.96238244
50	-0.52943480	-1.01487756	-1.53484154
7	-3.27282262	0.85513574	-1.60477209
6	-3.92070341	0.48151603	-2.86317015
1	-5.00795460	0.71066338	-2.86580348
1	-3.79866719	-0.59333616	-3.05007219
1	-3.44676018	1.01801169	-3.69604158
7	-1.97651982	-1.54767203	-0.08005135
6	-3.83599091	0.10584529	-0.47052780
1	-4.94906569	0.14629115	-0.50128734
1	-3.51271534	0.59403050	0.45865402
6	-3.39848161	-1.36436296	-0.40524855
1	-4.00822353	-1.84174550	0.37877473
1	-3.68606281	-1.86946452	-1.34743237
6	-1.70209777	-2.39847898	1.03134835
6	-1.84645963	-3.80620503	0.92344880
6	-1.56429732	-4.61801052	2.02900863
6	-1.13422406	-4.08598185	3.25017142
6	-0.99026829	-2.69769192	3.34114075
6	-1.26994777	-1.84619212	2.26268482
7	-0.93432832	2.59460521	-1.01688135
6	-3.36667609	2.30705786	-1.38416862
1	-4.36178064	2.59145617	-0.97655958
1	-3.27027464	2.80255795	-2.36279011
6	-2.27452540	2.85313535	-0.46239531
1	-2.43742990	3.93695068	-0.35981655
1	-2.37293696	2.41654944	0.54527920
6	-0.01223914	3.65109825	-1.17215538
6	0.38548508	4.42984486	-0.05748707
6	1.31709564	5.45875406	-0.24329725
6	1.89986122	5.72854471	-1.48612213
6	1.53482640	4.91096830	-2.56237793
6	0.59327251	3.88504195	-2.43291330
6	-2.26452231	-4.44134903	-0.37805575
1	-1.67072415	-5.70118952	1.92570055
6	-0.85845369	-4.98112345	4.43488455
1	-0.65627903	-2.25658703	4.28403616
6	-1.12975705	-0.35523459	2.44482565
6	-0.10624472	4.11353016	1.33503187
1	1.61740458	6.04943800	0.62622970
6	2.87782884	6.86522484	-1.66264880
1	1.98952842	5.08076572	-3.54176641
6	0.23480462	3.03669786	-3.62932539
1	-2.20917869	-5.53553581	-0.31058902
1	-1.60881007	-4.11203909	-1.19705737
1	-3.29512548	-4.17461634	-0.65691328
1	-0.50206822	0.08632617	1.66086578
1	-0.68490022	-0.12740411	3.42268562

1	-2.10879970	0.14565809	2.39659095
1	-1.79001117	-5.24465847	4.96050072
1	-0.19900708	-4.48984241	5.16302586
1	-0.38594669	-5.92374134	4.12433434
1	0.54720587	4.57918692	2.08406210
1	-0.11310255	3.02688241	1.50798297
1	-1.12922180	4.47310591	1.52365887
1	-0.84283215	3.08049273	-3.85747623
1	0.48634830	1.97333777	-3.47993159
1	0.77610850	3.37900233	-4.52010059
1	3.60986567	6.64684391	-2.45234108
1	3.42757535	7.06850100	-0.73322618
1	2.36125875	7.79655933	-1.94550955
1	-1.01198375	2.01515293	-1.85147941

Energy = -7584.942898 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 27

Atomic N.	X	Y	Z
8	0.49010593	-0.31745327	-0.42672288
8	1.96489477	1.14760077	0.87485397
6	2.53768134	2.41695619	0.62657088
1	2.18790555	3.15026116	1.37179399
1	2.27426243	2.80319357	-0.37344146
1	3.64007926	2.36398149	0.70720929
8	2.08064103	0.53601438	-1.71224546
6	1.75391173	-0.16406552	-0.59295648
6	2.69473243	-1.23463643	-0.05317971
1	2.66568613	-2.06217003	-0.78746182
1	2.19269729	-1.61949062	0.84425646
6	4.14345312	-0.87066019	0.29244792
1	4.12943220	0.01458165	0.94406968
1	4.55390358	-1.69518912	0.89650804
6	5.06697226	-0.64416742	-0.90659595
1	5.14370441	-1.58027184	-1.48770523
1	6.08313894	-0.42359000	-0.54327518
6	4.61085987	0.47439700	-1.84639871
1	4.58187723	1.44482243	-1.32684767
1	5.34353590	0.58062929	-2.66400170
6	3.25761771	0.22125597	-2.50267482
1	3.18168807	-0.82400721	-2.84726000
1	3.13374352	0.87390399	-3.37600708
50	-0.07774344	0.52245128	1.58693576
7	-3.02530193	0.03976645	2.29870486
6	-3.15188313	0.41471809	3.70832515
1	-4.20875263	0.56873596	4.01269913
1	-2.60046911	1.34261084	3.90619040
1	-2.71452951	-0.37140718	4.33842325
7	-1.30924225	2.07745218	0.76473475
6	-3.52224278	1.09992552	1.40951562
1	-4.54772425	1.41092753	1.71286368
1	-3.58155894	0.69110352	0.39120078
6	-2.62341547	2.33796835	1.36371005
1	-3.15281391	3.08368397	0.74607110
1	-2.56782293	2.78733778	2.37649894
6	-0.80584949	3.16595793	-0.01235223
6	-0.35200858	4.36118937	0.60116994

6	0.13114952	5.41047525	-0.19303577
6	0.18036392	5.32146120	-1.58680332
6	-0.29888278	4.14807987	-2.18182111
6	-0.79723310	3.07843733	-1.42845237
7	-1.75786185	-2.32572007	0.98887646
6	-3.69940782	-1.24404013	2.04469800
1	-4.79747438	-1.10697317	1.94160283
1	-3.54708099	-1.88079488	2.93135977
6	-3.18020725	-1.99445856	0.81946242
1	-3.79620481	-2.90485024	0.69704384
1	-3.32677650	-1.38765705	-0.08531459
6	-1.18536389	-3.43589044	0.33068150
6	-1.25656402	-3.58646059	-1.07494473
6	-0.64944667	-4.70103455	-1.66894186
6	0.05560605	-5.65916538	-0.93438929
6	0.15858322	-5.46350861	0.44813529
6	-0.44730693	-4.38038015	1.09087741
6	-0.37201133	4.53054714	2.10085034
1	0.48773867	6.32042646	0.29752585
6	0.74747330	6.44319487	-2.42369914
1	-0.29955009	4.06491041	-3.27205777
6	-1.36106455	1.87084460	-2.13316274
6	-1.89197874	-2.53889894	-1.95608807
1	-0.71137118	-4.80283594	-2.75566173
6	0.67419058	-6.86389399	-1.60215104
1	0.72020739	-6.18152714	1.05155790
6	-0.30481112	-4.22339630	2.58683968
1	0.34535858	5.29945850	2.41723776
1	-0.12754798	3.58935833	2.61520457
1	-1.36550176	4.84122086	2.46178818
1	-0.81594235	0.95864838	-1.85862958
1	-1.30887079	2.00350547	-3.22212052
1	-2.41469169	1.71133280	-1.85715258
1	0.20245841	6.55134153	-3.37208200
1	1.80344987	6.25626707	-2.67682362
1	0.70321882	7.40287304	-1.89110637
1	-1.57697368	-2.68033123	-2.99810386
1	-1.58670855	-1.53165543	-1.63867128
1	-2.99220204	-2.57959247	-1.94023657
1	-1.28135133	-4.22420692	3.09937739
1	0.20528276	-3.28484392	2.86210489
1	0.28456792	-5.04869556	3.00539160
1	1.64948523	-7.11386633	-1.16065776
1	0.82007271	-6.69297361	-2.67741251
1	0.03378139	-7.75420618	-1.49597287
1	-1.52376604	-2.33484411	1.97925103

Energy = -7584.938599 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 28

Atomic N.	X	Y	Z
8	2.33628058	-0.89296603	2.00708532
8	1.47547889	0.40323147	0.14996041
6	1.04887629	0.12200833	-1.16995835
1	-0.02270426	0.35272920	-1.27033567
1	1.20266426	-0.93998045	-1.42872727
1	1.59439135	0.74903083	-1.89843833

8	3.13746977	-1.58658946	0.04627124
6	2.93775964	-0.55467963	0.91917002
6	3.95377111	0.58199942	1.00061595
1	4.85569286	0.15223253	1.47609234
1	3.52823353	1.27495325	1.73804080
6	4.33281326	1.35702872	-0.26680699
1	3.40917659	1.67534554	-0.77110285
1	4.84352970	2.27988291	0.05068570
6	5.24728775	0.61060899	-1.24117076
1	6.20555782	0.38760918	-0.73918658
1	5.49048424	1.27189660	-2.08788896
6	4.66112423	-0.69946879	-1.77275968
1	3.73987842	-0.51726645	-2.34802341
1	5.37933969	-1.15856111	-2.47287464
6	4.37561560	-1.73850977	-0.69210994
1	5.21391106	-1.79388118	0.02345916
1	4.25803328	-2.73067760	-1.14634717
50	0.36069173	0.18053015	2.10504842
7	-2.55287743	0.65513426	2.64129806
6	-2.62852120	1.68751109	3.67498875
1	-3.55669332	1.60828888	4.27997875
1	-2.59418988	2.68718529	3.22472286
1	-1.76125562	1.59743440	4.34372377
7	-2.31110477	1.70659304	-0.27741247
6	-3.61549854	0.81729800	1.64252043
1	-4.60203218	0.95340317	2.13991976
1	-3.68640280	-0.11565942	1.06281126
6	-3.40851021	1.97850776	0.66775304
1	-4.36857033	2.15191031	0.14123361
1	-3.18525219	2.90459299	1.21204603
6	-2.02753496	2.71766448	-1.24099398
6	-1.39525604	3.91972899	-0.84649241
6	-1.09658682	4.88143826	-1.81955945
6	-1.38136506	4.68938065	-3.17569637
6	-1.97506249	3.47859931	-3.54974961
6	-2.30872464	2.49600506	-2.61102414
7	-0.70997447	-1.65508151	1.87591422
6	-2.56874013	-0.68114531	3.25898266
1	-3.58299446	-0.93715370	3.63796067
1	-1.89994287	-0.63814372	4.13398361
6	-2.08750558	-1.80768323	2.34750986
1	-2.17920375	-2.73903370	2.93979836
1	-2.79733038	-1.93726432	1.50342095
6	-0.21670139	-2.84847760	1.26166892
6	-0.58157307	-3.19609690	-0.06197668
6	-0.08063108	-4.37301254	-0.63552696
6	0.75998890	-5.23839235	0.06864623
6	1.07668495	-4.90665054	1.39133370
6	0.60708499	-3.73718214	1.99941826
6	-0.98772854	4.16036177	0.58558238
1	-0.59987044	5.80263472	-1.50389326
6	-1.07356405	5.75748158	-4.19745827
1	-2.19489288	3.29301071	-4.60419846
6	-2.95060897	1.20776784	-3.07329202
6	-1.52184296	-2.33452153	-0.86926305
1	-0.36076656	-4.61795378	-1.66403615
6	1.32023501	-6.48378563	-0.57620990
1	1.71032989	-5.58160305	1.97307289

6	0.97623998	-3.45185232	3.43339729
1	-0.14471400	4.86211777	0.63153923
1	-0.68877411	3.22201300	1.07479012
1	-1.80446303	4.59906721	1.18213379
1	-2.29216671	0.33563590	-2.92359161
1	-3.17897701	1.25653255	-4.14527893
1	-3.89302802	0.99882919	-2.54296160
1	-1.92218041	6.44993734	-4.31696987
1	-0.86722583	5.32178164	-5.18455696
1	-0.20362398	6.35841703	-3.89884734
1	-1.23067391	-2.31706190	-1.92895818
1	-1.52320230	-1.30707860	-0.48357654
1	-2.55480480	-2.71599841	-0.82171249
1	0.11736514	-3.07760191	4.00747824
1	1.75889397	-2.68166804	3.48433852
1	1.35490251	-4.36059904	3.92027450
1	2.33813667	-6.30905724	-0.96010262
1	0.70169097	-6.81010294	-1.42335236
1	1.38450074	-7.31336164	0.14202325
1	-2.51826692	0.83045065	-0.75827038

Energy = -7584.938156 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 29

Atomic N.	X	Y	Z
8	1.82924163	-1.86136329	1.83128560
8	1.46318543	0.07302854	0.42067981
6	1.24112093	0.29225025	-0.95967287
1	0.24225646	0.73003072	-1.10944498
1	1.29960167	-0.64771068	-1.53531718
1	1.98111022	1.00556290	-1.36588144
8	2.86762762	-2.03510046	-0.13373978
6	2.64441204	-1.30752516	1.00152111
6	3.75964212	-0.44167545	1.58287454
1	4.50725555	-1.14401889	1.99759495
1	3.29845881	0.05006162	2.44926476
6	4.44292164	0.61221081	0.70359790
1	3.66580987	1.22327137	0.22247127
1	4.99748278	1.29034376	1.37136018
6	5.41682339	0.06124161	-0.34080559
1	6.23963594	-0.46550831	0.17447416
1	5.88074923	0.90125871	-0.88168198
6	4.77982330	-0.90011799	-1.34704828
1	4.00141382	-0.39509857	-1.94026446
1	5.54895878	-1.23440886	-2.06359529
6	4.18813276	-2.15860891	-0.71844411
1	4.87641048	-2.57458186	0.03729314
1	4.03372622	-2.92593598	-1.48783815
50	0.00994725	-0.54994619	2.04041648
7	-2.87024999	0.19512802	2.38938999
6	-2.99218774	0.83185774	3.70057750
1	-4.01256371	0.72442347	4.12611151
1	-2.75677514	1.90115249	3.63358092
1	-2.27017570	0.37868163	4.39396000
7	-1.99379027	2.07404757	0.07641690
6	-3.71691799	0.85597640	1.39010203
1	-4.74940777	0.99572390	1.78196359

8	0.24198499	-0.17547296	0.79665130
8	2.63598180	-0.74219644	0.64166534
6	3.37729192	-1.64764953	-0.15511838
1	4.04274559	-1.10722971	-0.84739852
1	2.71833992	-2.29025769	-0.76550674
1	4.00824261	-2.29412651	0.48399591
8	0.50160468	-2.36877370	0.68057323
6	0.80282176	-1.20715189	1.31453776
6	1.13054717	-1.20052958	2.80148363
1	0.18377042	-1.44950473	3.31888461
1	1.33049762	-0.14712514	3.03940010
6	2.27814102	-2.06796956	3.33203435
1	3.17145896	-1.85833323	2.72707367
1	2.50366879	-1.72341847	4.35339642
6	1.99769878	-3.57141495	3.37910604
1	1.16081309	-3.76461601	4.07336664
1	2.87348676	-4.08809185	3.80210614
6	1.65409052	-4.18721056	2.02081394
1	2.48652601	-4.07405281	1.30909479
1	1.49617898	-5.27161169	2.14500308
6	0.38108662	-3.63253260	1.39208496
1	-0.41726598	-3.53343916	2.14651012
1	0.02055932	-4.30718803	0.60563725
50	1.89163971	1.33523166	0.31098869
7	-0.00448160	3.36441278	-0.37131709
6	0.92173678	4.49033356	-0.17317596
1	0.54239094	5.41785574	-0.64721876
1	1.90906787	4.26312494	-0.59456319
1	1.05165076	4.66759968	0.90243268
7	1.56740928	1.28511667	-1.80992424
6	-0.16635753	3.06195021	-1.80480039
1	-0.49973240	3.96627307	-2.35939312
1	-0.94568568	2.29509926	-1.90092778
6	1.10814261	2.51653624	-2.45416594
1	0.85686302	2.30425620	-3.50816345
1	1.87804079	3.31611967	-2.49376583
6	2.22963119	0.37208167	-2.68475676
6	3.55668068	0.59248823	-3.13252044
6	4.16410398	-0.33925429	-3.98680663
6	3.49881029	-1.48902524	-4.42214966
6	2.18047905	-1.68293130	-3.99146676
6	1.53578448	-0.77792639	-3.14045119
7	-2.21835136	1.56716979	1.14511240
6	-1.28849041	3.73675704	0.27275515
1	-1.66791523	4.66564798	-0.20803595
1	-1.06097317	3.97769761	1.32178116
6	-2.42981195	2.71976733	0.26295251
1	-3.31372857	3.26273608	0.62579626
1	-2.67943192	2.41903830	-0.77376121
6	-3.39219022	0.91719747	1.62325490
6	-3.81247950	-0.32925293	1.09796786
6	-4.94080305	-0.95600003	1.64030373
6	-5.68727970	-0.37981549	2.67529011
6	-5.25836992	0.85235965	3.17956543
6	-4.12440300	1.50657189	2.68156695
6	4.33611155	1.81524074	-2.71220541
1	5.19130802	-0.15968402	-4.31580210
6	4.18465567	-2.50144243	-5.30810881

1	1.63168049	-2.56476283	-4.33332253
6	0.10281582	-1.01761973	-2.73672438
6	-3.07110739	-0.97951072	-0.04619100
1	-5.25474644	-1.91815424	1.22652864
6	-6.92694569	-1.05515766	3.21171713
1	-5.80776834	1.31260431	4.00513697
6	-3.66728473	2.79843259	3.31190133
1	5.41509151	1.65139198	-2.83184052
1	4.13914251	2.08206558	-1.66330421
1	4.06739855	2.69464803	-3.31887770
1	-0.02012825	-0.99371630	-1.64670873
1	-0.24736510	-1.98755157	-3.11477947
1	-0.55806863	-0.23687284	-3.14465690
1	3.48302746	-2.94350934	-6.02933264
1	4.60393286	-3.32959437	-4.71462822
1	5.01306820	-2.04767179	-5.86865330
1	-3.61076236	-1.86919081	-0.39550164
1	-2.05243111	-1.28946650	0.23062259
1	-2.96322703	-0.29402080	-0.90039068
1	-3.98553467	3.68225694	2.73520231
1	-2.56975770	2.83074021	3.36608982
1	-4.08298969	2.90563989	4.32241869
1	-7.14215422	-0.73673522	4.24086142
1	-6.82393980	-2.14922571	3.20576692
1	-7.81097460	-0.80924016	2.60174036
1	-1.55526400	0.90078729	0.74524391

Energy = -7584.941902 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 31

Atomic N.	X	Y	Z
8	-0.10562796	-0.57914823	0.41177332
8	1.69670522	0.51634115	1.66492045
6	3.09555817	0.31307182	1.72070765
1	3.63024116	1.21658695	1.38425159
1	3.41934967	-0.52628660	1.08102202
1	3.41318035	0.10919876	2.76095200
8	1.29486668	-2.08081698	1.24457431
6	0.46832585	-1.02473748	1.47034347
6	-0.25476798	-0.88465673	2.80452347
1	-1.00531995	-1.69760442	2.82948256
1	-0.83118486	0.04531666	2.71247339
6	0.55192655	-0.85486478	4.10797215
1	1.34700549	-0.10296075	4.00307894
1	-0.11928660	-0.48952425	4.90118647
6	1.13467062	-2.19923925	4.54935551
1	0.30902395	-2.90613127	4.74550915
1	1.66100991	-2.06757379	5.50794220
6	2.08589554	-2.83388209	3.53213167
1	2.96266198	-2.19251037	3.35199857
1	2.47266746	-3.78219891	3.94162989
6	1.43262684	-3.16985607	2.19551110
1	0.44168672	-3.62903428	2.35135555
1	2.05269814	-3.88611531	1.64190876
50	0.38466325	1.61079502	0.19788225
7	-1.10669494	2.93734169	-2.13459849
6	-0.87517613	4.37442017	-1.97682071

1	-1.10419893	4.94478416	-2.90177631
1	0.17194870	4.56395435	-1.70886052
1	-1.50090039	4.76009750	-1.16076505
7	1.47326398	1.34305727	-1.63349903
6	-0.22988591	2.35698223	-3.16225338
1	-0.30230135	2.94096613	-4.10778284
1	-0.57726401	1.33519399	-3.36953402
6	1.24003041	2.27397203	-2.74366975
1	1.79562354	1.91744900	-3.62800336
1	1.62437546	3.29707122	-2.55292821
6	2.70964265	0.63284189	-1.72843432
6	3.95137525	1.28355122	-1.51493812
6	5.14496851	0.55589306	-1.62038493
6	5.15622377	-0.80560070	-1.93536663
6	3.92540312	-1.42918169	-2.17369676
6	2.70987082	-0.74000472	-2.08665586
7	-2.83046579	1.04566646	-0.59755343
6	-2.52675343	2.67179084	-2.41823244
1	-2.76232529	2.85234237	-3.48916173
1	-3.12283015	3.39770269	-1.84159839
6	-2.98873305	1.26483548	-2.04268527
1	-4.04497004	1.16321337	-2.35441852
1	-2.41666722	0.51591927	-2.60863495
6	-3.64609599	0.12448131	0.09454068
6	-3.74091506	-1.23131788	-0.30165344
6	-4.55113459	-2.09978151	0.44176376
6	-5.24853230	-1.69222414	1.58312142
6	-5.09950638	-0.36031654	1.98761964
6	-4.32059240	0.55056542	1.26837623
6	4.01944971	2.75113297	-1.16903532
1	6.09278774	1.07103491	-1.44127524
6	6.44847202	-1.58427370	-1.99896193
1	3.90833020	-2.48656869	-2.45150995
6	1.42455411	-1.45283496	-2.42244864
6	-2.92864180	-1.78400862	-1.44728625
1	-4.61274433	-3.14422035	0.12470629
6	-6.13687277	-2.64651513	2.34467840
1	-5.61329412	-0.01199455	2.88748813
6	-4.20005417	1.97678411	1.75227261
1	4.96723318	2.99152970	-0.66920257
1	3.18998075	3.04812956	-0.51026505
1	3.95341253	3.38456035	-2.06804585
1	0.73328793	-1.45105708	-1.56994557
1	1.62762833	-2.49174428	-2.71499538
1	0.90681922	-0.95650971	-3.25754714
1	6.41954374	-2.34560084	-2.79124212
1	6.64273071	-2.11107635	-1.05089140
1	7.30571985	-0.92413241	-2.18852401
1	-2.90624714	-2.88048768	-1.39973950
1	-1.89361238	-1.41673100	-1.39835656
1	-3.33881998	-1.50922430	-2.43143272
1	-4.55800295	2.70156455	1.00199115
1	-3.15921474	2.24923468	1.99578106
1	-4.79634428	2.12590671	2.66104436
1	-6.09312391	-2.46075869	3.42719436
1	-5.84753990	-3.69108152	2.16566610
1	-7.19096422	-2.54236174	2.04100847
1	-2.80983210	1.94146895	-0.11512707

Energy = -7584.938599 Hartree
 Number of imaginary frequencies = 0.

Compound TS2b isomer 32

Atomic N.	X	Y	Z
8	-1.22894204	0.75809377	2.73686767
8	0.68335772	0.70530772	1.14025974
6	1.81740689	1.45136309	1.57815981
1	2.13291025	2.14099979	0.77700758
1	2.66104960	0.77706426	1.79843307
1	1.60835099	2.05832434	2.47994900
8	-0.74653703	-1.21432769	1.70867765
6	-0.38019869	-0.17783415	2.54153728
6	0.61620384	-0.47671404	3.64851499
1	0.01135704	-0.76912630	4.52568960
1	1.06541300	0.48631296	3.92508340
6	1.69662678	-1.53158975	3.37448549
1	2.12580323	-1.36754549	2.37443852
1	2.51435113	-1.37340629	4.09456968
6	1.21180022	-2.98178005	3.49765944
1	0.75299180	-3.12090445	4.49246454
1	2.08065295	-3.65782905	3.46293139
6	0.20907354	-3.39926457	2.41842961
1	0.69665343	-3.42051339	1.43049908
1	-0.14286585	-4.42552328	2.61873484
6	-1.01863778	-2.50125670	2.32192349
1	-1.49058974	-2.35290980	3.30762601
1	-1.77363455	-2.94929028	1.66245091
50	-1.09681594	2.19675946	0.98330426
7	-0.79184437	2.70888162	-1.69251060
6	-0.08116148	3.97517586	-1.90715098
1	-0.25165632	4.38285112	-2.92291784
1	0.99392414	3.82990909	-1.75054884
1	-0.43649375	4.70919228	-1.17126179
7	1.84971344	1.16685188	-1.69783401
6	-0.39952505	1.65766025	-2.65821600
1	-0.87058157	1.86698985	-3.64213610
1	-0.81970495	0.70998043	-2.29217815
6	1.09467745	1.48051703	-2.91519594
1	1.17842269	0.67480749	-3.67196727
1	1.50741673	2.38495278	-3.38832974
6	3.13683391	0.58476388	-1.87010276
6	4.21944809	1.37294376	-2.32280350
6	5.48447418	0.78572345	-2.45840120
6	5.72128344	-0.55531353	-2.14159918
6	4.64119434	-1.31427026	-1.67371988
6	3.35633159	-0.77649081	-1.54316711
7	-2.62687683	1.14424384	-0.08371378
6	-2.25145578	2.92974257	-1.76694798
1	-2.54693890	3.24086738	-2.79024696
1	-2.48565245	3.76536608	-1.08665812
6	-3.06765223	1.70281053	-1.36002827
1	-4.12439775	2.03321695	-1.30928302
1	-3.03594685	0.95276487	-2.17591643
6	-3.48850822	0.12104648	0.40719983
6	-3.46953964	-1.17710102	-0.16266403
6	-4.36330938	-2.15264463	0.29929423

6	-5.27875233	-1.89581931	1.32485044
6	-5.28151512	-0.61431724	1.88618004
6	-4.41033745	0.39201725	1.45002162
6	4.04648638	2.84352493	-2.60820961
1	6.31498766	1.40889204	-2.80029726
6	7.08900023	-1.17102158	-2.31557226
1	4.79800987	-2.36471534	-1.41464484
6	2.21713209	-1.65008557	-1.07291639
6	-2.46967101	-1.54171598	-1.23035634
1	-4.33355999	-3.14805627	-0.15328600
6	-6.21282005	-2.97005415	1.82941902
1	-5.99166155	-0.38332513	2.68481898
6	-4.47562170	1.75063407	2.10273194
1	5.01302052	3.36244297	-2.56757951
1	3.36818337	3.30173898	-1.87360132
1	3.61898828	3.02850628	-3.60679412
1	1.74499631	-1.27063894	-0.15298752
1	2.57265949	-2.67011952	-0.87792587
1	1.41890001	-1.71314561	-1.82959914
1	7.16708565	-1.70362103	-3.27687883
1	7.30559111	-1.90076613	-1.52294350
1	7.87662840	-0.40557003	-2.30087590
1	-2.38225508	-2.63253546	-1.32504845
1	-1.48286974	-1.12845516	-0.97992188
1	-2.75338101	-1.15243948	-2.22153926
1	-4.40623331	2.56186199	1.36462557
1	-3.64717984	1.88780272	2.81554914
1	-5.41267729	1.86628604	2.66359758
1	-5.81259251	-3.45568323	2.73395896
1	-6.36522055	-3.75470877	1.07598054
1	-7.19525146	-2.55480886	2.09502864
1	1.28167593	0.61804605	-1.04647624

Energy = -7584.938155 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 33

Atomic N.	X	Y	Z
8	1.09712219	0.23978055	0.70318037
8	0.93756479	-0.07120984	-1.72294772
6	0.95588601	-1.17066002	-2.61396790
1	-0.07324683	-1.45223153	-2.90746284
1	1.40947843	-2.06368542	-2.14673924
1	1.51829839	-0.92115980	-3.53102016
8	2.41456890	-1.40652764	-0.03803847
6	2.03010702	-0.09316443	-0.11813488
6	3.04339552	0.97593647	-0.50464356
1	3.73134208	1.07822728	0.35622856
1	2.45636225	1.90099120	-0.53744447
6	3.83632851	0.83265460	-1.80892944
1	3.13054800	0.61774427	-2.62359881
1	4.27651119	1.81610727	-2.03580356
6	4.95920658	-0.20645773	-1.78039515
1	5.69943619	0.07932294	-1.01188135
1	5.49361277	-0.18880840	-2.74331546
6	4.48332262	-1.63209915	-1.49251103
1	3.80259705	-1.98802269	-2.28138399
1	5.35119295	-2.31288815	-1.50051236

6	3.80809617	-1.80394721	-0.13525301
1	4.38014364	-1.28140378	0.65060043
1	3.76719308	-2.86782885	0.13168471
50	-0.88691181	0.12892015	-0.40258613
7	-1.49852467	1.58448136	1.80001807
6	-0.40961125	2.46484947	2.25456142
1	-0.78111619	3.25320458	2.93853045
1	0.06933392	2.93263721	1.38958955
1	0.34884644	1.86394727	2.76847720
7	-1.13069427	2.19534755	-0.99716932
6	-2.52432823	2.34708071	1.05313134
1	-3.00615621	3.09495878	1.71596479
1	-3.30015826	1.63028049	0.73897833
6	-1.96053708	3.06798959	-0.17566852
1	-2.83440065	3.44947505	-0.74154317
1	-1.41757703	3.97380590	0.16496687
6	-0.74213517	2.73595119	-2.25210524
6	0.20016851	3.79472375	-2.34573531
6	0.56844127	4.29605389	-3.60139370
6	0.03596526	3.79239392	-4.79100037
6	-0.89339548	2.75117207	-4.69182062
6	-1.29174817	2.22273493	-3.45837450
7	-1.49070084	-1.45176435	2.43000889
6	-2.10279346	0.88350421	2.96352005
1	-2.93599629	1.48762023	3.37099504
1	-1.33851206	0.82610285	3.75311136
6	-2.60421205	-0.53133690	2.68088293
1	-3.18426418	-0.85902810	3.56057739
1	-3.30059457	-0.51199466	1.82456219
6	-1.50885701	-2.77814150	2.89879131
6	-2.59632325	-3.64241505	2.62447572
6	-2.56328130	-4.95309401	3.11789322
6	-1.47717261	-5.45929813	3.83877945
6	-0.38383114	-4.60787630	4.04041433
6	-0.37796974	-3.28489733	3.59025097
6	0.85463035	4.37269974	-1.11646020
1	1.30937147	5.09942102	-3.64703155
6	0.42645699	4.36660290	-6.13192320
1	-1.33309650	2.34003282	-5.60479641
6	-2.32227302	1.11985171	-3.43971300
6	-3.73609900	-3.21753669	1.72847569
1	-3.40858126	-5.61013889	2.89642763
6	-1.48387480	-6.86785030	4.38246775
1	0.49449879	-4.98103952	4.57372856
6	0.82898688	-2.40969348	3.83001637
1	1.82531178	4.82204533	-1.36622643
1	1.01002562	3.59187007	-0.35918921
1	0.24206977	5.16116285	-0.64995646
1	-1.86939466	0.12859289	-3.27131605
1	-2.85232520	1.06905365	-4.40046549
1	-3.05706143	1.26704800	-2.63613462
1	-0.32702777	5.08423185	-6.49425936
1	0.51715922	3.58110690	-6.89548922
1	1.38511932	4.89982414	-6.07391882
1	-4.28667355	-4.09858465	1.37406182
1	-3.35615373	-2.67311668	0.85097414
1	-4.46175241	-2.56033134	2.23210216
1	0.58162105	-1.52049673	4.43383503

1	1.27249742	-2.04694033	2.88771105
1	1.60590565	-2.96712780	4.36810923
1	-0.47558397	-7.30509710	4.38021660
1	-2.14059114	-7.52128649	3.79173446
1	-1.84718382	-6.89462280	5.42255974
1	-0.58600169	-1.00773978	2.56566381

Energy = -7584.941137 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 34

Atomic N.	X	Y	Z
8	0.92576975	-2.32320094	-0.11546301
8	1.73049593	-0.11843056	0.21091379
6	2.32458615	0.86375433	-0.63790005
1	1.54315650	1.53449094	-1.03062379
1	2.82265282	0.38743100	-1.49568045
1	3.06225586	1.46020222	-0.07445718
8	2.83832836	-1.84487283	-1.20345724
6	2.13026738	-1.82050717	-0.01155038
6	2.86771727	-2.14714217	1.28539693
1	3.09756660	-3.22680402	1.25363088
1	2.10628271	-2.03233576	2.06629348
6	4.12015009	-1.34013975	1.64854395
1	3.91132283	-0.26829654	1.50873363
1	4.30435038	-1.47578907	2.72586489
6	5.38795900	-1.73909926	0.88778692
1	5.62361574	-2.79363394	1.11539865
1	6.23940420	-1.14671934	1.25907636
6	5.28412867	-1.58046806	-0.63108897
1	5.14890718	-0.52250451	-0.90800899
1	6.23198795	-1.90301335	-1.09414756
6	4.17004490	-2.40515685	-1.27349293
1	4.15711641	-3.42933297	-0.86317706
1	4.34101295	-2.48391414	-2.35539722
50	-0.49280122	-0.66182077	-0.06632938
7	-1.12372339	1.81947565	1.14005101
6	-0.15434752	2.92318034	1.11324489
1	-0.50845927	3.80682945	1.68117070
1	0.04473277	3.21974564	0.07665656
1	0.78518206	2.57635522	1.56034541
7	-1.63366628	2.39859009	-1.81418002
6	-2.43112373	2.20503688	0.55978340
1	-3.00434828	2.80402565	1.29774332
1	-3.00577116	1.28054047	0.38625985
6	-2.39686823	3.03035641	-0.72818595
1	-3.45377994	3.19443130	-1.01557708
1	-1.98206913	4.02550507	-0.51123917
6	-1.88739622	2.83438587	-3.14253592
6	-1.56583405	4.15214920	-3.54395890
6	-1.81320715	4.54398489	-4.86638403
6	-2.34627795	3.67049122	-5.81844759
6	-2.62047720	2.35894847	-5.41214657
6	-2.40877938	1.92702091	-4.09905958
7	-0.99455559	-1.06643307	1.96738195
6	-1.30176914	1.33645165	2.52758789
1	-1.95243061	2.03526402	3.09433365
1	-0.30993810	1.33740234	2.99849510

6	-1.86358058	-0.08405738	2.61526155
1	-1.97949445	-0.32443920	3.68389082
1	-2.89404845	-0.10485514	2.20239568
6	-0.76732403	-2.27567220	2.67642093
6	-1.26803946	-3.51340461	2.19430065
6	-1.03512204	-4.68832970	2.91941643
6	-0.31448910	-4.69657660	4.11809206
6	0.18181077	-3.47455406	4.58206511
6	-0.02380245	-2.27498841	3.88862514
6	-0.89838254	5.12402773	-2.60214281
1	-1.55270791	5.56332445	-5.16327238
6	-2.62667799	4.12503338	-7.23061419
1	-3.02189922	1.64665389	-6.13752365
6	-2.73136902	0.50130379	-3.72008204
6	-2.05568576	-3.59634256	0.91046816
1	-1.43997729	-5.62862825	2.53555012
6	-0.05183321	-5.98333693	4.86348438
1	0.76327920	-3.45082879	5.50801229
6	0.60196507	-1.00926411	4.42102861
1	-0.37670505	5.90740776	-3.16729593
1	-0.16519862	4.60853672	-1.96454787
1	-1.61603475	5.62787342	-1.93522978
1	-1.83686244	-0.06134590	-3.40755725
1	-3.17445445	-0.03142809	-4.57079506
1	-3.44552946	0.44789034	-2.88282537
1	-3.68442917	4.40636539	-7.35687733
1	-2.41444492	3.32981205	-7.95882750
1	-2.02106118	5.00227165	-7.49565172
1	-2.64341378	-4.52355623	0.87566090
1	-1.38849580	-3.60331202	0.03341788
1	-2.74179363	-2.74461865	0.79854524
1	-0.12481132	-0.35840666	4.93326473
1	1.03738272	-0.41796979	3.60185623
1	1.39197862	-1.24475813	5.14645815
1	0.87524682	-6.46509933	4.51343298
1	-0.86752957	-6.70471239	4.71622086
1	0.05940914	-5.80726290	5.94223928
1	-1.69724512	1.38081324	-1.73907089

Energy = -7584.944306 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 35

Atomic N.	X	Y	Z
8	0.91883630	-0.51085246	-0.28483298
8	0.77079791	0.22246486	-2.63834143
6	1.24459064	-0.26506713	-3.87824035
1	0.46147940	-0.84792519	-4.40056133
1	2.10664320	-0.94476455	-3.74381924
1	1.54715335	0.56873691	-4.53638077
8	2.81131959	-0.89494783	-1.40235782
6	1.85885572	-0.00352874	-0.99941754
6	2.21950507	1.45620537	-0.76833737
1	2.83395481	1.48085833	0.15233053
1	1.26597452	1.93086350	-0.51016659
6	2.89901614	2.25585747	-1.88594425
1	2.32264280	2.11621499	-2.81115532
1	2.81122303	3.32217431	-1.62624097

6	4.37651491	1.93185461	-2.11609554
1	4.94683266	2.15949321	-1.19791663
1	4.77514458	2.59682655	-2.89827228
6	4.64207363	0.47641993	-2.50711298
1	4.15419865	0.22883405	-3.46262407
1	5.72448349	0.33452660	-2.66487598
6	4.22116232	-0.54125458	-1.45209134
1	4.53538227	-0.21168154	-0.44714335
1	4.69708300	-1.50974703	-1.65121663
50	-0.86087596	-0.97027606	-1.65020418
7	-1.96971595	-1.09771073	0.70327830
6	-1.42258501	-0.20756796	1.74426675
1	-2.16251755	-0.05285572	2.55230069
1	-1.15577638	0.75769359	1.30281842
1	-0.52340448	-0.65004653	2.17582011
7	-2.05627966	0.80184102	-1.41992986
6	-3.27365804	-0.58041269	0.22415964
1	-4.00147343	-0.51813298	1.05695832
1	-3.65866590	-1.30397594	-0.51238614
6	-3.13657999	0.79178381	-0.43863422
1	-4.11284351	1.01420546	-0.91217685
1	-3.00832748	1.56207395	0.34843293
6	-2.00310326	1.94192815	-2.26481700
6	-1.65758455	3.22366524	-1.76076341
6	-1.60753512	4.32479620	-2.62620234
6	-1.88910830	4.21491051	-3.99037957
6	-2.22997403	2.94882655	-4.47924566
6	-2.29761982	1.82343781	-3.64997983
7	0.34905025	-3.03542972	1.88931835
6	-2.09809899	-2.48905349	1.20285451
1	-2.85885620	-2.99082112	0.58440590
1	-2.47897649	-2.47778392	2.24177051
6	-0.83176154	-3.36544752	1.09320986
1	-1.15333390	-4.39576721	1.29449487
1	-0.50202483	-3.35120606	0.04348194
6	0.37940019	-2.88900781	3.28550839
6	-0.36585602	-3.70169830	4.18095016
6	-0.27662718	-3.45435762	5.55870676
6	0.55101955	-2.47212243	6.10671806
6	1.34937131	-1.74669945	5.21500397
6	1.28724170	-1.93611646	3.83305526
6	-1.30038083	3.42691517	-0.30975544
1	-1.32300746	5.29858971	-2.21735859
6	-1.85472834	5.42022181	-4.89941025
1	-2.46342254	2.83209872	-5.54115725
6	-2.70895362	0.50075585	-4.24947357
6	-1.17848325	-4.89720392	3.73674345
1	-0.86479139	-4.08654308	6.22931957
6	0.59209245	-2.21121335	7.59280920
1	2.05100465	-1.00456703	5.60503817
6	2.21942544	-1.15775955	2.93507028
1	-0.63641244	4.29376507	-0.18988518
1	-0.79836959	2.53688383	0.09447475
1	-2.18916059	3.61039662	0.31533673
1	-1.85053420	-0.17469147	-4.40226269
1	-3.17587733	0.65013379	-5.23233509
1	-3.41445613	-0.03485266	-3.59920287
1	-2.86658096	5.82162046	-5.06976843

1	-1.43707430	5.16973305	-5.88484716
1	-1.25017297	6.22908258	-4.46706676
1	-1.46054161	-5.49594307	4.61246538
1	-0.60115212	-5.54666233	3.06213856
1	-2.11061740	-4.62897444	3.21482110
1	1.68793011	-0.53984648	2.19306564
1	2.88531351	-1.82761252	2.36519408
1	2.85298014	-0.49094653	3.53318501
1	1.60917687	-1.96664047	7.93078327
1	0.24548806	-3.08504510	8.16138744
1	-0.05385887	-1.36276197	7.87093925
1	0.92737776	-2.34916687	1.40777111

Energy = -7584.945048 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 36

Atomic N.	X	Y	Z
8	2.08836651	0.72419655	1.48689950
8	1.94516075	1.17358208	-0.92376912
6	2.44937730	0.63795137	-2.13105369
1	1.69435787	-0.00580890	-2.62234902
1	3.33844566	0.00400389	-1.95460713
1	2.72015619	1.44424355	-2.83559775
8	3.97888303	0.21206342	0.40166342
6	3.02746940	1.14543760	0.71955407
6	3.39940500	2.61845517	0.80192286
1	3.99832559	2.73772001	1.72501349
1	2.44668436	3.12614298	0.98857504
6	4.10655403	3.28654480	-0.38309115
1	3.55165148	3.04805517	-1.30132365
1	4.01741838	4.37539005	-0.24602719
6	5.58795691	2.93752956	-0.54211169
1	6.13566017	3.25897598	0.36171812
1	6.00901890	3.51666045	-1.37902761
6	5.85694408	1.44881368	-0.77195102
1	5.39760399	1.10607815	-1.71222603
1	6.94292784	1.28764260	-0.87935299
6	5.39167500	0.54698414	0.36707288
1	5.67841244	0.97490406	1.34285975
1	5.86489725	-0.43978932	0.28225091
50	0.42880100	-0.09348807	0.17614454
7	-0.85250843	-0.34061813	2.47042370
6	-0.18509533	0.49144173	3.48725677
1	-0.82413656	0.61316597	4.38314199
1	0.05826321	1.47349274	3.07118011
1	0.75839841	0.01472826	3.77920055
7	-0.90801090	1.57782865	0.33713996
6	-2.13411689	0.24558087	2.02760124
1	-2.84008479	0.34960455	2.87683272
1	-2.56761837	-0.44702211	1.29192460
6	-1.94218326	1.61112404	1.36728621
1	-2.92103648	1.88875449	0.93142283
1	-1.74412441	2.36759925	2.15321445
6	-0.87083352	2.70392036	-0.52714419
6	-0.54240537	4.00119829	-0.05319099
6	-0.52153003	5.08419466	-0.94260716
6	-0.81195325	4.93933201	-2.30169225

6	-1.12780035	3.65582967	-2.76156282
6	-1.16694736	2.54764438	-1.90810382
7	-1.67163754	-2.89937377	0.91377246
6	-0.98527759	-1.71679580	3.01845431
1	-1.31315255	-1.65143228	4.07530117
1	0.02601896	-2.15535975	3.02422690
6	-1.96258068	-2.67137384	2.33395624
1	-1.91523242	-3.61457777	2.91178298
1	-2.98777437	-2.29050183	2.45588613
6	-2.11237097	-4.10349989	0.30981630
6	-3.49128270	-4.40496731	0.21453252
6	-3.88786387	-5.59928751	-0.40131521
6	-2.97039843	-6.49755669	-0.95429778
6	-1.61342549	-6.15848970	-0.89041489
6	-1.16739392	-4.98842144	-0.26816523
6	-0.16513360	4.24070168	1.38809562
1	-0.25156203	6.07183695	-0.55756003
6	-0.81079972	6.12574100	-3.23595738
1	-1.36381018	3.51122165	-3.81944513
6	-1.54506397	1.20090675	-2.47431183
6	-4.54468822	-3.43481350	0.69048196
1	-4.95698738	-5.81574965	-0.47334111
6	-3.42392993	-7.79081917	-1.58775008
1	-0.87253588	-6.83042002	-1.33125162
6	0.31012428	-4.67852354	-0.22429676
1	0.49419069	5.11526346	1.47523558
1	0.35197464	3.36480570	1.80492687
1	-1.04516685	4.43454027	2.02238631
1	-0.66846371	0.54548973	-2.61050320
1	-2.01503778	1.31366372	-3.46057534
1	-2.23417211	0.66308081	-1.80901933
1	-1.83175588	6.50574398	-3.40124226
1	-0.40138912	5.86204720	-4.22142458
1	-0.21536209	6.95413589	-2.82846069
1	-5.50780630	-3.65107989	0.21022464
1	-4.26016808	-2.40050626	0.44619235
1	-4.70566034	-3.48227859	1.77914155
1	0.67505962	-4.55234289	0.80787545
1	0.55870038	-3.75001836	-0.76383889
1	0.88657367	-5.49111557	-0.68389058
1	-2.77731419	-8.07487583	-2.42952847
1	-4.45504999	-7.71421146	-1.95893037
1	-3.39806747	-8.62076378	-0.86342192
1	-0.68675727	-2.72011137	0.71314341

Energy = -7584.943856 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 37

Atomic N.	X	Y	Z
8	1.96274209	-1.91819298	-0.50622779
8	2.08508015	0.17912357	0.66736376
6	2.35594726	1.53269577	0.31827146
1	1.41871476	2.06458354	0.07663973
1	2.99787116	1.58193886	-0.57615900
1	2.85782695	2.05457950	1.15192294
8	3.53132582	-0.50972271	-1.30150330
6	2.98430037	-1.18129015	-0.22439726

6	3.90386653	-1.67460144	0.88885295
1	4.42206430	-2.57035923	0.50027531
1	3.21686220	-2.03454280	1.66442072
6	4.91479540	-0.70137179	1.50826466
1	4.40383148	0.24334438	1.74783921
1	5.23634386	-1.12698388	2.47180700
6	6.16132355	-0.43234736	0.66063559
1	6.68877554	-1.38672340	0.48593354
1	6.85775709	0.20413087	1.22924769
6	5.86904955	0.22044884	-0.69203985
1	5.43638039	1.22478473	-0.55736762
1	6.81591320	0.36068758	-1.24032795
6	4.94737339	-0.59551537	-1.59436953
1	5.25178385	-1.65590942	-1.60927355
1	5.00365925	-0.21969198	-2.62448907
50	0.12375271	-0.68916643	-0.16611631
7	-0.85466927	0.55105269	2.01053834
6	-0.08225951	1.63353622	2.64278722
1	-0.55873168	1.97670805	3.58158445
1	0.01079986	2.48023462	1.95435214
1	0.92220896	1.25852454	2.87032056
7	-1.61554337	2.54551792	-0.17548788
6	-2.24000168	0.97767818	1.68161726
1	-2.85272908	0.97834486	2.60569263
1	-2.67182589	0.21648572	1.01366580
6	-2.40446091	2.36156440	1.05095732
1	-3.48874378	2.48255610	0.86024046
1	-2.13554883	3.13381815	1.78604841
6	-2.00622821	3.57989287	-1.06878328
6	-1.91260552	4.93820000	-0.68667752
6	-2.28910947	5.93232489	-1.59972620
6	-2.73297691	5.63310099	-2.89086699
6	-2.78009415	4.28417540	-3.26349735
6	-2.43324900	3.25626874	-2.38124585
7	-0.61513704	-2.24116445	1.13930964
6	-0.88836956	-0.61303455	2.93367100
1	-1.48116469	-0.35988203	3.83582401
1	0.15050443	-0.80221468	3.24046159
6	-1.43351305	-1.87663388	2.28510237
1	-1.39249766	-2.67246675	3.05497003
1	-2.51403379	-1.74857271	2.05620003
6	-0.91333157	-3.52384925	0.57984477
6	-2.08057117	-3.76284456	-0.19360638
6	-2.31720138	-5.04089928	-0.71961045
6	-1.44249487	-6.10832691	-0.50085652
6	-0.30682731	-5.86790752	0.28007665
6	-0.02789930	-4.60669947	0.81912059
6	-1.35311723	5.34474516	0.65445071
1	-2.20522189	6.97812223	-1.29272163
6	-3.15726113	6.72202206	-3.84672356
1	-3.10636902	4.01842356	-4.27220869
6	-2.51181030	1.81884170	-2.83813190
6	-3.09606791	-2.67884469	-0.46803287
1	-3.21525216	-5.20167446	-1.32246900
6	-1.69770801	-7.46685505	-1.10819960
1	0.38675037	-6.68916845	0.48036310
6	1.21636152	-4.41781664	1.64760029
1	-0.99297607	6.38121796	0.62057102

1	-0.51333839	4.69454861	0.94060606
1	-2.10203362	5.28731871	1.46037579
1	-1.52740049	1.32331729	-2.83390689
1	-2.90382600	1.76217628	-3.86124349
1	-3.17270970	1.21702361	-2.19390631
1	-4.25116539	6.85327911	-3.84114885
1	-2.86488104	6.48717499	-4.87968922
1	-2.71038747	7.68810940	-3.57570624
1	-3.67975092	-2.91401172	-1.36776793
1	-2.61591601	-1.70081604	-0.61857545
1	-3.80872297	-2.56872678	0.36528975
1	1.02541864	-3.78582597	2.52493691
1	1.98891616	-3.90944099	1.05388820
1	1.61124778	-5.38736677	1.98004997
1	-1.14892137	-7.58641195	-2.05601740
1	-2.76407433	-7.61551571	-1.32576799
1	-1.36734498	-8.27365017	-0.43897420
1	-1.52147412	1.65441811	-0.66817039

Energy = -7584.940396 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 38

Atomic N.	X	Y	Z
8	2.18773890	-1.10454035	0.78646207
8	2.20038438	-0.39616176	-1.49148846
6	2.83426237	-0.05036729	-2.71191931
1	2.07920432	0.03255821	-3.51048160
1	3.55030465	-0.84175682	-2.98744678
1	3.37013364	0.91371894	-2.65049100
8	3.69709563	-2.09237885	-0.65931761
6	3.13350654	-0.93978107	-0.02987622
6	4.13069773	0.20374408	0.23725489
1	4.25344324	0.23130122	1.33271050
1	3.61286139	1.13998055	-0.02126756
6	5.51351833	0.14849077	-0.42565140
1	5.41893768	-0.00631813	-1.51111495
1	5.98376513	1.13667345	-0.29445732
6	6.45430470	-0.91352850	0.16713484
1	6.46023226	-0.80724788	1.26636100
1	7.48412752	-0.70759851	-0.16629700
6	6.10262728	-2.35945845	-0.20112078
1	6.24114847	-2.51197410	-1.28437042
1	6.79817724	-3.04990458	0.30663991
6	4.67735386	-2.77431703	0.15215059
1	4.46139765	-2.61205339	1.22239959
1	4.53733301	-3.84673595	-0.05202826
50	0.34589738	0.33905452	-0.39032668
7	-0.48971960	-1.91365373	-1.12401295
6	0.43415925	-3.03683019	-0.84052706
1	0.04215196	-3.96788216	-1.28978479
1	0.55726004	-3.16578007	0.23818871
1	1.42219567	-2.80552983	-1.25069976
7	-1.79190600	-0.91161323	1.48088121
6	-1.84897053	-2.22439480	-0.60896027
1	-2.16558576	-3.20643425	-1.00910807
1	-2.53985906	-1.47365928	-1.01685166
6	-1.98831058	-2.25400019	0.91143632

1	-2.99418044	-2.65679574	1.14164829
1	-1.26458406	-2.94521379	1.35744357
6	-1.95146608	-0.74614137	2.89083004
6	-1.06228006	-1.35336828	3.80648875
6	-1.25485694	-1.13232446	5.17702293
6	-2.27412605	-0.31511277	5.67428780
6	-3.11499977	0.30939192	4.74625778
6	-2.97636652	0.10659360	3.36987972
7	-0.86814004	0.67957252	-2.18451905
6	-0.54263550	-1.70364511	-2.60097337
1	-0.99176753	-2.58995748	-3.08811498
1	0.50160766	-1.62521160	-2.92893004
6	-1.30862498	-0.44210824	-2.99759102
1	-1.10975313	-0.27474052	-4.07580376
1	-2.39896631	-0.63320369	-2.93257880
6	-1.46116829	1.94557846	-2.43430948
6	-2.85508132	2.18730283	-2.27844834
6	-3.38119435	3.46197343	-2.53297758
6	-2.58174372	4.53763533	-2.92280126
6	-1.20740795	4.30265808	-3.04487181
6	-0.64003342	3.04507399	-2.81624603
6	0.11631115	-2.18135715	3.35767102
1	-0.55855381	-1.60091126	5.87711287
6	-2.46748900	-0.11925755	7.15854502
1	-3.90722466	0.97335660	5.10093546
6	-3.90717363	0.81804043	2.41429496
6	-3.79695678	1.12449336	-1.77210915
1	-4.45505857	3.61871672	-2.39686131
6	-3.17080855	5.89821863	-3.20661473
1	-0.55078799	5.12433052	-3.34363174
6	0.84501398	2.87410498	-3.01937079
1	0.87459052	-2.21488714	4.15075731
1	0.59132701	-1.76933515	2.45696235
1	-0.16620877	-3.22591543	3.14567947
1	-3.37203598	1.53215396	1.76640344
1	-4.65992975	1.39098358	2.96961617
1	-4.44845343	0.11824493	1.75697744
1	-3.21445584	-0.82341558	7.55849743
1	-2.82235408	0.89513087	7.38731003
1	-1.53206992	-0.28773943	7.70894623
1	-4.67798996	1.58121979	-1.30209470
1	-3.29418111	0.49147925	-1.02652442
1	-4.16123152	0.45816916	-2.57047248
1	1.05736935	2.04464817	-3.70709968
1	1.37451243	2.64883041	-2.08042431
1	1.28381276	3.79260921	-3.43126416
1	-2.59999061	6.69611073	-2.70965075
1	-4.21231508	5.96066809	-2.86396122
1	-3.16243410	6.12063646	-4.28537369
1	-2.42733526	-0.26890579	1.00603068

Energy = -7584.936714 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 39

Atomic N.	X	Y	Z
8	1.73340964	-1.53501499	1.13414884
8	1.98292494	-0.33846480	-1.16115189

6	2.55374241	-0.79560786	-2.34788418
1	1.86550009	-0.71348178	-3.21951079
1	2.87068200	-1.86240947	-2.30379653
1	3.45617986	-0.21088932	-2.63876438
8	3.60333610	-2.19096565	0.15831591
6	2.85152149	-1.17753148	0.66271436
6	3.50238490	0.11212482	1.13436115
1	4.01010990	-0.13677813	2.08742046
1	2.66288018	0.76587242	1.40772116
6	4.45334911	0.87364829	0.20456436
1	3.94347119	1.00468135	-0.75987315
1	4.58909273	1.88035619	0.63013321
6	5.83288622	0.23975177	0.01338703
1	6.34972191	0.19021945	0.98848695
1	6.44578123	0.89491463	-0.62559390
6	5.79779434	-1.16545677	-0.59161592
1	5.36016655	-1.15117490	-1.60175347
1	6.82990980	-1.53859925	-0.70266896
6	5.05470467	-2.19005537	0.25767183
1	5.33343458	-2.09238839	1.32047594
1	5.31200457	-3.20674467	-0.06540840
50	-0.03470933	-0.18636075	0.38983953
7	-0.81067860	-2.09956741	-1.07981396
6	0.12074894	-3.23973656	-0.90649927
1	-0.24388650	-4.12114334	-1.46463561
1	0.21497910	-3.49051952	0.15344355
1	1.11251581	-2.95191932	-1.26905763
7	-1.50447750	-1.33652139	1.52442873
6	-2.14745426	-2.43942595	-0.52536321
1	-2.50756860	-3.38460398	-0.97627908
1	-2.83812642	-1.63168144	-0.80294377
6	-2.10862231	-2.54346180	0.99667025
1	-3.15415311	-2.65355277	1.34441102
1	-1.59707940	-3.48421645	1.29030931
6	-1.65868855	-1.07390821	2.91230059
6	-1.09615719	-1.91189837	3.91281366
6	-1.26820600	-1.58972836	5.26574612
6	-1.97020662	-0.45421413	5.68039179
6	-2.50843143	0.37246710	4.68797636
6	-2.37370825	0.08355031	3.32495737
7	-0.93730938	0.65734911	-2.27607203
6	-0.89259380	-1.79508328	-2.53287005
1	-1.40313566	-2.62951636	-3.05158877
1	0.13961421	-1.76690412	-2.90576982
6	-1.59367657	-0.49287277	-2.91066456
1	-1.57249904	-0.42565984	-4.01608801
1	-2.65169072	-0.51727414	-2.62239170
6	-1.36034024	1.97303593	-2.62511611
6	-2.66779137	2.42255425	-2.33201528
6	-3.02751184	3.73294902	-2.67508698
6	-2.13236356	4.62434340	-3.27243066
6	-0.82828611	4.17277718	-3.50831151
6	-0.42618474	2.86960244	-3.20122838
6	-0.27243972	-3.12291193	3.55033493
1	-0.81760484	-2.24254322	6.01884699
6	-2.16120768	-0.14204019	7.14546204
1	-3.06420255	1.26713967	4.98187923
6	-3.01830125	0.99895638	2.31176519

6	-3.66612267	1.55939555	-1.60067391
1	-4.03941679	4.07118607	-2.43781805
6	-2.55494070	6.02245617	-3.65356016
1	-0.09677742	4.85439348	-3.94951940
6	0.99667621	2.44019461	-3.47164583
1	0.36835918	-3.41687465	4.39244223
1	0.36633551	-2.91723418	2.68028927
1	-0.90249383	-3.99272823	3.30302739
1	-2.27416420	1.58098602	1.74592650
1	-3.68937087	1.71179438	2.80965948
1	-3.59537244	0.42516977	1.57317877
1	-3.13500428	-0.50810593	7.50880098
1	-2.13235426	0.94052696	7.33326006
1	-1.38399744	-0.61710566	7.75964355
1	-4.40550041	2.18634510	-1.08579588
1	-3.16987586	0.93106085	-0.84767085
1	-4.22529554	0.89352047	-2.27796650
1	1.04546380	1.60924947	-4.19387913
1	1.51184201	2.10329819	-2.55712199
1	1.57297170	3.27380848	-3.89175200
1	-1.73991179	6.74381876	-3.50245762
1	-3.41967368	6.35360575	-3.06290793
1	-2.84307981	6.07567692	-4.71559238
1	0.07814907	0.57209563	-2.37659597

Energy = -7584.933453 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 40

Atomic N.	X	Y	Z
8	1.71971023	-0.58054209	0.77871346
8	2.23471284	0.50788939	-1.22696900
6	3.10547090	1.05182993	-2.21460295
1	2.50705600	1.32660735	-3.09475517
1	3.84262657	0.28778341	-2.50356507
1	3.63326406	1.95101643	-1.85342264
8	3.48948455	-1.36380053	-0.50085109
6	2.81704736	-0.30740637	0.18790565
6	3.75871396	0.69160444	0.89549839
1	3.63619852	0.49251661	1.97245264
1	3.33424973	1.69531906	0.73594356
6	5.25338697	0.67386019	0.54602391
1	5.40137434	0.72694725	-0.54332703
1	5.70280313	1.58961201	0.96337390
6	6.01578522	-0.53583854	1.11167419
1	5.78390455	-0.62769032	2.18740463
1	7.09813690	-0.34005296	1.04733133
6	5.71817875	-1.86731946	0.41294679
1	6.09252596	-1.83611667	-0.62372690
1	6.26375580	-2.68101454	0.92107201
6	4.23958874	-2.24116516	0.36570039
1	3.79006863	-2.25205445	1.37352467
1	4.11975288	-3.24989653	-0.05736190
50	0.22151825	1.10583639	-0.40527135
7	-0.53538930	-0.97836721	-1.54808486
6	0.38755324	-2.14480853	-1.49057412
1	0.04459886	-2.90912533	-2.21069169
1	0.38960221	-2.57788396	-0.48923656

1	1.40267324	-1.82062232	-1.73811305
7	-1.20923102	-2.20377827	1.25082219
6	-1.88814020	-1.37736893	-1.05520964
1	-2.10985947	-2.39361048	-1.42724442
1	-2.62309551	-0.69023484	-1.49898279
6	-2.08083749	-1.31990266	0.46428892
1	-1.98008358	-0.26466987	0.79593068
1	-3.12595677	-1.59296179	0.66105402
6	-1.72984350	-2.70640540	2.47661400
6	-2.76286244	-3.67269921	2.45897126
6	-3.24296808	-4.17995739	3.67331076
6	-2.71810150	-3.78269935	4.90706968
6	-1.66862071	-2.85568905	4.89959621
6	-1.16923261	-2.30595183	3.71404910
7	-0.64379549	1.79541922	-2.27154016
6	-0.58997107	-0.53541929	-2.97551036
1	-1.10558832	-1.30392170	-3.58051157
1	0.45529449	-0.48331964	-3.31137466
6	-1.24604511	0.82401574	-3.17132783
1	-1.09667635	1.09983742	-4.23493624
1	-2.34515524	0.73821419	-3.04485416
6	-1.18077171	3.11562514	-2.32297349
6	-2.49955821	3.42049146	-1.88767469
6	-2.96855092	4.73961115	-1.95793188
6	-2.17900014	5.78871298	-2.43526530
6	-0.87760389	5.48270416	-2.84787965
6	-0.36960873	4.17969131	-2.79936719
6	-3.30670333	-4.21484137	1.15942013
1	-4.03609180	-4.93180370	3.64725256
6	-3.27010655	-4.32495403	6.20362854
1	-1.22760487	-2.53908467	5.84831190
6	-0.04218144	-1.30192316	3.76454377
6	-3.41352320	2.36859965	-1.30924368
1	-3.98359656	4.95192099	-1.61107981
6	-2.69510841	7.20704842	-2.46808076
1	-0.23634629	6.28217936	-3.22874260
6	1.04038835	3.92423749	-3.26985431
1	-3.75881958	-5.20302725	1.31533825
1	-2.50460029	-4.30623865	0.41262531
1	-4.08552837	-3.57015443	0.72074580
1	0.86986405	-1.66511869	3.26529074
1	0.21868411	-1.07248950	4.80540800
1	-0.30722708	-0.35618100	3.26755595
1	-4.01694775	-3.64030504	6.63653135
1	-2.47825789	-4.45632648	6.95416594
1	-3.76400089	-5.29457426	6.05336905
1	-4.15234280	2.82658362	-0.63875598
1	-2.84414864	1.62399304	-0.73413098
1	-3.97236753	1.82636380	-2.08891988
1	1.08747482	3.05351877	-3.93752480
1	1.71703124	3.71346521	-2.42773819
1	1.43484974	4.80044699	-3.80140352
1	-2.38356853	7.76371908	-1.56984961
1	-3.79238701	7.23374701	-2.50616956
1	-2.30764627	7.75454712	-3.33865666
1	-0.30167601	-1.75619829	1.39782739

Energy = -7584.936199 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 41

Atomic N.	X	Y	Z
8	1.91893399	-1.49755061	0.82367384
8	2.40985394	-0.26920435	-1.16166389
6	3.28633213	0.28647548	-2.12803769
1	2.70594072	0.63351411	-2.99829507
1	3.99406385	-0.48823372	-2.46544909
1	3.85638642	1.14743018	-1.73531556
8	3.61733484	-2.26170182	-0.54600310
6	3.01181006	-1.24162388	0.25064218
6	4.00306797	-0.30526632	0.96787715
1	3.91297936	-0.55343390	2.03845119
1	3.59970665	0.71425503	0.87057036
6	5.48254967	-0.34357661	0.56284529
1	5.59170580	-0.22268438	-0.52557349
1	5.97457504	0.52956617	1.02149928
6	6.22681856	-1.60937858	1.01894212
1	6.02364588	-1.77195966	2.09215093
1	7.31205654	-1.43844259	0.93467700
6	5.87110090	-2.87843585	0.23555271
1	6.20714331	-2.77586818	-0.80984610
1	6.41491985	-3.74040627	0.65922028
6	4.38342762	-3.21733308	0.21835551
1	3.97459745	-3.29895544	1.24045539
1	4.22560358	-4.18750620	-0.27679262
50	0.43188664	0.38170880	-0.23498210
7	-0.39434698	-1.52684510	-1.64420831
6	0.38609117	-2.77895880	-1.50758886
1	0.02597616	-3.52720094	-2.23751926
1	0.29706427	-3.17452860	-0.49225596
1	1.44613349	-2.56504941	-1.67653537
7	-2.09079051	-1.04049218	0.87966460
6	-1.84300542	-1.80114067	-1.45592713
1	-2.14267612	-2.61849499	-2.13922787
1	-2.39543128	-0.90372878	-1.76708031
6	-2.26483464	-2.17786598	-0.03739209
1	-3.32004476	-2.51131272	-0.08563273
1	-1.68330812	-3.03060102	0.33009875
6	-2.49850035	-1.20010138	2.23948097
6	-1.83986950	-2.10525012	3.10238385
6	-2.26998687	-2.19840574	4.43320990
6	-3.30596089	-1.41409254	4.94833899
6	-3.91374445	-0.49427316	4.08629274
6	-3.53412247	-0.37631267	2.74590659
7	-0.40254608	1.26876664	-2.05790591
6	-0.15704550	-0.96650428	-3.00729036
1	-0.56279743	-1.65714514	-3.77078342
1	0.93298453	-0.92586684	-3.12747145
6	-0.75246084	0.42883953	-3.19148254
1	-0.34392354	0.82621193	-4.14295864
1	-1.84565938	0.34784070	-3.35948944
6	-0.85346395	2.61554885	-2.07313871
6	-2.23280072	2.96507716	-2.08742428
6	-2.61689615	4.31375980	-2.09557438
6	-1.68931103	5.35633850	-2.06866241
6	-0.33435932	5.00743532	-2.03056359

6	0.09569452	3.67682672	-2.03543067
6	-0.65686989	-2.92878389	2.65681696
1	-1.75112140	-2.89644170	5.09472752
6	-3.76012158	-1.55894053	6.38062906
1	-4.71087837	0.15043466	4.46415234
6	-4.21881390	0.64348203	1.86443472
6	-3.32002258	1.92219508	-2.02915120
1	-3.68457413	4.55095720	-2.10151792
6	-2.12466574	6.80168056	-2.04966378
1	0.41937324	5.79938555	-2.01183581
6	1.57764113	3.39511490	-2.04052544
1	-0.06576449	-3.23794460	3.52866435
1	0.00620028	-2.36833072	1.98378563
1	-0.96469319	-3.85261083	2.13948464
1	-3.52398181	1.42564964	1.51586485
1	-5.01999426	1.14952981	2.41699576
1	-4.67580938	0.18668929	0.97151405
1	-4.63256121	-2.22744298	6.45619202
1	-4.05568695	-0.59094918	6.80858803
1	-2.96671057	-1.98386204	7.01003885
1	-4.24113083	2.34681201	-1.60846281
1	-3.00650620	1.07795751	-1.39806724
1	-3.57255673	1.51041389	-3.01947975
1	1.85153258	2.72853947	-2.86917710
1	1.91367197	2.90222383	-1.11490226
1	2.14535093	4.32987738	-2.13950777
1	-1.96446693	7.25489569	-1.05868220
1	-3.19125819	6.90034342	-2.29142451
1	-1.55447519	7.40260649	-2.77321696
1	-2.58360481	-0.23734371	0.48693940

Energy = -7584.936777 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 42

Atomic N.	X	Y	Z
8	1.41383624	-2.01539826	1.05752826
8	2.28590655	-0.66811734	-0.74970222
6	3.11126423	0.21988443	-1.45039845
1	2.67126393	0.47831652	-2.43859649
1	4.09965801	-0.22890221	-1.67540908
1	3.29175377	1.17899370	-0.91844654
8	3.27090549	-2.89887857	0.21629924
6	2.65773749	-1.84400284	0.83330530
6	3.43654847	-0.93851358	1.78144050
1	3.50994229	-1.50961161	2.72759771
1	2.74978852	-0.10790208	1.99797261
6	4.81382418	-0.37606668	1.40776980
1	4.75507450	0.13400419	0.43812367
1	5.05252123	0.40466103	2.14734983
6	5.95989037	-1.38941896	1.38735878
1	6.07659864	-1.83043504	2.39310813
1	6.90232134	-0.86177111	1.17138958
6	5.76519775	-2.52065206	0.37645924
1	5.68275881	-2.12551737	-0.64909488
1	6.65122271	-3.17732811	0.38899148
6	4.55392790	-3.40126705	0.66517627
1	4.49264097	-3.63626623	1.74174869

1	4.64068031	-4.35058784	0.12123998
50	0.14046244	-0.23321266	0.37440532
7	-0.54621679	-1.49353540	-1.69172871
6	0.21938512	-2.76589608	-1.72909367
1	-0.14121912	-3.39836502	-2.56016374
1	0.10722813	-3.30086350	-0.78236270
1	1.28200686	-2.53232336	-1.85405874
7	-1.66033685	-1.36558974	0.88448852
6	-1.98938417	-1.77247167	-1.47356248
1	-2.35038042	-2.49266386	-2.23334861
1	-2.53629208	-0.82846373	-1.59143698
6	-2.24022102	-2.29882264	-0.06193899
1	-3.33706808	-2.36831355	0.07121399
1	-1.86388314	-3.33980680	0.01521039
6	-2.05976868	-1.45679295	2.24314642
6	-1.86073959	-2.62565637	3.02837491
6	-2.27053237	-2.64052200	4.36872864
6	-2.86232328	-1.53398085	4.98399591
6	-3.04066157	-0.38304389	4.20832109
6	-2.66347384	-0.32644266	2.86187315
7	-0.51419950	1.55937386	-2.23149037
6	-0.29750523	-0.80129611	-2.98562980
1	-0.61775076	-1.46654236	-3.81129336
1	0.79425460	-0.69265145	-3.06716657
6	-0.96629679	0.55367130	-3.20408463
1	-0.73350424	0.85252655	-4.24580717
1	-2.05807185	0.46421438	-3.14985991
6	-0.97508025	2.89829469	-2.40858746
6	-2.33347321	3.22826958	-2.20561075
6	-2.74275064	4.55822325	-2.37463284
6	-1.85134244	5.58001661	-2.71125245
6	-0.50364029	5.23699188	-2.87622523
6	-0.05101178	3.92211318	-2.73541856
6	-1.16423857	-3.84267592	2.47046137
1	-2.09723783	-3.54710054	4.95586252
6	-3.31479359	-1.58485878	6.42384863
1	-3.50541425	0.49815491	4.65930080
6	-2.93965364	0.93187940	2.07482386
6	-3.34197068	2.19947290	-1.76050401
1	-3.79590178	4.80080414	-2.21184373
6	-2.31236815	7.01038170	-2.85563612
1	0.22034316	6.01550627	-3.13005090
6	1.41634548	3.61405540	-2.92337871
1	-0.77799106	-4.46849966	3.28634310
1	-0.32397127	-3.55171013	1.82518005
1	-1.84292793	-4.47229481	1.87238610
1	-2.01744938	1.47441041	1.81430101
1	-3.57637811	1.61486399	2.65320826
1	-3.44113636	0.69683957	1.12558877
1	-4.38780165	-1.82487249	6.49845552
1	-3.16373014	-0.61967438	6.92766523
1	-2.76861620	-2.35403347	6.98710442
1	-4.17345905	2.68221855	-1.23098898
1	-2.88063216	1.46756530	-1.08316278
1	-3.77883458	1.64544201	-2.60746121
1	1.58618999	2.84243703	-3.69110727
1	1.88707376	3.25900578	-1.99195135
1	1.95923197	4.51449585	-3.23639345

1	-2.01584554	7.61488199	-1.98418117
1	-3.40496254	7.07065058	-2.94413233
1	-1.87164438	7.48642397	-3.74337292
1	0.50630122	1.55456865	-2.20658064

Energy = -7584.933191 Hartree
Number of imaginary frequencies = 0.

Compound TS2b isomer 43

Atomic N.	X	Y	Z
8	0.39157352	-0.87215734	-0.41794547
8	1.59143353	-0.77671325	-2.53276539
6	2.32436562	-1.65170300	-3.37302327
1	1.84068334	-1.72186673	-4.36404324
1	2.37631178	-2.67567062	-2.96059942
1	3.34927964	-1.27013385	-3.52250528
8	2.05243254	-2.35179973	-0.51045650
6	1.64979625	-1.04827905	-0.64420795
6	2.62285924	0.05900546	-0.28559375
1	3.52359056	-0.00139357	-0.91368490
1	2.11530685	0.99263108	-0.55153108
6	3.01163673	0.04417520	1.20671010
1	2.12323642	-0.17756584	1.81889117
1	3.33235741	1.05882180	1.48710537
6	4.14854622	-0.93418491	1.52851677
1	5.04720926	-0.62332839	0.96727264
1	4.40978479	-0.85430402	2.59534836
6	3.84865427	-2.40172768	1.19848156
1	3.04773569	-2.79069543	1.84768617
1	4.74494886	-3.00855494	1.40909564
6	3.44797754	-2.66396093	-0.25185215
1	4.10082245	-2.12835765	-0.95844668
1	3.51283288	-3.73638773	-0.47799903
50	-0.64465863	-0.99967653	-2.41422844
7	-3.22834325	-0.38735008	-1.33247757
6	-4.05672884	-1.57944620	-1.55687201
1	-5.13242722	-1.32408845	-1.64377701
1	-3.93448019	-2.29379606	-0.73449427
1	-3.73286080	-2.07562208	-2.48188758
7	-1.97526157	-0.54105389	1.59197795
6	-3.61959481	0.30765587	-0.08504567
1	-4.69950533	0.56744748	-0.14545059
1	-3.05354977	1.24615312	-0.02963452
6	-3.39117932	-0.45414081	1.22002733
1	-3.91727948	0.11114734	2.00257921
1	-3.88503432	-1.44631016	1.18697655
6	-1.69585681	-1.07730889	2.88124800
6	-1.90244007	-0.27649048	4.02879286
6	-1.59849739	-0.79912496	5.29279280
6	-1.07549679	-2.08488989	5.46069098
6	-0.86572158	-2.85823560	4.31207895
6	-1.17132688	-2.38517547	3.03099728
7	-0.95283186	1.09161377	-2.61455703
6	-3.37350607	0.52881140	-2.48682666
1	-4.37921810	0.99881625	-2.48529100
1	-3.30646729	-0.08833955	-3.39822054
6	-2.31071115	1.62517345	-2.56332541
1	-2.53954363	2.21340275	-3.47501493

1	-2.44159055	2.33202171	-1.72099662
6	0.06927636	2.07961726	-2.68775535
6	0.40312669	2.88776875	-1.57092857
6	1.41442561	3.85219812	-1.69566107
6	2.11363459	4.05091143	-2.88900948
6	1.77140081	3.24901962	-3.98477292
6	0.77054858	2.27502012	-3.90581656
6	-2.39967895	1.14252663	3.90759635
1	-1.75643563	-0.16719428	6.17079592
6	-0.71552622	-2.61151934	6.82963943
1	-0.46541318	-3.87049341	4.41519260
6	-0.95175993	-3.27471256	1.83010066
6	-0.28254095	2.71490788	-0.23756234
1	1.66724730	4.45995045	-0.82226878
6	3.21527863	5.07879639	-2.99230576
1	2.29539514	3.38946414	-4.93418837
6	0.44434205	1.44764948	-5.12447739
1	-2.07392621	1.74135196	4.76843405
1	-3.50019574	1.19795561	3.87454867
1	-2.02305055	1.60506189	2.98444748
1	-1.86745679	-3.37816477	1.22726798
1	-0.64545113	-4.27939987	2.14872694
1	-0.17471755	-2.88396716	1.15531516
1	0.35803935	-2.47921038	7.03911638
1	-0.93135893	-3.68587351	6.91573620
1	-1.27037120	-2.08680701	7.61899281
1	0.36589584	3.06221151	0.57840133
1	-0.53928816	1.66304314	-0.05448621
1	-1.21407878	3.30140519	-0.17582253
1	-0.64005059	1.34469795	-5.26581240
1	0.84869277	0.42713436	-5.03614330
1	0.87997538	1.89779127	-6.02653837
1	4.20748091	4.60080957	-3.01283550
1	3.19772911	5.76993322	-2.13916278
1	3.12599897	5.67194843	-3.91405487
1	-1.42645180	-1.01087606	0.87077349

Energy = -7584.950533 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 44

Atomic N.	X	Y	Z
8	0.60620296	-0.27148703	0.00460263
8	1.20967436	0.06395081	-2.36795282
6	1.53918183	-0.73193741	-3.48805141
1	0.77231884	-0.62943810	-4.28081274
1	1.59327030	-1.80855989	-3.23634672
1	2.50889468	-0.41948619	-3.91679931
8	1.93223333	-1.89204526	-0.74448586
6	1.72058654	-0.55367780	-0.55495781
6	2.91544366	0.36033285	-0.35955423
1	3.57303619	0.32733929	-1.23975539
1	2.50373960	1.37421536	-0.30606058
6	3.71875668	0.02338903	0.91373497
1	3.02671981	-0.21791379	1.73678076
1	4.26343250	0.92787743	1.22485161
6	4.73042774	-1.11229563	0.71331942
1	5.46064997	-0.79624814	-0.05217412

1	5.30438614	-1.26194859	1.64158952
6	4.11864233	-2.45135427	0.28316790
1	3.49238110	-2.87078643	1.08698642
1	4.92984962	-3.17741656	0.10763063
6	3.27340317	-2.39055300	-0.98786157
1	3.76674128	-1.80182779	-1.77677083
1	3.10086250	-3.40204716	-1.37830901
50	-0.95373911	-0.05696292	-1.67708838
7	-3.62056684	0.68125582	-0.87144655
6	-4.64939451	-0.12989262	-1.52146339
1	-5.65962887	0.32028049	-1.42488039
1	-4.67587280	-1.13834178	-1.09307039
1	-4.41095543	-0.22976348	-2.58915377
7	-2.14940619	-1.00894415	1.13978255
6	-3.80697131	0.75622618	0.58183414
1	-4.83601952	1.09318185	0.83757311
1	-3.11888719	1.52170980	0.97004288
6	-3.53864098	-0.55765468	1.32011604
1	-3.78886414	-0.39617696	2.38770080
1	-4.21314764	-1.34717882	0.96488464
6	-1.78922117	-2.23608112	1.77529287
6	-2.24672651	-3.46848726	1.25737941
6	-1.86574876	-4.65700483	1.89280033
6	-1.02667582	-4.67055798	3.01167774
6	-0.55216855	-3.44135857	3.48369217
6	-0.92000675	-2.22806668	2.89200568
7	-1.04442799	2.06568265	-1.36533761
6	-3.53686762	2.00472879	-1.50647604
1	-4.43503857	2.62153411	-1.28246701
1	-3.52118659	1.83172488	-2.59444499
6	-2.28818989	2.79331088	-1.12475610
1	-2.31255436	3.71993756	-1.73098314
1	-2.37332177	3.13953900	-0.07321418
6	0.10629240	2.90134978	-1.23857391
6	0.59258711	3.30779338	0.02960489
6	1.71719265	4.14287853	0.10690384
6	2.38223076	4.60110855	-1.03356993
6	1.88188994	4.20662880	-2.28030634
6	0.76484621	3.37275696	-2.40349078
6	-3.08434153	-3.53246641	0.00461389
1	-2.21891475	-5.60481405	1.47812402
6	-0.65682226	-5.96556330	3.69423628
1	0.12145652	-3.42199397	4.34426594
6	-0.37145329	-0.93008316	3.43667388
6	-0.06515218	2.85031939	1.30758262
1	2.08466601	4.43682051	1.09413195
6	3.61041617	5.47363186	-0.92859340
1	2.37337255	4.56330585	-3.18953896
6	0.27125227	2.99460220	-3.77684283
1	-2.96690655	-4.50771904	-0.48567289
1	-2.78553677	-2.74637318	-0.70376605
1	-4.15947914	-3.40536451	0.21384165
1	0.27195588	-0.42192346	2.70024586
1	0.23282880	-1.11573482	4.33354187
1	-1.17156792	-0.22636032	3.71642423
1	-1.39348853	-6.23137999	4.46923733
1	0.32282451	-5.89485502	4.18625879
1	-0.62270236	-6.79943752	2.97953820

1	0.64968497	2.86508060	2.14122844
1	-0.44642967	1.82819295	1.19124770
1	-0.90957016	3.49967527	1.58991408
1	-0.82064462	3.08594441	-3.85528469
1	0.52026933	1.94735003	-4.00171137
1	0.73648965	3.62895536	-4.54315233
1	4.53117418	4.88544512	-1.07057643
1	3.67609954	5.95568609	0.05608629
1	3.61044049	6.26068115	-1.69611168
1	-1.51156557	-0.27485961	1.45071709

Energy = -7584.949795 Hartree
Number of imaginary frequencies = 0.

Compound TS2b isomer 45

Atomic N.	X	Y	Z
8	0.31635475	-2.81522918	-0.86516595
8	0.66521043	-0.47575837	-1.26118529
6	1.18601978	0.13907176	-2.44474745
1	0.42740694	0.83217710	-2.83809996
1	1.42820215	-0.60546005	-3.21862435
1	2.09332871	0.71832341	-2.20556498
8	2.26259065	-2.36233664	-1.84113193
6	1.37637234	-2.05212045	-0.83026499
6	1.95727491	-1.72420394	0.54110444
1	2.56764793	-0.80991024	0.49633989
1	1.09234703	-1.50752938	1.17846608
6	2.77959013	-2.88520145	1.13080871
1	2.28663063	-3.84066629	0.89276576
1	2.76603985	-2.79758191	2.22761416
6	4.23910761	-2.89331222	0.65689552
1	4.71474552	-1.94831264	0.97375739
1	4.78717995	-3.69935560	1.17009008
6	4.42353964	-3.05214787	-0.85745972
1	4.10789680	-4.05654383	-1.18253314
1	5.49507618	-2.96364069	-1.10323453
6	3.66661072	-2.03154254	-1.70575833
1	3.79383230	-1.00728953	-1.32055485
1	4.03824091	-2.04831481	-2.73942065
50	-1.38231254	-1.59685397	-1.51393878
7	-3.29622293	0.63204032	-1.21645582
6	-4.34821701	-0.02696662	-2.00284553
1	-5.34122896	0.43419403	-1.82546377
1	-4.41143847	-1.09379339	-1.75392556
1	-4.10639954	0.05120715	-3.07098103
7	-2.13099003	-1.54628432	0.49573913
6	-3.55294871	0.50716406	0.22644681
1	-4.56164503	0.90063149	0.48310074
1	-2.81020570	1.11819887	0.75570583
6	-3.43711734	-0.92797685	0.74600017
1	-3.62410259	-0.88280851	1.83139956
1	-4.27024269	-1.53906500	0.34046370
6	-1.66998732	-2.37118721	1.56454301
6	-1.70932555	-3.78548622	1.48170984
6	-1.24535143	-4.55569410	2.55695558
6	-0.73968226	-3.97979259	3.72593975
6	-0.70606953	-2.58282161	3.79865098
6	-1.16295218	-1.77482700	2.75075936

7	-0.80013102	2.53796816	-1.27330291
6	-3.22752309	2.04250503	-1.65744698
1	-4.22035217	2.52297211	-1.50752401
1	-3.02976465	2.02872801	-2.73997593
6	-2.18421340	2.94023085	-0.99465364
1	-2.33902621	3.94459462	-1.40983832
1	-2.37945867	3.03782654	0.09067034
6	0.19834214	3.54977942	-1.19556367
6	1.16491306	3.54029799	-0.16097614
6	2.16772199	4.51592588	-0.14925466
6	2.24020433	5.51947689	-1.12287116
6	1.28537381	5.50316811	-2.14474344
6	0.27579778	4.53440571	-2.20915413
6	-2.23369503	-4.49457216	0.25748742
1	-1.28475261	-5.64511776	2.47477603
6	-0.27274239	-4.83244038	4.88150883
1	-0.30390418	-2.10277510	4.69526434
6	-1.07691991	-0.27530065	2.88600683
6	1.12103081	2.49222827	0.92542827
1	2.90834308	4.49565506	0.65448850
6	3.30391479	6.58933163	-1.06290174
1	1.33968771	6.25293732	-2.93837762
6	-0.66818452	4.52091694	-3.38629532
1	-2.56798577	-5.50948095	0.51167190
1	-1.44766378	-4.59003782	-0.50778425
1	-3.07761168	-3.95608759	-0.19620842
1	-0.75782752	0.18149371	1.93914890
1	-0.36923653	0.00566332	3.67730665
1	-2.04969597	0.17412449	3.14433694
1	-1.06597447	-4.94930077	5.63710499
1	0.59235746	-4.38201427	5.38846064
1	0.01202343	-5.83898687	4.54677391
1	1.92117405	2.66286039	1.65676224
1	1.24294460	1.47193468	0.52730298
1	0.16355938	2.51178408	1.46877301
1	-1.62305868	5.02642822	-3.16896772
1	-0.90849131	3.48836541	-3.67792678
1	-0.21978703	5.03789568	-4.24474001
1	4.24276924	6.19963503	-0.64576012
1	2.98846912	7.42971945	-0.42407051
1	3.51569128	6.99912500	-2.05987120
1	-0.54112291	1.72514200	-0.71296418

Energy = -7584.947108 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 46

Atomic N.	X	Y	Z
8	0.41083360	-0.29522201	-0.08897133
8	0.58880538	-2.02646565	-1.87523007
6	1.05790317	-3.35725904	-1.96592009
1	0.22157860	-4.05759001	-2.15628529
1	1.54547024	-3.69366026	-1.03104985
1	1.77633595	-3.45767975	-2.79893708
8	2.19722652	-1.58402002	0.20061864
6	1.48063684	-0.76165515	-0.61920279
6	2.21329021	0.02739896	-1.68825173
1	2.71260953	-0.65649134	-2.38837743

1	1.43544853	0.54194361	-2.26091242
6	3.23679328	1.02511907	-1.10892570
1	2.81921935	1.51932526	-0.21738052
1	3.39677072	1.82024264	-1.85289085
6	4.59150171	0.38074139	-0.78611368
1	5.02061081	-0.01168476	-1.72448969
1	5.29083920	1.15279400	-0.42837077
6	4.53888655	-0.75808817	0.24042195
1	4.26280212	-0.37563121	1.23615408
1	5.54625559	-1.19425642	0.34399003
6	3.58367014	-1.89696693	-0.10973098
1	3.67962027	-2.20132256	-1.16290736
1	3.78977132	-2.77380657	0.51746041
50	-1.31574869	-1.71177363	-0.72871149
7	-3.06778789	-0.12637857	0.56350148
6	-3.80027485	-0.88181847	1.58760774
1	-4.69658422	-0.33940476	1.94636011
1	-3.13709402	-1.09716439	2.43156409
1	-4.12220097	-1.83848667	1.15460241
7	-0.92183983	0.27276748	2.73075104
6	-2.56254053	1.17938912	1.04704309
1	-3.37694073	1.93289685	1.00408828
1	-1.77919078	1.51042497	0.34909606
6	-2.02005529	1.21677208	2.47726560
1	-1.71178758	2.26753736	2.65437889
1	-2.83542824	1.01826692	3.18841100
6	-0.24210545	0.45404115	3.97249699
6	-0.84181416	0.02775428	5.18076468
6	-0.15808745	0.21395145	6.38944387
6	1.11461055	0.78997934	6.44666290
6	1.70654142	1.17568803	5.23854113
6	1.05221546	1.02754104	4.01060295
7	-2.02785611	-0.29922879	-2.17916107
6	-3.92093945	0.04244917	-0.63246202
1	-4.76730585	0.72455794	-0.40903214
1	-4.34138298	-0.94874799	-0.86642087
6	-3.16598916	0.55483294	-1.85286200
1	-3.89176488	0.57268327	-2.68862438
1	-2.88214755	1.61279023	-1.68561745
6	-1.41797948	-0.03956998	-3.43456054
6	-0.78186327	1.19699895	-3.72204542
6	-0.20881207	1.40629399	-4.98510551
6	-0.23439518	0.43424711	-5.98779678
6	-0.85594100	-0.78485185	-5.69075584
6	-1.44419599	-1.03625929	-4.44733095
6	-2.17053461	-0.68464661	5.18819571
1	-0.63119334	-0.12858997	7.31343174
6	1.81942356	1.00267637	7.76482821
1	2.70658684	1.61723912	5.24928665
6	1.73698688	1.46914315	2.74029469
6	-0.65241635	2.28358269	-2.68112659
1	0.28792015	2.36091685	-5.18121767
6	0.36810797	0.69132280	-7.34839058
1	-0.89390767	-1.56498790	-6.45597887
6	-2.11568928	-2.36525226	-4.20691013
1	-2.32060218	-1.21031249	6.14003801
1	-2.21628785	-1.41838765	4.37096691
1	-3.02212334	0.00231257	5.05834341

1	1.94838226	0.61616874	2.07779503
1	2.69017529	1.96301663	2.96917701
1	1.11973846	2.17315078	2.16146064
1	1.64812350	2.02119160	8.14853668
1	2.90600061	0.87224633	7.66563559
1	1.45843565	0.30096206	8.52898026
1	0.22090650	2.91596794	-2.89316297
1	-0.53582346	1.84968007	-1.67763758
1	-1.53122115	2.94791603	-2.65708256
1	-3.08323741	-2.24072599	-3.70127106
1	-1.50518680	-3.01937008	-3.56384110
1	-2.27338982	-2.89715385	-5.15475416
1	0.95349157	-0.17065199	-7.69978714
1	1.02849030	1.56886351	-7.33257246
1	-0.41245866	0.87911236	-8.10277271
1	-0.26889101	0.27066401	1.94214177

Energy = -7584.950461 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 47

Atomic N.	X	Y	Z
8	1.02736592	-2.00514317	1.92581499
8	0.41200274	-1.41494119	-0.31572607
6	0.33789396	-2.28099465	-1.45354366
1	-0.69129843	-2.25592637	-1.84185290
1	0.59921604	-3.31854081	-1.19456971
1	1.01613510	-1.92613888	-2.24725175
8	2.34544635	-2.90711164	0.37838936
6	1.71874785	-1.76892650	0.84260225
6	2.49859071	-0.45975846	0.78203404
1	2.71373343	-0.18314739	-0.26087737
1	1.82120955	0.30047569	1.18762839
6	3.80238414	-0.50648135	1.60036302
1	3.62976813	-1.06775367	2.53194880
1	4.05864668	0.51996034	1.90326560
6	4.98414469	-1.09757280	0.82005864
1	5.16654301	-0.46731478	-0.06827326
1	5.89724731	-1.03467441	1.43306947
6	4.79182529	-2.54853153	0.36144164
1	4.77116060	-3.22883511	1.22797751
1	5.65445662	-2.85064316	-0.25582400
6	3.52540064	-2.80022097	-0.45536929
1	3.38655162	-2.03660512	-1.23722339
1	3.58285594	-3.77904558	-0.95078516
50	-1.09883153	-1.88420749	1.41953897
7	-3.50963140	-0.46014819	0.48074213
6	-4.43842745	-1.32789767	1.21818435
1	-5.43988800	-0.86218113	1.32008708
1	-4.05396557	-1.54755163	2.22218871
1	-4.54357576	-2.28272629	0.68644607
7	-1.23107457	0.02992211	2.37829423
6	-3.29809999	0.81356478	1.18546903
1	-4.26822233	1.32301855	1.37904119
1	-2.70170569	1.46513653	0.53363228
6	-2.54809761	0.66129225	2.51110196
1	-2.43261147	1.67722952	2.92282248
1	-3.19116783	0.13034572	3.24359202

6	-0.23293228	0.59143752	3.22908211
6	0.20000632	-0.07364227	4.40473318
6	1.17765903	0.51745981	5.21489382
6	1.75675011	1.75310981	4.90703678
6	1.31611538	2.40552044	3.75155520
6	0.33725905	1.85334706	2.91507721
7	-1.95721781	0.01138120	-2.20976138
6	-4.06288671	-0.26801297	-0.87783945
1	-5.07790613	0.18229581	-0.80062914
1	-4.18082809	-1.26950562	-1.31860912
6	-3.25898361	0.58943206	-1.85360730
1	-3.86395431	0.65939772	-2.76696801
1	-3.16607046	1.62824559	-1.48241282
6	-1.39480317	0.40140373	-3.45827031
6	-0.24120332	1.22069383	-3.51271653
6	0.31841299	1.53696144	-4.75536156
6	-0.23627871	1.08238018	-5.95795918
6	-1.36689925	0.26269221	-5.88275814
6	-1.94941092	-0.09754071	-4.66080523
6	-0.36767024	-1.41066837	4.81291628
1	1.49305820	-0.00700598	6.12090540
6	2.83742666	2.34634304	5.77901125
1	1.74979246	3.37333131	3.48493147
6	-0.07869777	2.60369182	1.67482626
6	0.38470319	1.75597358	-2.24685454
1	1.20976889	2.16917014	-4.78235340
6	0.35803226	1.47584021	-7.28898096
1	-1.79958963	-0.13602614	-6.80403709
6	-3.11462927	-1.05613339	-4.64608955
1	-0.23772968	-1.57310915	5.89137506
1	0.15013108	-2.23184919	4.29308653
1	-1.43834293	-1.48957562	4.57757378
1	-0.21784981	1.91230369	0.83244151
1	0.67386585	3.35545659	1.40201676
1	-1.03474522	3.13485122	1.81222081
1	2.65441275	2.13759899	6.84241962
1	2.90439367	3.43506598	5.64982510
1	3.82455754	1.92396307	5.53173637
1	1.24488091	2.39486814	-2.48372293
1	0.73783833	0.95125437	-1.58202124
1	-0.32941762	2.36080074	-1.66672254
1	-4.08624840	-0.54007930	-4.58116579
1	-3.04935813	-1.73156881	-3.78094983
1	-3.13087630	-1.65592182	-5.56547403
1	1.45238721	1.55754125	-7.23252010
1	-0.02377784	2.45407677	-7.62236261
1	0.10867164	0.74476838	-8.06998825
1	-1.28654361	0.14005619	-1.45116246

Energy = -7584.947144 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 48

Atomic N.	X	Y	Z
8	0.79635805	0.01034985	0.26843500
8	1.35096443	1.59855902	-1.48199677
6	1.86260641	2.87722540	-1.81255949
1	1.68098152	3.63713360	-1.02813363

1	1.39363921	3.23027587	-2.74724507
1	2.94915199	2.82378864	-1.99880159
8	2.73557734	-0.42799044	-0.68408620
6	1.95325804	0.48526180	-0.04822985
6	2.62769866	1.50380349	0.85924238
1	3.25656152	2.19638300	0.28155124
1	1.81691706	2.09888244	1.29862642
6	3.48368835	0.83993781	1.95853519
1	2.97579908	-0.06107966	2.33733082
1	3.55526137	1.53528583	2.80843973
6	4.90495348	0.49910501	1.48689723
1	5.39832354	1.43388164	1.16789973
1	5.48975849	0.11872850	2.33893085
6	4.97924757	-0.51654083	0.33967739
1	4.65688038	-1.51179981	0.68563950
1	6.02822256	-0.62113535	0.01647531
6	4.14563560	-0.15957598	-0.88863045
1	4.29523611	0.88415551	-1.20371115
1	4.41446543	-0.80588979	-1.73403311
50	-0.77614450	1.26570475	-0.80519086
7	-2.55427384	-0.68958968	-0.17300998
6	-3.82092500	0.05429612	-0.30142358
1	-4.69280005	-0.62728417	-0.30037186
1	-3.83211231	0.63425970	-1.23288429
1	-3.91503596	0.75497890	0.53788579
7	-1.04030991	0.07127213	-2.54922223
6	-2.36741233	-1.60802889	-1.31881666
1	-3.24372554	-2.28350401	-1.40781116
1	-1.48020077	-2.22046590	-1.10844743
6	-2.14214945	-0.87680972	-2.63984752
1	-1.92405283	-1.64836264	-3.39903235
1	-3.09164500	-0.40489197	-2.97641778
6	-0.34607503	0.31033450	-3.76958561
6	-0.57708687	1.48116088	-4.53225231
6	0.13431038	1.68750131	-5.72274113
6	1.07081413	0.76333439	-6.19587755
6	1.29028964	-0.39036348	-5.43394327
6	0.60535264	-0.63298362	-4.23772049
7	-0.56295395	-1.27041721	2.63995242
6	-2.58698058	-1.45691264	1.10066795
1	-3.32708001	-2.27624822	0.98771757
1	-2.97634053	-0.78945053	1.88271296
6	-1.23381615	-2.03166175	1.57820761
1	-1.39404047	-3.06545258	1.90803170
1	-0.52176160	-2.07195854	0.74371201
6	-1.23028195	-0.95726091	3.84272170
6	-1.76152813	-1.97337365	4.67884779
6	-2.40245342	-1.61502624	5.87172127
6	-2.51394534	-0.28866619	6.29923296
6	-1.92926669	0.69559640	5.49433136
6	-1.29814553	0.39150727	4.28411388
6	-1.58385837	2.51882887	-4.09150505
1	-0.05923546	2.59505177	-6.30128336
6	1.79869139	0.98556262	-7.50035620
1	2.02960157	-1.12132573	-5.77333117
6	0.91164392	-1.87441862	-3.43945694
6	-1.58082891	-3.43877959	4.36603975
1	-2.80155706	-2.41357255	6.50303936

6	-3.23960328	0.06816162	7.57413244
1	-1.97171187	1.74092841	5.81153011
6	-0.68033427	1.50008786	3.46858644
1	-1.88405764	3.14986992	-4.93898869
1	-1.17755103	3.19131994	-3.31778169
1	-2.48284245	2.05573273	-3.66325068
1	1.02012491	-1.63413858	-2.37344146
1	1.83695364	-2.34611130	-3.79640675
1	0.10975086	-2.62602305	-3.52412915
1	1.26236486	0.51624757	-8.34069538
1	2.80687451	0.54892325	-7.47587252
1	1.89312351	2.05557728	-7.73066473
1	-1.69088399	-4.03648043	5.28045368
1	-0.58378327	-3.63027930	3.94327688
1	-2.32083035	-3.81690812	3.64180136
1	-1.07527542	1.53646410	2.43971944
1	0.41326010	1.38644052	3.38323259
1	-0.87216061	2.47483158	3.93474102
1	-2.79584193	0.95036584	8.05618000
1	-3.21669841	-0.76216274	8.29339790
1	-4.29888010	0.30205172	7.38004208
1	-0.07586491	-0.47622511	2.22547460

Energy = -7584.949492 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 49

Atomic N.	X	Y	Z
8	0.92194164	2.68324852	-0.15788183
8	2.89221334	1.55850399	0.87582707
6	3.59911561	1.28469634	2.06654263
1	3.89651179	0.22236979	2.11982131
1	3.00068426	1.50176895	2.97018480
1	4.52922535	1.88499951	2.10481787
8	1.44007242	3.67977428	1.74845254
6	1.82762098	3.26737905	0.51341170
6	2.96383286	3.99479508	-0.18488149
1	3.89592314	3.91051555	0.39082050
1	3.11926818	3.45761776	-1.12720370
6	2.63829207	5.48131418	-0.44646913
1	1.58890259	5.58270931	-0.76734978
1	3.25358891	5.82308769	-1.29254353
6	2.92332268	6.38551378	0.75989836
1	3.99959183	6.32013750	0.99675959
1	2.73273253	7.43481874	0.48481703
6	2.12192178	6.04709482	2.02303338
1	1.04935324	6.24857283	1.86914063
1	2.44833350	6.70664644	2.84402657
6	2.26595211	4.60574102	2.50523973
1	3.31410170	4.27116489	2.49818563
1	1.88590813	4.50445127	3.52982855
50	1.41224778	0.40629539	-0.30210757
7	-1.13655174	0.55182135	-1.02972054
6	-1.53651834	1.75445068	-1.77911174
1	-2.61444855	1.73310602	-2.03178549
1	-0.95602733	1.83885062	-2.70525265
1	-1.32083678	2.63708758	-1.16767931
7	-0.84050703	-2.09745336	-3.77523923

6	-1.44207442	-0.69005603	-1.77645743
1	-2.53955698	-0.82369733	-1.85456252
1	-1.05611861	-1.53397000	-1.18562257
6	-0.80939031	-0.75383717	-3.17828798
1	-1.29982793	-0.04404673	-3.85384226
1	0.24801712	-0.45598900	-3.11077714
6	-2.05980635	-2.81099772	-3.89730835
6	-2.17685056	-4.09993649	-3.31626606
6	-3.35922337	-4.82795715	-3.48144770
6	-4.44924021	-4.32371330	-4.19994688
6	-4.30178833	-3.06698227	-4.79528332
6	-3.13036418	-2.30849242	-4.67642021
7	0.26717359	-0.25563461	1.39385903
6	-1.79240358	0.54111522	0.29882726
1	-2.87824059	0.34466466	0.19057605
1	-1.65650773	1.54558063	0.72385627
6	-1.16811216	-0.47367701	1.25077140
1	-1.68141520	-0.35845035	2.22125292
1	-1.41032505	-1.50740898	0.92053336
6	0.82525676	-0.69737339	2.62285686
6	1.66096759	-1.84148109	2.68283534
6	2.20909882	-2.24208426	3.90998459
6	1.95677209	-1.55131280	5.09804773
6	1.12519789	-0.42657393	5.03060293
6	0.56104952	0.01232827	3.82825160
6	-1.03396153	-4.70322895	-2.53327441
1	-3.43057156	-5.81859255	-3.02518511
6	-5.73603964	-5.10358000	-4.32307243
1	-5.11735010	-2.66616035	-5.40307570
6	-3.01658869	-1.01246262	-5.44087267
6	1.96958196	-2.65642643	1.44851112
1	2.84479594	-3.13137817	3.93593264
6	2.57283664	-1.98638213	6.40642786
1	0.92002743	0.14061598	5.94309187
6	-0.27963510	1.26461411	3.82023454
1	-1.31630230	-5.68779850	-2.14059949
1	-0.73725843	-4.07879162	-1.67492378
1	-0.13349751	-4.84874392	-3.15364242
1	-3.20796824	-0.12938516	-4.80951023
1	-3.74869800	-0.98838973	-6.25855780
1	-2.01093316	-0.89549375	-5.87030315
1	-5.55331039	-6.18663597	-4.29769087
1	-6.25901079	-4.86694288	-5.25995302
1	-6.42626238	-4.86986780	-3.49660254
1	2.27675915	-3.67420459	1.72534800
1	2.79304242	-2.22097182	0.85858268
1	1.10071075	-2.71702623	0.77917349
1	-1.35905850	1.04179335	3.83408427
1	-0.08216279	1.85915983	2.91787553
1	-0.06749063	1.87677979	4.70734787
1	3.39060688	-1.31221616	6.70683718
1	2.99021673	-2.99947858	6.33299780
1	1.83429396	-1.97937572	7.22107172
1	-0.13482827	-2.68052578	-3.32986760

Energy = -7584.949631 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 50

Atomic N.	X	Y	Z
8	0.42970222	2.35021639	1.86074317
8	1.07706344	0.94717163	0.00116217
6	1.72195065	-0.25330779	-0.36767721
1	1.11797273	-0.79545230	-1.11343217
1	1.88002133	-0.91894782	0.49974158
1	2.70078635	-0.03783558	-0.83558255
8	2.11285520	1.00038421	2.39566803
6	1.60332406	1.93955886	1.54566121
6	2.56692052	2.90018249	0.86049843
1	3.28707194	2.35721660	0.23089987
1	1.94458079	3.50447917	0.19043466
6	3.31651855	3.79785061	1.86603987
1	2.62326527	4.11702871	2.66066003
1	3.63123822	4.71455717	1.34420288
6	4.55924416	3.12925768	2.46837115
1	5.26387024	2.90126133	1.64926124
1	5.07648563	3.84425235	3.12766385
6	4.28222990	1.83899474	3.24982762
1	3.69953609	2.05290604	4.16027451
1	5.24071312	1.40860617	3.58482456
6	3.54068184	0.76048261	2.46202588
1	3.96119618	0.63384014	1.45183074
1	3.61040854	-0.20519434	2.97966194
50	-1.05736482	1.56832731	0.31484339
7	-3.66681981	0.55113471	-0.70701885
6	-4.39366388	1.67636526	-1.29324198
1	-5.49123144	1.50620353	-1.30685580
1	-4.05956554	1.85673583	-2.32246757
1	-4.18428564	2.58680487	-0.71475971
7	-1.51255405	-0.74228925	-2.51555204
6	-3.79215360	-0.65840316	-1.52630389
1	-4.85439491	-0.83690619	-1.80665314
1	-3.48336506	-1.52041614	-0.91544998
6	-2.95522261	-0.64792687	-2.80707622
1	-3.29933691	-1.48845613	-3.44242263
1	-3.13981676	0.26848274	-3.38182521
6	-0.63953465	-0.78406024	-3.64354992
6	-0.40483820	0.38464114	-4.40392065
6	0.48348060	0.32435110	-5.48493338
6	1.16436553	-0.84750307	-5.83116102
6	0.93998402	-1.98534012	-5.04792070
6	0.04806719	-1.97811878	-3.96973109
7	-1.77700543	0.02559743	1.61464381
6	-4.09009647	0.33739156	0.68560034
1	-5.10617113	-0.11354159	0.73551768
1	-4.15391922	1.33151639	1.15671861
6	-3.13195753	-0.51821190	1.51008689
1	-3.58310151	-0.59541804	2.51846910
1	-3.12787175	-1.55901754	1.12133121
6	-1.01627815	-0.63071060	2.63217759
6	-0.41419306	-1.89092314	2.39894843
6	0.32265937	-2.50939727	3.41876435
6	0.46664861	-1.92929697	4.68153334
6	-0.16996405	-0.70394224	4.91300869
6	-0.90359789	-0.04632220	3.91964436
6	-1.04970777	1.69987011	-4.04482889

1	0.66476780	1.23641157	-6.05950022
6	2.09521723	-0.88840276	-7.01918411
1	1.46762145	-2.91236711	-5.28620529
6	-0.15909439	-3.23979139	-3.16305709
6	-0.56753397	-2.59827423	1.07479382
1	0.79279011	-3.47616100	3.21696162
6	1.29015124	-2.59335542	5.75946951
1	-0.09282542	-0.24115480	5.90065002
6	-1.56728113	1.26958489	4.23723221
1	-0.43698049	2.53781557	-4.40210867
1	-1.17425501	1.79677749	-2.95638514
1	-2.04607272	1.81112945	-4.50341511
1	0.22306865	-3.14518070	-2.13285518
1	0.37161389	-4.08131790	-3.62551665
1	-1.22233665	-3.51766443	-3.09133315
1	1.55999696	-1.19175231	-7.93314600
1	2.91105366	-1.60800660	-6.86594820
1	2.53908181	0.09742393	-7.21388721
1	0.33453372	-3.17479253	0.82691669
1	-0.75776571	-1.87071550	0.27513412
1	-1.41203761	-3.30632305	1.09324062
1	-2.60033607	1.30499434	3.86401200
1	-1.02402329	2.09823322	3.76088524
1	-1.58111572	1.44118822	5.32190514
1	2.30066109	-2.15745211	5.81490946
1	1.40652132	-3.66906500	5.56980705
1	0.83092541	-2.46733928	6.75021410
1	-1.36117637	-1.57317233	-1.94196522

Energy = -7584.942546 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 51

Atomic N.	X	Y	Z
8	0.14339292	0.96350741	0.87556648
8	1.00279546	2.65289521	-0.63921905
6	1.53803611	3.94220042	-0.87627929
1	1.13099778	4.71637774	-0.19647937
1	1.31752002	4.24881268	-1.91351306
1	2.63686442	3.93134308	-0.77129710
8	2.32797217	0.79575521	0.61816210
6	1.26800573	1.58631217	0.94167340
6	1.47307253	2.68103027	1.98048556
1	2.16412401	3.45376444	1.61414695
1	0.49354035	3.16068172	2.10748386
6	1.99118805	2.13564038	3.32739186
1	1.49297237	1.18156123	3.56224561
1	1.69655776	2.84018183	4.11996174
6	3.51736426	1.97342980	3.36438346
1	3.97432590	2.96338797	3.19073606
1	3.82736778	1.66605306	4.37548828
6	4.08896017	0.98041403	2.34452724
1	3.79126740	-0.04938735	2.59931302
1	5.19018173	1.00812495	2.39239502
6	3.68021369	1.24041092	0.89652300
1	3.80077767	2.29779601	0.61678797
1	4.29566288	0.64137977	0.21317334
50	-1.21532428	2.27695775	-0.45429730

7	-3.12698483	0.40005630	-0.30777791
6	-4.29676390	1.16778541	-0.77555490
1	-5.17025042	0.51099575	-0.94842350
1	-4.06015444	1.68592584	-1.71319425
1	-4.56004190	1.92536521	-0.02605015
7	-1.07715929	1.10552669	-2.22183847
6	-2.68323421	-0.55809915	-1.34947205
1	-3.53071737	-1.20729256	-1.65169430
1	-1.91523480	-1.19643879	-0.89706755
6	-2.11167932	0.14324310	-2.57939315
1	-1.69396293	-0.64567041	-3.23027015
1	-2.93270159	0.59986967	-3.17556119
6	-0.12165789	1.36598849	-3.24705839
6	-0.21815228	2.51405025	-4.06877661
6	0.74376923	2.73879814	-5.06464052
6	1.80540049	1.85557568	-5.28083897
6	1.89166820	0.72484189	-4.45898342
6	0.95562518	0.46556798	-3.45200920
7	-1.42904437	-1.75602186	1.38098896
6	-3.49535298	-0.29522723	0.95363837
1	-4.14001083	-1.16024292	0.70806772
1	-4.11014938	0.41022372	1.53454459
6	-2.35498667	-0.72346514	1.88584268
1	-1.77414978	0.17302470	2.15498519
1	-2.82533455	-1.08397043	2.81196117
6	-1.16043317	-2.90134287	2.16939163
6	-2.19122672	-3.80696249	2.52421331
6	-1.87567258	-4.93890905	3.28744316
6	-0.57053387	-5.23456907	3.69083261
6	0.44198683	-4.35835934	3.28351951
6	0.17544813	-3.20469642	2.54006839
6	-1.34107435	3.51069140	-3.89440846
1	0.65274751	3.62831950	-5.69407368
6	2.81180859	2.09541869	-6.38108683
1	2.72247934	0.02703648	-4.59622669
6	1.11800754	-0.74503154	-2.56919956
6	-3.60537291	-3.63828063	2.02452636
1	-2.68303442	-5.62834740	3.54836750
6	-0.26464993	-6.44643402	4.53768492
1	1.47786057	-4.57122564	3.56083322
6	1.31052649	-2.29632854	2.13655043
1	-1.44810283	4.13293791	-4.79323292
1	-1.16068530	4.19340706	-3.04761815
1	-2.29991293	3.01301217	-3.69700027
1	1.00091553	-0.47129911	-1.51214290
1	2.10609555	-1.20144725	-2.71438503
1	0.36280590	-1.51738083	-2.78678393
1	2.57861018	1.49206603	-7.27291346
1	3.82755804	1.82035065	-6.06302881
1	2.82314157	3.14909244	-6.69096851
1	-4.16038322	-4.57933807	2.13137889
1	-3.60823202	-3.35363913	0.96181709
1	-4.17008829	-2.86456013	2.56693745
1	1.15337753	-1.26474452	2.48558927
1	1.43797398	-2.23837733	1.04368138
1	2.25740981	-2.65747094	2.55813980
1	0.70688778	-6.88707733	4.27344370
1	-1.03456092	-7.22118330	4.41958427

1 -0.22297746 -6.18717241 5.60789585
 1 -0.56527555 -1.29719627 1.09038675
 Energy = -7584.949275 Hartree
 Number of imaginary frequencies = 0.

Compound TS2b isomer 52

Atomic N.	X	Y	Z
8	0.51875764	-0.07138209	0.21719864
8	1.05365145	1.80593204	-1.12949860
6	1.54859757	3.12376595	-1.28784323
1	1.26968229	3.79665446	-0.45442739
1	1.14990759	3.55322075	-2.22239947
1	2.64789200	3.11542106	-1.37941194
8	2.63891673	-0.06874122	-0.40480831
6	1.60948682	0.62435275	0.17217949
6	1.94008243	1.55286813	1.33733809
1	2.58493996	2.38640356	1.02122867
1	0.98183894	1.98824930	1.65149248
6	2.60271263	0.80824906	2.51385880
1	2.12873006	-0.17683744	2.64365220
1	2.39939165	1.37026954	3.43793082
6	4.12283468	0.66527033	2.35597491
1	4.56466961	1.67574143	2.29591060
1	4.54094124	0.20179313	3.26358485
6	4.57226944	-0.14174362	1.13152587
1	4.28901720	-1.20084214	1.24290740
1	5.67276955	-0.11491922	1.06379139
6	4.00864983	0.35042906	-0.20045571
1	4.10352993	1.44258773	-0.30486789
1	4.54984188	-0.11207300	-1.03632379
50	-1.10261905	1.23944080	-0.61156934
7	-3.61772180	-0.18361247	-0.66204810
6	-4.56571054	0.78870302	-1.21696985
1	-5.51666737	0.31385118	-1.53390014
1	-4.12510967	1.29493546	-2.08440399
1	-4.78780890	1.55252814	-0.45987129
7	-1.25636518	0.12609728	-2.42498946
6	-3.22688460	-1.19313991	-1.65941823
1	-4.12190008	-1.72832179	-2.04665613
1	-2.58056092	-1.92690015	-1.15729821
6	-2.45016289	-0.60441691	-2.83484960
1	-2.16644812	-1.45769501	-3.47747731
1	-3.13410449	0.00815800	-3.46258330
6	-0.25234124	0.17675351	-3.44152784
6	-0.16605198	1.28485250	-4.31669521
6	0.82051843	1.30812705	-5.31130886
6	1.73049653	0.25784603	-5.47303581
6	1.63063347	-0.83372748	-4.60312939
6	0.65948111	-0.89568406	-3.59576154
7	-2.21821833	-0.51060909	1.99581265
6	-4.18864775	-0.80153990	0.54839349
1	-4.97558594	-1.53736615	0.27755067
1	-4.69207096	-0.00256994	1.11726892
6	-3.18118095	-1.48681009	1.46897519
1	-3.75523400	-1.97648227	2.27930450
1	-2.65400982	-2.28583074	0.93182886
6	-1.45395613	-0.80665576	3.14935303

6	-0.61110049	-1.94175816	3.21665382
6	0.13575281	-2.16118383	4.38232279
6	0.11072525	-1.28800130	5.47365522
6	-0.69019705	-0.14498603	5.36563396
6	-1.47128487	0.10790382	4.23453236
6	-1.12514985	2.44600797	-4.19622898
1	0.87564707	2.17088223	-5.98100615
6	2.76530385	0.28495613	-6.57305479
1	2.33597851	-1.66329694	-4.70384312
6	0.60376072	-2.08989525	-2.67719626
6	-0.42403656	-2.87157774	2.04271889
1	0.78649503	-3.03883147	4.41814995
6	0.91118312	-1.56694138	6.72307825
1	-0.71791130	0.57135427	6.19087648
6	-2.31799436	1.35841298	4.17727947
1	-1.01373839	3.12926340	-5.04884148
1	-0.95341188	3.02968168	-3.27811980
1	-2.17094016	2.10961723	-4.15911055
1	0.56982082	-1.76963031	-1.62736046
1	1.48072958	-2.73348093	-2.82653666
1	-0.29298988	-2.70332527	-2.86367369
1	2.39144158	-0.20996392	-7.48383474
1	3.68315840	-0.23957998	-6.27300406
1	3.03226566	1.31463456	-6.84798336
1	0.48398945	-3.47287416	2.18073916
1	-0.31407243	-2.29710746	1.11175001
1	-1.26236141	-3.57504845	1.91929102
1	-3.38908887	1.13000429	4.04781199
1	-2.02438760	2.02423859	3.34833622
1	-2.21725702	1.93288398	5.10647869
1	1.34681571	-0.64622271	7.13665485
1	1.72959936	-2.27169514	6.52297401
1	0.28244463	-2.00960422	7.51212597
1	-2.68006921	0.39056239	2.10520029

Energy = -7584.943832 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 53

Atomic N.	X	Y	Z
8	0.31190792	1.95454824	2.28048015
8	0.53001302	1.38092494	-0.07305014
6	0.74044478	2.43057203	-1.02198887
1	0.63294983	3.43543959	-0.57612354
1	-0.00833701	2.32924223	-1.82324517
1	1.74273694	2.34992886	-1.47363007
8	1.61180782	0.21662518	1.79674709
6	1.30964887	1.53492570	1.55851078
6	2.48092008	2.49614477	1.36910319
1	2.99516106	2.31705737	0.41345114
1	2.04391861	3.50093603	1.32352436
6	3.50353241	2.41204858	2.52105880
1	2.97488785	2.27256799	3.47675943
1	4.02182913	3.38057089	2.59088540
6	4.55576992	1.31296885	2.31675673
1	5.08557701	1.51201415	1.36850476
1	5.31471157	1.38330781	3.11196065
6	3.99927831	-0.11570458	2.28470206

1	3.63779807	-0.40939358	3.28304911
1	4.81020927	-0.81613362	2.02371716
6	2.85228872	-0.33159003	1.29993379
1	3.07987928	0.07232344	0.30029336
1	2.64875054	-1.40542579	1.18823242
50	-1.52547765	1.76120138	1.07573044
7	-3.30115151	0.35167214	-0.64015925
6	-4.05023098	1.29691494	-1.47238004
1	-4.99241590	0.86093634	-1.86237884
1	-3.43157315	1.62771881	-2.31474328
1	-4.29776621	2.18117595	-0.86955327
7	-1.04490447	0.06094237	-2.66443610
6	-2.94738865	-0.88595957	-1.36011767
1	-3.85824442	-1.50524616	-1.51525748
1	-2.27420974	-1.46252048	-0.70940781
6	-2.29163647	-0.71405441	-2.72832704
1	-2.12027431	-1.73649991	-3.11994815
1	-2.99101448	-0.23259300	-3.42716956
6	-0.16873635	-0.03361784	-3.78211093
6	-0.50724065	0.58180773	-5.00921202
6	0.38502344	0.49586973	-6.08603001
6	1.61541247	-0.16090256	-5.98591709
6	1.94594514	-0.73736739	-4.75335407
6	1.07792509	-0.69502044	-3.65725160
7	-1.99832129	-0.12447984	1.95085382
6	-4.07000875	0.02665670	0.57617140
1	-4.98769617	-0.54494387	0.32113469
1	-4.39287043	0.98407465	1.01790881
6	-3.27284431	-0.75792527	1.61862051
1	-3.92304230	-0.83422601	2.51311231
1	-3.13461804	-1.80213547	1.27306104
6	-1.31965852	-0.77331471	3.02588630
6	-0.61598134	-1.98364699	2.81242037
6	0.00150764	-2.62768459	3.89207721
6	-0.04393618	-2.10846400	5.18944645
6	-0.73458457	-0.90766358	5.38578224
6	-1.36652684	-0.23230644	4.33448982
6	-1.78008616	1.37638390	-5.16100407
1	0.11455915	0.98295557	-7.02652454
6	2.54817152	-0.26001465	-7.16903353
1	2.90565372	-1.24864221	-4.64180279
6	1.47304285	-1.35399091	-2.35673642
6	-0.48330837	-2.57090592	1.43027687
1	0.54392701	-3.55941916	3.70810413
6	0.65464795	-2.80119133	6.33536053
1	-0.78737038	-0.48074439	6.39096880
6	-2.07663822	1.06838179	4.61693335
1	-1.69583905	2.08449125	-5.99561071
1	-1.99605012	1.94014180	-4.24157667
1	-2.65289569	0.73567730	-5.36496067
1	1.51583600	-0.63577294	-1.52214265
1	2.46139050	-1.82193589	-2.44911504
1	0.75765944	-2.13899422	-2.06417656
1	2.39650559	-1.20313346	-7.71803808
1	3.60075641	-0.23338462	-6.85481977
1	2.38177705	0.56121826	-7.87933969
1	0.34031367	-3.29672694	1.39415061
1	-0.28865573	-1.77617574	0.69695127

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1 -1.39585793 -3.10047889 1.11102676
1 -3.04001570 1.13294733 4.09227419
1 -1.46735013 1.92493570 4.28773165
1 -2.25541735 1.18632591 5.69403934
1 1.64512861 -2.35751748 6.52531576
1 0.80787629 -3.86835623 6.12487316
1 0.07866624 -2.71492720 7.26756430
1 -0.54557127 -0.15344420 -1.79926360

```

Energy = -7584.944832 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 54

Atomic N.	X	Y	Z
8	1.11195910	0.02037840	1.83984840
8	2.02917981	1.33096421	0.10147862
6	2.97903323	1.38198197	-0.95870119
1	2.53985524	1.93155408	-1.80612957
1	3.25792813	0.37489539	-1.31183457
1	3.88952398	1.91829658	-0.63805521
8	2.89438319	-0.91391474	0.85494548
6	2.32158232	0.22052227	1.45349562
6	3.23596644	1.06331873	2.34347439
1	4.07956409	1.47484994	1.76796091
1	2.62524486	1.91803682	2.65878534
6	3.76066089	0.29578686	3.57162499
1	2.95647836	-0.34335798	3.97032404
1	4.00024796	1.02284420	4.36307526
6	5.01678610	-0.53683269	3.28389049
1	5.82155132	0.14644159	2.95958114
1	5.36878538	-1.00194478	4.21856356
6	4.83899498	-1.62447608	2.21815467
1	4.14730453	-2.40597677	2.57218862
1	5.80973768	-2.11834145	2.04395461
6	4.32354975	-1.11771178	0.87038928
1	4.86269569	-0.20854920	0.55717647
1	4.48555613	-1.88065398	0.09607175
50	-0.03446890	0.26971051	-0.37676242
7	-1.29195821	1.67344284	1.31212091
6	-0.40917996	2.76303101	1.78954458
1	-0.98356718	3.49159217	2.39013982
1	0.05140687	3.27391100	0.93864053
1	0.38514817	2.31977010	2.39725852
7	-0.97081470	1.95719135	-1.43703306
6	-2.39946079	2.23395419	0.49875253
1	-2.97524762	2.96507382	1.09903896
1	-3.06546736	1.40437734	0.22299859
6	-1.86521649	2.88614178	-0.77486706
1	-2.73812151	3.12509298	-1.41332769
1	-1.40919578	3.86652040	-0.51948059
6	-0.61203480	2.24962306	-2.77829623
6	0.18853222	3.37482142	-3.11616206
6	0.53907484	3.60621428	-4.45301723
6	0.13015828	2.75946164	-5.48757696
6	-0.65463597	1.65210736	-5.14631510
6	-1.03643203	1.38626778	-3.82591438
7	-1.60791290	-1.31978679	1.57165253
6	-1.79537535	0.94388062	2.50720263

1	-2.47329068	1.60655010	3.07862663
1	-0.91599286	0.74079776	3.13379574
6	-2.51409340	-0.37368712	2.23316455
1	-2.87130165	-0.75443560	3.21019030
1	-3.40831447	-0.21871941	1.61562812
6	-2.02577353	-2.66829181	1.39494419
6	-3.11291361	-2.99108481	0.55169451
6	-3.47233915	-4.33620501	0.39177632
6	-2.77738118	-5.37613297	1.01524568
6	-1.67440259	-5.03607559	1.80822265
6	-1.28733325	-3.70845890	2.01257467
6	0.70963168	4.30773783	-2.05095267
1	1.16670680	4.47070885	-4.68789148
6	0.49776480	3.04293394	-6.92456150
1	-0.99457681	0.97608501	-5.93571472
6	-1.91790116	0.19314377	-3.54212666
6	-3.85168934	-1.93581879	-0.23414300
1	-4.31047344	-4.57442951	-0.26814571
6	-3.20050025	-6.81512165	0.84424770
1	-1.09525275	-5.82887745	2.28846431
6	-0.08217312	-3.39925504	2.86988139
1	1.59665620	4.84826660	-2.40777206
1	0.97811997	3.75043821	-1.14158988
1	-0.03723785	5.06402922	-1.76046693
1	-1.35141349	-0.64319175	-3.10325575
1	-2.38256598	-0.17094892	-4.46835518
1	-2.70738745	0.44772199	-2.82175660
1	-0.32015216	3.56037760	-7.45121765
1	0.70297366	2.11577702	-7.47799921
1	1.38677025	3.68492913	-6.99021578
1	-4.33813906	-2.38383961	-1.11018479
1	-3.16321874	-1.15412533	-0.58720517
1	-4.64121723	-1.44381547	0.35681698
1	-0.33663315	-2.74827552	3.72154427
1	0.71078533	-2.88659596	2.30199718
1	0.34421095	-4.32499409	3.27607799
1	-2.33144426	-7.48500586	0.78285062
1	-3.80113626	-6.94937754	-0.06542099
1	-3.81231713	-7.15481806	1.69517076
1	-0.68685281	-1.27842534	2.01720095

Energy = -7584.948035 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 55

Atomic N.	X	Y	Z
8	1.18633926	-2.01312804	0.32604721
8	1.48769271	0.18224736	1.19700110
6	2.31962633	1.29906690	0.89980656
1	1.68699718	2.15578365	0.62063330
1	2.99708796	1.08917248	0.05656184
1	2.91629553	1.57919836	1.78504956
8	3.28569555	-1.27456403	0.17460658
6	2.16876602	-1.44805348	0.97109729
6	2.38470721	-1.87163234	2.41950178
1	2.94380760	-1.10230267	2.97360325
1	1.38017106	-1.92203212	2.85478187
6	3.08805275	-3.23637509	2.54272318

1	2.69808578	-3.91757298	1.77022421
1	2.81311631	-3.68030572	3.51142597
6	4.61721230	-3.14388108	2.46258759
1	4.97420931	-2.51247215	3.29542637
1	5.05414057	-4.14184618	2.62578964
6	5.15830278	-2.57191658	1.14678228
1	4.95025969	-3.25828362	0.31031230
1	6.25542355	-2.48214579	1.21531487
6	4.60377693	-1.19870448	0.77118903
1	4.60746908	-0.51245129	1.63347197
1	5.21817827	-0.74606776	-0.01909234
50	-0.25201067	-0.43636540	-0.18353245
7	-1.77755201	1.82218802	0.63078773
6	-1.11151302	3.06177068	1.05043912
1	-1.83146286	3.83322024	1.39034426
1	-0.51924783	3.46543002	0.21999033
1	-0.43465784	2.83340120	1.88305664
7	-1.02178490	2.58993888	-2.22784162
6	-2.73605275	2.04349923	-0.47631812
1	-3.68030882	2.46583891	-0.07358361
1	-2.98605418	1.05897415	-0.90477026
6	-2.28927350	2.98414588	-1.59710050
1	-3.11925530	3.00343537	-2.33000183
1	-2.20831895	4.00727415	-1.20158315
6	-0.74179119	3.08576035	-3.52850795
6	-0.55187142	4.47043753	-3.74886346
6	-0.25987035	4.92378426	-5.04211855
6	-0.12293143	4.05354548	-6.12733507
6	-0.27449563	2.68366289	-5.88133240
6	-0.58548629	2.18502355	-4.61233282
7	-1.57797527	-1.09248245	1.34767580
6	-2.45937896	1.19551539	1.78333557
1	-3.39291263	1.74784386	2.02254152
1	-1.78242445	1.28160071	2.64370608
6	-2.77714396	-0.28738508	1.57794571
1	-3.29790568	-0.63530493	2.48444319
1	-3.51808405	-0.40110585	0.75914848
6	-1.49907446	-2.32118630	2.05734015
6	-1.58991194	-3.56361842	1.37721372
6	-1.51753104	-4.75924301	2.10148144
6	-1.35039127	-4.78163719	3.49056339
6	-1.25345826	-3.55334711	4.15088272
6	-1.32033277	-2.33204174	3.46657777
6	-0.58487540	5.46308470	-2.61273956
1	-0.10891772	5.99573278	-5.19464922
6	0.16626595	4.57056236	-7.51607084
1	-0.15662275	1.97558999	-6.70560980
6	-0.74448866	0.69681668	-4.41280460
6	-1.76281250	-3.62592340	-0.11996987
1	-1.60128331	-5.70531368	1.55981171
6	-1.24586177	-6.08735800	4.24203539
1	-1.10791659	-3.53947067	5.23467779
6	-1.14568210	-1.04828525	4.23992014
1	-0.04251066	6.37709379	-2.88784432
1	-0.11788955	5.03994131	-1.71118069
1	-1.60969853	5.76248360	-2.34123731
1	0.01149390	0.28323299	-3.72592163
1	-0.64433748	0.16820347	-5.36904287

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1 -1.72851348  0.43953314 -3.98923492
1 -0.76063740  4.68382549 -8.10090923
1  0.81875426  3.88387275 -8.07311440
1  0.65371883  5.55443954 -7.48282576
1 -2.15640044 -4.60493755 -0.42476857
1 -0.79872006 -3.48785305 -0.63523036
1 -2.44558811 -2.84489059 -0.48271161
1 -2.09945607 -0.52283967  4.40873384
1 -0.48956990 -0.35478762  3.69332051
1 -0.70737666 -1.24801695  5.22675514
1 -0.22859955 -6.50553703  4.17639542
1 -1.93135548 -6.84236956  3.83165908
1 -1.47924769 -5.95622969  5.30727005
1 -0.90682119  1.57509410 -2.18181205

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Energy = -7584.948468 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 56

Atomic N.	X	Y	Z
8	1.44261372	0.09648208	1.61437488
8	2.35307479	0.29263166	-0.55595767
6	2.98181963	-0.39235577	-1.63502884
1	2.59580016	0.00811642	-2.58560300
1	2.77647734	-1.47584403	-1.61169755
1	4.07390070	-0.23012446	-1.61363101
8	2.47291803	-1.76072741	0.90009487
6	2.51587796	-0.36786678	1.08008683
6	3.85626698	0.22714379	1.51393604
1	4.63518095	0.04164645	0.75816596
1	3.69663167	1.31195891	1.53946900
6	4.32667923	-0.27907449	2.89055824
1	3.45798922	-0.35805279	3.56383586
1	4.99404573	0.47700450	3.33257842
6	5.08203983	-1.61303067	2.82815981
1	5.98470545	-1.47407854	2.20720696
1	5.44163275	-1.87672532	3.83563900
6	4.27350903	-2.78568053	2.26107359
1	3.44319749	-3.04772782	2.93668103
1	4.92386007	-3.67456317	2.20165277
6	3.68677330	-2.54152536	0.86996979
1	4.43659353	-2.09327483	0.19748877
1	3.37139630	-3.49501419	0.42350060
50	-0.00845817	0.12792644	-0.43080020
7	-0.22244368	2.37733459	0.70936906
6	1.08664572	3.06910729	0.66632468
1	0.98134387	4.11815929	0.99776208
1	1.49079216	3.04629469	-0.35020125
1	1.77856052	2.53583288	1.32482302
7	-0.47441390	1.64069653	-1.96165979
6	-1.20050633	3.08204842	-0.15598735
1	-1.30559778	4.13426542	0.17298214
1	-2.17145824	2.58016801	-0.04152601
6	-0.77799529	3.01700544	-1.62248755
1	-1.62374258	3.40068293	-2.22597170
1	0.05526150	3.73140526	-1.79427707
6	-0.35738507	1.32355714	-3.33968568
6	0.69857162	1.83286941	-4.14362812

6	0.78727704	1.46731925	-5.49363375
6	-0.13384745	0.60383421	-6.09362459
6	-1.16888595	0.10442832	-5.29470301
6	-1.30233061	0.44901350	-3.94454217
7	-1.56879711	0.05298990	2.08113670
6	-0.66454583	2.33635139	2.12943625
1	-0.88953638	3.36513829	2.47038364
1	0.19635896	1.97091091	2.70602965
6	-1.86709154	1.44686270	2.43003678
1	-2.09464312	1.56641603	3.50757432
1	-2.75845742	1.78475773	1.88599348
6	-2.49875164	-0.96433794	2.43510938
6	-3.78743267	-1.00829172	1.85625219
6	-4.65747595	-2.04693723	2.21400642
6	-4.28984261	-3.05756354	3.10698962
6	-2.99290133	-3.01875043	3.63297105
6	-2.09360027	-1.99539053	3.31852651
6	1.75951898	2.73178601	-3.55808449
1	1.61569107	1.86114442	-6.08950806
6	-0.03339966	0.24248311	-7.55641985
1	-1.90831935	-0.56758463	-5.73904085
6	-2.46973252	-0.09905201	-3.15849042
6	-4.22769785	-0.01197312	0.81198549
1	-5.64841175	-2.07551217	1.75361586
6	-5.25729179	-4.14927435	3.49562931
1	-2.66740036	-3.80924320	4.31389332
6	-0.70135999	-2.01064968	3.90567231
1	2.67320514	2.70239758	-4.16686010
1	2.00905061	2.42393184	-2.53212547
1	1.43263805	3.78306413	-3.51204157
1	-2.16565871	-0.91188782	-2.48043442
1	-3.23497176	-0.50101256	-3.83613658
1	-2.92259002	0.67961270	-2.52941203
1	-0.72694492	0.84466213	-8.16495991
1	-0.28646022	-0.81323868	-7.72870350
1	0.97965437	0.41906652	-7.94259548
1	-5.03146744	-0.43561718	0.19621253
1	-3.39362669	0.25716031	0.14758435
1	-4.61689186	0.91922987	1.25481093
1	-0.48781833	-1.09964490	4.48734236
1	0.07631212	-2.08298850	3.12841749
1	-0.58075261	-2.86909127	4.57817984
1	-4.73828840	-5.10128212	3.67325401
1	-6.01247215	-4.31115532	2.71450925
1	-5.79509544	-3.89381599	4.42269278
1	-0.62707192	-0.18493629	2.40547991

Energy = -7584.948070 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 57

Atomic N.	X	Y	Z
8	0.40511423	-2.12129998	0.95032811
8	1.67785370	-0.10909839	0.91057509
6	2.76711154	0.39579815	0.14447425
1	2.44576216	1.30864322	-0.38040608
1	3.10290885	-0.33041415	-0.61303115
1	3.61400461	0.65175277	0.80426073

8	2.53688216	-2.42645717	0.36972287
6	1.64429379	-1.85505152	1.25786471
6	2.00984979	-1.85957587	2.73789263
1	2.92081261	-1.26878977	2.91837811
1	1.18206811	-1.34378302	3.23775434
6	2.17324567	-3.28151011	3.30689478
1	1.39838755	-3.93613887	2.87804842
1	1.97986400	-3.24454880	4.38962460
6	3.57024193	-3.87287545	3.07872558
1	4.31061459	-3.22793436	3.58432484
1	3.63636661	-4.85729456	3.56864619
6	3.97297120	-4.02072239	1.60656261
1	3.34656334	-4.77688551	1.10666978
1	5.01229620	-4.38555717	1.55062950
6	3.88942432	-2.73277116	0.78896278
1	4.33716679	-1.88251579	1.32847273
1	4.43223619	-2.85067797	-0.15886249
50	-0.43404442	-0.32560298	0.01030577
7	-0.79563290	2.49550819	0.05440843
6	0.35654321	3.39785290	-0.06572183
1	0.06785877	4.46462250	0.02177991
1	0.85414058	3.23929787	-1.03040206
1	1.06902993	3.16798210	0.73618424
7	-0.47222173	1.96034336	-2.93654203
6	-1.82603896	2.75602341	-0.97694582
1	-2.43086076	3.63999820	-0.68539602
1	-2.51153755	1.89285827	-0.99024296
6	-1.32713866	3.02741480	-2.39751410
1	-2.23296237	3.17482376	-3.01737738
1	-0.78640914	3.98501801	-2.41569519
6	-0.32807869	1.87187350	-4.34641314
6	0.31169510	2.90364480	-5.07339668
6	0.45197609	2.77689409	-6.46159077
6	0.00346141	1.65183091	-7.15969849
6	-0.59022266	0.62403095	-6.41756725
6	-0.76966339	0.71300018	-5.03333187
7	-1.52447176	0.14113796	1.77875161
6	-1.38519931	2.59925675	1.40641510
1	-1.97251511	3.53760791	1.49688530
1	-0.55083764	2.64938951	2.11860633
6	-2.26179028	1.40430081	1.78820491
1	-2.65905142	1.60287213	2.79649758
1	-3.15446901	1.36966741	1.12918496
6	-1.74514651	-0.72533774	2.88323379
6	-2.43111825	-1.95646060	2.71929359
6	-2.64104724	-2.78792548	3.82622862
6	-2.19081068	-2.45307016	5.10751295
6	-1.50958443	-1.24106646	5.25836849
6	-1.27574921	-0.37894061	4.17915249
6	0.90967029	4.10375929	-4.38113594
1	0.95499003	3.57916474	-7.00793505
6	0.14229605	1.55338776	-8.65987110
1	-0.93576485	-0.27650303	-6.93164825
6	-1.42486477	-0.42651364	-4.29018736
6	-2.94309831	-2.39490819	1.36983633
1	-3.18163371	-3.72702479	3.68050337
6	-2.40155959	-3.38410020	6.27765846
1	-1.13333881	-0.95872408	6.24567509

6	-0.47852230	0.88158083	4.40766811
1	1.67834258	4.56647205	-5.01383543
1	1.37353075	3.81338978	-3.42700577
1	0.16116649	4.88080168	-4.15846062
1	-0.74513263	-0.89726460	-3.56167698
1	-1.74762917	-1.20682931	-4.99074984
1	-2.31125641	-0.09595211	-3.72544098
1	-0.76397103	1.91839170	-9.16933346
1	0.29922560	0.51461834	-8.98171329
1	0.98568827	2.15588188	-9.02411270
1	-3.72692966	-3.15622663	1.48078489
1	-2.13662767	-2.84342980	0.76778197
1	-3.35245562	-1.55100882	0.79706037
1	0.24945731	1.03037310	3.59638095
1	0.06053712	0.83016676	5.36295605
1	-1.11203647	1.78255832	4.44032478
1	-1.57574296	-4.10854673	6.36413527
1	-3.32938385	-3.96236086	6.16723680
1	-2.45208955	-2.83227968	7.22630978
1	-0.73700994	1.05998802	-2.53089809

Energy = -7584.948490 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 58

Atomic N.	X	Y	Z
8	2.83960032	-1.21166825	0.16661698
8	2.72266722	-0.14645264	-1.84608281
6	2.57823014	-0.23911986	-3.25862908
1	1.80480158	0.47704369	-3.56444144
1	2.26322532	-1.25391686	-3.54803276
1	3.51991487	0.01580197	-3.77506495
8	3.01079226	-2.55892444	-1.64080274
6	3.41760874	-1.36279452	-0.99070185
6	4.91834497	-1.04390216	-1.05033028
1	5.26400566	-0.92655057	-2.09033847
1	5.00904036	-0.06048527	-0.57078999
6	5.79067945	-2.07321596	-0.31213069
1	5.27225685	-2.38133121	0.60955793
1	6.72253847	-1.58028579	0.00523037
6	6.15460062	-3.29431224	-1.16551900
1	6.73829412	-2.95171404	-2.03844333
1	6.82272768	-3.95631051	-0.59178108
6	4.95550919	-4.10625505	-1.66765749
1	4.42774677	-4.58133793	-0.82499903
1	5.31967974	-4.92319345	-2.31339717
6	3.92956018	-3.30155492	-2.46778631
1	4.42818499	-2.64698625	-3.20346522
1	3.27744460	-3.98702407	-3.02867079
50	1.61520708	0.77996415	0.00861821
7	-0.33269319	-0.76078743	-0.30946958
6	-0.00288506	-2.20560956	-0.33921707
1	-0.92435086	-2.79915214	-0.47960147
1	0.49770704	-2.50183558	0.58672512
1	0.70027775	-2.40455031	-1.15336382
7	-1.99438083	-0.43420771	3.13997531
6	-1.38499033	-0.49424148	0.70881665
1	-2.27407455	-1.10940349	0.47324178

1	-1.67706013	0.55923182	0.61540753
6	-0.95021808	-0.76027924	2.15999365
1	-0.65523028	-1.80632782	2.28980947
1	-0.06321373	-0.15106323	2.39965963
6	-3.20311475	-1.18054688	3.15690351
6	-3.19665194	-2.55856228	3.48130631
6	-4.41222239	-3.25424528	3.51876855
6	-5.64225864	-2.63317728	3.28240895
6	-5.63184881	-1.25767696	3.02227521
6	-4.44342613	-0.52438056	2.95103741
7	0.24899794	1.83335054	-1.35073268
6	-0.81298667	-0.34415236	-1.66146302
1	-1.77409792	-0.84405273	-1.88463366
1	-0.06386339	-0.70907938	-2.37697625
6	-0.96072638	1.16910458	-1.80768442
1	-1.16438925	1.36234200	-2.88156176
1	-1.87457955	1.50786066	-1.27721810
6	0.23778263	3.25781226	-1.33856416
6	-0.58826679	4.01138544	-0.45776758
6	-0.55669743	5.41264582	-0.49044690
6	0.28722492	6.12139177	-1.34800267
6	1.12222588	5.37647438	-2.18746471
6	1.11324358	3.97728157	-2.19858980
6	-1.92705822	-3.28021431	3.86337185
1	-4.39227152	-4.31690264	3.77448225
6	-6.93342638	-3.41510940	3.30406356
1	-6.57857895	-0.73568046	2.86146379
6	-4.49897575	0.95888829	2.66903949
6	-1.46532547	3.34832239	0.57400465
1	-1.20117855	5.96510839	0.19896537
6	0.33221751	7.63029337	-1.33915746
1	1.79982662	5.90028191	-2.86723471
6	2.02826548	3.25510478	-3.15513945
1	-2.15912986	-4.14217806	4.50254488
1	-1.24467015	-2.61378908	4.40971184
1	-1.37830305	-3.66862345	2.98999810
1	-4.08297253	1.55921030	3.49544787
1	-5.53743458	1.28309929	2.52810192
1	-3.94154191	1.23097861	1.75842285
1	-7.22996330	-3.72399044	2.28888965
1	-7.75900078	-2.81744504	3.71484447
1	-6.83780622	-4.32745361	3.90820694
1	-1.74953771	4.06524754	1.35522926
1	-0.93019563	2.51408148	1.05203342
1	-2.39675021	2.94394016	0.14578483
1	1.45679808	2.61506844	-3.84267449
1	2.74101663	2.60175371	-2.63246059
1	2.60197234	3.97447920	-3.75448322
1	1.19842660	7.99929047	-0.76717132
1	-0.57071716	8.05481720	-0.88035333
1	0.42200693	8.03549862	-2.35716653
1	-2.19158792	0.56489778	3.11670399

Energy = -7584.938180 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 59

Atomic N. X Y Z

8	1.94869554	-1.29784918	-0.15354633
8	1.93146515	0.07464297	-2.00426745
6	2.48097110	0.65648413	-3.17558408
1	1.66496003	1.09545791	-3.76834178
1	2.97204089	-0.11898468	-3.78755808
1	3.20853400	1.45595706	-2.94868565
8	3.24278569	-1.99731767	-1.86355126
6	2.85513258	-0.94539970	-1.00024223
6	3.97904587	-0.03566409	-0.48719734
1	4.54059267	0.43207672	-1.31150377
1	3.46233702	0.77136499	0.05074144
6	4.94747543	-0.75988793	0.46447873
1	4.36692572	-1.43171132	1.11611354
1	5.41506672	-0.01309185	1.12467480
6	6.05785894	-1.53145599	-0.25906566
1	6.67131758	-0.81209904	-0.83036989
1	6.73246622	-1.98464668	0.48493347
6	5.56358480	-2.62002754	-1.21853495
1	5.05546570	-3.42601228	-0.66486192
1	6.43355083	-3.07930183	-1.71775556
6	4.60831881	-2.12463403	-2.30677366
1	4.97662306	-1.18440092	-2.75285745
1	4.54825115	-2.86875892	-3.11388063
50	0.26817408	0.44189173	-0.37385184
7	-0.89622211	-1.41612101	-1.67027664
6	-0.06950447	-2.61526942	-1.93460441
1	-0.63436967	-3.33120441	-2.56058764
1	0.22979014	-3.09065771	-0.99724197
1	0.84993786	-2.31639767	-2.44615650
7	-1.60634375	-1.24887490	1.30189586
6	-2.17745042	-1.80911446	-1.03133941
1	-2.66380644	-2.59102488	-1.64583588
1	-2.83998322	-0.93235904	-1.04337645
6	-2.05794096	-2.32319856	0.40163738
1	-3.04924989	-2.71762228	0.69790971
1	-1.35500479	-3.16113234	0.45922092
6	-1.48819709	-1.53864622	2.69708967
6	-0.54104501	-2.47044921	3.17960191
6	-0.45936689	-2.68895364	4.56171131
6	-1.25707960	-2.00532842	5.48375034
6	-2.15676880	-1.05721021	4.98438692
6	-2.28995275	-0.81495571	3.61389065
7	-1.16311944	1.38762546	-1.77634442
6	-1.16179669	-0.73176599	-2.96791101
1	-1.76667786	-1.38885570	-3.62212849
1	-0.17994294	-0.58948267	-3.43838525
6	-1.84946287	0.62096173	-2.79855227
1	-1.81692684	1.12146115	-3.78823018
1	-2.92926502	0.46709368	-2.59132648
6	-1.62781060	2.70300794	-1.51989555
6	-2.93125725	2.97484207	-1.01749074
6	-3.32774520	4.29618311	-0.76672792
6	-2.47801971	5.38415861	-0.97479242
6	-1.19075382	5.11088276	-1.45211768
6	-0.75648689	3.81051731	-1.72790551
6	0.41993952	-3.19497347	2.26921129
1	0.27978709	-3.40679145	4.92626953
6	-1.15865660	-2.28515005	6.96385098

1	-2.77853489	-0.48805305	5.67982817
6	-3.27087212	0.23112889	3.13498330
6	-3.89835572	1.86778557	-0.68301463
1	-4.33335161	4.47327900	-0.37456006
6	-2.91447639	6.79710150	-0.67091835
1	-0.50188696	5.94094896	-1.63187897
6	0.62959921	3.61098361	-2.28989601
1	1.29327846	-3.53336644	2.84192944
1	0.78299516	-2.55361462	1.45414472
1	-0.03170080	-4.09543037	1.82091701
1	-2.76817083	1.07346320	2.63134575
1	-3.82670283	0.64978045	3.98291397
1	-4.01209021	-0.17985409	2.43018079
1	-1.89530110	-3.04290843	7.27525568
1	-1.35192275	-1.38100898	7.55740499
1	-0.16441464	-2.66642380	7.23326206
1	-4.62641001	2.20181203	0.06811586
1	-3.35798144	0.99736214	-0.28274056
1	-4.46831274	1.51927912	-1.55925143
1	0.59760290	3.01772046	-3.21405363
1	1.29086876	3.07279897	-1.59375346
1	1.09718966	4.58000612	-2.51013136
1	-2.41939998	7.18314981	0.23408721
1	-3.99868965	6.85306120	-0.50585246
1	-2.65952754	7.48213387	-1.49288678
1	-2.24431872	-0.45896274	1.19285727

Energy = -7584.940072 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 60

Atomic N.	X	Y	Z
8	1.88308525	-1.82311261	0.31452280
8	1.95493245	-0.25382251	-1.62705362
6	2.49549198	0.96190405	-2.07253027
1	2.45093203	1.76990020	-1.30898094
1	1.96199286	1.32872427	-2.97502685
1	3.55719113	0.86181349	-2.37459683
8	3.26590204	-2.53522515	-1.24549663
6	2.90680933	-1.53806996	-0.38940296
6	3.98510814	-0.61671573	0.15212367
1	4.45174789	-0.02641873	-0.64907831
1	3.46947551	0.08886102	0.81639773
6	5.08138466	-1.38596606	0.92038339
1	4.62384176	-2.18975925	1.51833010
1	5.54728508	-0.69372094	1.63794744
6	6.17678642	-1.94657552	0.00307194
1	6.65490198	-1.10183251	-0.52324855
1	6.96478128	-2.41126132	0.61635447
6	5.69110584	-2.96365213	-1.03730249
1	5.36342096	-3.89329767	-0.54456300
1	6.53293133	-3.23749375	-1.69477069
6	4.54563618	-2.47928834	-1.92378807
1	4.72344494	-1.46722925	-2.31815600
1	4.41627645	-3.15515184	-2.77914143
50	0.31601533	-0.14085758	0.21356355
7	-0.91993910	-1.29437506	-1.63296199
6	-0.13143818	-2.48693705	-2.03580117

1	-0.71365833	-3.10069728	-2.74639654
1	0.12646025	-3.08459425	-1.15715444
1	0.80210084	-2.15097857	-2.49848747
7	-1.12921166	-1.47225893	1.15891051
6	-2.19427156	-1.71593261	-0.99720138
1	-2.74190259	-2.40302730	-1.67109036
1	-2.80264950	-0.81751901	-0.83496803
6	-1.93665838	-2.37294221	0.35776389
1	-2.92198420	-2.54678226	0.83117408
1	-1.49839902	-3.38015366	0.20150314
6	-1.05635929	-1.70704663	2.55716348
6	-0.53798521	-2.91076517	3.10861850
6	-0.48600897	-3.07103252	4.50004768
6	-0.91436750	-2.07798505	5.38536549
6	-1.40880263	-0.89083529	4.83389235
6	-1.49558115	-0.69144034	3.45133924
7	-1.33203733	1.77895713	-1.83948469
6	-1.13300490	-0.48238266	-2.86253548
1	-1.62215292	-1.11782420	-3.62638974
1	-0.12706248	-0.23952803	-3.23782802
6	-1.95926499	0.79488671	-2.73454475
1	-2.08068633	1.19110405	-3.76275015
1	-2.97113872	0.57287228	-2.37353945
6	-1.95574570	3.05989742	-1.74336231
6	-3.20281434	3.20681834	-1.09574294
6	-3.77730370	4.48186207	-1.00675273
6	-3.15009260	5.62331009	-1.51349688
6	-1.90206039	5.45990753	-2.12650561
6	-1.29719782	4.20574474	-2.25404882
6	0.01431571	-4.00737476	2.23124051
1	-0.07276586	-4.00074148	4.90180349
6	-0.86816382	-2.28647327	6.88029432
1	-1.75562477	-0.09621281	5.50031710
6	-2.08992577	0.59532601	2.93147874
6	-3.90381742	2.03654099	-0.45374984
1	-4.74060345	4.58222914	-0.50030333
6	-3.77324057	6.99085188	-1.36921012
1	-1.38313806	6.33471537	-2.52655482
6	0.05207237	4.09394693	-2.92499590
1	0.68250865	-4.65894079	2.81035209
1	0.58054423	-3.58657146	1.38899672
1	-0.78115356	-4.64652395	1.81483710
1	-1.33679676	1.24299359	2.45606899
1	-2.54933786	1.16465747	3.75069761
1	-2.85350680	0.39348328	2.16738081
1	-1.83737433	-2.64267755	7.26532173
1	-0.63360393	-1.35236895	7.40997076
1	-0.11283004	-3.03528476	7.15586853
1	-4.57254124	2.38103843	0.34553581
1	-3.17591071	1.33784747	-0.01861772
1	-4.52311611	1.47297192	-1.17065406
1	0.04652268	3.37258077	-3.75743461
1	0.83831125	3.77517581	-2.22120595
1	0.35845318	5.06526756	-3.33268189
1	-3.33934379	7.53773117	-0.51720810
1	-4.85566378	6.92107010	-1.19849610
1	-3.60648370	7.60438156	-2.26580715
1	-0.35704866	1.89828610	-2.11753821

Energy = -7584.942755 Hartree
 Number of imaginary frequencies = 0.

Compound TS2b isomer 61

Atomic N.	X	Y	Z
8	2.03071594	-0.21930736	-0.99814600
8	1.55298316	2.05209208	-0.31997499
6	1.69326174	3.12052059	0.59869933
1	1.86808920	2.78243637	1.63869691
1	0.77528840	3.73342490	0.59134382
1	2.52739167	3.78016090	0.30188382
8	3.47077131	1.21156621	-1.85946655
6	2.86868310	0.72368944	-0.73915786
6	3.66832590	0.68981022	0.55581522
1	3.90566492	1.70441258	0.90713716
1	3.00566602	0.23585592	1.30417705
6	4.97324181	-0.12271835	0.42288119
1	4.79293299	-1.01806056	-0.19307493
1	5.25553274	-0.48677757	1.42239678
6	6.14014769	0.69897068	-0.14249097
1	6.32814789	1.54768944	0.53824085
1	7.05645227	0.08800354	-0.13049243
6	5.92234087	1.24270427	-1.56010127
1	5.90408897	0.41840664	-2.29127932
1	6.77418804	1.88663030	-1.83495176
6	4.64315319	2.05589223	-1.74508548
1	4.50571680	2.79851079	-0.94437230
1	4.66928482	2.59510589	-2.70084095
50	0.05323865	0.37539530	-0.07361945
7	-0.61213160	-1.75139451	-1.41930163
6	0.37310767	-2.84766245	-1.39974272
1	0.06649982	-3.68228054	-2.05805635
1	0.49570310	-3.21596456	-0.37423253
1	1.33540666	-2.45177197	-1.74199510
7	-1.40216827	-2.66781616	1.41054428
6	-1.96696877	-2.18967438	-0.98884857
1	-2.47520661	-2.68565083	-1.83923340
1	-2.54783320	-1.28417957	-0.75194615
6	-2.03982496	-3.16666436	0.18494686
1	-3.11656523	-3.36908269	0.34428054
1	-1.58897197	-4.12482309	-0.11265936
6	-1.82944810	-3.18800712	2.65827632
6	-1.66349709	-4.55859280	2.96763110
6	-2.08544540	-5.03327322	4.21670723
6	-2.64286661	-4.19590378	5.18716335
6	-2.75831747	-2.83507419	4.87829685
6	-2.37076473	-2.31773829	3.63846493
7	-0.94836992	1.08078206	-1.81685448
6	-0.67775047	-1.15600395	-2.77949905
1	-1.11806715	-1.88452280	-3.48949504
1	0.35882953	-0.94909447	-3.07973623
6	-1.46434069	0.15054996	-2.80782604
1	-1.36877680	0.55815935	-3.83010125
1	-2.54993987	-0.05367624	-2.67700219
6	-1.14994192	2.46421266	-2.06471348
6	-2.06188679	3.21450472	-1.28010905
6	-2.22996807	4.58499813	-1.52511644

6	-1.52411318	5.25030804	-2.53126001
6	-0.62545514	4.50065899	-3.30018067
6	-0.42015517	3.13347530	-3.08535838
6	-0.97411239	-5.50493240	2.01541829
1	-1.94479144	-6.09348345	4.44312429
6	-3.11359334	-4.73818922	6.51528120
1	-3.17387056	-2.15067458	5.62240314
6	-2.52882719	-0.84172434	3.36106801
6	-2.87430429	2.56163383	-0.18574044
1	-2.94588876	5.14451265	-0.91666043
6	-1.70310974	6.73129988	-2.76722980
1	-0.04852886	4.99972773	-4.08407164
6	0.60511261	2.39932227	-3.91122460
1	-0.60647428	-6.38775730	2.55443597
1	-0.11805589	-5.01417732	1.52904499
1	-1.64178252	-5.86568880	1.21706164
1	-1.56231344	-0.34479260	3.17724824
1	-3.00111961	-0.33920580	4.21447802
1	-3.15443778	-0.65293598	2.47380543
1	-4.19800711	-4.93300390	6.50525665
1	-2.91993380	-4.02816534	7.33146048
1	-2.61356974	-5.68515301	6.75998926
1	-3.75427389	3.17226243	0.05827215
1	-2.29477739	2.44035983	0.74416327
1	-3.20852399	1.55742192	-0.47910169
1	0.14345464	1.82672334	-4.73251915
1	1.16706240	1.68864596	-3.29072595
1	1.30970097	3.10663557	-4.36876011
1	-0.85414356	7.30577564	-2.36355686
1	-2.61461592	7.10520506	-2.28181982
1	-1.76728189	6.96331835	-3.84004951
1	-1.38507307	-1.64617276	1.41768622

Energy = -7584.950189 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 62

Atomic N.	X	Y	Z
8	0.39366522	-0.30250940	0.21547368
8	2.58239675	-0.02477086	-0.92172968
6	3.50435519	1.04127443	-1.03674841
1	3.63978434	1.33310974	-2.09080219
1	4.49522448	0.73578119	-0.64936441
1	3.17173028	1.93897879	-0.48583034
8	1.80233455	0.80230266	1.51740909
6	1.53947568	-0.31221783	0.78852606
6	2.16138577	-1.65019453	1.16713607
1	1.68307638	-1.94626987	2.12139034
1	1.78400493	-2.35551095	0.41512293
6	3.68514895	-1.78372180	1.27051091
1	4.12465096	-1.39498591	0.34133613
1	3.91747093	-2.85978842	1.30039334
6	4.32138729	-1.11691618	2.49179697
1	3.93790460	-1.59651673	3.40989089
1	5.40687466	-1.30265176	2.47908425
6	4.06726933	0.38927600	2.58804011
1	4.49024916	0.92189592	1.72244847
1	4.58182812	0.78598082	3.47929931

6	2.59710956	0.76429963	2.73524690
1	2.09662628	0.09856620	3.45885611
1	2.50407648	1.79337251	3.10411525
50	0.74300116	-0.59081250	-2.06090307
7	-1.99115872	-0.68731272	-2.30753589
6	-2.42157578	-2.01297235	-2.76740813
1	-3.45238113	-2.00315762	-3.17343903
1	-2.36126971	-2.72941804	-1.94077384
1	-1.73864079	-2.34906816	-3.55935407
7	-2.24862862	-1.77455926	0.57665563
6	-2.84790421	-0.13787615	-1.23104179
1	-3.76024485	0.31005794	-1.67936587
1	-2.29054594	0.67925501	-0.74967700
6	-3.33429241	-1.11746812	-0.16271269
1	-3.99089766	-0.52588385	0.50781190
1	-3.98144364	-1.88166046	-0.61997020
6	-2.63595295	-2.43243074	1.78054821
6	-3.25903940	-3.70109844	1.72042251
6	-3.62255883	-4.34418106	2.91026258
6	-3.37557435	-3.78132939	4.16697550
6	-2.73951650	-2.53548312	4.20806456
6	-2.37657595	-1.84748280	3.04383826
7	0.08971093	1.37164938	-2.59937429
6	-1.94457948	0.24702150	-3.45150304
1	-2.96906590	0.45002079	-3.82796884
1	-1.38652802	-0.25826573	-4.25646782
6	-1.25371206	1.56945419	-3.13390899
1	-1.22215891	2.14170909	-4.08262444
1	-1.89109647	2.16990662	-2.45165157
6	0.85204107	2.57230210	-2.51574421
6	0.67308855	3.48777843	-1.44882476
6	1.43794096	4.66188812	-1.41259038
6	2.37664866	4.97056866	-2.40225005
6	2.53285384	4.06551456	-3.45875621
6	1.79178524	2.88007474	-3.53222775
6	-3.48249364	-4.39396286	0.40027538
1	-4.09338427	-5.32886124	2.84891081
6	-3.80178094	-4.48353672	5.43398857
1	-2.53124595	-2.07333302	5.17669201
6	-1.72180474	-0.49059382	3.15127802
6	-0.31931913	3.21409416	-0.34659606
1	1.29612076	5.35400295	-0.57789862
6	3.21428657	6.22456932	-2.32184100
1	3.25112438	4.28907728	-4.25226641
6	2.00928020	1.93856013	-4.69261503
1	-3.64544654	-5.46928501	0.54896480
1	-2.61310959	-4.25337124	-0.25761253
1	-4.36199665	-4.00185537	-0.13542183
1	-0.67900461	-0.50112510	2.79987025
1	-1.71897209	-0.14756745	4.19376373
1	-2.24255371	0.26604515	2.54565096
1	-4.82897568	-4.20352221	5.71750689
1	-3.14834189	-4.22249651	6.27759171
1	-3.78504395	-5.57534170	5.31192303
1	-0.07703978	3.80228186	0.54841197
1	-0.32368883	2.14946079	-0.07864362
1	-1.34336829	3.48801732	-0.64923567
1	1.05898559	1.59415519	-5.12248707

1	2.55581498	1.03184485	-4.38601065
1	2.59756351	2.42640376	-5.48121834
1	4.19253063	6.02007437	-1.85797334
1	2.72082305	6.99791098	-1.71778977
1	3.41023922	6.64103365	-3.31983161
1	-1.47895718	-1.11820459	0.73250502

Energy = -7584.943901 Hartree
Number of imaginary frequencies = 0.

Compound TS2b isomer 63

Atomic N.	X	Y	Z
8	0.72310162	-3.06866860	0.27815679
8	1.33839917	-1.32460737	-1.35781312
6	2.13225722	-1.96188486	-2.34931684
1	1.70144475	-1.77839518	-3.35086608
1	2.17625976	-3.06049562	-2.21835375
1	3.16442966	-1.57078612	-2.34620261
8	0.98814237	-0.94560719	1.02070332
6	1.51062477	-2.05677271	0.39815137
6	2.99215436	-2.36269379	0.56231391
1	3.08778429	-2.87181711	1.53811193
1	3.21801782	-3.13607192	-0.18365332
6	3.99866080	-1.20828164	0.46600688
1	3.75316691	-0.58121377	-0.40393379
1	4.99013424	-1.64377236	0.26528940
6	4.09591579	-0.33053130	1.71775806
1	4.36211252	-0.96646833	2.58064961
1	4.92535782	0.38353631	1.59385121
6	2.81161666	0.43616095	2.04018307
1	2.58327794	1.16861165	1.24969935
1	2.95418763	1.01262438	2.96975732
6	1.59068370	-0.45492631	2.24182463
1	1.81905615	-1.30365229	2.90877223
1	0.77881610	0.11843365	2.70702958
50	-0.72731060	-2.62735677	-1.37858593
7	-2.04605508	-0.72173035	-2.72934318
6	-2.80848718	-1.60380793	-3.62978768
1	-3.57924151	-1.03781068	-4.18674564
1	-3.29947495	-2.40512633	-3.06279969
1	-2.12308645	-2.07507777	-4.34725332
7	-2.17166543	-1.82094717	-0.03172237
6	-2.90775537	-0.12187865	-1.69179666
1	-3.81010914	0.34278503	-2.13888144
1	-2.31458330	0.64981538	-1.18781447
6	-3.32403469	-1.15696192	-0.64173305
1	-3.91111851	-0.62619847	0.12410219
1	-4.03173208	-1.88589871	-1.09051740
6	-2.25617671	-2.04926801	1.36824846
6	-2.34544086	-3.36342311	1.89353311
6	-2.43949699	-3.55386591	3.27864337
6	-2.45072126	-2.48532367	4.17985106
6	-2.34464431	-1.19358516	3.65269351
6	-2.24297523	-0.95620698	2.27697420
7	-0.02942577	1.50236320	-1.77554512
6	-1.29750121	0.25403357	-3.56968808
1	-1.91341853	0.51158428	-4.45375490
1	-0.40458930	-0.26903772	-3.95192146

6	-0.89449310	1.59376061	-2.95489621
1	-0.40764269	2.15329814	-3.77997160
1	-1.80258417	2.16449285	-2.70298100
6	0.66046268	2.69627571	-1.41801810
6	-0.03682258	3.76708221	-0.81159353
6	0.66474831	4.92472744	-0.44846565
6	2.04183364	5.05736732	-0.64837313
6	2.71586609	3.98838305	-1.25119090
6	2.05281067	2.82274771	-1.64984298
6	-2.34024692	-4.57502604	0.99414957
1	-2.51460862	-4.57502604	3.66199136
6	-2.59699726	-2.71393418	5.66537285
1	-2.32286549	-0.33855438	4.33465195
6	-2.06172490	0.45704547	1.78462934
6	-1.51225126	3.67443895	-0.51544416
1	0.11303751	5.73975801	0.02726884
6	2.78362989	6.29473448	-0.20283499
1	3.79063487	4.06902075	-1.43462861
6	2.82024002	1.72448564	-2.34385538
1	-2.75207901	-5.44809914	1.51825452
1	-1.31716454	-4.83902645	0.68103737
1	-2.92960596	-4.40649796	0.08155128
1	-1.31531954	0.48896056	0.97781283
1	-1.73522329	1.11345482	2.60287690
1	-2.99478030	0.88703710	1.38480735
1	-3.65347648	-2.66468334	5.97467279
1	-2.05510592	-1.95244575	6.24383211
1	-2.21719646	-3.70216084	5.95871878
1	-1.79102767	4.36996078	0.28691542
1	-1.78275847	2.65537047	-0.20803143
1	-2.12885666	3.92749381	-1.39322627
1	2.40682817	1.51062799	-3.34211946
1	2.78253078	0.78043348	-1.78074062
1	3.87311554	2.00788808	-2.46850801
1	3.23948812	6.15039492	0.78970850
1	2.11183333	7.16068363	-0.13202474
1	3.59640002	6.54738808	-0.89824432
1	0.59281385	0.68834603	-1.81753516

Energy = -7584.934244 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 64

Atomic N.	X	Y	Z
8	0.23567806	-0.48590729	-0.08380977
8	2.34837437	-0.35712302	-1.37788534
6	3.62636399	0.20443247	-1.15264308
1	3.86378121	0.96175706	-1.91734087
1	4.40630198	-0.57872653	-1.21198905
1	3.69590569	0.69760430	-0.16675827
8	1.97399354	-0.82502443	1.24473107
6	1.28637028	-1.18635297	0.13157256
6	1.32745612	-2.62333465	-0.37200201
1	0.77626389	-3.22224188	0.37939164
1	0.69656563	-2.62148190	-1.27044535
6	2.67280841	-3.28315806	-0.69600034
1	3.22584915	-2.61583233	-1.37151706
1	2.45777225	-4.19910383	-1.26832938

6	3.52858567	-3.65893459	0.51551217
1	2.99120235	-4.40930080	1.12226748
1	4.45080853	-4.14973450	0.16685891
6	3.89422536	-2.47706246	1.41659367
1	4.48892498	-1.72794807	0.87165856
1	4.52915621	-2.83678985	2.24359560
6	2.69470596	-1.79061139	2.05973268
1	1.97492313	-2.53743601	2.43588877
1	3.02000761	-1.17831087	2.91002059
50	0.43639091	0.46851328	-2.18937898
7	-2.10494518	1.44225097	-1.80972052
6	-3.03403401	0.84292805	-2.77504802
1	-3.97480059	1.42063773	-2.86833739
1	-3.26467943	-0.18593514	-2.47736311
1	-2.54615235	0.81120163	-3.75866890
7	-2.78309202	-0.92255700	0.06864475
6	-2.66471004	1.53362167	-0.44099969
1	-3.31604481	2.43056321	-0.36905739
1	-1.82354951	1.68992877	0.25044557
6	-3.50800276	0.35460976	0.04479717
1	-3.86950040	0.64186537	1.05342448
1	-4.40836287	0.25413692	-0.58047152
6	-3.39981294	-1.96932709	0.81348163
6	-4.49580669	-2.67542076	0.26492870
6	-5.08106518	-3.71416640	1.00036323
6	-4.60857344	-4.09315825	2.26087904
6	-3.51158977	-3.39596486	2.78047013
6	-2.90805745	-2.33862996	2.08978415
7	0.62998849	2.47138500	-1.46781003
6	-1.68753135	2.77887893	-2.28188777
1	-2.54349518	3.48522496	-2.25207829
1	-1.38295782	2.66693234	-3.33518243
6	-0.52043813	3.36863732	-1.49626935
1	-0.26319048	4.32695103	-1.99037647
1	-0.85876930	3.64749408	-0.47648001
6	1.81107521	3.07437086	-0.94726843
6	2.01327896	3.21859241	0.44869542
6	3.18703198	3.82455254	0.91604733
6	4.17485619	4.30336761	0.04874458
6	3.95564318	4.17005205	-1.32687449
6	2.79821658	3.56851339	-1.83663702
6	-5.00641060	-2.36441422	-1.11901164
1	-5.92045116	-4.25771475	0.55879039
6	-5.27243090	-5.19963455	3.04511905
1	-3.11979985	-3.67141891	3.76326966
6	-1.74893975	-1.60161376	2.71791744
6	0.99025244	2.72116542	1.43899655
1	3.33368611	3.91912913	1.99563766
6	5.44787550	4.91812372	0.57990903
1	4.70615959	4.54811811	-2.02634811
6	2.62128162	3.44752574	-3.33143663
1	-5.59411573	-3.20349264	-1.51342189
1	-4.16768599	-2.16641498	-1.80154908
1	-5.65647459	-1.47484338	-1.13571751
1	-0.80797201	-1.75821483	2.16935587
1	-1.59347522	-1.94015300	3.75022840
1	-1.91580057	-0.51429641	2.73776054
1	-6.01930285	-4.79666615	3.74777293

1	-4.54183912	-5.76659107	3.63862419
1	-5.79446650	-5.90244818	2.38165665
1	1.44844818	2.56471896	2.42453837
1	0.54684818	1.77509284	1.10227740
1	0.17205887	3.44803190	1.57199287
1	1.61166108	3.74219584	-3.64791226
1	2.76268482	2.41051769	-3.67721581
1	3.35386252	4.07265520	-3.85919166
1	6.21546221	4.14844751	0.76001459
1	5.27641010	5.43548393	1.53391111
1	5.87140942	5.64022970	-0.13154162
1	-1.81227946	-0.77294779	0.35567343

Energy = -7584.943911 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 65

Atomic N.	X	Y	Z
8	-0.32107133	-2.55583453	0.38810325
8	0.74227840	-0.49053934	0.95297474
6	0.77262509	0.36466172	2.08427906
1	0.06614610	1.19970810	1.94874847
1	1.78482592	0.78148055	2.23379588
1	0.47101504	-0.18059321	2.99304533
8	0.35657766	-2.41688180	2.52656984
6	0.66495585	-2.28557110	1.18824041
6	2.05647707	-2.69592643	0.70452929
1	2.07616353	-3.80079937	0.71718729
1	2.07047939	-2.41109157	-0.35578781
6	3.29555440	-2.12918687	1.40798759
1	3.18125820	-1.04008460	1.51621568
1	4.15699387	-2.27920318	0.73832870
6	3.62056971	-2.76833606	2.76102304
1	3.81001377	-3.84596372	2.61150265
1	4.55971146	-2.34233689	3.14838624
6	2.51976967	-2.60803914	3.81205559
1	2.36885500	-1.54608011	4.06458712
1	2.83432055	-3.10662603	4.74444389
6	1.17711461	-3.21539211	3.41187644
1	1.31661904	-4.21845150	2.97406578
1	0.53770840	-3.32643723	4.29737139
50	-0.92257780	-0.69542950	-0.64973152
7	-1.64161932	1.97292197	-0.66713554
6	-2.31474185	2.08078599	-1.97555459
1	-2.96229696	2.97766662	-2.01377463
1	-2.93451262	1.19334018	-2.16063643
1	-1.56496310	2.15722394	-2.76996207
7	-2.63600469	-0.49442351	0.61069906
6	-2.63234973	1.98389304	0.42927846
1	-3.30671287	2.86111355	0.34135407
1	-2.07927942	2.06878948	1.37589288
6	-3.46514010	0.70334101	0.47592202
1	-4.14378977	0.79442263	1.34000623
1	-4.13390589	0.65886176	-0.40967911
6	-3.25002050	-1.55943847	1.33371544
6	-3.71040225	-2.72996545	0.68023562
6	-4.31872177	-3.74857068	1.42493188
6	-4.49396610	-3.65708280	2.80888677

6	-4.02658987	-2.50315261	3.44574499
6	-3.41151381	-1.46163905	2.74117279
7	0.84544909	2.36933947	-2.47199440
6	-0.62207425	3.03892612	-0.51629996
1	-0.52091920	3.25763059	0.55754435
1	-0.97282964	3.96729422	-1.00662529
6	0.77581137	2.67430472	-1.02861261
1	1.43300450	3.52871299	-0.82115716
1	1.16259301	1.82581198	-0.43521050
6	2.05008626	2.69622326	-3.15435171
6	2.87209964	1.67411304	-3.68828583
6	4.02587271	2.02228427	-4.39867640
6	4.40576220	3.35573101	-4.59211063
6	3.56720948	4.35037899	-4.07840967
6	2.39250255	4.05100250	-3.37693262
6	-3.55558181	-2.91724586	-0.80929166
1	-4.66942358	-4.64185667	0.90112144
6	-5.18640709	-4.75223398	3.58445144
1	-4.12851906	-2.41323614	4.53094959
6	-2.89825010	-0.26572081	3.50281048
6	2.51101518	0.21842013	-3.50756621
1	4.65093517	1.22322917	-4.80553055
6	5.68110180	3.70645618	-5.32025099
1	3.81727529	5.40056419	-4.25042725
6	1.48314345	5.17216730	-2.93633032
1	-4.25495291	-3.67984128	-1.17783868
1	-2.54032183	-3.26047206	-1.06654954
1	-3.73851967	-1.98427856	-1.36094928
1	-1.95039427	0.08701993	3.07587433
1	-2.74219775	-0.51807600	4.56011772
1	-3.60210776	0.58252394	3.47275662
1	-6.27134037	-4.57044935	3.64908338
1	-4.80651855	-4.81599808	4.61368227
1	-5.04838562	-5.73169327	3.10635805
1	3.30301213	-0.42693573	-3.90776086
1	1.57835948	-0.04979603	-4.03088188
1	2.36575747	-0.04422246	-2.44798374
1	1.62296045	5.44471169	-1.87801385
1	0.42828032	4.88642311	-3.05857658
1	1.67441893	6.07602978	-3.52933455
1	5.90076113	2.98326874	-6.11778641
1	6.54392815	3.70724392	-4.63505745
1	5.62203550	4.70640326	-5.77125406
1	0.62551367	1.38070834	-2.60559464

Energy = -7584.941693 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 66

Atomic N.	X	Y	Z
8	-0.68503976	-3.08457780	-1.19790816
8	0.90510708	-1.33290172	-0.72816271
6	1.38032198	-0.71765321	0.45254236
1	1.05367172	0.33386880	0.48116106
1	2.48488545	-0.72250235	0.48212940
1	0.99540836	-1.22053504	1.35606658
8	0.56096202	-3.50603509	0.60534322
6	0.51174426	-3.17170429	-0.72179848

6	1.60528374	-3.66343141	-1.66823399
1	1.44289327	-4.75114489	-1.78632843
1	1.34775841	-3.21588039	-2.63713837
6	3.07577133	-3.37092280	-1.34718299
1	3.17987442	-2.29953647	-1.12217534
1	3.65661430	-3.54850984	-2.26602983
6	3.67999554	-4.21706581	-0.22378708
1	3.64825463	-5.28152418	-0.51680255
1	4.74539232	-3.96126103	-0.11048666
6	2.97520471	-4.06354046	1.12606478
1	3.05286646	-3.02976537	1.49825346
1	3.48030496	-4.70046759	1.87168992
6	1.50650787	-4.47897530	1.11447656
1	1.37586355	-5.42731810	0.56564033
1	1.15290189	-4.63671780	2.14146137
50	-1.03637743	-0.97067750	-1.86529648
7	-2.17069077	1.74869120	-2.12983608
6	-3.07372546	1.36900353	-3.21975183
1	-3.87726235	2.11878514	-3.37240958
1	-3.54033136	0.39547294	-3.02049136
1	-2.49823689	1.27601695	-4.15074873
7	-2.41719079	-0.58656824	-0.26556769
6	-2.86801410	1.83130467	-0.84355700
1	-3.71019149	2.55883026	-0.87739933
1	-2.15402627	2.18936753	-0.08828648
6	-3.41822529	0.48339635	-0.36917627
1	-3.86023831	0.66580838	0.62538588
1	-4.27589178	0.18926379	-1.01003873
6	-2.73197675	-1.52168536	0.77256757
6	-3.42203712	-2.72787237	0.49656981
6	-3.71346641	-3.61087012	1.54416168
6	-3.34831262	-3.34445834	2.86763096
6	-2.68688273	-2.14095712	3.13044930
6	-2.38596463	-1.22467470	2.11494184
7	0.50197768	2.82328963	-0.95815092
6	-1.46969211	2.98363185	-2.52822304
1	-2.20845771	3.74706721	-2.86255550
1	-0.85016227	2.72564077	-3.40133166
6	-0.58688575	3.66517687	-1.48385823
1	-0.13415132	4.53189516	-1.98383510
1	-1.20824361	4.08623552	-0.67030615
6	1.67108941	3.51384091	-0.51792818
6	1.94988585	3.69391441	0.85683799
6	3.13223314	4.34119940	1.23731136
6	4.04513311	4.83138227	0.29736665
6	3.74883747	4.64621067	-1.05817688
6	2.58898592	3.98905349	-1.48421037
6	-3.85688281	-3.09264255	-0.90188509
1	-4.24478292	-4.53841782	1.31424379
6	-3.69545364	-4.30475664	3.98055816
1	-2.39475155	-1.90361667	4.15724897
6	-1.71000957	0.07492124	2.47314954
6	0.99154955	3.20737624	1.91936612
1	3.33590388	4.47855139	2.30239630
6	5.32460070	5.50677443	0.72980607
1	4.45314693	5.00462770	-1.81336546
6	2.35197902	3.75671983	-2.95558667
1	-4.71402311	-3.77886295	-0.87157130

1	-3.04212260	-3.59618902	-1.44264126
1	-4.14306879	-2.20718813	-1.48571479
1	-1.00777674	0.38006073	1.68760765
1	-1.17117047	-0.01107351	3.42632914
1	-2.44096446	0.89325774	2.58394814
1	-4.71720934	-4.12960100	4.35396051
1	-3.01245952	-4.19213581	4.83368111
1	-3.64986277	-5.34831524	3.63935518
1	1.27301455	3.60785651	2.90140462
1	0.98910117	2.10900855	2.00972366
1	-0.04473974	3.51757431	1.71734035
1	1.64808154	4.48659754	-3.38729930
1	1.92199504	2.75898886	-3.12268806
1	3.29120207	3.84275937	-3.51718187
1	6.16552639	4.79522991	0.74186605
1	5.23423815	5.92378521	1.74191248
1	5.59971857	6.32194424	0.04630048
1	0.14116570	2.22815299	-0.21314660

Energy = -7584.933343 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 67

Atomic N.	X	Y	Z
8	0.66468108	-0.14490952	-0.31226745
8	1.63014495	0.74594498	1.77209973
6	2.45026922	0.20327154	2.78890991
1	1.84049165	-0.13665903	3.64857626
1	3.16992927	0.95749593	3.15402985
1	3.01170444	-0.67889035	2.42938519
8	2.74605823	-0.87032557	0.02244562
6	1.89091063	0.18546462	-0.10221746
6	2.37807894	1.51144588	-0.66303986
1	2.54808259	1.34613955	-1.74424112
1	1.50798678	2.17279124	-0.58693111
6	3.59118390	2.20115280	-0.02795783
1	3.43284392	2.24886346	1.05860960
1	3.59631133	3.24318337	-0.38295913
6	4.94751596	1.56972635	-0.34770703
1	5.12012243	1.60798180	-1.43798304
1	5.74542379	2.17428184	0.11142442
6	5.08319235	0.11785598	0.11635619
1	4.99403667	0.04258359	1.21136236
1	6.08978605	-0.25345325	-0.13957129
6	4.09062147	-0.83951086	-0.53406179
1	4.01535273	-0.64672416	-1.61725652
1	4.42147779	-1.87716353	-0.39961624
50	-0.47105843	-0.04888447	1.65695930
7	-2.78787470	-0.40384695	0.21032229
6	-3.67258573	-0.91002643	1.27409315
1	-4.73177671	-0.91556317	0.95240432
1	-3.58562851	-0.28859934	2.17483568
1	-3.37392831	-1.93233979	1.53868341
7	-1.28139484	1.90090859	1.31806409
6	-3.11170053	1.00188911	-0.11449428
1	-4.19885349	1.10258436	-0.31723610
1	-2.57071900	1.26233482	-1.03389239
6	-2.70183063	1.98715615	0.98192519

1	-2.94614625	2.99706721	0.61479396
1	-3.35036826	1.84319520	1.87204111
6	-0.62867153	3.13500667	1.57830751
6	-0.18874182	3.47096324	2.88459277
6	0.47245589	4.68536282	3.10684395
6	0.71376389	5.60195351	2.07834530
6	0.27206188	5.26519966	0.79465747
6	-0.39151716	4.06142473	0.52598906
7	-0.77471280	-2.13852882	-2.01020145
6	-2.94653487	-1.26447964	-0.99116939
1	-3.93692684	-1.04954493	-1.44427919
1	-2.97717452	-2.31027818	-0.65312129
6	-1.84080625	-1.13310719	-2.06293869
1	-2.32000422	-1.15143573	-3.04991603
1	-1.34308970	-0.15803374	-1.97434831
6	-1.06707382	-3.51758957	-2.05966949
6	-1.76834691	-4.08579874	-3.15414453
6	-2.01908803	-5.46441793	-3.16799903
6	-1.57217801	-6.32136202	-2.15863132
6	-0.82861340	-5.75337601	-1.11716366
6	-0.57242978	-4.38092327	-1.04452133
6	-0.43457654	2.54880381	4.05355501
1	0.80003077	4.92544365	4.12202406
6	1.39641798	6.92134905	2.34953165
1	0.45906618	5.95616436	-0.03233695
6	-0.81002223	3.75760722	-0.89196795
6	-2.17858791	-3.26396132	-4.35182619
1	-2.55847001	-5.88265610	-4.02223253
6	-1.87983358	-7.79924107	-2.18663430
1	-0.43998161	-6.39742756	-0.32377148
6	0.23082687	-3.83285666	0.10863912
1	-0.35373899	3.09637213	5.00226116
1	0.30100927	1.72938251	4.09108162
1	-1.42898238	2.08461785	3.99911427
1	-0.67681414	2.69032669	-1.11897814
1	-0.22276080	4.35080767	-1.60566747
1	-1.87136781	3.99350238	-1.07305384
1	0.66515154	7.70186186	2.61441898
1	1.94514239	7.27731705	1.46652257
1	2.10525513	6.84277678	3.18526268
1	-2.32566309	-3.91447639	-5.22408342
1	-1.40809536	-2.51920223	-4.59955597
1	-3.12290120	-2.71732211	-4.19404793
1	-0.33712682	-3.09017634	0.69388461
1	1.15231395	-3.32587433	-0.21971700
1	0.52297837	-4.64053631	0.79177994
1	-1.03082538	-8.39457130	-1.82177234
1	-2.12179995	-8.13739586	-3.20348239
1	-2.74334526	-8.04164696	-1.54636800
1	-0.09801193	-1.88644528	-1.28910148

Energy = -7584.947785 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 68

Atomic N.	X	Y	Z
8	1.33052480	-2.76258492	1.20839202
8	1.18590271	-0.44957185	0.63789248

6	1.57857049	0.80294704	1.19520259
1	0.69614476	1.30622351	1.62194502
1	2.01291418	1.45365882	0.41675323
1	2.31763148	0.66430575	2.00050855
8	3.08908534	-1.53185129	1.88487065
6	2.25174069	-1.91759205	0.85348082
6	2.83229113	-2.10452724	-0.54337990
1	3.45772099	-3.01486826	-0.50164360
1	1.96877182	-2.36259794	-1.16785145
6	3.61091256	-0.95131248	-1.18768525
1	3.03309894	-0.02141423	-1.07743478
1	3.66035771	-1.15094018	-2.26957417
6	5.03699398	-0.75739020	-0.66496742
1	5.62014294	-1.67264903	-0.86973548
1	5.52670908	0.05203012	-1.22954631
6	5.12020683	-0.45239019	0.83268005
1	4.63329649	0.50744098	1.06735039
1	6.17920971	-0.34164220	1.12117267
6	4.52815866	-1.53952324	1.72717786
1	4.84999275	-2.53926730	1.38860023
1	4.88231230	-1.40819275	2.75827813
50	-0.49583185	-1.61316288	1.68914413
7	-3.25222945	-0.43938652	1.44493484
6	-3.75970626	-0.20403291	2.79647017
1	-4.86989307	-0.20616104	2.83751154
1	-3.39791560	0.75608581	3.18261313
1	-3.38238454	-0.99063838	3.46406651
7	-1.74714184	2.13536882	0.71619582
6	-3.69540095	0.59474277	0.50232822
1	-4.80816507	0.62701249	0.45487154
1	-3.34764481	0.30505231	-0.50043744
6	-3.21253872	2.01640272	0.79123878
1	-3.71590972	2.67972898	0.05921893
1	-3.55025887	2.34529901	1.78261316
6	-1.20755208	3.45023894	0.80543292
6	-1.21036196	4.13627815	2.04265404
6	-0.64934254	5.41747761	2.11371636
6	-0.06204891	6.03960609	1.00715637
6	-0.03399013	5.32878256	-0.19820899
6	-0.59856206	4.05438232	-0.32166940
7	-1.44654000	-2.30523515	-0.08406130
6	-3.64886689	-1.78063655	0.98493552
1	-4.74096966	-1.82722330	0.77775043
1	-3.44855452	-2.47656512	1.81626284
6	-2.89804816	-2.27865815	-0.24912383
1	-3.28738022	-3.29660463	-0.45290101
1	-3.19265103	-1.68218708	-1.13722086
6	-0.78186595	-2.89852238	-1.19955540
6	-0.45743024	-2.12600207	-2.34170079
6	0.16975667	-2.73640847	-3.43662024
6	0.49117452	-4.09795713	-3.44054627
6	0.16597816	-4.84869003	-2.30499339
6	-0.45817474	-4.27770090	-1.18861330
6	-1.74594569	3.48967099	3.29566979
1	-0.65115726	5.93325663	3.07749605
6	0.50865114	7.43385172	1.10569286
1	0.43350998	5.78173351	-1.07624221
6	-0.53704447	3.33520770	-1.64900041

6	-0.74054933	-0.64485425	-2.37678528
1	0.41774535	-2.12568855	-4.30899334
6	1.19533384	-4.73152876	-4.61685705
1	0.40640420	-5.91499090	-2.28371882
6	-0.75233084	-5.13293123	0.01784652
1	-1.29344046	3.94426203	4.18659496
1	-1.52695954	2.41200209	3.29950905
1	-2.83756113	3.60540843	3.39366150
1	0.11303018	2.44573498	-1.60997701
1	-0.13193531	3.99689770	-2.42475176
1	-1.52924919	2.99607277	-1.98517132
1	-0.24789901	8.19238472	0.84861070
1	1.35423815	7.57172060	0.41801402
1	0.85576558	7.65298653	2.12469602
1	-0.29633951	-0.18577801	-3.26977921
1	-0.32126758	-0.16072839	-1.48308516
1	-1.82080150	-0.43112344	-2.39573097
1	-1.75710309	-4.94581079	0.42028067
1	-0.03578309	-4.91328096	0.82366186
1	-0.66734171	-6.19873714	-0.23226240
1	2.28405786	-4.77324581	-4.45300293
1	1.02443731	-4.16233253	-5.54058075
1	0.85382557	-5.76309872	-4.78072834
1	-1.42653048	1.68396378	-0.14101666

Energy = -7584.944057 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 69

Atomic N.	X	Y	Z
8	0.58341181	-0.36318767	-0.29101461
8	1.94711280	0.90626997	1.32077551
6	2.79172230	0.54337603	2.39593267
1	3.66820025	1.21361816	2.44713759
1	3.14678907	-0.49925610	2.29856062
1	2.25183868	0.60663539	3.36074710
8	2.54293656	-1.34920847	0.10628207
6	1.86418545	-0.23320226	-0.28764555
6	2.48442388	0.73827291	-1.27847612
1	2.48200750	0.22393000	-2.25860476
1	1.75189948	1.54924893	-1.35568786
6	3.86657977	1.33495617	-0.98832071
1	3.86158228	1.73921990	0.03369885
1	3.99597335	2.19842386	-1.65882659
6	5.04745531	0.38246086	-1.18532264
1	5.08004665	0.05442902	-2.23950195
1	5.98675156	0.92809355	-1.00378716
6	5.00263500	-0.85791200	-0.29025403
1	5.04556847	-0.57923794	0.77421796
1	5.89280605	-1.47950351	-0.48475701
6	3.79062247	-1.75265527	-0.52540988
1	3.60775971	-1.88577259	-1.60476053
1	3.96180582	-2.74474192	-0.08869843
50	-0.25391734	0.54856735	1.61720324
7	-2.76634383	0.24111108	0.52954876
6	-3.57640481	0.26628506	1.75985229
1	-4.65447378	0.37588525	1.53366363
1	-3.26975822	1.09963739	2.40528822

1	-3.42086935	-0.66687077	2.31608963
7	-0.76621705	2.42489028	0.72788984
6	-2.89151239	1.51821256	-0.20519473
1	-3.96381760	1.76705611	-0.35138148
1	-2.43923903	1.37594926	-1.19564795
6	-2.18410921	2.68637371	0.48463163
1	-2.30309033	3.56572008	-0.16881792
1	-2.72558808	2.94999290	1.41786754
6	0.11115718	3.52421474	0.53183085
6	0.76819837	4.14263487	1.62606454
6	1.64754212	5.20933676	1.39906502
6	1.90258801	5.70533562	0.11696483
6	1.24556971	5.09357214	-0.95622355
6	0.35996822	4.02413130	-0.77644575
7	-1.37581372	-2.44541049	-1.15541375
6	-3.22122359	-0.89232945	-0.31778443
1	-4.21278238	-0.63189369	-0.74364120
1	-3.38045144	-1.75956392	0.33907616
6	-2.25826669	-1.31241870	-1.45137751
1	-2.85798454	-1.53191745	-2.34375548
1	-1.59820068	-0.47510263	-1.71523428
6	-1.89593363	-3.68965030	-0.74167502
6	-1.42707634	-4.28635740	0.45986965
6	-1.91254473	-5.53952980	0.84608358
6	-2.86316633	-6.23804045	0.09260748
6	-3.28563857	-5.65469360	-1.10535121
6	-2.81265783	-4.41248703	-1.54814029
6	0.52705026	3.68486762	3.04365492
1	2.14121151	5.67316341	2.25733542
6	2.82894969	6.87784195	-0.10088397
1	1.43567371	5.45107555	-1.97231603
6	-0.28706455	3.39867783	-1.98820686
6	-0.40657604	-3.58496809	1.32127547
1	-1.53911507	-5.97781610	1.77544534
6	-3.41257858	-7.56511831	0.55789274
1	-3.98826551	-6.19722557	-1.74377120
6	-3.22839594	-3.92475390	-2.91462588
1	0.81769878	4.46715164	3.75778842
1	1.11742842	2.78804159	3.29087019
1	-0.52852142	3.43023300	3.21143460
1	-0.36494067	2.30841875	-1.87146556
1	0.29140845	3.62023878	-2.89507270
1	-1.30865061	3.77646422	-2.15695834
1	2.26820540	7.82418108	-0.16384108
1	3.39333606	6.77448034	-1.03848255
1	3.54865479	6.97823429	0.72276837
1	-0.16958788	-4.18966627	2.20590067
1	-0.76586366	-2.60376835	1.67449820
1	0.53804022	-3.39242315	0.78774315
1	-2.38260317	-3.45500135	-3.43774366
1	-4.04181719	-3.18164635	-2.87556815
1	-3.58954334	-4.76492214	-3.52236104
1	-3.76455140	-8.17113876	-0.28836119
1	-4.26772261	-7.42858458	1.23951793
1	-2.65455723	-8.14567280	1.10206902
1	-0.57935882	-2.12726212	-0.60233253

Energy = -7584.947796 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 70

Atomic N.	X	Y	Z
8	0.56997663	-0.15960088	-0.25039077
8	1.39119959	0.44238785	1.95717287
6	2.04314780	-0.19018327	3.04176188
1	2.82204628	0.46555826	3.47115397
1	2.51118231	-1.14339089	2.73458600
1	1.31650507	-0.43196520	3.84167480
8	2.42541170	-1.27660096	0.33050224
6	1.79319096	-0.07197333	0.13867219
6	2.58786678	1.14008570	-0.32411084
1	2.84715533	0.95560694	-1.38391912
1	1.86063981	1.96047521	-0.32522792
6	3.83320141	1.56615365	0.46208107
1	3.57626343	1.61327374	1.53009284
1	4.07305431	2.59781909	0.16113771
6	5.07307720	0.69536698	0.24550143
1	5.35760593	0.73103189	-0.82123160
1	5.92069483	1.12315428	0.80427176
6	4.88722610	-0.76873839	0.65064877
1	4.68884516	-0.85678732	1.73046505
1	5.82386684	-1.31990457	0.46082908
6	3.78706694	-1.49566770	-0.11804621
1	3.84922028	-1.26506639	-1.19513857
1	3.90299273	-2.58107781	-0.00247126
50	-0.74936831	-0.25715685	1.56155860
7	-3.65776396	-0.36026439	1.06111383
6	-4.27605867	-0.39864504	2.38859963
1	-5.36733818	-0.19960015	2.35121298
1	-3.81247568	0.34787241	3.04533768
1	-4.11340284	-1.38707662	2.83898401
7	-1.48925233	1.71794295	1.20588136
6	-3.76222610	0.97098958	0.44827929
1	-4.82202387	1.31119740	0.42307556
1	-3.40719795	0.89273721	-0.58871287
6	-2.91754103	2.03190255	1.15573502
1	-3.07123470	2.97234964	0.59886777
1	-3.33853984	2.22893906	2.16463876
6	-0.64435315	2.86047792	1.07809842
6	-0.03895033	3.44955969	2.21488118
6	0.80059421	4.56025267	2.05561566
6	1.06218946	5.12092113	0.80139709
6	0.44685391	4.53944254	-0.31315303
6	-0.40079838	3.43002844	-0.19894841
7	-2.07755566	-2.27124882	-0.64888018
6	-4.23100948	-1.41298616	0.20708290
1	-5.25765419	-1.14219832	-0.12266847
1	-4.33290911	-2.31758714	0.82902497
6	-3.40754128	-1.76923823	-1.02964771
1	-3.98143387	-2.52532959	-1.59904277
1	-3.30504966	-0.89534414	-1.68694770
6	-1.34153831	-3.06366539	-1.56732440
6	-0.95358890	-2.55887961	-2.83008909
6	-0.21673322	-3.38085294	-3.69250107
6	0.17990932	-4.67522192	-3.34291983
6	-0.16956897	-5.13606977	-2.06832838

6	-0.92067063	-4.36060333	-1.18000829
6	-0.27658799	2.89961696	3.59943986
1	1.26322293	5.00008821	2.94334650
6	1.96128261	6.32608128	0.65603185
1	0.64123178	4.95203161	-1.30708146
6	-1.01199853	2.82937551	-1.43957567
6	-1.24219131	-1.13512516	-3.23526025
1	0.07963331	-2.97613811	-4.66380501
6	0.94733560	-5.54761791	-4.30709219
1	0.14551324	-6.13430643	-1.75362635
6	-1.26157904	-4.90867138	0.18620189
1	-0.05346354	3.65872407	4.36124039
1	0.37170619	2.03153086	3.79141831
1	-1.31301689	2.56133366	3.72891808
1	-0.89435416	1.73736060	-1.43202174
1	-0.53723687	3.23473525	-2.34290695
1	-2.09073329	3.04216409	-1.51138771
1	1.39136732	7.26726389	0.72486305
1	2.47361231	6.32439899	-0.31641605
1	2.72742653	6.34836245	1.44349575
1	-0.57666254	-0.83110964	-4.05361366
1	-1.07684124	-0.45651507	-2.38662195
1	-2.27623081	-0.99512011	-3.58830714
1	-2.34992194	-4.95243311	0.35786092
1	-0.82567137	-4.30084419	0.99644119
1	-0.87177330	-5.92797852	0.29872426
1	1.64588785	-6.21227217	-3.77994084
1	1.52295411	-4.94349957	-5.02178049
1	0.26926532	-6.18832922	-4.89359856
1	-2.14938211	-2.75570917	0.24482566

Energy = -7584.942614 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 71

Atomic N.	X	Y	Z
8	1.33536923	-2.51068354	1.59877002
8	1.24216342	-0.37099186	0.54889381
6	1.73403609	0.94802284	0.77532786
1	2.11347389	1.38603413	-0.16388743
1	2.54249787	0.94599819	1.52392268
1	0.91783178	1.58337593	1.15481579
8	3.19439435	-1.26826072	1.86239815
6	2.25940847	-1.81843352	1.00330925
6	2.71495771	-2.33582044	-0.35599205
1	3.29909444	-3.25347018	-0.16016988
1	1.79246235	-2.66674209	-0.84742159
6	3.49047089	-1.39838994	-1.28925097
1	2.96774387	-0.43172076	-1.34434879
1	3.44103956	-1.82719302	-2.30239892
6	4.96225548	-1.18777442	-0.92311895
1	5.48301792	-2.16089010	-0.96309853
1	5.44125462	-0.55130869	-1.68419015
6	5.18272114	-0.57419974	0.46169502
1	4.76391983	0.44339597	0.51331264
1	6.26593494	-0.47312808	0.64464831
6	4.61383200	-1.40233254	1.61192787
1	4.85949469	-2.47008801	1.48048866

1	5.05642414	-1.07437027	2.56191492
50	-0.39175743	-1.17046452	1.95519125
7	-3.16350031	-0.01493346	1.78727937
6	-3.54049230	0.45286816	3.12062573
1	-4.64196396	0.47706148	3.26383090
1	-3.14361382	1.45827627	3.30410695
1	-3.10308528	-0.21603090	3.87440395
7	-1.64844179	2.28729677	0.42385650
6	-3.67366171	0.86639309	0.73131800
1	-4.78149414	0.96158707	0.80279082
1	-3.46306348	0.38779435	-0.23673736
6	-3.09342933	2.28097081	0.70790619
1	-3.66345096	2.85032129	-0.05375702
1	-3.27238059	2.78868270	1.66449773
6	-1.04225492	3.56472349	0.24900745
6	-0.82938379	4.40664053	1.36603105
6	-0.20601998	5.64608908	1.17657971
6	0.23608090	6.07730675	-0.07878749
6	0.04975763	5.21429348	-1.16457641
6	-0.58335435	3.97386336	-1.02650142
7	-1.52129972	-2.15862799	0.44649220
6	-3.61560464	-1.40208840	1.59340560
1	-4.72226429	-1.45438111	1.49006736
1	-3.35087252	-1.95586371	2.50920367
6	-2.98121715	-2.11695838	0.40187812
1	-3.40044570	-3.14315653	0.40389478
1	-3.34407353	-1.66768205	-0.54614985
6	-0.97082305	-2.97293591	-0.58954656
6	-0.71537262	-2.43306780	-1.87347031
6	-0.20292602	-3.25935745	-2.88341689
6	0.06902467	-4.61399460	-2.66414976
6	-0.18677562	-5.13350105	-1.38978040
6	-0.69602400	-4.34209442	-0.35214987
6	-1.20390940	3.96792459	2.75978398
1	-0.03985727	6.28339911	2.04902411
6	0.87701398	7.43249846	-0.25768459
1	0.39953998	5.51663065	-2.15494704
6	-0.75344783	3.08276629	-2.23487377
6	-0.95078963	-0.97015971	-2.15580702
1	-0.00798799	-2.82755136	-3.86882234
6	0.64838678	-5.48193884	-3.75593734
1	0.01782166	-6.18924522	-1.19290614
6	-0.91787732	-4.95168257	1.00895274
1	-0.59695888	4.49741745	3.50573921
1	-1.04850566	2.88615060	2.88138008
1	-2.25979161	4.17902613	2.99506569
1	-0.13724349	2.17109919	-2.16804957
1	-0.44930822	3.61146379	-3.14690137
1	-1.79729152	2.75936341	-2.36988831
1	0.11833417	8.20935726	-0.44393113
1	1.56833518	7.44034290	-1.11123753
1	1.43569577	7.73305655	0.63940966
1	-0.60803962	-0.71025383	-3.16606450
1	-0.40381062	-0.35411724	-1.42735004
1	-2.01664424	-0.70279855	-2.08584046
1	-1.88965321	-4.66750908	1.43512380
1	-0.14402273	-4.60627651	1.71074319
1	-0.86682534	-6.04723644	0.95558274

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1  1.74079847 -5.57813931 -3.65039659
1  0.45042214 -5.06011438 -4.75050116
1  0.23109327 -6.49816275 -3.72460532
1 -1.47509122  1.70463014 -0.39595288
Energy = -7584.944060 Hartree
Number of imaginary frequencies = 0.

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Compound TS2b isomer 72

Atomic N.	X	Y	Z
8	1.13398600	-2.87941885	1.07159507
8	1.16451168	-0.54454100	0.58471709
6	1.64108813	0.65889317	1.18281853
1	2.12022471	1.30386555	0.42613122
1	2.36710906	0.44292712	1.98293364
1	0.79485452	1.20718741	1.62688446
8	2.96740174	-1.80311882	1.81233120
6	2.11853456	-2.09160924	0.75820059
6	2.70322680	-2.27104640	-0.63791335
1	3.25738239	-3.22725272	-0.62293416
1	1.83147717	-2.43991852	-1.28107488
6	3.57532477	-1.15782034	-1.23053932
1	3.06778049	-0.19123583	-1.09316444
1	3.62451315	-1.32174027	-2.31843686
6	5.00451231	-1.09141016	-0.68515527
1	5.51940298	-2.04072165	-0.91628718
1	5.56203938	-0.30245802	-1.21473825
6	5.08969021	-0.84607893	0.82322770
1	4.67446661	0.13976304	1.08638239
1	6.14989805	-0.82703936	1.12756193
6	4.40387917	-1.91460073	1.67199457
1	4.65467691	-2.92386532	1.30289936
1	4.75178242	-1.84521568	2.71124983
50	-0.60961336	-1.61512434	1.58169210
7	-3.31498909	-0.31373113	1.40782237
6	-3.82378912	-0.14090142	2.76815557
1	-4.93338013	-0.09635339	2.80163836
1	-3.42457747	0.77647942	3.21640873
1	-3.48748016	-0.98328674	3.38796735
7	-1.63756967	2.18916821	0.79941005
6	-3.69239950	0.80245841	0.53352231
1	-4.80043983	0.91516000	0.50067556
1	-3.37323499	0.55071479	-0.48881057
6	-3.10625386	2.16589093	0.90187681
1	-3.57612014	2.91024852	0.22777463
1	-3.39925575	2.45028162	1.92074704
6	-1.00656652	3.45246363	0.98609316
6	-0.93261445	4.02392387	2.27825952
6	-0.28353098	5.25361681	2.44403887
6	0.31784070	5.93194962	1.37862563
6	0.26756850	5.33154726	0.11545117
6	-0.38554761	4.11313200	-0.10175848
7	-1.58820391	-2.16699100	-0.22543824
6	-3.77326608	-1.60052466	0.85929924
1	-4.86412048	-1.57914805	0.64118427
1	-3.61652017	-2.35753608	1.64535046
6	-3.03483915	-2.05557895	-0.39822149
1	-3.47235799	-3.03726029	-0.67012674

1	-3.28988504	-1.38955200	-1.24865282
6	-0.94722152	-2.73544288	-1.36784291
6	-0.55925584	-1.91957021	-2.45844984
6	0.04164108	-2.50350976	-3.58229899
6	0.27600396	-3.88023162	-3.66416693
6	-0.11106923	-4.67414570	-2.57832646
6	-0.71309751	-4.13099861	-1.43623888
6	-1.48223519	3.30513954	3.48512006
1	-0.22651391	5.68028069	3.44883728
6	0.98454708	7.27118874	1.58169734
1	0.74344677	5.82939863	-0.73325545
6	-0.40577647	3.51244164	-1.48803747
6	-0.74747503	-0.42381895	-2.40775847
1	0.33783999	-1.85982811	-4.41503334
6	0.95222574	-4.48803616	-4.87007236
1	0.06108764	-5.75304747	-2.61814713
6	-1.07734692	-5.03458214	-0.28548571
1	-0.97390234	3.64218521	4.39790392
1	-1.34498489	2.21867156	3.38534951
1	-2.55907440	3.49095321	3.62871003
1	0.18634509	2.58444715	-1.54748714
1	0.02058796	4.21403217	-2.21592355
1	-1.42652905	3.26712298	-1.82025850
1	0.26720172	8.09678650	1.44884431
1	1.79883337	7.42806196	0.86124885
1	1.40018630	7.36203814	2.59465265
1	-0.29442185	0.05409896	-3.28635669
1	-0.27721271	-0.01639096	-1.50105906
1	-1.81175590	-0.14205192	-2.38665819
1	-2.08135962	-4.82041883	0.10546749
1	-0.37031686	-4.89518833	0.54603517
1	-1.03943944	-6.08798122	-0.59309721
1	2.03025126	-4.62988138	-4.69248915
1	0.84696877	-3.84574294	-5.75476456
1	0.53240633	-5.47483015	-5.11036396
1	-1.36720085	1.79425859	-0.10196432

Energy = -7584.944074 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 73

Atomic N.	X	Y	Z
8	1.73827016	-0.14647914	1.55167866
8	1.97504115	1.12897360	-0.51246041
6	2.64551854	1.39632809	-1.73528171
1	1.94776714	1.86435199	-2.44900393
1	3.04169869	0.48027074	-2.21071362
1	3.48199296	2.09255242	-1.55889964
8	3.53154802	1.27465940	1.36154664
6	2.77024984	0.17115347	0.90336061
6	3.56476831	-0.93705803	0.19730189
1	3.55961061	-1.78960645	0.89770144
1	2.96019864	-1.26653564	-0.66139781
6	5.00907135	-0.64587969	-0.23080204
1	5.05829048	0.28237727	-0.81888133
1	5.32491684	-1.45771575	-0.90576011
6	6.00851822	-0.56983280	0.93463719
1	5.87987900	-1.46148193	1.57354057

1	7.03285694	-0.62606686	0.53304636
6	5.89042044	0.69343370	1.79447770
1	6.16378546	1.57819426	1.19639850
1	6.60986328	0.64134663	2.62985229
6	4.50240135	0.93447578	2.37903261
1	4.15195847	0.06557948	2.96303463
1	4.52602434	1.79931736	3.05862522
50	-0.05453534	0.14936680	-0.44514340
7	-0.67102802	1.76672757	1.34364939
6	0.34830180	2.84498000	1.41123044
1	-0.00046053	3.65021348	2.08239841
1	0.53068268	3.25211167	0.41301250
1	1.29023910	2.42523909	1.77916002
7	-1.21699440	1.73310411	-1.40570951
6	-1.95928311	2.30669951	0.83405143
1	-2.30143046	3.13240266	1.48688328
1	-2.70028591	1.49641204	0.87585634
6	-1.82759368	2.78441978	-0.60956460
1	-2.84738755	3.01330757	-0.97396332
1	-1.28256285	3.75025988	-0.62412524
6	-1.34202445	1.82873011	-2.81613898
6	-0.78253764	2.91012597	-3.55102301
6	-0.91224396	2.94828057	-4.94584703
6	-1.57817173	1.94954705	-5.66138601
6	-2.12848020	0.89050537	-4.93098116
6	-2.03405142	0.81493133	-3.53646302
7	-1.12898374	-1.14896345	2.10396957
6	-0.81784731	1.21517003	2.72170854
1	-1.22610128	2.00800180	3.37657881
1	0.19982018	0.98276126	3.06298995
6	-1.68738163	-0.02927303	2.87099099
1	-1.73604238	-0.25207055	3.95546842
1	-2.71972322	0.16307504	2.55039835
6	-1.70277429	-2.44028068	2.27168798
6	-3.01743889	-2.71405220	1.83115661
6	-3.53445697	-4.00624895	1.99445522
6	-2.78788519	-5.04561758	2.55647540
6	-1.47350490	-4.76287079	2.94828200
6	-0.91970700	-3.48539901	2.82217121
6	-0.00922726	4.01110983	-2.86706591
1	-0.46009961	3.78262329	-5.48960924
6	-1.72566092	2.02391124	-7.16232061
1	-2.66672254	0.10015819	-5.46134710
6	-2.70427918	-0.33446270	-2.82250929
6	-3.85212779	-1.67035139	1.13145387
1	-4.54961157	-4.20766735	1.64287591
6	-3.37713265	-6.42311239	2.74164939
1	-0.85776746	-5.56013823	3.37236404
6	0.50402784	-3.23660493	3.26260853
1	0.68771768	4.48798418	-3.56926394
1	0.56426966	3.62119460	-2.01443958
1	-0.67075998	4.80167389	-2.47787905
1	-1.98445404	-1.10421634	-2.50149465
1	-3.43470478	-0.82218117	-3.48193574
1	-3.21828246	0.01145722	-1.91497564
1	-2.70734763	2.43507624	-7.44730711
1	-1.64523911	1.02991068	-7.62434864
1	-0.95791018	2.67132282	-7.60745192

1	-4.61427212	-2.14797282	0.50230050
1	-3.22542048	-1.03379107	0.49022043
1	-4.38307858	-1.01204073	1.83819914
1	0.56674105	-2.44978118	4.03084183
1	1.14793956	-2.91661048	2.42800689
1	0.93821621	-4.15070868	3.68640232
1	-2.63338256	-7.20818186	2.54604840
1	-4.23114491	-6.58566475	2.07050085
1	-3.73722124	-6.56747007	3.77278495
1	-0.11584151	-1.17941988	2.24242830

Energy = -7584.942216 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 74

Atomic N.	X	Y	Z
8	2.31210876	0.19172093	2.17581248
8	3.02448034	0.90198487	-0.02460620
6	3.31284475	1.70978189	-1.13078272
1	2.72197080	1.38806415	-2.01372933
1	4.37824583	1.66100454	-1.43653512
1	3.06992817	2.77973771	-0.95343751
8	3.07249832	2.26367617	2.31247544
6	3.30654502	0.96070147	1.99254990
6	4.71344280	0.38419199	2.07994080
1	4.98260641	0.41224349	3.15421247
1	4.59222460	-0.67608929	1.82576489
6	5.84550619	0.97731024	1.23497844
1	5.51949263	0.98918474	0.18681271
1	6.69504499	0.27843609	1.28878713
6	6.33148623	2.36421537	1.66016924
1	6.78568697	2.29962516	2.66489077
1	7.13577986	2.68721390	0.98071682
6	5.23460245	3.43174744	1.69423008
1	4.77468586	3.56513739	0.70261776
1	5.68546629	4.40178156	1.96209240
6	4.13977814	3.15936399	2.72136998
1	4.57561970	2.78285360	3.66256309
1	3.59555149	4.08412027	2.95091915
50	1.54209483	-0.90391654	0.28426722
7	-0.27473792	0.84443069	0.27681273
6	0.18761192	2.24120975	0.12731721
1	-0.65649533	2.94034743	0.26897863
1	0.61949092	2.39978647	-0.86513942
1	0.96559107	2.44161439	0.87162769
7	-1.86536574	0.10291289	-3.13970542
6	-1.32193494	0.51535118	-0.72538239
1	-2.16085410	1.23023593	-0.62481499
1	-1.69870329	-0.48570567	-0.47772625
6	-0.82698107	0.50319034	-2.18120003
1	-0.44270787	1.48670304	-2.47118115
1	0.01154347	-0.20690435	-2.27630782
6	-2.97917199	0.95571709	-3.36473322
6	-2.80294299	2.22876310	-3.95847917
6	-3.92685294	3.03041983	-4.19679642
6	-5.22701788	2.60855150	-3.90291929
6	-5.38458681	1.32314861	-3.37124658
6	-4.29262733	0.49479154	-3.09405851

7	-0.10250894	-1.64653909	1.49109983
6	-0.81409138	0.67611122	1.65906549
1	-1.70462894	1.31930315	1.78923738
1	-0.02231808	1.02336121	2.33583212
6	-1.15393591	-0.77734232	1.98479354
1	-1.27514243	-0.83599794	3.08639765
1	-2.15076184	-1.04174161	1.56863606
6	-0.21254624	-3.02025604	1.84537792
6	-1.04097688	-3.90324640	1.10331511
6	-1.12342560	-5.25333261	1.46469986
6	-0.40548083	-5.77639437	2.54585338
6	0.40979436	-4.90079451	3.26958013
6	0.52097911	-3.54289627	2.94120908
6	-1.44698095	2.71300745	-4.41206217
1	-3.77587318	4.00929642	-4.65953255
6	-6.41681767	3.50538969	-4.14597797
1	-6.38992357	0.95203710	-3.15629816
6	-4.52849388	-0.88364530	-2.52251196
6	-1.81653869	-3.41418815	-0.09475907
1	-1.76316810	-5.91741943	0.87683469
6	-0.48228166	-7.24316835	2.89633226
1	0.97630036	-5.28260374	4.12351608
6	1.42479086	-2.65555930	3.76249075
1	-1.55721343	3.43832445	-5.22893429
1	-0.82976532	1.87582421	-4.76760244
1	-0.88553417	3.21833801	-3.60929179
1	-4.16980457	-1.68269694	-3.19276953
1	-5.60055780	-1.05454040	-2.36484694
1	-4.02474308	-1.02370191	-1.55289435
1	-6.69301128	4.05790424	-3.23361492
1	-7.29932451	2.92811060	-4.45473719
1	-6.20407867	4.24902773	-4.92597389
1	-2.22645020	-4.25828838	-0.66467375
1	-1.16983533	-2.82228994	-0.75887603
1	-2.66167927	-2.76973557	0.19601895
1	0.99016958	-1.66099131	3.91980815
1	2.38870907	-2.48611975	3.25830770
1	1.63572454	-3.11704159	4.73673677
1	0.25845695	-7.82705975	2.32669210
1	-1.47211766	-7.66048384	2.66513968
1	-0.27905002	-7.41109514	3.96285987
1	-2.17681336	-0.84551930	-2.93560243

Energy = -7584.931826 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 75

Atomic N.	X	Y	Z
8	1.93761289	-0.66619736	2.12306380
8	2.32726312	0.27920216	-0.05482220
6	2.67415881	1.14089203	-1.10756373
1	1.79761732	1.31435275	-1.76155806
1	3.47796035	0.73015589	-1.75117612
1	3.01413035	2.13406014	-0.74418122
8	3.54730749	0.84432781	2.27786446
6	3.09120893	-0.31446457	1.72312760
6	4.07024765	-1.38717890	1.26321495
1	4.57166433	-1.74899566	2.18239236

1	3.43245101	-2.21179438	0.92170429
6	5.10997629	-1.07497787	0.18203424
1	4.58616400	-0.66453999	-0.69093621
1	5.54550314	-2.03404355	-0.13988964
6	6.24784279	-0.14481103	0.60693526
1	6.85170698	-0.64016050	1.38793862
1	6.92286921	0.01166470	-0.24907599
6	5.78357315	1.21160138	1.14403832
1	5.20724773	1.76610291	0.38706386
1	6.66806364	1.82791305	1.37619126
6	4.96457005	1.11895072	2.42818046
1	5.39957809	0.37000230	3.11202741
1	4.96328068	2.08539462	2.94792819
50	0.32101798	-0.78927827	0.45875099
7	-0.46132743	1.47333848	1.29988086
6	0.51861012	2.56606507	1.15066564
1	0.15631716	3.48796010	1.64247680
1	0.69735962	2.76522541	0.08969267
1	1.46588814	2.25556707	1.60472012
7	-1.22476768	1.54689062	-1.66675842
6	-1.79223454	1.84379208	0.74517703
1	-2.26406217	2.58691144	1.41723180
1	-2.41178036	0.93613702	0.77450126
6	-1.81410301	2.44195533	-0.66112214
1	-2.87597585	2.66773653	-0.88339770
1	-1.28692269	3.40481329	-0.66863465
6	-1.45771194	1.82288957	-3.04226708
6	-0.96790761	3.00316501	-3.64791751
6	-1.20113826	3.21483469	-5.01372433
6	-1.87859285	2.28956151	-5.81247568
6	-2.31779003	1.10811341	-5.20270967
6	-2.12681770	0.86042237	-3.84047031
7	-1.12937152	-1.12038779	2.05167031
6	-0.60528386	1.15131593	2.75043249
1	-1.01640570	2.02957916	3.28405952
1	0.40811977	0.95083761	3.12152672
6	-1.48335862	-0.07540494	2.99337745
1	-1.32249296	-0.37755054	4.04914522
1	-2.55778265	0.20495448	2.92982030
6	-1.75956583	-2.38011861	2.25276518
6	-3.07154155	-2.62892580	1.76663625
6	-3.66610026	-3.88014960	1.96599495
6	-3.00566578	-4.91720676	2.63471437
6	-1.71541190	-4.66528034	3.10906720
6	-1.08358395	-3.42635417	2.93163252
6	-0.14505775	4.01076412	-2.88287044
1	-0.81202132	4.12896824	-5.46961117
6	-2.13527966	2.55493593	-7.27625370
1	-2.83339310	0.35451648	-5.80331039
6	-2.62593651	-0.43207914	-3.23772264
6	-3.82885933	-1.57096219	1.00349617
1	-4.67463636	-4.05114079	1.57906008
6	-3.65469837	-6.26942301	2.80913019
1	-1.18005121	-5.45540857	3.64293885
6	0.31190977	-3.22899055	3.47234631
1	0.45472205	4.61622524	-3.57477140
1	0.53900814	3.50981522	-2.18260694
1	-0.76590180	4.70737553	-2.29719400

1	-1.80833900	-1.04471946	-2.82282877
1	-3.13245583	-1.03924310	-3.99810743
1	-3.34676933	-0.25669959	-2.42275691
1	-3.15146756	2.94825649	-7.43868685
1	-2.04493499	1.63669360	-7.87323475
1	-1.42969596	3.29473543	-7.67780113
1	-4.74387407	-1.98795521	0.56289929
1	-3.20842505	-1.15951264	0.19395763
1	-4.12469101	-0.72586942	1.64489841
1	0.45901224	-2.21679211	3.86716819
1	1.07069921	-3.35799599	2.68503237
1	0.52555442	-3.96237659	4.26187134
1	-3.52240157	-6.89312077	1.91051102
1	-4.73602629	-6.17739391	2.98282337
1	-3.21650672	-6.81683826	3.65461898
1	-1.50109696	0.58536977	-1.46196043

Energy = -7584.931404 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 76

Atomic N.	X	Y	Z
8	1.46322334	1.00154757	0.74709302
8	1.65692365	0.76716506	-1.73742473
6	1.69369411	1.66803110	-2.82723260
1	0.80603695	1.55260324	-3.47094154
1	2.58664775	1.47840071	-3.45330977
1	1.72016501	2.72119761	-2.49194264
8	2.82108545	2.55125237	-0.05405304
6	2.52388000	1.23672056	0.07364675
6	3.61990356	0.18206751	0.02716116
1	4.20557547	0.31437248	0.95803612
1	3.09066367	-0.77291584	0.13794883
6	4.55548191	0.10474257	-1.18523753
1	3.93387699	0.06523925	-2.09036922
1	5.08669806	-0.85818821	-1.12687254
6	5.59245062	1.22478127	-1.28810155
1	6.26608372	1.18099332	-0.41377923
1	6.22519445	1.04872489	-2.17200947
6	4.99049377	2.62948346	-1.36900830
1	4.35699654	2.74149942	-2.26227832
1	5.80467558	3.36649942	-1.47018158
6	4.19172335	3.03526068	-0.13617747
1	4.71986961	2.74082613	0.78635252
1	4.05428457	4.12342024	-0.11395251
50	-0.08784373	0.00287685	-0.57182288
7	-1.44259536	0.20072415	1.86540580
6	-0.59584743	0.77548397	2.92687798
1	-1.19256341	1.00291634	3.83211422
1	-0.11080329	1.69034898	2.57317924
1	0.19343773	0.06103240	3.19032741
7	-1.36318159	1.73112953	-0.69945478
6	-2.46298122	1.18589151	1.43197966
1	-2.95209694	1.63120532	2.32422996
1	-3.23093605	0.64985466	0.85691273
6	-1.88744450	2.28789806	0.54596227
1	-2.71189141	2.98616385	0.31988993
1	-1.14389598	2.86889076	1.12525249

6	-1.50353265	2.50543380	-1.87379074
6	-1.08251476	3.86315179	-1.94805431
6	-1.27107430	4.58506203	-3.13333201
6	-1.84472227	4.01768112	-4.27544165
6	-2.22846746	2.67431879	-4.20233393
6	-2.07699466	1.91614521	-3.03561997
7	-1.67980087	-3.04428864	0.90343720
6	-2.11185050	-1.01772320	2.39152241
1	-2.95038843	-0.70408380	3.04695868
1	-1.39642060	-1.55214691	3.03302026
6	-2.62517524	-1.99932361	1.31864715
1	-3.53848696	-2.47558713	1.69511235
1	-2.91673517	-1.44706905	0.41234475
6	-1.25780070	-4.01425838	1.84538758
6	-2.18746233	-4.92646980	2.40718007
6	-1.73666239	-5.89123011	3.31634903
6	-0.39029729	-6.01751757	3.67307281
6	0.52126133	-5.14840841	3.06393671
6	0.11721424	-4.15441227	2.16591167
6	-0.34728053	4.52323198	-0.80628884
1	-0.92863941	5.62326193	-3.16979146
6	-2.06234646	4.82914639	-5.52991915
1	-2.67873883	2.19989419	-5.07851934
6	-2.54694295	0.48174006	-3.03351521
6	-3.63755465	-4.94022369	1.98857975
1	-2.46684289	-6.58936548	3.73449850
6	0.06080085	-7.04901123	4.67889833
1	1.58519077	-5.23858976	3.29816890
6	1.15409648	-3.25543237	1.53782964
1	0.19574174	5.40721941	-1.16690588
1	0.37608007	3.83102822	-0.35188085
1	-1.02208650	4.85968828	-0.00379540
1	-1.71373367	-0.23630066	-3.12413788
1	-3.22057962	0.29395339	-3.88032174
1	-3.06964040	0.23697960	-2.09806609
1	-3.04659462	5.32476377	-5.52050972
1	-2.02493048	4.19805670	-6.42859173
1	-1.30374491	5.61761093	-5.63331366
1	-4.06614637	-5.93979502	2.13959789
1	-3.74156427	-4.67037487	0.92794073
1	-4.25492239	-4.23545456	2.56938004
1	0.94635952	-2.18874431	1.72030115
1	1.20493257	-3.37785721	0.44335487
1	2.15054703	-3.47790337	1.94072092
1	1.09111702	-7.37660313	4.48348618
1	-0.58884555	-7.93508816	4.66271114
1	0.03545876	-6.64580965	5.70410490
1	-0.89626354	-2.61743641	0.40345517

Energy = -7584.943910 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 77

Atomic N.	X	Y	Z
8	0.95997840	0.42437923	0.89262664
8	1.09545112	0.61454672	-1.56019700
6	1.44725406	1.61787307	-2.49407029
1	0.58247191	1.89020753	-3.11989617

1	2.24922633	1.25763333	-3.16600442
1	1.79547095	2.53847337	-1.99274302
8	2.72323895	1.62240410	0.27079207
6	2.02508974	0.45391393	0.18158039
6	2.75356722	-0.85856849	-0.08871268
1	3.32959199	-1.08191252	0.83044922
1	1.95556462	-1.61145902	-0.13465981
6	3.65026999	-0.99701697	-1.32435906
1	3.07501245	-0.67543685	-2.20369411
1	3.85436058	-2.07030439	-1.46282411
6	4.98679304	-0.25536951	-1.25196087
1	5.58690453	-0.66809618	-0.42145014
1	5.55949211	-0.45326811	-2.17173076
6	4.85644865	1.25652838	-1.05248034
1	4.32376099	1.72502160	-1.89441109
1	5.86355448	1.70598555	-1.03231382
6	4.17496014	1.65600538	0.25226605
1	4.55328035	1.04547215	1.09011006
1	4.38766956	2.70800543	0.48126489
50	-0.83059686	0.11427540	-0.51628065
7	-1.99695528	0.56486088	1.92649782
6	-1.24962437	1.52616978	2.75374389
1	-1.87991321	1.94655979	3.56263995
1	-0.87388486	2.33778667	2.12362528
1	-0.38075057	1.02404857	3.19365191
7	-1.67321241	2.09917426	-0.49163982
6	-3.16414547	1.20665705	1.28561985
1	-3.88787770	1.54943061	2.05421042
1	-3.66600156	0.43916476	0.67412519
6	-2.78410029	2.39741182	0.40270746
1	-3.70075655	2.67596459	-0.15769902
1	-2.56725502	3.27240849	1.05201209
6	-1.42288351	3.12501454	-1.44678378
6	-0.61331850	4.24274921	-1.11855721
6	-0.38146481	5.23655415	-2.07716298
6	-0.92901492	5.17081642	-3.36379504
6	-1.72357571	4.06352139	-3.67797565
6	-1.98038745	3.04683280	-2.74788618
7	-1.07193422	-2.39993143	1.72419119
6	-2.42432261	-0.59916228	2.74233007
1	-3.42973208	-0.41177952	3.16619134
1	-1.73590159	-0.68248028	3.59728289
6	-2.43774414	-1.93677175	2.00390434
1	-2.97461629	-2.66573501	2.63648558
1	-3.01383567	-1.83472180	1.06874979
6	-0.75571340	-3.77342176	1.74273384
6	-1.44230092	-4.69252586	0.91286677
6	-1.08480668	-6.04568005	0.95662522
6	-0.04740012	-6.52467299	1.76393747
6	0.65364796	-5.59112024	2.53611612
6	0.31824657	-4.23355246	2.54667330
6	0.03408733	4.35134077	0.23923361
1	0.25594211	6.08451557	-1.81128931
6	-0.68996751	6.27224970	-4.36892223
1	-2.15893030	3.98554349	-4.67794228
6	-2.83103490	1.86807871	-3.15885234
6	-2.48422170	-4.22952604	-0.07681270
1	-1.62028635	-6.74331331	0.30716059

6	0.29497790	-7.99448586	1.80849683
1	1.48326552	-5.92916918	3.16255713
6	1.09775686	-3.27311373	3.41353583
1	0.78137296	5.15593815	0.24908444
1	0.52581495	3.40889263	0.51711118
1	-0.70327610	4.57820988	1.02584088
1	-2.21770906	0.97563666	-3.36433601
1	-3.39236546	2.09644437	-4.07478094
1	-3.54076624	1.58184028	-2.37134051
1	-1.39454722	7.10610342	-4.22036219
1	-0.82203847	5.91134930	-5.39788389
1	0.32420331	6.68582153	-4.27736807
1	-2.64859271	-4.99816513	-0.84306341
1	-2.16052890	-3.30425620	-0.57698727
1	-3.45848560	-4.02330542	0.39333051
1	0.45263690	-2.76537991	4.14937353
1	1.59612978	-2.48436999	2.82543373
1	1.87860775	-3.80566835	3.97064734
1	1.35778189	-8.15343094	2.03727484
1	0.07444518	-8.48620796	0.85086846
1	-0.28728905	-8.51771736	2.58408308
1	-0.38426295	-1.84671736	2.22918558

Energy = -7584.939381 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 78

Atomic N.	X	Y	Z
8	2.27561212	-0.93095505	1.63033140
8	2.20481133	0.79355091	-0.04651711
6	2.24345279	2.02987170	-0.71061981
1	1.27772152	2.21944785	-1.21814442
1	3.02959371	2.07305360	-1.49112904
1	2.41977954	2.87698579	-0.01395222
8	3.55425262	0.75319928	2.28296900
6	3.27865171	-0.20293282	1.35086453
6	4.39199257	-0.78241944	0.48759484
1	5.06137562	-1.32321846	1.18523419
1	3.89717102	-1.55322826	-0.11604655
6	5.21187878	0.12756908	-0.43282288
1	4.51644707	0.69081491	-1.06849432
1	5.79007339	-0.52404076	-1.10677171
6	6.18159676	1.07943356	0.27007520
1	6.96072912	0.49089450	0.78635806
1	6.70533562	1.68308580	-0.48768964
6	5.52100086	2.00749493	1.29288292
1	4.75992537	2.64761662	0.81994772
1	6.28480434	2.68574119	1.70840359
6	4.89467096	1.27534544	2.47607780
1	5.54928541	0.45358929	2.81372929
1	4.75987434	1.96372414	3.31999397
50	0.52320611	-0.81205213	0.10850843
7	-0.57949150	0.75963265	1.76714516
6	0.13994271	2.02651167	1.99902487
1	-0.33457756	2.60396862	2.81415033
1	0.14568222	2.62575150	1.08352697
1	1.17780662	1.79953969	2.26594162
7	-1.69817054	1.71692967	-0.92152476

6	-2.01482749	0.98834848	1.44485271
1	-2.53973722	1.31114960	2.36505413
1	-2.43342638	0.01435443	1.15381956
6	-2.32579732	2.02952576	0.37010550
1	-3.43035889	2.07059479	0.29127899
1	-2.00416875	3.02386022	0.70602119
6	-2.14591455	2.41149545	-2.07895255
6	-1.97456670	3.80930066	-2.20848370
6	-2.41084218	4.44311523	-3.37996697
6	-2.98707461	3.74266171	-4.44311714
6	-3.10716534	2.35378742	-4.31296253
6	-2.70521235	1.67889941	-3.15677643
7	-0.62882465	-2.00998569	1.51821291
6	-0.47912413	-0.08202726	2.99600005
1	-0.98657596	0.42992616	3.83594942
1	0.59151518	-0.16516225	3.22342539
6	-1.06254113	-1.48007739	2.79694176
1	-0.71767277	-2.09373522	3.65507722
1	-2.17076063	-1.44850135	2.88686395
6	-0.96947294	-3.36732769	1.26023746
6	-2.25129986	-3.71747804	0.75761485
6	-2.56027842	-5.05860376	0.50186312
6	-1.63762057	-6.08727455	0.72304082
6	-0.37834886	-5.73473740	1.21679533
6	-0.02830345	-4.40439749	1.48655188
6	-1.27686954	4.62979364	-1.15124941
1	-2.26730490	5.52314711	-3.46830440
6	-3.47024369	4.45552444	-5.68303347
1	-3.53436708	1.77338660	-5.13461113
6	-2.86129260	0.17833205	-3.07395315
6	-3.28381395	-2.65795898	0.46303865
1	-3.55159664	-5.30482769	0.11117042
6	-1.98173094	-7.52375698	0.40944290
1	0.35868096	-6.51999807	1.40681791
6	1.35128450	-4.09948540	2.01781940
1	-0.89507014	5.56327486	-1.58472669
1	-0.42839414	4.07805347	-0.72128445
1	-1.94552529	4.90773344	-0.32095793
1	-1.89381588	-0.33778346	-2.95760274
1	-3.32808352	-0.20946880	-3.98778915
1	-3.49577141	-0.12564567	-2.22568345
1	-4.55442858	4.64589834	-5.63686037
1	-3.28464675	3.85975194	-6.58762932
1	-2.97228551	5.42691088	-5.80491734
1	-4.14468145	-3.08867121	-0.06486059
1	-2.85428572	-1.86183333	-0.16243891
1	-3.66219378	-2.17938185	1.38002872
1	1.33370697	-3.30341911	2.77175426
1	2.02027988	-3.74210358	1.22004187
1	1.80376780	-5.00107288	2.45272326
1	-1.79798841	-7.75426435	-0.65227908
1	-3.04145670	-7.73598671	0.60857403
1	-1.37444854	-8.21939468	1.00449836
1	-1.75345981	0.71062946	-1.08622253

Energy = -7584.931393 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 79

Atomic N.	X	Y	Z
8	1.88031101	-1.44473362	0.86214358
8	2.72296309	-0.10939191	-0.95789534
6	3.00037718	-1.15627408	-1.88000882
1	2.32508993	-1.07118285	-2.74529862
1	2.84889507	-2.15053844	-1.41975689
1	4.03913069	-1.09779096	-2.24826169
8	2.62195063	0.58610648	1.37895846
6	2.88105321	-0.64286190	0.76870114
6	4.28844070	-1.23277450	0.91717541
1	4.45817757	-1.32907605	2.00452018
1	4.20963430	-2.26063371	0.53822017
6	5.48773098	-0.53960925	0.25305113
1	5.27812433	-0.40574762	-0.81682223
1	6.34529448	-1.22869849	0.31802195
6	5.89640999	0.81081349	0.84355611
1	6.25290060	0.67147470	1.87965631
1	6.75372410	1.20120692	0.27229720
6	4.76709890	1.84355175	0.84953338
1	4.34516335	1.97472286	-0.15896551
1	5.17226839	2.82073188	1.16055810
6	3.64453292	1.50052714	1.82471585
1	4.07278395	1.11332870	2.76778388
1	3.06896162	2.40347004	2.06959605
50	0.34897754	0.02004716	-0.41316050
7	-0.60545397	-2.38140869	-0.84080386
6	0.10125401	-3.49932718	-0.18065330
1	-0.36459506	-4.46526480	-0.45404154
1	0.08773062	-3.37479568	0.90502763
1	1.15074527	-3.49561048	-0.48773485
7	-2.12311864	-0.92691231	1.46031880
6	-2.05429125	-2.43488908	-0.51225883
1	-2.46044278	-3.40564990	-0.86059922
1	-2.55865574	-1.65257537	-1.09751904
6	-2.42610502	-2.27591896	0.96166182
1	-3.50523472	-2.51636124	1.04565561
1	-1.89952695	-3.01233697	1.58006895
6	-2.43253899	-0.64657408	2.82556224
6	-1.66060209	-1.20787537	3.86775756
6	-1.98271024	-0.88749051	5.19324970
6	-3.02140212	-0.01156848	5.52390528
6	-3.74388337	0.56635553	4.47350836
6	-3.47323871	0.26210117	3.13560104
7	-0.23527747	-0.08553157	-2.54582691
6	-0.43132436	-2.50772977	-2.31617785
1	-0.97442049	-3.40059090	-2.68352365
1	0.64071631	-2.66880703	-2.49141407
6	-0.87965536	-1.26969385	-3.08582997
1	-0.59865385	-1.44168985	-4.14560652
1	-1.98886240	-1.21351099	-3.08955073
6	-0.57954001	1.15454721	-3.15786266
6	-1.88879716	1.70927155	-3.08147097
6	-2.16943049	2.93891764	-3.69342613
6	-1.19625938	3.67071581	-4.37688112
6	0.09377595	3.13166690	-4.43179464
6	0.41742584	1.90397143	-3.84346986
6	-0.46798867	-2.08688307	3.58595872

1	-1.37631953	-1.32091486	5.99266052
6	-3.35851622	0.29508388	6.96315765
1	-4.54684591	1.27259386	4.69917250
6	-4.27848721	0.92326927	2.04005837
6	-2.99591541	1.03375459	-2.31180167
1	-3.18249154	3.34329581	-3.61358047
6	-1.51021361	5.01017332	-4.99857473
1	0.87843835	3.67975187	-4.96062613
6	1.82685637	1.38487995	-3.97029138
1	0.20857216	-2.09605217	4.45036316
1	0.09686204	-1.73207009	2.71170592
1	-0.75712574	-3.13454151	3.39879894
1	-3.66015625	1.58953369	1.41552341
1	-5.07864666	1.53804338	2.47051001
1	-4.75160933	0.18934989	1.36842608
1	-4.17808008	-0.34588757	7.32546902
1	-3.68344998	1.33747554	7.08678150
1	-2.49525023	0.12479620	7.62049437
1	-3.74089146	1.76889932	-1.97962868
1	-2.58843541	0.52613026	-1.42477059
1	-3.52663374	0.27571061	-2.91031790
1	1.83832955	0.36833763	-4.38845539
1	2.33310843	1.33124518	-2.99526024
1	2.41693377	2.03659940	-4.62849045
1	-1.17321312	5.83744383	-4.35369873
1	-2.58977652	5.13495207	-5.15735006
1	-1.00516677	5.13084793	-5.96758604
1	-2.60150838	-0.24792023	0.86716276

Energy = -7584.928445 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 80

Atomic N.	X	Y	Z
8	0.88714361	1.30079007	1.62632847
8	2.16838598	-0.60650516	0.96312833
6	3.25223875	-0.91571045	0.09737867
1	2.87258267	-1.43886435	-0.79808408
1	3.97917366	-1.57506371	0.60177267
1	3.76900673	-0.00248007	-0.24219620
8	3.04362679	1.75331128	1.17150009
6	2.12675500	0.99512941	1.87097573
6	2.44194555	0.56248361	3.29642749
1	2.37824035	1.47390950	3.91871119
1	1.58907676	-0.06138256	3.58866835
6	3.74987197	-0.18615267	3.57775211
1	3.86055946	-1.00329721	2.84941506
1	3.64535046	-0.67100763	4.56077194
6	5.00848198	0.68546891	3.59808612
1	4.90856695	1.43922222	4.39897060
1	5.87821960	0.06508858	3.86688590
6	5.29199409	1.41062140	2.28025937
1	5.49538755	0.69223940	1.47023690
1	6.20536900	2.01915789	2.39100671
6	4.18103933	2.35849881	1.83509171
1	3.82206845	2.96336126	2.68506551
1	4.56181383	3.04992342	1.07201612
50	0.16975704	-0.00770508	0.00454704

7	-1.53419745	-2.10030675	-1.55914986
6	-0.87348408	-3.38956475	-1.34934127
1	-1.58099651	-4.24455261	-1.40336871
1	-0.37454960	-3.40618038	-0.37294188
1	-0.10897518	-3.53088713	-2.12567639
7	-1.01743913	-1.17844987	1.30851269
6	-2.58760142	-1.83813453	-0.56793129
1	-3.45646167	-2.51732850	-0.72391766
1	-2.94167542	-0.80713731	-0.72484249
6	-2.16132689	-1.99266636	0.89151973
1	-3.05339718	-1.72642136	1.49175382
1	-1.98137319	-3.06491446	1.10689318
6	-0.81413966	-1.23081851	2.72453737
6	-0.05870080	-2.27484655	3.31240153
6	0.10758080	-2.30586028	4.70434856
6	-0.45659751	-1.33752835	5.54131413
6	-1.19718182	-0.31065962	4.94477797
6	-1.38610053	-0.23851763	3.55881548
7	-1.86249650	0.42473549	-3.18229127
6	-2.05738831	-2.05021596	-2.93495464
1	-2.79484367	-2.86950231	-3.09716535
1	-1.20880580	-2.24069452	-3.61141992
6	-2.73618412	-0.74337995	-3.34543014
1	-3.02185369	-0.85996193	-4.40419531
1	-3.67727017	-0.61884332	-2.78390217
6	-1.77109873	1.38668585	-4.20940161
6	-2.92904758	2.06082749	-4.66803741
6	-2.80665398	3.01322246	-5.68759775
6	-1.57327521	3.35117269	-6.25344706
6	-0.43436429	2.71077013	-5.75031805
6	-0.50732237	1.73791027	-4.74854422
6	0.59536541	-3.33931494	2.46710086
1	0.70134836	-3.11180162	5.14383554
6	-0.29340756	-1.40961850	7.04094505
1	-1.64169359	0.46346015	5.57576084
6	-2.16987920	0.91061234	2.97619963
6	-4.27206421	1.84082913	-4.01407576
1	-3.70882583	3.52970004	-6.02612543
6	-1.47356498	4.36194086	-7.37070990
1	0.54732633	2.96769905	-6.15686083
6	0.75477666	1.07589984	-4.25129604
1	1.26668358	-3.95780754	3.07719707
1	1.17828465	-2.88486505	1.65429032
1	-0.14644292	-4.01212358	2.00912690
1	-1.49091887	1.63944638	2.50863743
1	-2.73644257	1.42897534	3.76094222
1	-2.87122369	0.57907468	2.19880962
1	-1.17239869	-1.87518501	7.51425409
1	-0.18161947	-0.40903184	7.48160362
1	0.58422762	-2.00835133	7.31976509
1	-4.95436382	2.66543722	-4.25797367
1	-4.16449165	1.79026413	-2.92005777
1	-4.75953770	0.90660059	-4.33299208
1	0.70975548	-0.02124979	-4.34843063
1	0.94687700	1.29240263	-3.18752432
1	1.62396598	1.42692184	-4.82171440
1	-0.53231126	4.92670250	-7.31925774
1	-2.30475831	5.07966375	-7.33578968

1 -1.50600290 3.87301493 -8.35784245
 1 -0.95809847 0.16171534 -2.79353309
 Energy = -7584.941423 Hartree
 Number of imaginary frequencies = 0.

Compound TS2b isomer 81

Atomic N.	X	Y	Z
8	1.85465217	-1.09711289	-1.14815855
8	2.15665531	1.31047153	-0.81738621
6	2.62647510	2.23135257	0.14845626
1	3.16846299	1.72706997	0.97104639
1	1.77931607	2.77650404	0.60478544
1	3.29758644	2.97818780	-0.31244156
8	3.60376906	-0.63488615	0.16762838
6	2.97673130	-0.48634294	-1.03742123
6	3.79062176	-0.28426215	-2.30636835
1	4.29760742	-1.24806535	-2.50418258
1	3.03797770	-0.16931747	-3.09523058
6	4.79941368	0.86814088	-2.37940311
1	4.30083895	1.79229665	-2.05381584
1	5.05627823	1.01356399	-3.44019437
6	6.09337711	0.65129709	-1.59169185
1	6.61939478	-0.23160043	-1.99631786
1	6.76409674	1.50968039	-1.75370002
6	5.88494825	0.44920820	-0.08901653
1	5.43460274	1.34208131	0.37150288
1	6.86554861	0.31033903	0.39645433
6	5.04643440	-0.77383173	0.26882106
1	5.35896873	-1.64721859	-0.32871756
1	5.18260765	-1.02640522	1.32802153
50	0.23655976	0.21445701	-0.28048787
7	-1.09045303	-1.87383807	-1.12154484
6	-0.41476941	-3.17706108	-0.98788136
1	-1.01285541	-3.99277496	-1.43671024
1	-0.23565044	-3.39233756	0.07199369
1	0.55474889	-3.11824918	-1.49328494
7	-1.66438234	-2.07441425	1.89039648
6	-2.43597269	-1.86613536	-0.48807755
1	-3.16327047	-2.34471703	-1.17365503
1	-2.74518371	-0.81509316	-0.37695548
6	-2.57406402	-2.58243132	0.85584742
1	-3.63400030	-2.46422362	1.15429449
1	-2.41537094	-3.66109729	0.71119940
6	-2.00270915	-2.28204751	3.25175810
6	-2.08379865	-3.58898687	3.78734827
6	-2.40572405	-3.75387383	5.14113283
6	-2.62459302	-2.67027831	5.99650335
6	-2.49673605	-1.38426137	5.45757246
6	-2.19786716	-1.16919243	4.10874796
7	-0.70637894	0.83986032	-2.10536170
6	-1.20219934	-1.50818729	-2.55761766
1	-1.90440166	-2.19540763	-3.07052231
1	-0.20111401	-1.63734126	-2.99234533
6	-1.63930440	-0.06234105	-2.76414013
1	-1.64495015	0.11637332	-3.85786557
1	-2.69630623	0.06205665	-2.44262886
6	-0.90374708	2.22729850	-2.37862301

6	-1.96082044	2.97379684	-1.79493356
6	-2.10311961	4.33492327	-2.10167050
6	-1.23522317	4.99430323	-2.97616243
6	-0.20356555	4.24663401	-3.55587244
6	-0.02302650	2.88762593	-3.27449036
6	-1.75672269	-4.80455256	2.95509839
1	-2.45811057	-4.76960754	5.54198027
6	-2.99472833	-2.87663722	7.44563961
1	-2.64372873	-0.51555312	6.10450411
6	-2.08190989	0.24161248	3.58273864
6	-2.94737387	2.34168482	-0.84272623
1	-2.91865516	4.89521694	-1.63609493
6	-1.38689995	6.46837854	-3.26645637
1	0.48226297	4.73444843	-4.25407076
6	1.10808694	2.13465714	-3.92587519
1	-1.49816275	-5.65233040	3.60287905
1	-0.90399414	-4.60319185	2.28997564
1	-2.59887648	-5.12456131	2.32114840
1	-1.07203567	0.46503615	3.20189714
1	-2.30299091	0.96655846	4.37610865
1	-2.78218985	0.43054307	2.75317764
1	-4.08512592	-2.81661987	7.59221840
1	-2.53915477	-2.11189270	8.09016132
1	-2.67068458	-3.86315870	7.80406427
1	-3.45511055	3.10910630	-0.24387763
1	-2.44966483	1.64199233	-0.15506148
1	-3.72601390	1.77397227	-1.37708580
1	0.76540357	1.18269217	-4.35440969
1	1.87267184	1.88744974	-3.17540240
1	1.56887734	2.73791695	-4.71984768
1	-0.70977443	7.06913137	-2.63841796
1	-2.41071939	6.81284475	-3.06758332
1	-1.14449441	6.69778347	-4.31372404
1	-1.42629910	-1.09711027	1.71041012

Energy = -7584.945577 Hartree

Number of imaginary frequencies = 0.

Compound TS2b isomer 82

Atomic N.	X	Y	Z
8	1.80206883	0.00552522	1.67441320
8	2.14644575	-1.10824335	-0.39315486
6	2.85328579	-0.90229219	-1.61047435
1	2.17799187	-0.45812038	-2.36304784
1	3.24010777	-1.85877132	-2.00210786
1	3.69144106	-0.20295472	-1.46536183
8	3.83990288	0.31220967	0.74010998
6	2.84718132	-0.57063013	1.15392923
6	3.26694345	-1.88387084	1.80726278
1	3.62081885	-1.62845278	2.82188082
1	2.32608747	-2.42724347	1.95438159
6	4.29146576	-2.77380729	1.09344137
1	4.01832724	-2.86712599	0.03118313
1	4.20626926	-3.78690529	1.51678181
6	5.74675798	-2.31523824	1.23059928
1	6.01581812	-2.30418468	2.30149031
1	6.41040230	-3.05454946	0.75441700
6	6.02875757	-0.93030161	0.64258575

1	5.88288498	-0.93136638	-0.44984359
1	7.08770752	-0.67271310	0.81382519
6	5.18908834	0.19379562	1.24681687
1	5.16399002	0.11681558	2.34712934
1	5.63170719	1.16652429	0.99332035
50	0.28139427	0.18930137	0.08866385
7	-1.19989610	-1.03497028	-1.90560925
6	-0.56609941	-2.31216550	-2.26182246
1	-1.28043032	-2.99764562	-2.76022100
1	-0.16196106	-2.79574871	-1.36637747
1	0.26598537	-2.12252617	-2.95280313
7	-0.87371260	-1.38200068	0.96206534
6	-2.37018514	-1.21993291	-1.02777326
1	-3.17433333	-1.78457069	-1.54490399
1	-2.75318241	-0.21721812	-0.78533369
6	-2.02859855	-1.95124745	0.27086177
1	-2.93449450	-1.89528155	0.90524805
1	-1.88994253	-3.02847242	0.05075619
6	-0.66371822	-1.90720773	2.26907825
6	-0.23828508	-3.24699426	2.46766925
6	-0.07334280	-3.73868060	3.77016449
6	-0.30877045	-2.94992232	4.89930487
6	-0.70471591	-1.62390387	4.69147825
6	-0.88399094	-1.09159458	3.40987825
7	-1.98874426	1.94099987	-2.15389371
6	-1.51992512	-0.30904821	-3.15856767
1	-1.99140084	-1.01167619	-3.87714839
1	-0.56065744	0.00511905	-3.60264564
6	-2.46090317	0.89067137	-3.06290483
1	-2.56727886	1.27489614	-4.09495258
1	-3.46119332	0.54213876	-2.76275420
6	-2.34619188	3.28740096	-2.40581298
6	-3.70356154	3.68595076	-2.42479753
6	-4.01721478	5.02985907	-2.66710424
6	-3.03497076	6.00492811	-2.86318922
6	-1.69680309	5.59831667	-2.79436398
6	-1.33403325	4.26587772	-2.57608914
6	0.10763327	-4.14439106	1.30451095
1	0.26643726	-4.77001715	3.90098310
6	-0.15837802	-3.51053929	6.29327679
1	-0.88407844	-0.97913146	5.55595732
6	-1.29739034	0.35220489	3.26848960
6	-4.81419277	2.71414733	-2.10815620
1	-5.07007742	5.32394838	-2.67230415
6	-3.40122247	7.44190073	-3.14697313
1	-0.90474963	6.34039116	-2.92368269
6	0.12639058	3.88620305	-2.51899815
1	0.78381515	-4.94811296	1.62594903
1	0.60082865	-3.56944203	0.50727481
1	-0.77987140	-4.62613916	0.86352336
1	-0.43471703	0.98831284	3.01071906
1	-1.70682681	0.73267734	4.21379280
1	-2.04828477	0.48579225	2.47788858
1	-1.13259768	-3.81615233	6.70726538
1	0.26643062	-2.76705170	6.98231506
1	0.49229404	-4.39562607	6.29993534
1	-5.72434425	3.25583434	-1.81991684
1	-4.52683592	2.05282283	-1.27702844

1	-5.07437325	2.07034802	-2.96303344
1	0.38140559	3.11668372	-3.26596451
1	0.41511112	3.48227143	-1.53488111
1	0.75874555	4.76138258	-2.71373940
1	-2.68770552	8.13777542	-2.68407035
1	-4.40493679	7.68022490	-2.76956606
1	-3.40066910	7.64857626	-4.22928572
1	-0.99213374	1.84235442	-1.95995951

Energy = -7584.941434 Hartree

Number of imaginary frequencies = 0.

Intermediate 3a (I3a)

Compound I3a isomer 1

Atomic N.	X	Y	Z
8	-0.57537860	-0.18576698	0.91929739
8	0.06751063	-0.99705145	-1.05404672
6	0.93408841	-1.76380053	-1.89680804
1	0.99465804	-1.21739770	-2.84420967
1	0.52213069	-2.77141102	-2.07091948
1	1.94081866	-1.83738594	-1.46323338
8	1.32124911	-1.42942985	0.90289597
6	-0.01165051	-1.30847572	0.40236025
6	-0.90197900	-2.55041841	0.57807492
1	-0.50126247	-3.39835201	-0.00073523
1	-1.85326669	-2.27178179	0.10421999
6	-1.13720970	-2.97337794	2.03651463
1	-1.26346765	-2.07286920	2.65814478
1	-2.09004897	-3.52157401	2.09258011
6	-0.02901011	-3.86455174	2.60947278
1	0.02533585	-4.78928214	2.00806145
1	-0.30339404	-4.17856101	3.62901458
6	1.35858481	-3.21588272	2.63795955
1	1.37696018	-2.36660052	3.34003442
1	2.09158743	-3.95048157	3.01205879
6	1.85318111	-2.71323386	1.28018154
1	1.67818967	-3.46973068	0.49516479
1	2.93842197	-2.53873001	1.32579712
50	-0.69451056	1.34973242	-0.62384961
7	-0.55686654	2.75958899	1.53056463
6	-1.00560858	4.11839726	1.17056271
1	-0.86417236	4.82391181	2.00985779
1	-2.06552517	4.09787688	0.89225142
1	-0.43840699	4.47927714	0.30413370
6	-1.28947377	2.24084736	2.71444795
1	-1.11803655	2.91706088	3.57530809
1	-0.84047275	1.26728048	2.95450455
6	-2.79761037	2.06708435	2.56034047
1	-3.17152860	1.70532206	3.53476683
1	-3.30820990	3.01541352	2.35070945
6	0.89483738	2.73471991	1.85839335
1	1.11296160	1.72012327	2.21987895
1	1.11573044	3.45548384	2.66922750
6	1.78116166	3.02113136	0.65302273
1	1.70411119	4.07309281	0.32955595
1	2.82675627	2.86369602	0.97514875
1	-2.51835333	0.27762636	1.52630051

7	-3.09834905	1.13094832	1.45930689
16	-4.75429357	0.69029440	1.37884378
8	-5.08458647	-0.33433638	2.39633545
8	-5.49998623	1.96528650	1.34971406
6	-4.80721140	-0.09768885	-0.23871559
6	-4.63255094	0.67792789	-1.38861277
6	-4.69427556	0.05824359	-2.63371168
6	-4.92574040	-1.32447959	-2.74729812
6	-5.10345659	-2.07326514	-1.57491258
6	-5.04364525	-1.46952786	-0.31640444
1	-4.45345916	1.74880778	-1.30389692
1	-4.55155030	0.65555986	-3.53574566
6	-4.96502203	-1.98143755	-4.10360513
1	-5.29103132	-3.14603312	-1.64539048
1	-5.18586255	-2.04327410	0.59886664
1	-5.62937571	-1.43804604	-4.79013393
1	-3.96428431	-1.98737980	-4.56181357
1	-5.31242341	-3.02002771	-4.03746956
7	1.40521297	2.08960379	-0.41183394
16	2.14004797	2.29180276	-1.86582905
8	1.35927295	1.42314492	-2.79703397
8	2.35248895	3.71549100	-2.22932774
6	3.79553073	1.56999385	-1.67595628
6	4.86858165	2.14817726	-2.35678350
6	6.13587028	1.57466174	-2.24256667
6	6.34832006	0.43472574	-1.45131420
6	5.25312835	-0.11373316	-0.76438391
6	3.97704983	0.44249365	-0.87161198
1	4.70474558	3.04444100	-2.95421577
1	6.97756141	2.02606829	-2.77152109
6	7.71586663	-0.19490736	-1.35524608
1	5.40436563	-0.98910190	-0.12894816
1	3.13167172	0.02202727	-0.32340986
1	8.51142616	0.55434185	-1.46278247
1	7.85374239	-0.71195757	-0.39635157
1	7.85938906	-0.94036525	-2.15324643

Energy = -8524.641097 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 2

Atomic N.	X	Y	Z
8	-0.24859506	-1.12966805	1.18234003
8	1.24531279	-1.87706846	-0.30233944
6	2.59551040	-2.26067050	-0.60078473
1	2.78563017	-1.91885738	-1.62340760
1	2.70796330	-3.35617984	-0.54615609
1	3.30527170	-1.76844243	0.07690713
8	1.76354969	-1.71620565	2.01493837
6	0.73628488	-2.06238722	1.09319234
6	0.20053031	-3.49888284	1.20496946
1	0.97639207	-4.21941165	0.89903574
1	-0.59358645	-3.55423683	0.44821309
6	-0.34913550	-3.87468147	2.59002499
1	-0.89310825	-3.01377909	3.01054361
1	-1.09282334	-4.67676605	2.46491249
6	0.72505602	-4.35991652	3.57189565
1	1.21362619	-5.25275086	3.14312339

1	0.24321575	-4.69371739	4.50466764
6	1.80222542	-3.32250518	3.90589980
1	1.36843588	-2.48454951	4.47555988
1	2.56153950	-3.78707283	4.55750865
6	2.52196145	-2.73881302	2.68933682
1	2.83032378	-3.53783537	1.99387357
1	3.43583326	-2.21836320	3.01035419
50	-0.07482214	0.25342913	-0.48453689
7	-0.59012671	1.80452965	1.51690692
6	-0.95491846	3.12963221	0.98254871
1	-1.02791929	3.88304455	1.78851505
1	-1.91764743	3.06833083	0.46208908
1	-0.20007369	3.45627238	0.25709631
6	-1.60109984	1.31246016	2.48580613
1	-1.73188390	2.05993370	3.29300753
1	-1.18312585	0.40097276	2.93446184
6	-2.98176060	0.99431091	1.91788030
1	-3.61358350	0.69196175	2.77181342
1	-3.45650817	1.87000802	1.45704292
6	0.72448415	1.83791713	2.21659311
1	0.88831787	0.82606911	2.61266369
1	0.69051960	2.55335642	3.06079446
6	1.88051459	2.19304362	1.28578268
1	1.87046684	3.27352173	1.04541617
1	2.82150236	1.99110831	1.82452332
1	-2.32636029	-0.86374877	1.23315322
7	-2.88238355	-0.06277849	0.89177611
16	-4.41333406	-0.62667723	0.35409232
8	-5.04712508	-1.49633253	1.37166425
8	-5.12514084	0.57138427	-0.13598252
6	-3.90858184	-1.66022569	-1.02942954
6	-3.47671262	-1.05761665	-2.21433108
6	-3.09419211	-1.86820220	-3.27987845
6	-3.13191084	-3.27028792	-3.17714933
6	-3.57710757	-3.84342096	-1.97683952
6	-3.96577532	-3.04714974	-0.89706157
1	-3.44934717	0.02808022	-2.29548396
1	-2.75072039	-1.40627316	-4.20698105
6	-2.68610526	-4.13134490	-4.33141646
1	-3.62111061	-4.92984120	-1.88380228
1	-4.32154528	-3.48539330	0.03478918
1	-3.14082718	-3.79950865	-5.27524802
1	-1.59461360	-4.07157996	-4.46069789
1	-2.94922623	-5.18458226	-4.17280286
7	1.75945722	1.37056399	0.08672403
16	2.89611806	1.53191150	-1.08312273
8	4.27149078	1.44397478	-0.53709092
8	2.45486489	0.59479283	-2.15634428
6	2.72435688	3.21494819	-1.74444643
6	1.65303704	3.51164690	-2.59271386
6	1.50789978	4.80834412	-3.08242024
6	2.41858771	5.82270686	-2.73600156
6	3.48212660	5.49874961	-1.88194893
6	3.64324471	4.20152246	-1.38597629
1	0.95307925	2.72500115	-2.87763109
1	0.67601568	5.03934701	-3.75096376
6	2.26761796	7.21474325	-3.29719416
1	4.20114261	6.27151640	-1.60309391

1	4.48068615	3.94246402	-0.73883930
1	2.64709857	7.26316024	-4.32977294
1	1.21360619	7.52367580	-3.32598237
1	2.82793998	7.94928900	-2.70456555

Energy = -8524.641411 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 3

Atomic N.	X	Y	Z
8	0.87550319	-1.76923069	-0.21602763
8	2.06179984	-0.88480262	-1.86030195
6	3.17897388	-0.29216531	-2.53324275
1	2.81866060	-0.03763966	-3.53629657
1	4.02708085	-0.98942775	-2.61129299
1	3.49063866	0.62652592	-2.01481210
8	2.24401623	-0.06189740	0.34647213
6	2.12922173	-1.25468738	-0.40032904
6	3.25760266	-2.28180566	-0.21073898
1	4.20808657	-1.88478198	-0.60196105
1	2.98027536	-3.12360949	-0.86247651
6	3.46210096	-2.77289124	1.23043214
1	2.49024219	-2.90833945	1.72564076
1	3.93100839	-3.76807079	1.18768302
6	4.35704949	-1.85213003	2.06872187
1	5.35356507	-1.79615142	1.59401313
1	4.51071863	-2.30541093	3.05983513
6	3.81294898	-0.43183924	2.25386896
1	2.89969298	-0.45356153	2.86686968
1	4.55516633	0.16868208	2.80701838
6	3.50761145	0.30740427	0.95357257
1	4.33501878	0.20230319	0.23134408
1	3.38417068	1.38121408	1.15468132
50	0.12377958	-2.28607412	-2.18925171
7	-2.15495132	-2.65976924	-0.97108725
6	-2.91190875	-3.24727971	-2.09964008
1	-3.99506288	-3.27036662	-1.88237244
1	-2.74494468	-2.67378301	-3.01970368
1	-2.56325792	-4.27437621	-2.26813718
7	-1.14880094	-0.48744375	-2.41818108
6	-2.63005735	-1.28914141	-0.66198141
1	-3.68541278	-1.29983227	-0.32656590
1	-2.01021453	-0.90191707	0.15631395
6	-2.49686352	-0.35302001	-1.86037290
1	-2.67989685	0.67299032	-1.49346591
1	-3.27000033	-0.56262159	-2.61782365
16	-0.84464598	0.31604263	-3.81869962
7	-0.65937602	-2.83120048	1.93098245
6	-2.30118833	-3.59939516	0.18730960
1	-3.34174709	-3.97608398	0.18315933
1	-1.64156515	-4.46022353	0.00079116
6	-2.07102449	-3.05937730	1.59577431
1	-2.44985720	-3.82695882	2.28498299
1	-2.69536296	-2.16219740	1.75765663
16	-0.40279374	-2.14293847	3.44981430
8	1.05935142	-2.00957423	3.59449126
8	-1.20824696	-2.91690007	4.41562716
6	-1.11144236	-0.47461520	3.37976546

6	-2.20668747	-0.16028686	4.18382650
6	-2.75018021	1.12628271	4.12015976
6	-2.21787197	2.09626279	3.25931072
6	-1.11855311	1.74591438	2.45420974
6	-0.55686291	0.47142065	2.50936508
1	-2.61629231	-0.91790829	4.85116470
1	0.29406381	0.21591799	1.87383558
1	-0.69640398	2.48432409	1.76918136
6	-2.79547718	3.48842650	3.20319607
1	-3.60519685	1.37772969	4.75044470
8	0.41592551	-0.30600918	-4.32741418
8	-2.02367715	0.38630565	-4.71594000
6	-0.46782018	2.02324326	-3.33416365
6	-0.97883261	3.07520123	-4.09528450
6	-0.66120915	4.38813197	-3.74069360
6	0.15694895	4.66331684	-2.63455785
6	0.64437325	3.58304331	-1.87907020
6	0.34065468	2.26474777	-2.21987648
1	-1.62382847	2.85767213	-4.94593498
1	-1.06106857	5.21385973	-4.33239077
6	0.52236635	6.08243292	-2.27663287
1	1.27157460	3.77793582	-1.00649031
1	0.71470233	1.43167410	-1.62243613
1	-3.76431078	3.54195374	3.71565803
1	-2.12070846	4.21175486	3.68616274
1	-2.93422995	3.82123062	2.16493500
1	1.47199752	6.37221189	-2.75331915
1	-0.24344088	6.79232500	-2.61567900
1	0.65275529	6.20313343	-1.19285205
1	-0.07837250	-2.35387905	1.20922635

Energy = -8524.639579 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 4

Atomic N.	X	Y	Z
8	2.44691343	-2.19806188	-0.66660718
8	3.80279547	-1.31568342	0.88368749
6	4.39247268	-1.39739177	2.18933364
1	4.43566878	-0.37056553	2.56714348
1	5.41131084	-1.81382233	2.12678961
1	3.77242043	-1.99996724	2.86596500
8	2.89702278	-3.50690933	1.11552026
6	3.43830593	-2.59268718	0.16959075
6	4.68961427	-3.07314756	-0.58038098
1	5.54051570	-3.16808379	0.11386138
1	4.93060812	-2.24895425	-1.26438626
6	4.49810670	-4.37994797	-1.36611748
1	3.49801053	-4.37688057	-1.82772836
1	5.22131252	-4.39625330	-2.19599501
6	4.70024840	-5.64523696	-0.52272907
1	5.72934455	-5.63880562	-0.12166933
1	4.63213985	-6.53270500	-1.17212391
6	3.71961922	-5.80031180	0.64458423
1	2.69579417	-5.96405948	0.27060060
1	3.99007430	-6.69728942	1.22720306
6	3.68189306	-4.61097147	1.60540994
1	4.70271537	-4.29166032	1.87640492

1	3.17403001	-4.89933879	2.53709952
50	1.77421371	-0.25772863	-0.06574685
7	-0.43019482	-1.43040553	-0.77478722
6	-0.33764894	-2.11555977	-2.08016485
1	-1.25872580	-2.68623947	-2.30164568
1	-0.16148429	-1.38711739	-2.87965813
1	0.51660167	-2.80055450	-2.04175754
7	-0.62317524	1.18878999	-2.24384584
6	-1.58641715	-0.50681613	-0.69299317
1	-2.52105816	-1.08788575	-0.56037128
1	-1.45745905	0.10535417	0.21281627
6	-1.81561262	0.40455132	-1.90076421
1	-2.68799526	1.03909736	-1.65766085
1	-2.07572678	-0.18476014	-2.78912574
16	-0.65264591	2.08105268	-3.69366577
7	0.61395135	-0.84875788	1.72283008
6	-0.51892442	-2.45068224	0.30709729
1	-1.44861059	-3.04170405	0.19615502
1	0.34580450	-3.11375303	0.17548322
6	-0.46610569	-1.83212461	1.70468875
1	-0.29000350	-2.64380278	2.42972150
1	-1.43800161	-1.36907275	1.96304247
16	0.90376217	-0.02155918	3.10594454
8	2.08362797	0.83211076	2.78779489
8	0.91814074	-0.90831607	4.29338776
6	-0.50682119	1.10024644	3.33369995
6	-1.54942892	0.74536926	4.19114712
6	-2.64425171	1.60348046	4.32882305
6	-2.70840507	2.81737087	3.62959727
6	-1.64212790	3.15270646	2.77650161
6	-0.54641566	2.30414580	2.62356033
1	-1.48598978	-0.18401021	4.75644799
1	0.29062468	2.57613120	1.97935500
1	-1.66777504	4.09976003	2.23324304
6	-3.87102933	3.76020041	3.81725149
1	-3.45943793	1.32736628	5.00059977
8	0.64157435	2.78103040	-3.73442917
8	-1.08326157	1.13026313	-4.73573642
6	-1.95128314	3.32678074	-3.51926999
6	-3.24043946	3.05335631	-3.98067678
6	-4.23612916	4.01979042	-3.82302937
6	-3.96067101	5.25481160	-3.21649433
6	-2.65238152	5.50219957	-2.76543530
6	-1.64578365	4.54934944	-2.91326857
1	-3.44839887	2.10502433	-4.47505720
1	-5.24441424	3.81289814	-4.18610553
6	-5.03085034	6.30853559	-3.08399817
1	-2.41678420	6.46151738	-2.30095545
1	-0.62575320	4.75350794	-2.58776279
1	-4.77358961	3.22555635	4.14097142
1	-3.64175425	4.51411149	4.58661360
1	-4.10205513	4.30296961	2.89067153
1	-4.96868667	7.03074217	-3.91292460
1	-6.03521010	5.86668031	-3.10698369
1	-4.92116989	6.87671365	-2.15058611
1	-0.25914987	1.77601303	-1.48800065

Energy = -8524.636618 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 5

Atomic N.	X	Y	Z
8	2.05657159	-2.13694398	-0.61508082
8	3.17970848	-1.75294960	1.30182833
6	3.31837224	-2.01053487	2.70695599
1	3.58703577	-1.05445786	3.17076772
1	4.12410763	-2.74168899	2.88192859
1	2.37302438	-2.36305711	3.13935627
8	1.60908435	-3.54797828	1.09073163
6	2.61421144	-2.85374185	0.37762142
6	3.81535349	-3.69442001	-0.07679019
1	4.37871205	-4.07012768	0.79306080
1	4.46955076	-2.98153979	-0.59511863
6	3.44467876	-4.85517910	-1.01385004
1	2.65401332	-4.51762436	-1.70211238
1	4.31955120	-5.09192077	-1.63867191
6	3.01617235	-6.13052200	-0.27702749
1	3.85560880	-6.46934079	0.35589096
1	2.84182508	-6.93487903	-1.00948400
6	1.77071942	-5.97463990	0.60245079
1	0.87979728	-5.78569268	-0.01804406
1	1.58707351	-6.92045180	1.13988174
6	1.86110717	-4.85629659	1.64140298
1	2.82572313	-4.88946028	2.17595082
1	1.06766301	-4.97798663	2.39258848
50	2.10307207	-0.07411296	-0.01126422
7	-2.09762693	-0.42129251	-1.26803939
6	-3.22638411	0.06711081	-0.47436375
1	-2.87365892	0.48953789	0.47419492
1	-3.73775250	0.86617088	-1.02791150
1	-3.97095743	-0.72820537	-0.24720000
7	-1.01912504	0.30380207	-4.19736214
6	-2.57440220	-0.84027363	-2.59170720
1	-3.12448261	-1.80921143	-2.52340170
1	-3.29195323	-0.08814949	-2.95112876
6	-1.48494305	-0.99447860	-3.65594873
1	-1.90977680	-1.55574193	-4.50102017
1	-0.63519857	-1.57788222	-3.27708355
16	0.53328336	0.87156179	-3.76900915
7	0.06467240	-0.25721358	0.97487169
6	-1.40664540	-1.54339756	-0.60867041
1	-2.07735270	-2.43477260	-0.57873109
1	-0.53083079	-1.82293170	-1.21027090
6	-0.94722590	-1.32417004	0.83201539
1	-0.53916414	-2.28698431	1.17660162
1	-1.81575010	-1.10042527	1.47270167
16	0.31317918	0.26724063	2.50779981
8	1.68178257	0.89519353	2.43973570
8	0.04062249	-0.75937013	3.54257278
6	-0.84077361	1.62449880	2.84238966
6	-2.00724606	1.36943287	3.56544840
6	-2.90149362	2.41500321	3.80951839
6	-2.63799010	3.71611234	3.35795507
6	-1.44933389	3.94546945	2.64266059
6	-0.55318244	2.91095582	2.37851982
1	-2.19634658	0.36622824	3.94582071

1	0.37232395	3.09442152	1.83291023
1	-1.21993066	4.95507741	2.29450303
6	-3.58457986	4.85078092	3.66093677
1	-3.81571612	2.21682035	4.37226646
8	1.04654835	-0.02507488	-2.70358820
8	1.29417078	1.07407105	-5.02043915
6	0.21956966	2.49841119	-3.06318460
6	0.70640872	3.62095826	-3.73225253
6	0.47310440	4.88462482	-3.18536853
6	-0.23938900	5.03422557	-1.98684282
6	-0.71718569	3.88028275	-1.34092669
6	-0.48861276	2.60863449	-1.86335513
1	1.25915281	3.49756199	-4.66241928
1	0.85271448	5.76836702	-3.70121981
6	-0.46532997	6.39885144	-1.38568173
1	-1.27480953	3.97626170	-0.40758321
1	-0.86116105	1.71127967	-1.36192751
1	-4.58389918	4.48004773	3.92278791
1	-3.21979420	5.44832021	4.51089360
1	-3.68176165	5.53267652	2.80484665
1	0.28048093	6.60644803	-0.60225510
1	-0.37863075	7.19070026	-2.14075898
1	-1.45691781	6.47124051	-0.91852224
1	-1.05343638	0.34674041	-5.21674975

Energy = -8524.622556 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 6

Atomic N.	X	Y	Z
8	3.26600735	-3.04109988	-1.65220533
8	3.72846180	-1.90270439	-3.56098859
6	4.21929451	-0.68292984	-4.13819283
1	3.54377540	-0.42985094	-4.96325201
1	5.23704408	-0.83668448	-4.53054463
1	4.20769874	0.13431035	-3.40513736
8	4.64869794	-1.27742120	-1.42035291
6	4.32296511	-2.41092286	-2.18142971
6	5.48371381	-3.33680420	-2.56053888
1	6.19478487	-2.81738964	-3.22317574
1	5.02063005	-4.13503532	-3.15453747
6	6.22092222	-3.93081825	-1.34871134
1	5.48381407	-4.18597184	-0.57118337
1	6.68795124	-4.87885181	-1.65647295
6	7.31251096	-3.01392939	-0.78221064
1	8.06428229	-2.83418982	-1.57107175
1	7.84162154	-3.53562327	0.03099766
6	6.80982915	-1.66133859	-0.26553871
1	6.17199285	-1.79816090	0.62249743
1	7.67285736	-1.05437169	0.05601104
6	6.01976290	-0.84336155	-1.28671736
1	6.53145877	-0.82506031	-2.26367813
1	5.92755084	0.19702726	-0.94496789
50	1.59155309	-2.56094327	-2.93606429
7	-0.40643259	0.64571814	0.77134691
6	0.25588789	1.86630651	1.22728848
1	1.13088717	2.08103704	0.60022063
1	-0.43582676	2.71453323	1.13631969

1	0.59509953	1.80123226	2.28530194
7	-3.80443150	-0.85651503	1.48611528
6	-1.64303425	0.39546627	1.51905456
1	-1.45454078	-0.13798144	2.47537627
1	-2.08478767	1.36846742	1.77816780
6	-2.65222377	-0.39445385	0.67764985
1	-2.18142033	-1.30595907	0.28334828
1	-2.97478795	0.21123319	-0.18066583
16	-5.12842096	0.20800992	1.68821931
7	1.05592342	-0.83363018	-1.61839046
6	0.49895981	-0.50664046	0.82278669
1	1.01710653	-0.55761359	1.80973299
1	-0.09711965	-1.42638158	0.73090042
6	1.56511552	-0.52475031	-0.27499243
1	2.29640010	-1.31309820	-0.03737074
1	2.13340637	0.41769865	-0.29567291
16	0.80666305	0.36723884	-2.70256010
8	1.00994607	-0.38775974	-4.01196426
8	1.60869205	1.58617804	-2.44928593
6	-0.92867341	0.86940532	-2.74602689
6	-1.28163413	2.15467349	-2.33519776
6	-2.62252906	2.53718501	-2.38031913
6	-3.61877145	1.65323488	-2.82499786
6	-3.22886272	0.37081936	-3.24692769
6	-1.89269444	-0.02684635	-3.21084614
1	-0.50729828	2.84121063	-1.99632840
1	-1.59979726	-1.01832168	-3.55707755
1	-3.98525232	-0.32652408	-3.61142629
6	-5.06919626	2.05997298	-2.81812866
1	-2.90332687	3.54122601	-2.05738125
8	-5.07069995	1.30950326	0.70013658
8	-6.30505769	-0.68256638	1.77996075
6	-4.84078176	0.93580449	3.31380110
6	-4.90461936	0.12191273	4.44872113
6	-4.72111021	0.69702981	5.70297521
6	-4.48066416	2.07638689	5.84332303
6	-4.42931669	2.86643181	4.68674443
6	-4.60983098	2.30573460	3.41926772
1	-5.10016479	-0.94482336	4.34554812
1	-4.76748985	0.06640845	6.59273585
6	-4.29783627	2.68398519	7.21118615
1	-4.24749950	3.93881261	4.77603245
1	-4.57485773	2.91664088	2.51808161
1	-5.19053205	3.11655135	-3.09303149
1	-5.66157342	1.44904700	-3.51139611
1	-5.49185448	1.93102915	-1.80954532
1	-5.23060292	2.62960140	7.79262147
1	-3.52957467	2.14661409	7.78544385
1	-4.00283785	3.73863221	7.14555387
1	-4.22530173	-1.71498194	1.12303654

Energy = -8524.625726 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 7

Atomic N.	X	Y	Z
8	0.91864450	-1.69333501	-0.47255268
8	1.95875712	-0.58578815	-2.08040105

6	3.00689896	0.12282069	-2.75240134
1	3.87098475	-0.52595651	-2.96204776
1	3.32145536	0.99117106	-2.15493011
1	2.57084421	0.47066884	-3.69557687
8	2.26102663	-0.00009585	0.18776358
6	2.13796069	-1.10880838	-0.67822359
6	3.31254378	-2.10096950	-0.67584281
1	4.22001238	-1.62223669	-1.07765688
1	3.02317119	-2.87640806	-1.40064549
6	3.63050449	-2.74021689	0.68418455
1	2.69965405	-2.97267372	1.22026941
1	4.13185684	-3.70274433	0.49908886
6	4.54498520	-1.87985415	1.56451939
1	5.50561075	-1.72937276	1.03908564
1	4.77931670	-2.43238344	2.48710461
6	3.96408121	-0.51299479	1.94123293
1	3.09431628	-0.64097914	2.60259446
1	4.71916488	0.05379723	2.51227466
6	3.54834246	0.35186824	0.75383306
1	4.32962805	0.36176996	-0.02514082
1	3.40148245	1.39081861	1.08211015
50	0.05246692	-2.02423981	-2.43842860
7	-2.12611836	-2.62061979	-1.12639644
6	-2.93749358	-3.11223282	-2.26295663
1	-4.00234258	-3.20163302	-1.98172400
1	-2.85131843	-2.43657604	-3.12280798
1	-2.56767805	-4.10052040	-2.56528009
7	-1.29383313	-0.26548852	-2.38690779
6	-2.62376233	-1.31148830	-0.63819551
1	-3.65256291	-1.40069047	-0.23810185
1	-1.96216022	-0.99001365	0.17589709
6	-2.60437200	-0.24716783	-1.73216457
1	-2.79625096	0.72506790	-1.24353950
1	-3.42002546	-0.40560726	-2.45675814
16	-1.11481301	0.69255000	-3.70969768
7	-0.42762459	-3.05357379	1.63396031
6	-2.16481472	-3.68470121	-0.07191338
1	-3.19233806	-4.09509060	-0.04876469
1	-1.49599926	-4.49628561	-0.39575697
6	-1.85232675	-3.29297679	1.36933265
1	-2.16060706	-4.14396881	1.99261888
1	-2.48848791	-2.44128606	1.67077893
16	-0.08464291	-2.53870480	3.20372223
8	1.37926731	-2.36586442	3.26464425
8	-0.79445388	-3.45180248	4.12182588
6	-0.84779031	-0.90277628	3.38267611
6	-1.88757649	-0.72732450	4.29581497
6	-2.47262680	0.53538548	4.42574751
6	-2.03656494	1.61964330	3.65079516
6	-0.99367345	1.40831482	2.73098358
6	-0.39126435	0.15858160	2.59258525
1	-2.22224183	-1.57332885	4.89530846
1	0.41489254	0.01243119	1.87005709
1	-0.64863753	2.23721197	2.10930799
6	-2.65342057	2.98652275	3.81153891
1	-3.28452479	0.67781223	5.14139896
8	0.13221970	0.18403148	-4.35876402
8	-2.35253969	0.80270489	-4.51966093

6	-0.77211576	2.35480332	-3.06906073
6	-1.37825312	3.45629100	-3.67407298
6	-1.08880405	4.73757817	-3.19945447
6	-0.20497659	4.93174629	-2.12731798
6	0.37874495	3.80142715	-1.52955835
6	0.10437068	2.51423761	-1.99192679
1	-2.07346539	3.30027053	-4.49826417
1	-1.56292363	5.60186332	-3.66850375
6	0.12758255	6.32010235	-1.64005077
1	1.05869893	3.93171287	-0.68490288
1	0.55291055	1.64069890	-1.51586998
1	-3.63839720	2.92867866	4.29223990
1	-2.01621319	3.63025445	4.43768922
1	-2.76862443	3.49052280	2.84221455
1	1.04097627	6.69577811	-2.12741762
1	-0.67942763	7.02928429	-1.86594491
1	0.30865872	6.33345799	-0.55683201
1	0.08605581	-2.47310058	0.93721634

Energy = -8524.639574 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 8

Atomic N.	X	Y	Z
8	2.38867772	-2.29442518	-0.86129881
8	3.82276927	-1.33950535	0.57578621
6	4.47790707	-1.38039942	1.85197889
1	5.50790432	-1.75760783	1.74317649
1	3.91610021	-1.99897708	2.56384142
1	4.49804306	-0.34809324	2.21657425
8	3.02800542	-3.56913247	0.88475093
6	3.45646237	-2.64290352	-0.10162457
6	4.66931318	-3.07171854	-0.94004489
1	5.57408426	-3.11061388	-0.31164744
1	4.81484749	-2.24836062	-1.65141394
6	4.48848571	-4.40117090	-1.68960689
1	3.45689065	-4.46238798	-2.07088780
1	5.14481927	-4.39411780	-2.57337318
6	4.82818538	-5.63494282	-0.84342233
1	5.87912257	-5.55013429	-0.51486502
1	4.77278751	-6.53845133	-1.47127427
6	3.94193024	-5.82435828	0.39208894
1	2.90591133	-6.05351277	0.09384976
1	4.30413824	-6.69304848	0.96768524
6	3.90345225	-4.62185826	1.33591767
1	4.92096561	-4.24326648	1.53216931
1	3.47517433	-4.92003946	2.30369155
50	1.72582609	-0.36112517	-0.24059007
7	-0.50594064	-1.55909514	-0.78805195
6	-0.49970080	-2.26145621	-2.08728722
1	-1.42833821	-2.84316391	-2.23549652
1	-0.38860418	-1.53989894	-2.90461115
1	0.36187670	-2.93832481	-2.10234441
7	-0.82463156	1.03447732	-2.28360463
6	-1.66017678	-0.64017131	-0.63795009
1	-2.57782326	-1.22535351	-0.42888859
1	-1.47049601	-0.01277480	0.24609649
6	-1.98589030	0.25499394	-1.83442753

1	-2.83089332	0.89537755	-1.51909646
1	-2.32830120	-0.33894817	-2.69116571
16	-1.06293754	2.12022317	-3.57233015
7	0.72443843	-0.95462174	1.63966765
6	-0.51255346	-2.56180846	0.31361074
1	-1.44223671	-3.16181777	0.27529601
1	0.34666473	-3.22160371	0.13577570
6	-0.37404772	-1.91825564	1.69372745
1	-0.17429676	-2.71812832	2.42535448
1	-1.32393067	-1.43554678	1.99335337
16	0.97324994	0.01760773	2.93657766
8	2.17248614	0.82404929	2.57344058
8	0.92767560	-0.74227924	4.20716198
6	-0.42894852	1.17280563	2.98670835
6	-1.52166922	0.91284745	3.81485438
6	-2.61496386	1.78517558	3.79954987
6	-2.62907556	2.91851366	2.97470217
6	-1.51090678	3.16223993	2.15664034
6	-0.41605888	2.29987221	2.15739600
1	-1.49982963	0.04764368	4.47689871
1	0.45988576	2.50189757	1.53948322
1	-1.49668484	4.04740365	1.51685137
6	-3.79576367	3.87500900	2.98371799
1	-3.46940308	1.58325109	4.44843064
8	0.24691241	2.75675549	-3.78553679
8	-1.76067435	1.35071896	-4.61902326
6	-2.20242008	3.38943643	-2.97062333
6	-3.57088872	3.26609201	-3.21423640
6	-4.43843280	4.24632672	-2.72437556
6	-3.95728851	5.34500957	-1.99792256
6	-2.57146875	5.44773580	-1.77843290
6	-1.69171201	4.47995653	-2.25816227
1	-3.94198365	2.42669250	-3.80134696
1	-5.50862804	4.15905641	-2.91963786
6	-4.89547456	6.39771921	-1.46367779
1	-2.17575153	6.30760641	-1.23433316
1	-0.61577012	4.57603041	-2.11163456
1	-4.67831039	3.42725459	3.45810010
1	-3.54699953	4.79186754	3.54024466
1	-4.06906097	4.18100527	1.96386003
1	-4.56687827	7.40614723	-1.75254663
1	-5.91729292	6.25040630	-1.83463515
1	-4.92858242	6.37332540	-0.36373077
1	-0.30327247	1.50086838	-1.53385110

Energy = -8524.636556 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 9

Atomic N.	X	Y	Z
8	2.24087398	-1.85025293	0.68177046
8	3.51856420	-0.24774976	1.59029261
6	4.05468287	0.36763674	2.77181512
1	5.08475281	0.01893824	2.95217116
1	3.42123199	0.16582258	3.64530714
1	4.05798105	1.44524125	2.57733818
8	2.68276393	-2.07142042	2.88331529
6	3.21776598	-1.73028910	1.61134618

6	4.51023324	-2.46059813	1.21634139
1	5.34214700	-2.14887350	1.86871830
1	4.73992000	-2.08426479	0.21093193
6	4.39532761	-3.99309892	1.20090893
1	3.40950879	-4.27477187	0.79803447
1	5.14261675	-4.39172975	0.49732555
6	4.62464482	-4.64491176	2.57065554
1	5.64010797	-4.38338662	2.91736259
1	4.61256602	-5.74120472	2.46086014
6	3.61681935	-4.23730162	3.65073872
1	2.61297061	-4.62235164	3.40799859
1	3.90838481	-4.69860518	4.60951477
6	3.49747294	-2.72883008	3.87292284
1	4.49407797	-2.26207907	3.95071167
1	2.97196364	-2.53138213	4.81864866
50	1.48644364	0.11863159	0.25277225
7	-0.67905738	-1.37802380	0.20631349
6	-0.48676571	-2.61321172	-0.57940359
1	-1.35387595	-3.29226189	-0.47276906
1	-0.35375545	-2.37468814	-1.64123482
1	0.42165610	-3.11261789	-0.22390070
7	-3.02597920	0.71127406	-1.89695883
6	-1.88902757	-0.64159350	-0.21749878
1	-2.76736053	-1.31892359	-0.18281674
1	-2.07118220	0.16925319	0.49813085
6	-1.77444169	-0.00640957	-1.60932363
1	-1.54722178	-0.75454765	-2.38590091
1	-0.95970366	0.73105572	-1.59976810
16	-2.96746685	2.05521095	-2.94016218
7	0.30771563	0.40238410	2.07815861
6	-0.75960129	-1.73019331	1.65105835
1	-1.67095003	-2.32575312	1.85314439
1	0.12354731	-2.34723123	1.86200366
6	-0.73206461	-0.49984694	2.56214058
1	-0.52555338	-0.84698129	3.58846276
1	-1.71969579	-0.00144314	2.58200541
16	0.54971186	1.83627129	2.83608069
8	1.66380256	2.45292022	2.05259359
8	0.67620198	1.68638119	4.30540535
6	-0.93812889	2.82964396	2.54628881
6	-1.79189593	3.12798336	3.60791569
6	-2.94865381	3.87410586	3.36150692
6	-3.26245226	4.32285649	2.07087236
6	-2.38392615	4.00653265	1.01854117
6	-1.22728115	3.26592509	1.24908358
1	-1.53934136	2.78458945	4.61051946
1	-0.54988013	3.03827615	0.42524317
1	-2.60659291	4.33370292	0.00156606
6	-4.50144170	5.14224658	1.80937627
1	-3.61897480	4.11049353	4.19025768
8	-4.37849254	2.44334727	-3.11615985
8	-1.95529550	2.96689002	-2.37638905
6	-2.34330399	1.46925046	-4.53082696
6	-0.97472288	1.53041486	-4.80037318
6	-0.50491405	1.05759438	-6.02767150
6	-1.38121368	0.52733194	-6.98644592
6	-2.75526249	0.49029269	-6.69015800
6	-3.24291665	0.95560983	-5.47043101

1	-0.29569848	1.96735792	-4.06885947
1	0.56275876	1.11174973	-6.24682333
6	-0.86721941	0.00293627	-8.30320200
1	-3.45483260	0.10189558	-7.43268871
1	-4.31109178	0.95286289	-5.25377460
1	-5.19049217	5.11287620	2.66317168
1	-4.24101415	6.19579265	1.62424677
1	-5.03465401	4.78340354	0.91808784
1	-1.50280614	0.32893487	-9.13800963
1	0.15861652	0.34035265	-8.49682825
1	-0.86363810	-1.09803347	-8.31059734
1	-3.79799189	0.10859130	-2.19100158

Energy = -8524.638410 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 10

Atomic N.	X	Y	Z
8	1.73846544	-2.35701484	1.05119671
8	3.11315717	-0.59913093	1.00492341
6	4.06298376	0.28084789	1.63729464
1	5.08452934	-0.06950890	1.42582700
1	3.87897816	0.33980221	2.71645895
1	3.90755143	1.26691167	1.19239279
8	2.98138224	-2.02292167	2.90385602
6	2.98870378	-2.03018754	1.50048224
6	4.08707176	-2.85175888	0.81702607
1	5.07557097	-2.40933957	1.01968320
1	3.89840403	-2.72797095	-0.25721931
6	4.08820103	-4.34149721	1.19615143
1	3.04844342	-4.69986626	1.25623878
1	4.56199222	-4.90427712	0.37754421
6	4.84098321	-4.64911167	2.49673103
1	5.89234925	-4.33354563	2.37652620
1	4.86575824	-5.73897578	2.65406984
6	4.26438160	-3.97475845	3.74617187
1	3.26708948	-4.38010861	3.98163156
1	4.90946799	-4.20471927	4.61065011
6	4.14146004	-2.45481780	3.64970826
1	5.06527975	-2.00596244	3.24757224
1	3.97594730	-2.02643307	4.64764299
50	0.84302281	-0.56320144	0.48536941
7	-1.17034539	-1.86853064	0.77976046
6	-1.03153976	-3.28647471	0.36435387
1	-1.97282488	-3.83262740	0.54680036
1	-0.78257002	-3.34037622	-0.70071654
1	-0.21491334	-3.74415830	0.93075679
7	-3.40129015	-0.47771688	-1.96528457
6	-2.34082617	-1.23052826	0.10504936
1	-3.26848522	-1.72123822	0.45068926
1	-2.37847820	-0.18053753	0.42587493
6	-2.27057584	-1.26381536	-1.42624531
1	-2.41245534	-2.28901389	-1.79669766
1	-1.27359524	-0.91040219	-1.75187856
16	-3.15389823	1.27487553	-1.88726994
7	0.01284999	0.22281781	2.27056761
6	-1.32634013	-1.80472991	2.26465258
1	-2.29550766	-2.24243124	2.56066200

1	-0.51608240	-2.41355330	2.68880476
6	-1.21271291	-0.37728956	2.80115217
1	-1.16903468	-0.42967866	3.90041421
1	-2.10888975	0.21175957	2.53399070
16	0.35638380	1.80437786	2.67176291
8	1.63658508	2.07348116	1.96861844
8	0.23103530	1.96670820	4.13563273
6	-0.91191426	2.83236917	1.90487568
6	-2.03395974	3.21582084	2.64333305
6	-3.03121558	3.96866369	2.01870497
6	-2.91830196	4.34980701	0.67303546
6	-1.76066026	3.97579935	-0.03202618
6	-0.76260752	3.20997065	0.56617017
1	-2.10862395	2.94268350	3.69547428
1	0.11846400	2.89985033	0.00373866
1	-1.64744977	4.27679296	-1.07516265
6	-4.02176169	5.10633714	-0.01898727
1	-3.91350908	4.26574482	2.58831822
8	-4.53286868	1.89407504	-1.99359949
8	0.69459989	0.17126816	-1.24606882
6	-2.35975263	1.54970308	-3.51488590
6	-0.97912259	1.36800798	-3.64468244
6	-0.39463455	1.59962091	-4.89323555
6	-1.15916916	2.01499374	-5.99525667
6	-2.54010765	2.20904145	-5.81961572
6	-3.14605854	1.98443745	-4.58301120
1	-0.36371879	1.05309048	-2.79084514
1	0.68291933	1.46342439	-5.00547896
6	-0.51596835	2.23781874	-7.34199614
1	-3.14571454	2.55297740	-6.66097382
1	-4.21161371	2.15767679	-4.42197987
1	-4.71796476	5.55286366	0.70238338
1	-3.61943384	5.90428496	-0.65835940
1	-4.59281009	4.42372619	-0.66827789
1	-1.02862453	3.02835234	-7.90650419
1	0.54164821	2.51433312	-7.23993014
1	-0.55769479	1.32165112	-7.95216181
1	-3.58003368	-0.72855810	-2.94237486

Energy = -8524.610776 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 11

Atomic N.	X	Y	Z
8	0.15668338	-0.17247320	0.31245971
8	2.06118079	0.86642921	0.93139048
6	3.46078016	0.70868902	1.19078689
1	3.67202233	1.31963618	2.07697402
1	4.06284324	1.08500685	0.34715841
1	3.71725599	-0.33971333	1.39474784
8	2.07212909	-1.22977548	-0.22214527
6	1.41582734	0.02681985	-0.15116717
6	1.45100252	0.87160832	-1.43430812
1	2.47834695	1.21942385	-1.63220990
1	0.85864141	1.76276542	-1.18847880
6	0.88093530	0.17226964	-2.67799106
1	-0.00218214	-0.41897299	-2.38723776
1	0.52023380	0.94272000	-3.37686064

6	1.89916919	-0.70946996	-3.41233647
1	2.74678187	-0.07631008	-3.72898992
1	1.44633510	-1.09838973	-4.33826760
6	2.44099377	-1.88228301	-2.58824532
1	1.64235451	-2.61618078	-2.39313214
1	3.21647648	-2.40677636	-3.17192060
6	3.05550238	-1.48732105	-1.24465468
1	3.74659453	-0.63590157	-1.36480325
1	3.64022430	-2.32611035	-0.84006366
50	0.09339162	0.43410612	2.42044221
7	-2.51318571	0.22791804	2.06466280
6	-3.11635392	-0.40737969	3.25449618
1	-4.21834573	-0.45023761	3.17560680
1	-2.72254653	-1.42166274	3.38479304
1	-2.85038550	0.17941195	4.14224919
7	-1.28634612	-2.33880232	1.28502575
6	-2.87265559	-0.49181063	0.81701064
1	-3.94714742	-0.33351766	0.59425140
1	-2.28791469	-0.04852761	0.00038555
6	-2.64245943	-2.00698605	0.84276479
1	-2.86281669	-2.38044715	-0.17480220
1	-3.34390011	-2.49570540	1.53080318
16	-0.95390956	-3.93417461	1.72025387
7	-0.61745324	2.41322315	1.70654895
6	-2.94467080	1.64975406	1.97118557
1	-3.97032555	1.71089445	1.55762967
1	-2.96323982	2.06204460	2.98909231
6	-1.97006784	2.49620549	1.14948803
1	-2.34039762	3.53357650	1.14523068
1	-1.93691259	2.15831635	0.10121026
16	-0.12296647	3.63223856	2.69680468
8	1.02697935	3.04188086	3.44373451
8	-1.23756547	4.26917838	3.44539308
6	0.54504658	4.91432555	1.60183126
6	0.05746510	6.21717190	1.68517086
6	0.59722261	7.20094777	0.85052789
6	1.61717350	6.89855535	-0.06143239
6	2.08679886	5.57350549	-0.12485993
6	1.55941326	4.58148708	0.69821131
1	-0.73324553	6.44732422	2.39838186
1	1.91971816	3.55320059	0.64418527
1	2.87841293	5.31886745	-0.83289834
6	2.21239687	7.96485206	-0.94720906
1	0.21753086	8.22259898	0.91241600
8	0.44674602	-3.93543607	2.17378946
8	-2.06813310	-4.36300773	2.59087717
6	-1.04327286	-4.92281963	0.20746019
6	-2.21589078	-5.61330968	-0.10301984
6	-2.27176222	-6.36163316	-1.28128766
6	-1.17222327	-6.43201581	-2.14957520
6	-0.00453583	-5.72693990	-1.80904553
6	0.06915646	-4.97491845	-0.63777189
1	-3.06066296	-5.57720266	0.58408518
1	-3.18515056	-6.90692039	-1.52609418
6	-1.22573385	-7.27074106	-3.40178182
1	0.86280465	-5.77437329	-2.47061626
1	0.98011456	-4.44188905	-0.36498592
1	1.63063826	8.89419470	-0.90162803

1	3.24359699	8.19919382	-0.64147771
1	2.25457834	7.63641813	-1.99561496
1	-0.76501942	-8.25612107	-3.23035040
1	-2.26017272	-7.44273332	-3.72582876
1	-0.67740043	-6.79576273	-4.22651017
1	-0.53454730	-1.90200656	0.72008566

Energy = -8524.643139 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 12

Atomic N.	X	Y	Z
8	2.95370402	-0.29317377	1.51170463
8	3.83682092	-0.75461450	-0.49031130
6	4.72126785	-0.43988720	-1.57341533
1	4.23158119	-0.82218104	-2.47679672
1	5.68589838	-0.95487712	-1.44330145
1	4.88050247	0.64442894	-1.65819994
8	4.63038933	1.06178310	0.81609010
6	4.16969082	-0.27685742	0.91270532
6	5.14387454	-1.28811685	1.52809110
1	6.03024951	-1.40763477	0.88411474
1	4.60228421	-2.24239538	1.49923926
6	5.57468630	-0.95451756	2.96533787
1	4.70669832	-0.56162543	3.51801002
1	5.86566803	-1.89048906	3.46670773
6	6.75140795	0.02589891	3.04784619
1	7.62009989	-0.42386360	2.53503473
1	7.04920544	0.15014972	4.10122626
6	6.47930832	1.40488574	2.43738054
1	5.71048696	1.94128066	3.01631072
1	7.39885161	2.01168190	2.49329932
6	6.02738642	1.37598058	0.97671704
1	6.66478577	0.69981382	0.38056995
1	6.11806777	2.38076122	0.53995790
50	1.54111499	-0.12965396	-0.07648813
7	-0.19407975	-0.62451784	1.97795072
6	0.56728960	-0.54415677	3.24507357
1	-0.07200353	-0.82545020	4.10309754
1	1.44132518	-1.20071801	3.20197487
1	0.93260402	0.47961926	3.38536420
7	1.06904518	-2.25636539	-0.03442607
6	-0.61449361	-2.02901024	1.72756735
1	-1.01219329	-2.47193560	2.66240539
1	-1.42690682	-2.01790360	0.98903998
6	0.52345754	-2.88495888	1.16397561
1	0.14249311	-3.89584305	0.94802107
1	1.32638597	-3.00856697	1.90898792
16	0.97767346	-2.99153054	-1.49654483
7	-1.60787375	1.64418416	-0.03808570
6	-1.38846473	0.25617287	2.10599712
1	-2.09635410	-0.21419040	2.81811268
1	-1.06879617	1.20435581	2.55601760
6	-2.14333660	0.56553745	0.80312784
1	-3.17358999	0.83872515	1.06991284
1	-2.21990227	-0.32933910	0.16688719
16	-1.91551996	3.25313266	0.41554572
8	-0.77961684	4.02654234	-0.12214783

8	-2.29930875	3.31840365	1.84460761
6	-3.39148686	3.66316298	-0.53997563
6	-4.62116156	3.77854246	0.10667924
6	-5.75178305	4.11548526	-0.64282239
6	-5.66529663	4.34433263	-2.02315466
6	-4.40869966	4.22607745	-2.64496475
6	-3.27211731	3.88948177	-1.91451001
1	-4.68140084	3.61910876	1.18257625
1	-2.29770490	3.81230477	-2.39611073
1	-4.32130698	4.40675904	-3.71796119
6	-6.88122743	4.73610674	-2.82434432
1	-6.71714356	4.20827860	-0.14207158
8	1.62298784	-2.01067733	-2.41744139
8	1.43668949	-4.39725528	-1.43467288
6	-0.77642021	-3.06773172	-1.96687580
6	-1.47877027	-4.26680414	-1.83803155
6	-2.83677110	-4.30304345	-2.16795283
6	-3.50197095	-3.16052866	-2.63540246
6	-2.76835905	-1.96756980	-2.76412759
6	-1.41525742	-1.91428545	-2.43372828
1	-0.95471661	-5.16063561	-1.50077140
1	-3.38667912	-5.24091354	-2.06800416
6	-4.95782946	-3.21398943	-3.02655826
1	-3.26482321	-1.06811800	-3.13405135
1	-0.84892060	-0.98953570	-2.55219234
1	-7.80770121	4.54120443	-2.26961119
1	-6.85812994	5.80928069	-3.06897954
1	-6.92570948	4.18977106	-3.77671907
1	-5.06552530	-3.31458038	-4.11783419
1	-5.46631569	-4.06998934	-2.56452321
1	-5.48602387	-2.29637159	-2.73340132
1	-0.61228999	1.55316910	-0.28675441

Energy = -8524.632438 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 13

Atomic N.	X	Y	Z
8	0.22386316	-0.07561548	0.30671294
8	1.89673643	1.43285098	0.42474523
6	3.31568770	1.62211531	0.46591182
1	3.69767824	1.95531070	-0.51338749
1	3.83526891	0.70583292	0.77728074
1	3.49130200	2.41521572	1.20300022
8	2.24915561	-0.79785453	-0.36413450
6	1.33254221	0.28601369	-0.38636739
6	1.00604021	0.85484750	-1.77603709
1	1.89080188	1.35978813	-2.19772218
1	0.26052068	1.63700843	-1.58141276
6	0.45808573	-0.17425847	-2.77684848
1	-0.21844324	-0.86606060	-2.24987024
1	-0.15873941	0.35521402	-3.51935143
6	1.54979341	-0.95379440	-3.52112738
1	2.17876195	-0.23391633	-4.07411728
1	1.08429927	-1.59978141	-4.28251107
6	2.45112298	-1.80723693	-2.62258094
1	1.87719478	-2.63738788	-2.17991599
1	3.24537770	-2.26432573	-3.23690325

6	3.12507580	-1.04116698	-1.48330987
1	3.57781814	-0.10574333	-1.85339252
1	3.93599681	-1.64729341	-1.05413943
50	0.28653843	0.89918135	2.27146872
7	-2.22232207	0.09215915	2.38753454
6	-2.50736354	-0.41032997	3.74749712
1	-3.56974543	-0.69541412	3.85921297
1	-1.87410334	-1.27560820	3.97357262
1	-2.27781613	0.38021584	4.47241974
7	-0.53494008	-2.26363036	1.84199798
6	-2.55603773	-0.91545854	1.34952331
1	-3.65684842	-1.03071881	1.28534230
1	-2.19865402	-0.52761421	0.38665622
6	-1.97508517	-2.31492011	1.58116846
1	-2.22590625	-2.91645988	0.68741970
1	-2.45098861	-2.79621615	2.44489356
16	0.21552438	-3.63809210	2.46918677
7	-0.94988650	2.51232345	1.37628231
6	-2.98288495	1.34742841	2.13734366
1	-4.03728230	1.11222526	1.89325229
1	-2.97168274	1.93678681	3.06414745
6	-2.34217415	2.20182098	1.04137826
1	-2.94301412	3.11813238	0.92884939
1	-2.35893000	1.68050658	0.07077543
16	-0.63874957	3.97388995	2.06792184
8	0.70039065	3.79187300	2.70213343
8	-1.77176882	4.49345028	2.87713629
6	-0.43108715	5.13437182	0.68982467
6	-1.18968643	6.30253039	0.65020345
6	-1.00136975	7.20132556	-0.40467923
6	-0.06599900	6.94658115	-1.41623732
6	0.68590016	5.75881020	-1.34869982
6	0.50995451	4.85256888	-0.30605012
1	-1.91250568	6.49756679	1.44163139
1	1.08957942	3.92968109	-0.25678797
1	1.42092084	5.54479607	-2.12767592
6	0.13221526	7.91340230	-2.55725820
1	-1.59232777	8.11858753	-0.43824541
8	1.61886120	-3.25352988	2.69323169
8	-0.65703643	-4.11990691	3.56004169
6	0.19003011	-4.89265626	1.16563947
6	-0.81163822	-5.86433478	1.15584712
6	-0.81881058	-6.82205039	0.13861283
6	0.15931857	-6.82087102	-0.86662707
6	1.16092956	-5.83482652	-0.82452823
6	1.18396999	-4.87149071	0.18229489
1	-1.55466300	-5.88080059	1.95252128
1	-1.59347530	-7.59101237	0.13323742
6	0.13627522	-7.84439806	-1.97397047
1	1.941111902	-5.82982318	-1.58841021
1	1.97150332	-4.11912207	0.22693147
1	-0.46006859	8.82623190	-2.41585649
1	1.18874969	8.20287854	-2.65409914
1	-0.16648787	7.46190313	-3.51548863
1	1.14841886	-8.19925004	-2.21174560
1	-0.48020586	-8.71176009	-1.70579271
1	-0.28110357	-7.41267749	-2.89701288
1	0.01650900	-1.79801789	1.09751198

Energy = -8524.643128 Hartree
 Number of imaginary frequencies = 0.

Compound I3a isomer 14

Atomic N.	X	Y	Z
8	3.38598039	0.34488878	0.41456774
8	3.63328692	0.55653373	-1.80422598
6	3.84134727	1.41723541	-2.93375989
1	3.20842063	1.02396184	-3.73611959
1	4.89805266	1.39186538	-3.24631994
1	3.53271063	2.44613509	-2.70763145
8	4.09600892	2.35875237	-0.31248672
6	4.21831726	0.95242327	-0.46696015
6	5.64855569	0.39615309	-0.41405245
1	6.22764090	0.74381009	-1.28509568
1	5.52440134	-0.68841188	-0.53021232
6	6.40517144	0.71050511	0.88618914
1	5.70831672	0.62759688	1.73518799
1	7.17145207	-0.06499959	1.03882656
6	7.09568631	2.08027746	0.88534037
1	7.82466768	2.10513731	0.05604457
1	7.68232132	2.19464738	1.81088567
6	6.14736769	3.27537154	0.74125168
1	5.50551312	3.36975739	1.63228113
1	6.74143296	4.20298831	0.68068143
6	5.23762970	3.22091700	-0.48672428
1	5.81105734	2.95290168	-1.39040887
1	4.79214499	4.21005351	-0.66588562
50	1.64625369	-0.30420240	-0.64082983
7	0.66053730	0.46275315	1.63255686
6	1.39207367	-0.06095472	2.80382489
1	1.00732611	0.37176596	3.74587268
1	1.30634097	-1.15275763	2.84381036
1	2.44980120	0.20022591	2.68684158
7	-0.60100180	-2.25214910	1.31127855
6	-0.79743682	0.20144339	1.70244148
1	-1.26777208	0.90109054	2.42182291
1	-1.22113489	0.42583037	0.71175407
6	-1.22389176	-1.20358440	2.13014726
1	-2.32842625	-1.22070938	2.07313277
1	-0.94803623	-1.40016500	3.17388288
16	-1.05420287	-3.86221351	1.62598951
7	0.66268099	1.66014550	-0.88096404
6	0.90595906	1.92729914	1.51413603
1	0.49987665	2.45307161	2.39983401
1	1.99577331	2.05679865	1.48902383
6	0.30113366	2.52310301	0.24216720
1	0.70444374	3.54130055	0.11670005
1	-0.79691111	2.61930258	0.34292406
16	0.01310423	1.97480637	-2.35278289
8	0.61612233	0.94958535	-3.25095677
8	0.08901329	3.41483920	-2.69147230
6	-1.75564179	1.57727293	-2.22667855
6	-2.68474591	2.58990419	-1.98224024
6	-4.03522673	2.25872004	-1.83614339
6	-4.47329667	0.93064838	-1.93974791
6	-3.51760865	-0.06916616	-2.19393508

6	-2.16684676	0.24481593	-2.33701684
1	-2.34863355	3.62505424	-1.92879658
1	-1.42955609	-0.52876578	-2.55589967
1	-3.84035246	-1.10823772	-2.28940346
6	-5.93670398	0.58369989	-1.82155799
1	-4.76251314	3.05043672	-1.64576881
8	-0.29865406	-4.67039678	0.65519656
8	-0.92782358	-4.03596390	3.08483214
6	-2.80878331	-3.99119058	1.20648429
6	-3.77363863	-3.84479245	2.20380892
6	-5.12531421	-3.92629406	1.85740916
6	-5.52320324	-4.15346668	0.53228085
6	-4.52699407	-4.30665781	-0.44940839
6	-3.17508597	-4.22761934	-0.12311580
1	-3.46401934	-3.69423400	3.23748539
1	-5.88388063	-3.81989459	2.63480467
6	-6.98178672	-4.24453697	0.16053441
1	-4.81699630	-4.50407786	-1.48332650
1	-2.40445200	-4.37438975	-0.88006450
1	-6.48626339	1.34695044	-1.25549794
1	-6.40271933	0.51169729	-2.81676536
1	-6.07984748	-0.38649382	-1.32613298
1	-7.20950247	-5.21107718	-0.31207679
1	-7.62786868	-4.13487964	1.04024880
1	-7.25517641	-3.46161062	-0.56255644
1	-0.62597478	-2.08058065	0.30053956

Energy = -8524.636546 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 15

Atomic N.	X	Y	Z
8	3.00692931	0.28635758	0.51470363
8	3.95155126	1.83429616	-0.82009511
6	5.07758691	2.56761659	-1.30925592
1	4.67403516	3.36498609	-1.94607015
1	5.74710179	1.93725347	-1.91704718
1	5.64307827	3.01696716	-0.47896736
8	4.68615342	1.61481911	1.33225203
6	4.22496036	0.84066174	0.21917324
6	5.23190666	-0.21548093	-0.29569921
1	6.24857324	0.20858355	-0.32938024
1	4.93375088	-0.41559435	-1.33672982
6	5.22063822	-1.53927417	0.48177831
1	4.17750744	-1.87216946	0.57740664
1	5.74261842	-2.29824963	-0.12214880
6	5.87734945	-1.47334699	1.86433283
1	6.96572331	-1.32375324	1.74605510
1	5.75332822	-2.44678207	2.36450190
6	5.33662048	-0.36146392	2.77155582
1	4.25196598	-0.47090289	2.92411130
1	5.81104440	-0.45215223	3.76281143
6	5.63358934	1.05013737	2.25578767
1	6.65020690	1.07816956	1.81726739
1	5.62032485	1.76499750	3.09094671
50	1.50216584	0.30437529	-0.93305016
7	0.44665118	2.32265662	0.31737865
6	1.43112218	2.75259311	1.33871787

8	3.28297471	0.31319773	0.40077637
8	3.62831560	0.75546427	-1.76850683
6	3.91110424	1.71588558	-2.79633508
1	4.98431345	1.70626268	-3.04847879
1	3.59714793	2.72326325	-2.49294177
1	3.32403409	1.40857685	-3.66801086
8	4.01941957	2.39059377	-0.08060825
6	4.15097609	1.00544207	-0.37727089
6	5.57927027	0.44347618	-0.31537962
1	6.19767709	0.87675054	-1.11841249
1	5.46239662	-0.62310536	-0.54776890
6	6.27483363	0.62015854	1.04345905
1	5.53949654	0.45350329	1.84644506
1	7.03424874	-0.16958830	1.15121280
6	6.96317263	1.98026128	1.21463615
1	7.72854382	2.08782879	0.42564741
1	7.50769655	1.99677159	2.17235179
6	6.02080645	3.18700089	1.15216969
1	5.34027325	3.19139859	2.01922216
1	6.61596302	4.11395246	1.21344059
6	5.16550690	3.26228422	-0.11357863
1	5.77917614	3.08834063	-1.01396459
1	4.72807917	4.26698399	-0.20822025
50	1.57784825	-0.22434446	-0.77500497
7	0.53227534	0.32471465	1.53581040
6	1.23550289	-0.31542241	2.66643614
1	0.82541505	0.02016020	3.63719479
1	1.15491189	-1.40602142	2.59664920
1	2.29454188	-0.04211546	2.60259569
7	-0.72030914	-2.33717021	0.90552180
6	-0.92620707	0.06210551	1.54540210
1	-1.41409076	0.68483239	2.32198031
1	-1.32743994	0.38765530	0.57330817
6	-1.35357468	-1.38136468	1.82170239
1	-2.45756221	-1.40332211	1.76458193
1	-1.07105719	-1.68130079	2.83870501
16	-0.86528574	-3.99559608	1.26192910
7	0.57597412	1.74823348	-0.83632492
6	0.78448372	1.79251052	1.57317798
1	0.35719064	2.22762704	2.49731891
1	1.87503587	1.91594174	1.58894237
6	0.21745119	2.51786489	0.35231319
1	0.65025516	3.53154411	0.32724210
1	-0.88003259	2.63314992	0.44226476
16	0.13516460	2.31887012	-2.30639243
8	0.71015552	1.34025212	-3.27269058
8	0.41614560	3.76720791	-2.44958732
6	-1.67067690	2.14618342	-2.39980507
6	-2.49114705	3.24301614	-2.13252746
6	-3.87951105	3.08617477	-2.17823810
6	-4.46086907	1.85085867	-2.49790487
6	-3.61082268	0.76341009	-2.76714565
6	-2.22450461	0.90239327	-2.71871376
1	-2.03917236	4.20989218	-1.91307386
1	-1.56625826	0.06426133	-2.95052462
1	-4.04457308	-0.20378946	-3.03007087
6	-5.95886853	1.69815856	-2.59059844
1	-4.52215744	3.94423727	-1.97142501

8	-0.17280894	-4.68175699	0.15908053
8	-0.45955015	-4.13338572	2.67337995
6	-2.62207500	-4.40802134	1.15492180
6	-3.41560227	-4.36487633	2.30235529
6	-4.77385869	-4.67553800	2.19951138
6	-5.34731200	-5.02900722	0.96933901
6	-4.51987341	-5.07361336	-0.16709191
6	-3.16351645	-4.76602776	-0.08427816
1	-2.96517787	-4.11897964	3.26338638
1	-5.39672307	-4.65330155	3.09539519
6	-6.81499791	-5.35661293	0.85981952
1	-4.94370703	-5.36744201	-1.12924219
1	-2.51744460	-4.82990468	-0.95979438
1	-6.47802028	2.47115199	-2.00922132
1	-6.29662058	1.78840842	-3.63487132
1	-6.28567571	0.71358314	-2.22910177
1	-6.97228558	-6.29830227	0.31528926
1	-7.28064626	-5.44923307	1.84881832
1	-7.35242738	-4.57130583	0.30669831
1	-0.91533471	-2.18134693	-0.08732643

Energy = -8524.636615 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 17

Atomic N.	X	Y	Z
8	2.98856900	0.31015635	0.64629334
8	3.89469006	1.94950066	-0.60328850
6	5.00073037	2.73903621	-1.04799458
1	5.54626252	3.16576698	-0.19270377
1	4.57747361	3.55320491	-1.64982039
1	5.69358309	2.15891748	-1.67922498
8	4.61440804	1.65155715	1.54566330
6	4.19066849	0.91650256	0.39200387
6	5.23653990	-0.08088252	-0.16084172
1	6.23856063	0.37784881	-0.16872312
1	4.95169696	-0.24518110	-1.21181322
6	5.26601967	-1.43649811	0.55933155
1	4.23337051	-1.80425217	0.64093646
1	5.80954072	-2.15325893	-0.07624799
6	5.92334320	-1.40856647	1.94286754
1	7.00562941	-1.21664198	1.82976738
1	5.83409511	-2.40639915	2.40055784
6	5.34730225	-0.35607618	2.89773626
1	4.26811863	-0.51155774	3.04970724
1	5.82956393	-0.47071668	3.88272891
6	5.58774323	1.08618136	2.44102719
1	6.60062600	1.17199164	2.00145428
1	5.55047263	1.76409829	3.30568752
50	1.50923597	0.35111718	-0.82853114
7	0.37496433	2.27865045	0.49782542
6	1.31559920	2.66532288	1.57603348
1	0.83569864	3.39192435	2.25690975
1	1.64264853	1.78207904	2.13119360
1	2.21432372	3.10960257	1.13326035
7	0.01508750	-0.50814451	0.56551121
6	-0.85730363	1.67686592	1.06751239
1	-1.28196501	2.33278349	1.85163146

1	-1.58990469	1.57693467	0.25834678
6	-0.60029588	0.27855973	1.63333889
1	-1.57897296	-0.13758851	1.93255152
1	0.02923594	0.31219302	2.53742950
16	0.37617477	-2.08743986	0.81936652
7	-0.96191675	2.29321559	-2.22883405
6	0.10760936	3.49509215	-0.31788587
1	-0.10334356	4.34850579	0.35575823
1	1.04666309	3.73194104	-0.84179045
6	-1.04951433	3.44332235	-1.31628585
1	-1.06148891	4.40650988	-1.85367291
1	-2.00893882	3.37048858	-0.78405034
16	-2.24936181	2.15241338	-3.35903329
8	-1.73950834	1.21688664	-4.37890560
8	-2.77087017	3.48338128	-3.74195616
6	-3.50788374	1.34597426	-2.35115735
6	-4.75852232	1.94891848	-2.22009964
6	-5.74467884	1.30116112	-1.47167915
6	-5.49305190	0.06706559	-0.85470065
6	-4.21940477	-0.51261527	-1.00190418
6	-3.22584206	0.11545249	-1.74934921
1	-4.94575922	2.90931588	-2.69926815
1	-2.24012035	-0.33779390	-1.85285741
1	-3.99896779	-1.46869107	-0.52349870
6	-6.56452435	-0.63743943	-0.06137144
1	-6.72568821	1.76691962	-1.36367062
8	1.39259079	-2.36270654	-0.24987622
8	0.66458177	-2.40913027	2.23534644
6	-1.10086118	-3.03620806	0.36612154
6	-1.97378937	-3.47885797	1.36049576
6	-3.11755839	-4.19537785	0.99396544
6	-3.39564920	-4.48473288	-0.35019514
6	-2.48909858	-4.03917224	-1.32894653
6	-1.34942129	-3.31672994	-0.98078044
1	-1.74148816	-3.28488722	2.40726567
1	-3.79834354	-4.54868228	1.77089436
6	-4.63523580	-5.24832302	-0.74373683
1	-2.67014815	-4.26535176	-2.38164228
1	-0.64024931	-2.98882043	-1.74067234
1	-7.40000916	0.03446062	0.17197241
1	-6.96974832	-1.49070969	-0.62685414
1	-6.16466671	-1.03672756	0.88094470
1	-4.40103445	-6.04803925	-1.46019691
1	-5.12238702	-5.70043945	0.12945504
1	-5.36747743	-4.58626698	-1.23170453
1	-0.09842708	2.26908655	-2.78312732

Energy = -8524.632268 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 18

Atomic N.	X	Y	Z
8	2.80423983	-1.33739876	0.04587763
8	2.97581153	0.88373665	0.16381437
6	3.60213539	2.07711820	0.64636805
1	4.00454965	1.93615005	1.66006294
1	2.81621751	2.84144061	0.65332579
1	4.40425606	2.39758623	-0.03697238

8	4.50831705	-0.51872627	1.30005193
6	3.77344164	-0.39206233	0.08384527
6	4.60626287	-0.35117129	-1.20393186
1	5.23740816	0.55193658	-1.22558057
1	3.86540470	-0.23304570	-2.00533255
6	5.46579233	-1.60290331	-1.44110687
1	4.89266600	-2.49348608	-1.13801098
1	5.64553324	-1.70194517	-2.52286975
6	6.82249944	-1.57067468	-0.72594084
1	7.39460096	-0.70210273	-1.09763308
1	7.40473772	-2.46283151	-1.00720721
6	6.73972917	-1.48603527	0.80209000
1	6.29882607	-2.40575203	1.21913228
1	7.76012952	-1.40813524	1.21419187
6	5.92982178	-0.29957431	1.32786366
1	6.20865855	0.62760431	0.79696987
1	6.14890571	-0.14255347	2.39417866
50	1.08083470	-0.45746674	0.98685095
7	0.01884841	-2.80600227	0.02581757
6	1.15371230	-3.70285033	-0.29382270
1	0.78991656	-4.64475661	-0.74669940
1	1.84436564	-3.20080121	-0.97660369
1	1.71085215	-3.93111985	0.62287879
7	0.05051495	-0.11582610	-0.93188172
6	-0.65781095	-2.39452047	-1.23540751
1	-0.71823860	-3.25842179	-1.92568336
1	-1.68076230	-2.08023244	-0.99138710
6	0.03937481	-1.21077381	-1.90359107
1	-0.53407688	-0.94035512	-2.80599202
1	1.05794485	-1.47678764	-2.23281994
16	0.06099845	1.43042148	-1.48412259
7	-1.55373463	-1.95840141	2.67485659
6	-0.91812913	-3.56746610	0.89283633
1	-1.37673749	-4.38140371	0.29642648
1	-0.31375557	-4.05971121	1.67116949
6	-2.05174629	-2.79472157	1.56762439
1	-2.79046325	-3.53274233	1.92115664
1	-2.56774396	-2.14000084	0.85056271
16	-2.74030519	-1.36503172	3.77221617
8	-2.00115121	-1.19171595	5.03864535
8	-3.96732488	-2.19062697	3.70893750
6	-3.13380761	0.24993901	3.08210248
6	-4.45909513	0.55091887	2.77124818
6	-4.76487660	1.82829743	2.29268590
6	-3.76525611	2.79545194	2.11399593
6	-2.43681636	2.45702013	2.43265718
6	-2.11518548	1.19488444	2.92268008
1	-5.23060746	-0.20566148	2.90978094
1	-1.08370939	0.93722873	3.16267455
1	-1.64039306	3.18491568	2.27220206
6	-4.09197082	4.16747428	1.58334458
1	-5.80059819	2.07438420	2.05161951
8	0.22542880	2.25728333	-0.25241612
8	0.96716357	1.65149133	-2.63743333
6	-1.61970096	1.70967745	-2.11809078
6	-1.79304570	2.19108435	-3.41547417
6	-3.08692409	2.42365190	-3.89045495
6	-4.20962808	2.18258381	-3.08580061

6	-4.00539122	1.69116275	-1.78402138
6	-2.72124859	1.45456918	-1.29638320
1	-0.91671776	2.37378784	-4.03652648
1	-3.22488804	2.79749490	-4.90689473
6	-5.60278555	2.46266473	-3.59222893
1	-4.86595712	1.49002538	-1.14247797
1	-2.57044578	1.07461648	-0.28576336
1	-3.80619489	4.94693690	2.30485047
1	-3.53563809	4.37011746	0.65655135
1	-5.16348088	4.27330237	1.37242776
1	-5.95964893	3.44090137	-3.23358443
1	-5.63434459	2.48277835	-4.68923546
1	-6.31798533	1.70760366	-3.23831292
1	-0.88157793	-2.45244651	3.27112373

Energy = -8524.631692 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 19

Atomic N.	X	Y	Z
8	3.19949515	0.46150400	1.56375720
8	3.33172223	-0.87431070	-0.34403445
6	4.03652350	-0.39669048	-1.50364843
1	3.33901594	-0.46706022	-2.34911904
1	4.91575807	-1.02557162	-1.70768743
1	4.36133673	0.64726443	-1.39031549
8	5.26654564	0.03229294	0.83833123
6	4.00072238	-0.49792172	1.07336328
6	3.94229929	-1.82304335	1.84325362
1	4.36200919	-2.64008928	1.23623633
1	2.87223051	-2.03329618	1.97229596
6	4.63579718	-1.75853193	3.21429487
1	4.43597385	-0.77848683	3.67456344
1	4.17386137	-2.50809491	3.87424611
6	6.14395783	-2.03349672	3.14524217
1	6.29666317	-3.04376598	2.72568914
1	6.55775914	-2.06014951	4.16569442
6	6.94412749	-1.02703552	2.31015948
1	6.95465885	-0.04050523	2.80040573
1	7.99372189	-1.36020056	2.24620765
6	6.42852226	-0.82657980	0.88591792
1	6.23159766	-1.79055498	0.38751423
1	7.17753773	-0.28960281	0.28700031
50	1.52147414	0.61374143	0.28891714
7	0.34883179	-1.80062632	-1.58957496
6	1.02710293	-2.32680575	-2.77895434
1	0.52833329	-3.23431038	-3.17993167
1	1.06363648	-1.56497473	-3.56700953
1	2.05674227	-2.59609673	-2.51066764
7	-0.33225201	0.59783462	-3.03164934
6	-1.05623574	-1.46515529	-1.85498741
1	-1.66578076	-2.37755226	-2.04152256
1	-1.45907390	-0.98412248	-0.95141407
6	-1.27361668	-0.53194205	-3.05126403
1	-2.32503656	-0.19725309	-3.01145651
1	-1.14434332	-1.06884466	-4.00080545
16	-0.73554432	2.01150163	-3.85984839
7	0.31750533	-1.02259918	1.21177160

6	0.47713434	-2.77990371	-0.49649893
1	0.02331725	-3.75519870	-0.78090883
1	1.55409353	-2.94385964	-0.34613447
6	-0.15219171	-2.35185183	0.82963472
1	0.12684555	-3.10940054	1.58271402
1	-1.25466304	-2.37148341	0.74986033
16	-0.27132862	-0.31777697	2.55737653
8	0.34823336	1.06279352	2.43779076
8	-0.08309893	-1.08562733	3.80580671
6	-2.05970343	-0.11350558	2.35026636
6	-2.93260173	-0.84542379	3.15555595
6	-4.31013436	-0.70264793	2.97091025
6	-4.82602428	0.16095375	1.99372729
6	-3.92241743	0.88521993	1.19566543
6	-2.54574785	0.75427094	1.36797771
1	-2.52761180	-1.50656821	3.92080411
1	-1.85475487	1.33254572	0.75281507
1	-4.30086648	1.56152319	0.42661626
6	-6.31382999	0.33397532	1.81832163
1	-4.99568390	-1.27378523	3.59956549
8	0.43249984	2.89617146	-3.70745293
8	-1.25072175	1.58474910	-5.17454420
6	-2.10967052	2.77295639	-2.96013274
6	-3.41942430	2.59492513	-3.40683054
6	-4.46648470	3.18879054	-2.69520547
6	-4.22162186	3.95886570	-1.54928787
6	-2.89019046	4.12170697	-1.12384507
6	-1.83503209	3.53644534	-1.81988134
1	-3.60628162	2.02069346	-4.31372140
1	-5.49197645	3.05899736	-3.04586586
6	-5.34984073	4.62026935	-0.79790787
1	-2.67774001	4.72358399	-0.23818430
1	-0.80289929	3.68500704	-1.50131803
1	-6.86780732	-0.52775585	2.21210128
1	-6.66756810	1.22757113	2.35601946
1	-6.57958974	0.46515317	0.76067340
1	-5.29690013	5.71514643	-0.89417088
1	-6.32791818	4.29693510	-1.17583121
1	-5.30159318	4.39217002	0.27677637
1	0.07821494	0.81450084	-2.11422828

Energy = -8524.624085 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 20

Atomic N.	X	Y	Z
8	2.83365147	-1.28075988	0.08297893
8	2.94477749	0.93394754	0.33472677
6	3.54140077	2.11265933	0.88502428
1	4.32919111	2.49619303	0.21772402
1	3.95502670	1.92214964	1.88602247
1	2.73539523	2.85365147	0.94223783
8	4.53509603	-0.49298262	1.35876073
6	3.77679122	-0.31170212	0.16511591
6	4.58446667	-0.16367154	-1.13089953
1	5.18867801	0.75757502	-1.10426203
1	3.82583243	-0.01541101	-1.91040182
6	5.47615094	-1.37020164	-1.46309725

1	4.93672531	-2.29621103	-1.20800404
1	5.63786195	-1.39426933	-2.55195053
6	6.84431775	-1.33968272	-0.77035518
1	7.38170512	-0.43096224	-1.09485774
1	7.44920336	-2.19263972	-1.11770445
6	6.78672506	-1.35566115	0.76092896
1	6.38277079	-2.31438135	1.12429233
1	7.81157159	-1.27174761	1.16075012
6	5.95043934	-0.23319840	1.37866117
1	6.19116872	0.73755821	0.91078558
1	6.18333475	-0.14520504	2.44982586
50	1.07982179	-0.49608488	1.05074043
7	0.08702343	-2.82065834	-0.00832562
6	1.24700424	-3.68624022	-0.32445385
1	0.91340396	-4.62117976	-0.81335929
1	1.94446783	-3.15092786	-0.97435580
1	1.78496567	-3.93123282	0.59949919
7	0.06888677	-0.09920385	-0.86979330
6	-0.56545573	-2.38350515	-1.27403579
1	-0.58223170	-3.22392687	-1.99481933
1	-1.60328635	-2.10569966	-1.04956871
6	0.11763285	-1.15887185	-1.87988072
1	-0.43633610	-0.87209928	-2.78937802
1	1.15262808	-1.38599994	-2.18614872
16	0.07325189	1.46480136	-1.37207752
7	-1.57735269	-2.06568546	2.60955334
6	-0.85600907	-3.62354797	0.81385127
1	-1.27954842	-4.43247711	0.18563840
1	-0.26189815	-4.12104124	1.59675112
6	-2.02543117	-2.89354983	1.47507937
1	-2.75211812	-3.65785709	1.79635655
1	-2.54175798	-2.23918187	0.75796198
16	-2.80505986	-1.52832880	3.69062311
8	-2.09979091	-1.35928847	4.97678358
8	-4.00598095	-2.38717704	3.58369767
6	-3.22995229	0.08815560	3.02284470
6	-4.55882813	0.36170122	2.70181722
6	-4.89130999	1.64025637	2.24477809
6	-3.91455086	2.63561695	2.09679882
6	-2.58175040	2.32464245	2.42499115
6	-2.23401300	1.06151058	2.89426630
1	-5.31269604	-0.41623839	2.81638879
1	-1.19909346	0.82558629	3.14202355
1	-1.80175396	3.07475545	2.28806969
6	-4.26960418	4.00749771	1.58435573
1	-5.93016857	1.86505820	1.99654611
8	0.17146360	2.25547918	-0.11032169
8	1.02175192	1.73934121	-2.47932765
6	-1.58499707	1.73146753	-2.06767356
6	-1.71400692	2.25611919	-3.35343122
6	-2.99148891	2.47833965	-3.87528317
6	-4.14162102	2.18428572	-3.12897884
6	-3.98176789	1.64997223	-1.83799062
6	-2.71431753	1.42312076	-1.30405882
1	-0.81647997	2.47920585	-3.92938465
1	-3.09471721	2.88579055	-4.88289519
6	-5.51797181	2.45326645	-3.68496023
1	-4.86407369	1.40754775	-1.24180761

1	-2.59755803	1.00942642	-0.30227268
1	-3.95504463	4.78748368	2.29273792
1	-3.75524095	4.21310040	0.63387314
1	-5.34954911	4.10881613	1.41900993
1	-5.90598595	3.41672601	-3.31866935
1	-5.50577540	2.49934879	-4.78161109
1	-6.23346926	1.67823144	-3.37809840
1	-0.90454040	-2.55169421	3.21162192

Energy = -8524.631696 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 21

Atomic N.	X	Y	Z
8	3.16603975	0.48395573	1.65103131
8	3.36920902	-0.77654181	-0.30227179
6	4.08295908	-0.22758342	-1.42429976
1	4.98584313	-0.81966433	-1.63472943
1	4.37210444	0.82000733	-1.25907362
1	3.40634147	-0.28249482	-2.28770389
8	5.25726970	0.12514881	0.95861176
6	3.99845515	-0.43948927	1.14469576
6	3.95184146	-1.79443453	1.86171040
1	4.40121936	-2.57862302	1.23303761
1	2.88407212	-2.03125690	1.95979469
6	4.61552570	-1.76922830	3.24874166
1	4.38637408	-0.81184889	3.74187613
1	4.15553883	-2.55266862	3.86953760
6	6.13006522	-2.01172048	3.20121384
1	6.31180627	-3.00159820	2.74612776
1	6.52341864	-2.07025604	4.22839573
6	6.92634917	-0.95786120	2.42283653
1	6.90694468	0.00867693	2.95117471
1	7.98357792	-1.26767347	2.36802205
6	6.43563149	-0.71166797	0.99697423
1	6.26860344	-1.65884220	0.45718324
1	7.18533827	-0.13662409	0.43543953
50	1.50606373	0.63395072	0.35111851
7	0.43518176	-1.72182576	-1.63623186
6	1.14273114	-2.17341595	-2.83913131
1	0.67495566	-3.07494049	-3.28799517
1	1.16733498	-1.37516848	-3.59074138
1	2.17615113	-2.42624870	-2.56935023
7	-0.30410999	0.71563841	-2.98986590
6	-0.97603631	-1.41496397	-1.90397557
1	-1.55718893	-2.33581683	-2.13440888
1	-1.40174032	-0.98337626	-0.98601862
6	-1.20966810	-0.44096004	-3.06376884
1	-2.27156483	-0.14099961	-3.02211977
1	-1.05423737	-0.93435737	-4.03267733
16	-0.73610398	2.13742826	-3.78977948
7	0.33740097	-1.07035897	1.19143264
6	0.57824546	-2.74579678	-0.58677792
1	0.15844727	-3.72026433	-0.92163013
1	1.65748568	-2.88398032	-0.42717165
6	-0.08342388	-2.39631904	0.74687479
1	0.20940637	-3.17595468	1.47155026
1	-1.18335448	-2.44907185	0.64842704

16	-0.30944796	-0.43152932	2.54371859
8	0.27651053	0.96743926	2.49451642
8	-0.13897031	-1.24244380	3.76718056
6	-2.09551041	-0.26426576	2.28833000
6	-2.97296023	-1.06358122	3.02151215
6	-4.34721678	-0.94814052	2.79760836
6	-4.85561251	-0.04534495	1.85240025
6	-3.94773460	0.74696619	1.12731286
6	-2.57421312	0.64387975	1.33946153
1	-2.57470342	-1.75482924	3.76337108
1	-1.88024390	1.27468003	0.78197123
1	-4.32023751	1.45492975	0.38427421
6	-6.34132802	0.09670421	1.63611584
1	-5.03614023	-1.57205852	3.36988427
8	0.40324809	3.05183536	-3.60114707
8	-1.22058585	1.72524473	-5.12073020
6	-2.14421669	2.83725470	-2.89249926
6	-3.44133321	2.63218599	-3.36370556
6	-4.51601558	3.17728264	-2.65425461
6	-4.31102117	3.92521807	-1.48615033
6	-2.99130511	4.11701065	-1.03671812
6	-1.90886911	3.58051534	-1.73014879
1	-3.59749751	2.07543945	-4.28713390
1	-5.53190657	3.02627680	-3.02383403
6	-5.46938109	4.53198636	-0.73453844
1	-2.81006865	4.70302841	-0.13364491
1	-0.88644026	3.75182278	-1.39234401
1	-6.88112403	-0.80622336	1.94912476
1	-6.74085005	0.93949307	2.22166458
1	-6.57506331	0.29424025	0.58127124
1	-5.44063018	5.63059316	-0.78856589
1	-6.43173362	4.20038932	-1.14426609
1	-5.43723174	4.26436501	0.33167275
1	0.07932980	0.91872616	-2.05779474

Energy = -8524.624090 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 22

Atomic N.	X	Y	Z
8	-0.34218984	-0.28898683	0.19753944
8	1.79992835	-0.19732006	-0.54105177
6	3.12082981	-0.42447529	-0.01107756
1	3.65773195	-0.94224884	-0.81570320
1	3.09866913	-1.05264695	0.88860114
1	3.62326906	0.52345360	0.22185330
8	1.32391691	0.54450882	1.59333911
6	0.77522815	0.50044890	0.28647110
6	0.49901070	1.87425141	-0.35167722
1	-0.48366701	2.21381504	0.01227933
1	0.37084821	1.66554157	-1.42268037
6	1.54412661	2.97563235	-0.12635618
1	2.56221429	2.56412379	-0.21572383
1	1.44562389	3.71482282	-0.93703062
6	1.37885248	3.70661256	1.21421672
1	0.35713922	4.12322323	1.25480533
1	2.06293843	4.56948949	1.24893465
6	1.61012258	2.83809777	2.45601111

1	2.67598049	2.56972726	2.54070231
1	1.36141925	3.42103205	3.35912941
6	0.80270441	1.54097029	2.49559950
1	-0.26796497	1.71967354	2.30091726
1	0.88059784	1.08425124	3.49235507
50	0.18845194	-2.14000715	-0.81719851
7	-2.38061954	-2.27171199	-1.14588113
6	-2.50702665	-3.49683545	-1.97102674
1	-3.51807222	-3.57655587	-2.40943601
1	-1.76791581	-3.49671012	-2.78117332
1	-2.32631406	-4.37216312	-1.33522129
7	-0.34143771	-1.18794075	-2.76197083
6	-2.64530741	-1.05510744	-1.95467582
1	-3.70041605	-1.04034819	-2.29289323
1	-2.47135402	-0.18839823	-1.30449657
6	-1.72868253	-0.95480494	-3.17565945
1	-1.85803105	0.05780473	-3.59963680
1	-2.03795890	-1.67204469	-3.95364797
16	0.72930978	-1.60770243	-3.94116535
7	-2.29866604	-1.14023146	1.96569197
6	-3.35715256	-2.39966705	-0.02622016
1	-4.37150000	-2.48513971	-0.46747369
1	-3.14806590	-3.35338421	0.47716490
6	-3.42539143	-1.28773181	1.03253049
1	-4.32763493	-1.49363164	1.62551820
1	-3.56637715	-0.30043771	0.57081345
16	-1.96499015	-2.49751747	2.92354654
8	-0.93239064	-3.35479366	2.28802835
8	-3.27562169	-3.07678996	3.29629838
6	-1.21563738	-1.75170535	4.38440008
6	-2.03861729	-1.18660527	5.36214153
6	-1.45487625	-0.64297273	6.50405125
6	-0.06026956	-0.65915638	6.68560098
6	0.73775769	-1.23632632	5.68708317
6	0.16969557	-1.78642226	4.53518705
1	-3.11988174	-1.18832538	5.22822785
1	0.78577159	-2.24281429	3.76145817
1	1.82199104	-1.25788181	5.81068086
6	0.55470936	-0.09235467	7.94057858
1	-2.09171469	-0.20173484	7.27305743
8	1.91233885	-2.11728029	-3.18669812
8	0.11324088	-2.44960101	-4.99812429
6	1.22758335	-0.06285850	-4.74747950
6	0.87594277	0.17022686	-6.07592138
6	1.26971902	1.36602298	-6.68475688
6	2.01159183	2.32661951	-5.98422259
6	2.35246456	2.06265609	-4.64471087
6	1.96685707	0.87761373	-4.02253990
1	0.31179407	-0.58579698	-6.62090744
1	0.99803990	1.55149289	-7.72568541
6	2.45318448	3.60715645	-6.64825416
1	2.93215579	2.79874475	-4.08340983
1	2.23163428	0.67328945	-2.98448825
1	0.41478865	-0.77994684	8.78896903
1	1.63307134	0.07188317	7.82058158
1	0.08715134	0.86221777	8.21922750
1	3.54456251	3.62018929	-6.79079605
1	1.98524005	3.72973167	-7.63322386

1 2.19874935 4.48364294 -6.03509688
 1 -1.43320366 -0.81185209 1.48180092
 Energy = -8524.640851 Hartree
 Number of imaginary frequencies = 0.

Compound I3a isomer 23

Atomic N.	X	Y	Z
8	2.77426569	-2.04143667	0.28893903
8	3.81121392	-0.51864310	1.52327308
6	4.92256121	0.29381466	1.93827140
1	4.47440252	1.15151632	2.45287306
1	5.51568766	0.62826463	1.07748641
1	5.55728459	-0.26260150	2.64429441
8	4.82392619	-1.16656139	-0.41109393
6	4.03343981	-1.69316024	0.66946600
6	4.72337737	-2.84463980	1.44243958
1	4.26196813	-3.77814401	1.08505374
1	4.41166961	-2.73486533	2.49163277
6	6.25157629	-2.97122959	1.34307246
1	6.73751399	-1.99708536	1.50663891
1	6.58440680	-3.62199617	2.16786935
6	6.74545348	-3.57999273	0.02075444
1	6.19512572	-4.52050600	-0.15897084
1	7.80573992	-3.86056720	0.12711461
6	6.60015376	-2.66685464	-1.20190856
1	7.28341493	-1.80670866	-1.10881006
1	6.90555366	-3.21475760	-2.10987859
6	5.19092867	-2.12223073	-1.42163874
1	4.44103791	-2.93039209	-1.46688093
1	5.14350609	-1.57711026	-2.37645959
50	1.69889777	-0.15307310	0.22687671
7	-0.21691923	-1.96019714	-0.03224707
6	0.13260999	-2.91401677	-1.10452438
1	-0.56086070	-3.77629108	-1.11333654
1	0.09459344	-2.41748096	-2.08144847
1	1.15758662	-3.26422193	-0.93863631
7	-1.30517638	0.75960854	-1.19241828
6	-1.60791132	-1.47654098	-0.18542287
1	-2.28675194	-2.35086120	-0.25418070
1	-1.88058381	-0.93355254	0.73002490
6	-1.89237874	-0.57184042	-1.38513484
1	-2.99000760	-0.53031094	-1.50972241
1	-1.47278662	-0.98568091	-2.31093061
16	-1.25610305	1.80917783	-2.53024911
7	0.65664251	-0.48491262	2.15413862
6	-0.07278554	-2.62823929	1.29209029
1	-0.83038383	-3.42827814	1.40560226
1	0.92690804	-3.08054560	1.29894827
6	-0.18078934	-1.64156745	2.45769243
1	0.15649817	-2.15700767	3.37212948
1	-1.23562826	-1.35244346	2.63230913
16	0.67934281	0.76976260	3.20624509
8	1.76201177	1.66296801	2.70884341
8	0.65477162	0.30771180	4.61331472
6	-0.87987778	1.66810834	2.94067203
6	-1.99020955	1.39569425	3.74194798
6	-3.19833282	2.05283245	3.48678083

6	-3.31106877	2.99030924	2.45022086
6	-2.17430575	3.25383893	1.66390429
6	-0.96449799	2.60029192	1.90006743
1	-1.89522609	0.69361934	4.57006917
1	-0.08454312	2.82184200	1.29493498
1	-2.22774746	3.99618316	0.86447973
6	-4.60269874	3.73219961	2.21014972
1	-4.06573948	1.84109490	4.11525936
8	-0.73091701	3.07641946	-1.99275140
8	-0.59130254	1.05598851	-3.60878329
6	-2.96814685	2.09086739	-3.04449937
6	-3.52942095	1.29463364	-4.04483578
6	-4.85666156	1.51194833	-4.42093271
6	-5.62842069	2.51587058	-3.81646954
6	-5.03464348	3.30471148	-2.81576370
6	-3.71184124	3.10063911	-2.42659268
1	-2.92287713	0.53273949	-4.53327879
1	-5.29801974	0.89462182	-5.20538398
6	-7.04898685	2.76972541	-4.25299681
1	-5.61626912	4.09797020	-2.34226759
1	-3.24464750	3.73071562	-1.67010745
1	-5.46092197	3.19049008	2.62850191
1	-4.57627981	4.72586954	2.68401152
1	-4.78206442	3.89184718	1.13782730
1	-7.08922217	3.59296073	-4.98318670
1	-7.48682861	1.88409197	-4.73088014
1	-7.68425615	3.05765735	-3.40467243
1	-1.66902893	1.26793885	-0.37892649

Energy = -8524.634985 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 24

Atomic N.	X	Y	Z
8	0.46384453	0.19352851	0.59636080
8	1.99288369	-1.01298984	-0.45791879
6	3.28823102	-1.31143732	-0.99536356
1	3.98228126	-1.58075091	-0.18646310
1	3.67964616	-0.46940524	-1.58307666
1	3.14138605	-2.16578780	-1.66456671
8	2.38392192	-0.51980745	1.71673050
6	1.83567858	0.04213447	0.52742225
6	2.50104024	1.37346282	0.09539879
1	1.87983069	2.17631487	0.52151134
1	2.36726721	1.44461420	-0.99444890
6	3.96780186	1.62589710	0.48267545
1	4.58675097	0.73657427	0.29242213
1	4.35439543	2.41415683	-0.18270847
6	4.15807923	2.08110332	1.93681752
1	3.50953388	2.95615621	2.11932260
1	5.19324244	2.43234059	2.07464847
6	3.85505838	1.00398914	2.98313956
1	4.60521743	0.19817051	2.92446318
1	3.93729470	1.43765723	3.99446764
6	2.47418917	0.36598792	2.85228920
1	1.67939110	1.12960819	2.80838438
1	2.27020785	-0.26615217	3.72878928
50	-0.46838816	-0.98292814	-0.96728761

7	-2.40401697	0.71453902	-0.51795142
6	-3.37287358	0.36780920	-1.58309646
1	-4.14636204	1.15015933	-1.68794124
1	-2.85574465	0.24388076	-2.54165999
1	-3.86073716	-0.58006639	-1.32435912
7	-0.31878039	0.75505192	-2.34084294
6	-1.73607978	2.01033863	-0.80590881
1	-2.47215535	2.83779270	-0.77182372
1	-0.98743615	2.16767023	-0.02003861
6	-1.03369947	2.01794842	-2.16798525
1	-0.34817360	2.88190675	-2.19185150
1	-1.77557766	2.17211349	-2.97416422
16	0.61513615	0.55333776	-3.67082132
7	-1.45402043	0.11398940	2.57875211
6	-3.17010485	0.76852644	0.76010244
1	-3.96541367	1.53474500	0.65121714
1	-3.67525197	-0.20047563	0.87347204
6	-2.42490239	1.09028419	2.06502412
1	-3.20504023	1.22501609	2.82765767
1	-1.88392573	2.04447807	1.99281514
16	-2.06921521	-1.43351635	2.89137596
8	-1.86723979	-2.31515868	1.71137322
8	-3.42859890	-1.24856512	3.44840989
6	-0.97247727	-2.02300969	4.19332468
6	-1.35623027	-1.86754228	5.52634474
6	-0.51488452	-2.34583674	6.53048123
6	0.70232506	-2.97416222	6.21949504
6	1.05966387	-3.11180335	4.86865193
6	0.22847946	-2.64570237	3.84929346
1	-2.30619559	-1.38929335	5.76253155
1	0.51070478	-2.75627219	2.80281911
1	2.00442799	-3.59189089	4.60759531
6	1.58978817	-3.51687907	7.31142842
1	-0.80932155	-2.23143574	7.57530746
8	1.52465674	1.70481922	-3.89124595
8	1.17670196	-0.81927018	-3.51418714
6	-0.50796164	0.51428219	-5.09513018
6	-1.27194651	-0.63349312	-5.33174654
6	-2.15120000	-0.65694070	-6.41200575
6	-2.28519468	0.45373027	-7.26525751
6	-1.50798910	1.59060009	-7.00489402
6	-0.61791938	1.62827634	-5.92696014
1	-1.15776485	-1.50356316	-4.68433433
1	-2.74148583	-1.55539963	-6.60350925
6	-3.22699767	0.40508137	-8.44257202
1	-1.59368601	2.46070759	-7.65859963
1	0.00277457	2.50299407	-5.73560501
1	1.50723659	-2.92032270	8.22962939
1	1.30549942	-4.54983258	7.56647280
1	2.64268957	-3.53459852	7.00104535
1	-2.85108170	-0.27994262	-9.21785829
1	-4.22008769	0.03925803	-8.14500458
1	-3.34787131	1.39490109	-8.90060902
1	-0.61322442	0.03829828	1.96033447

Energy = -8524.640848 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 25

Atomic N.	X	Y	Z
8	2.84597947	-1.95003088	0.24441589
8	3.76315820	-0.52228834	1.67215143
6	4.81856911	0.29191331	2.21156722
1	5.45606842	-0.30593548	2.88022358
1	4.31155585	1.06946327	2.79438241
1	5.42270355	0.74162199	1.41324546
8	4.87430543	-0.91566606	-0.27679860
6	4.07244114	-1.58863706	0.71024702
6	4.78942445	-2.78378750	1.38606627
1	4.38483178	-3.69390993	0.91702999
1	4.43847848	-2.79833433	2.42851521
6	6.32437579	-2.83233882	1.33270986
1	6.75762514	-1.86065410	1.61558684
1	6.65962863	-3.55160029	2.09745110
6	6.89100681	-3.27561039	-0.02576983
1	6.39159812	-4.21438532	-0.32412773
1	7.95894744	-3.52033892	0.09184471
6	6.74524561	-2.24485971	-1.15100601
1	7.38402363	-1.37101761	-0.94192915
1	7.10674458	-2.67968134	-2.09869110
6	5.32046307	-1.74103532	-1.36733899
1	4.61138137	-2.57127279	-1.52668170
1	5.28028482	-1.09939178	-2.26050435
50	1.69037651	-0.11133521	0.32393488
7	-0.12680799	-1.95402134	-0.21576871
6	0.31409731	-2.77805956	-1.35953770
1	-0.34173998	-3.65926556	-1.49297254
1	0.30399378	-2.18446222	-2.28140441
1	1.34326954	-3.10606963	-1.17561777
7	-1.27538333	0.81648592	-1.18143453
6	-1.52909940	-1.51112823	-0.38925650
1	-2.16706684	-2.40064868	-0.56735144
1	-1.86282248	-1.06487091	0.55769892
6	-1.80138534	-0.51263032	-1.51501196
1	-2.89418817	-0.49998289	-1.68157855
1	-1.33053347	-0.82646853	-2.45529520
16	-1.21894079	1.98255510	-2.41878501
7	0.58027315	-0.68325230	2.15497625
6	-0.01623055	-2.74916583	1.03994188
1	-0.74154197	-3.58625243	1.03190714
1	1.00142633	-3.15934083	1.05381706
6	-0.22502104	-1.89339885	2.29195462
1	0.08410871	-2.48851697	3.16700944
1	-1.29852515	-1.66159235	2.43384983
16	0.48761966	0.46051085	3.32349819
8	1.56225579	1.43515296	2.98862092
8	0.39379312	-0.14116308	4.67369840
6	-1.08588362	1.33008978	3.04418815
6	-2.23166974	0.94796125	3.74419093
6	-3.44591183	1.58822539	3.47492698
6	-3.53082737	2.61579088	2.52484494
6	-2.35916484	2.98859405	1.84030651
6	-1.14235237	2.35413473	2.09158110
1	-2.16083194	0.17361311	4.50779657
1	-0.23621594	2.66000638	1.56719928
1	-2.39178237	3.80124964	1.11122661

6	-4.83238226	3.33588268	2.27235903
1	-4.34110173	1.29082938	4.02482260
8	-0.76394081	3.21510217	-1.75219566
8	-0.48618789	1.35271475	-3.53184480
6	-2.92116795	2.24683929	-2.97295204
6	-3.41898196	1.51370135	-4.05187263
6	-4.74045396	1.71426049	-4.45732368
6	-5.56872327	2.63944716	-3.80445047
6	-5.03764749	3.36757094	-2.72528636
6	-3.72193501	3.17912404	-2.30610961
1	-2.76884595	0.81451525	-4.57670647
1	-5.13233475	1.14632256	-5.30295029
6	-6.98428219	2.87579375	-4.26646453
1	-5.66325967	4.10085844	-2.21274335
1	-3.30348340	3.76346508	-1.48696220
1	-5.69219835	2.73958170	2.60407405
1	-4.86224010	4.29187624	2.81801935
1	-4.96292773	3.56998095	1.20657657
1	-7.04663038	3.79012371	-4.87666798
1	-7.35120471	2.04302144	-4.87961307
1	-7.66626319	3.00788531	-3.41549759
1	-1.68993553	1.23613636	-0.34195470

Energy = -8524.634945 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 26

Atomic N.	X	Y	Z
8	3.33754721	1.41411577	0.24581506
8	3.08276019	3.64387907	0.33436921
6	3.41595211	4.97668162	-0.05778456
1	2.72159277	5.63431767	0.48185137
1	3.28948383	5.12682631	-1.14068730
1	4.44561148	5.24318021	0.23336208
8	3.24244386	2.70309993	-1.71697687
6	3.73862783	2.56931880	-0.38095142
6	5.29045841	2.65877791	-0.27598644
1	5.65376424	1.62183971	-0.23065740
1	5.50143973	3.09022618	0.71400300
6	6.07037140	3.41005891	-1.36783482
1	5.60884415	4.38376769	-1.59074700
1	7.07127261	3.63200747	-0.96218413
6	6.24266677	2.61804864	-2.67223220
1	6.66125233	1.62539339	-2.43024462
1	6.99162311	3.12188038	-3.30469835
6	4.95222240	2.43855183	-3.47721932
1	4.60823337	3.41392083	-3.86014873
1	5.15147433	1.80752085	-4.35977180
6	3.80132471	1.80526836	-2.70060572
1	4.10827535	0.86031537	-2.22164873
1	2.97410055	1.56936280	-3.38447969
50	1.84877976	-0.04316606	0.26368675
7	0.00530939	1.67266066	0.85982686
6	0.44768830	2.47756130	2.02021457
1	-0.24593848	3.31926435	2.20186805
1	0.49020598	1.85179095	2.91991280
1	1.45118226	2.87020374	1.81586245
7	-0.99035716	-1.24400245	1.54175473

6	-1.36445383	1.14643096	1.07066456
1	-2.02057899	1.98135330	1.38655907
1	-1.74418224	0.79255700	0.10206314
6	-1.50974596	0.01618898	2.09011622
1	-2.57934827	-0.05435484	2.35899971
1	-0.95131686	0.22980377	3.01069433
16	-0.81482194	-2.56332606	2.60907547
7	0.69080528	0.49711326	-1.53155854
6	0.02891524	2.51408675	-0.37290365
1	-0.75519036	3.29385629	-0.31719948
1	1.00917309	3.00797775	-0.39742854
6	-0.15070310	1.68391725	-1.64734347
1	0.14964183	2.31158573	-2.50208162
1	-1.21377006	1.41473426	-1.80347375
16	0.77765659	-0.56751052	-2.77317429
8	1.90362659	-1.46873050	-2.39623201
8	0.75596489	0.11419793	-4.08894643
6	-0.73678863	-1.56549037	-2.68907861
6	-1.83714888	-1.22930668	-3.47971406
6	-3.01302599	-1.97771955	-3.36932257
6	-3.10215925	-3.06546859	-2.48857889
6	-1.97602779	-3.38633532	-1.70903549
6	-0.79744121	-2.64576226	-1.80194573
1	-1.75851554	-0.40443511	-4.18747995
1	0.07435847	-2.91392804	-1.20414945
1	-2.01076410	-4.24047210	-1.02934757
6	-4.35678549	-3.89957806	-2.40977300
1	-3.87293061	-1.71736073	-3.98968092
8	-0.39875382	-3.68380415	1.74751596
8	0.00012214	-2.06596507	3.73108634
6	-2.46182679	-2.93694954	3.25590199
6	-2.85869682	-2.40030062	4.48213410
6	-4.13725029	-2.68640658	4.96577858
6	-5.02147864	-3.50286374	4.24467392
6	-4.59212073	-4.03140584	3.01451345
6	-3.32013607	-3.75618018	2.51609247
1	-2.16324183	-1.78725982	5.05437756
1	-4.45006595	-2.27342130	5.92635988
6	-6.38715401	-3.83697600	4.78865671
1	-5.26254294	-4.67719529	2.44436457
1	-2.98040553	-4.18800094	1.57489933
1	-5.23597825	-3.33685519	-2.74957289
1	-4.27111150	-4.79374482	-3.04675677
1	-4.54315019	-4.25082396	-1.38550477
1	-6.38347840	-4.83112250	5.26197808
1	-6.70624667	-3.11113071	5.54725126
1	-7.14170910	-3.86139883	3.99085421
1	-1.47743029	-1.56489157	0.69800375

Energy = -8524.628249 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 27

Atomic N.	X	Y	Z
8	0.79473646	0.04788861	0.62605609
8	0.62633937	-0.75213666	-1.55386457
6	-0.35942312	-1.77925380	-1.34724579
1	-1.07775086	-1.68270416	-2.17240505

1	-0.87621482	-1.64504674	-0.38438333
1	0.10018684	-2.77564430	-1.37588618
8	1.92518798	-1.83371743	-0.02725970
6	1.50801796	-0.52510988	-0.40583771
6	2.65300493	0.34927010	-0.95398408
1	3.14851478	0.83347576	-0.09698555
1	2.18868997	1.15426174	-1.54300136
6	3.70966273	-0.38600889	-1.79229059
1	3.22006637	-1.13587340	-2.43300874
1	4.18052158	0.34310359	-2.46949094
6	4.81078633	-1.03767066	-0.94035233
1	5.25685707	-0.25881920	-0.29763400
1	5.62055971	-1.39034261	-1.59907852
6	4.34502687	-2.20570519	-0.06181461
1	4.11255291	-3.08025267	-0.69140885
1	5.16533013	-2.50923962	0.61067289
6	3.10997748	-1.91480867	0.78969472
1	3.22544063	-1.00372568	1.39922499
1	2.93239894	-2.74948120	1.48436233
50	0.78266613	2.06993024	1.24154792
7	-1.82865482	2.69301426	1.19950416
6	-1.83241753	4.03684421	1.81264879
1	-2.86117749	4.38275151	2.02340022
1	-1.26458746	4.02773892	2.75113249
1	-1.35199444	4.74479118	1.12659918
7	-0.26782485	1.34974963	3.04463261
6	-2.45334732	1.69650804	2.10105173
1	-3.49835852	1.98525752	2.32976562
1	-2.47155280	0.73490197	1.56962975
6	-1.66852182	1.51928280	3.40168360
1	-2.07038573	0.62749378	3.91524645
1	-1.82479346	2.37539275	4.08009876
16	0.84972269	1.03948233	4.19423251
7	-0.77419572	1.74401986	-1.55155885
6	-2.53228322	2.74204867	-0.10455728
1	-3.62770058	2.73193134	0.06165020
1	-2.28152809	3.69120990	-0.59428250
6	-2.15795114	1.61253978	-1.06488159
1	-2.88921930	1.60797458	-1.89145070
1	-2.23111251	0.63184281	-0.57406692
16	-0.53138167	2.63461688	-2.97535888
8	0.92803651	2.64797411	-3.17863937
8	-1.31589820	3.88016795	-2.84068594
6	-1.27239572	1.66986703	-4.31377090
6	-2.45720379	2.10571750	-4.90644987
6	-3.01403070	1.35174056	-5.94382282
6	-2.40335316	0.17239875	-6.39191330
6	-1.20692538	-0.23929711	-5.77561982
6	-0.63606571	0.49887377	-4.74206999
1	-2.91869414	3.03279152	-4.56810109
1	0.29594144	0.17880706	-4.27488140
1	-0.71213511	-1.15025863	-6.11777854
6	-3.00636670	-0.64253652	-7.50818789
1	-3.93699930	1.69208747	-6.41650274
8	2.13080331	1.20909467	3.42038887
8	0.66047896	1.80440946	5.44843811
6	0.68498187	-0.71191484	4.62321809
6	0.64826257	-1.08892952	5.96557446

6	0.53485114	-2.44418526	6.28553284
6	0.45732026	-3.42139318	5.28231768
6	0.48691347	-3.00680274	3.93884674
6	0.60121850	-1.65961197	3.59852465
1	0.70287104	-0.32433418	6.73969354
1	0.50350003	-2.74596921	7.33419755
6	0.36580398	-4.88574304	5.63264109
1	0.41909799	-3.75290912	3.14416885
1	0.62015907	-1.33848835	2.55368938
1	-3.88552027	-0.14630448	-7.93760055
1	-2.27825379	-0.80908231	-8.31511237
1	-3.31862354	-1.63425036	-7.14785144
1	1.35670330	-5.36289523	5.57512107
1	-0.01161756	-5.03213576	6.65297809
1	-0.29305161	-5.42420321	4.93780637
1	-0.26367934	0.83553314	-1.61489572

Energy = -8524.642724 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 28

Atomic N.	X	Y	Z
8	3.32092539	1.43381845	0.29929525
8	3.03776429	3.65208110	0.50952008
6	3.35145853	5.00839158	0.18886429
1	3.21449574	5.21632850	-0.88318048
1	4.38004757	5.27166899	0.48665175
1	2.65351115	5.62657237	0.76902333
8	3.19451688	2.82500641	-1.59053447
6	3.70229103	2.62624534	-0.26685693
6	5.25346093	2.73110586	-0.16795218
1	5.63096701	1.69833889	-0.18135824
1	5.46652226	3.11139182	0.84237498
6	6.01472041	3.55103637	-1.22300434
1	5.53797761	4.52857687	-1.39002562
1	7.01542585	3.76511854	-0.81266995
6	6.18827542	2.83288887	-2.56927378
1	6.62289115	1.83494858	-2.38399434
1	6.92507186	3.38095702	-3.17881399
6	4.89437884	2.67804724	-3.37390161
1	4.53415848	3.66740385	-3.70214702
1	5.09572063	2.09758851	-4.29005527
6	3.75806202	1.98834455	-2.62434485
1	4.08113245	1.02379436	-2.19809911
1	2.92908771	1.77752306	-3.31424057
50	1.84560887	-0.03716159	0.25843677
7	-0.01538780	1.62766517	0.94270163
6	0.42231674	2.38188854	2.13831948
1	-0.27846049	3.20790145	2.36002861
1	0.47231736	1.71540621	3.00791981
1	1.42171028	2.79286510	1.95061792
7	-0.97608440	-1.33212763	1.47763744
6	-1.37758999	1.07526669	1.13392061
1	-2.04136705	1.88506917	1.49581811
1	-1.75918592	0.76647630	0.15076103
6	-1.50270817	-0.10735159	2.09509335
1	-2.56887598	-0.20290399	2.36975880
1	-0.93740730	0.06434153	3.02026862

16	-0.76973078	-2.70109954	2.47460012
7	0.66949521	0.57271117	-1.50252635
6	-0.00690360	2.52684907	-0.24877208
1	-0.79940037	3.29416820	-0.15298896
1	0.96762897	3.03247467	-0.25367773
6	-0.18289527	1.75590110	-1.56035913
1	0.10899195	2.42568482	-2.38555815
1	-1.24395203	1.48447710	-1.72604066
16	0.77298495	-0.42390509	-2.79800638
8	1.91052311	-1.32841167	-2.46598813
8	0.74474035	0.32507023	-4.07666128
6	-0.72782918	-1.44533707	-2.77093992
6	-1.82773808	-1.08751404	-3.55240299
6	-2.99324084	-1.85719446	-3.48607925
6	-3.07233433	-2.98635593	-2.65824729
6	-1.94692539	-3.32746197	-1.88610813
6	-0.77860827	-2.56692441	-1.93585859
1	-1.75645376	-0.22876305	-4.21947047
1	0.09302829	-2.85074134	-1.34508407
1	-1.97402649	-4.21292675	-1.24736504
6	-4.31517535	-3.84100408	-2.62742236
1	-3.85270044	-1.58033019	-4.09987708
8	-0.35534978	-3.77225296	1.55166206
8	0.05793964	-2.25118993	3.60713999
6	-2.40259978	-3.12421102	3.12658850
6	-2.78204415	-2.66089838	4.38723305
6	-4.04875673	-2.98831477	4.87729932
6	-4.93859924	-3.77066183	4.12687040
6	-4.52398668	-4.23096681	2.86404961
6	-3.26494222	-3.91390649	2.35904694
1	-2.08071809	-2.07678507	4.98210206
1	-4.34589381	-2.63742436	5.86702544
6	-6.30862538	-4.11414575	4.65397660
1	-5.19482684	-4.85872072	2.27449899
1	-2.93515600	-4.29545283	1.39289510
1	-5.19603648	-3.28229029	-2.96936578
1	-4.20307488	-4.71623743	-3.28619110
1	-4.51636873	-4.22295296	-1.61694484
1	-6.51879677	-5.18741927	4.54543622
1	-6.40939186	-3.84867143	5.71359274
1	-7.08963500	-3.57509249	4.09627102
1	-1.47036526	-1.61628449	0.62508851

Energy = -8524.628244 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 29

Atomic N.	X	Y	Z
8	3.14647024	1.92260942	1.64575075
8	1.81538957	2.14321835	-0.23244463
6	2.16319081	3.30401454	-1.00920485
1	2.60204750	3.01130091	-1.97109810
1	2.84326671	3.97156936	-0.45630511
1	1.22164126	3.83359039	-1.20224802
8	2.31065995	0.10089990	0.46583509
6	2.94803060	1.37708578	0.42285963
6	4.23958690	1.37974206	-0.40788783
1	5.04512596	1.11940322	0.29485520

1	4.44829006	2.41651752	-0.70316427
6	4.26916602	0.43629277	-1.61999980
1	3.29569652	0.44244255	-2.13522129
1	5.00409255	0.82435066	-2.34265812
6	4.67311352	-1.00036548	-1.24912321
1	5.64221120	-0.96035988	-0.72183276
1	4.85000474	-1.57718198	-2.17083731
6	3.66018152	-1.75579490	-0.37885563
1	2.77214800	-2.01559496	-0.97840969
1	4.10314110	-2.70862089	-0.04285952
6	3.17518570	-0.99325462	0.85176264
1	3.99919325	-0.62236515	1.48011980
1	2.56632348	-1.64834216	1.48957952
50	1.41340428	2.97463631	2.23551335
7	-1.45125475	2.83188599	1.39241803
6	-1.72648697	4.26561377	1.59573229
1	-2.81541768	4.46894708	1.62360115
1	-1.28340312	4.61448327	2.53707506
1	-1.27966268	4.84611720	0.77821203
7	0.28197424	1.59899874	3.47519495
6	-1.96980273	2.04776860	2.53413798
1	-2.99011320	2.39395038	2.80133494
1	-2.04804249	0.99712032	2.22926533
6	-1.06697044	2.11070419	3.76934634
1	-1.52809936	1.52953632	4.58153681
1	-1.00298426	3.14491210	4.15032004
16	0.79163735	0.29535705	4.38179847
7	-0.59869380	0.86398533	-1.24855277
6	-2.11570056	2.42103580	0.12856470
1	-3.21550985	2.48200528	0.27408397
1	-1.86241812	3.15287684	-0.64916172
6	-1.78354026	1.01314746	-0.39825892
1	-2.65076149	0.66233722	-0.97662303
1	-1.67031028	0.30015969	0.43114394
16	-0.71624842	1.32213895	-2.86399658
8	0.67952925	1.44655600	-3.33644696
8	-1.67498135	2.43891592	-3.04951435
6	-1.46232133	-0.13167830	-3.63448013
6	-2.69772873	-0.01641054	-4.26902416
6	-3.24352863	-1.13796261	-4.90072512
6	-2.56820023	-2.36589033	-4.90895749
6	-1.32210511	-2.45033963	-4.25993264
6	-0.76476774	-1.34391968	-3.62516798
1	-3.21450789	0.94256538	-4.26699613
1	0.20268327	-1.41081158	-3.12784477
1	-0.78153082	-3.39877434	-4.25673851
6	-3.14697535	-3.56857923	-5.61076454
1	-4.21110803	-1.05319061	-5.39853643
8	2.21653126	0.09520538	4.05127442
8	0.36753938	0.45403399	5.79413682
6	-0.15196746	-1.12142667	3.74197546
6	-0.88067253	-1.91300402	4.63000465
6	-1.58378998	-3.01744348	4.14073960
6	-1.56796130	-3.34262577	2.77667732
6	-0.83148225	-2.52217011	1.90394573
6	-0.12438749	-1.41640075	2.37566989
1	-0.89154263	-1.65569885	5.68859470
1	-2.15623540	-3.63673993	4.83409229

6	-2.30083015	-4.55532350	2.25917619
1	-0.81242150	-2.75322996	0.83657381
1	0.44250422	-0.78248889	1.69085450
1	-4.19111206	-3.39934325	-5.90216549
1	-2.57690511	-3.80035208	-6.52340710
1	-3.10706223	-4.46180014	-4.97144739
1	-1.62074711	-5.41810263	2.18186580
1	-3.12249555	-4.84347684	2.92770681
1	-2.71394564	-4.37721383	1.25709138
1	0.30677367	1.17824557	-0.85952900

Energy = -8524.613554 Hartree
Number of imaginary frequencies = 0.

Compound I3a isomer 30

Atomic N.	X	Y	Z
8	4.81622146	-0.50668496	-2.02915883
8	5.09876868	0.59970722	-0.10305341
6	5.31044721	1.77316940	0.69144555
1	5.12199705	1.47878787	1.73162938
1	4.62492144	2.58137682	0.40148300
1	6.35250343	2.11937348	0.60657214
8	4.17427458	1.72649610	-1.85100536
6	5.15992612	0.72703967	-1.57198094
6	6.58163720	1.11526482	-2.05661857
1	6.76490993	0.51948487	-2.96301735
1	7.28464281	0.73280480	-1.30117969
6	6.86480560	2.59465695	-2.36067092
1	6.51841756	3.23979345	-1.53809527
1	7.95906316	2.71784356	-2.40832738
6	6.26718563	3.08915032	-3.68859362
1	6.55848965	2.38552372	-4.48790055
1	6.72497869	4.05690104	-3.94952049
6	4.74248602	3.25114383	-3.68736208
1	4.45607416	4.07844022	-3.01668915
1	4.40078859	3.53273236	-4.69795940
6	3.97647994	2.00505045	-3.25503010
1	4.25056845	1.12060414	-3.85145369
1	2.89427344	2.15481237	-3.37886293
50	3.85057807	-1.64714207	-0.55394028
7	0.42845572	0.23261390	2.12733420
6	0.83119200	0.05002208	3.52204017
1	0.95039070	1.01257326	4.06840596
1	0.09435686	-0.56394272	4.05439148
1	1.79097332	-0.48213842	3.55079610
7	-2.21353874	-1.05132015	2.48396598
6	-0.83312810	0.96465556	2.01627669
1	-0.72416810	2.01740113	2.37258887
1	-1.10308958	1.02380615	0.95046469
6	-2.01299085	0.37377170	2.79024268
1	-2.89882975	0.98576512	2.53814459
1	-1.85749782	0.45724458	3.87339531
16	-3.58979297	-1.78945270	3.13609132
7	1.85179844	-0.56977770	-0.56716918
6	1.48115929	0.92313134	1.37167831
1	1.49213236	2.01271579	1.60818734
1	2.44926788	0.52214169	1.70857636
6	1.41327039	0.76945998	-0.15125428

1	2.06967104	1.53092442	-0.60320181
1	0.39431402	0.96928339	-0.51915982
16	1.24324173	-1.23171702	-1.91434481
8	2.30502693	-2.31217332	-2.18038723
8	0.90328287	-0.31579838	-3.02387838
6	-0.26703704	-2.14589016	-1.52208247
6	-1.28882896	-2.20193824	-2.47109546
6	-2.42282693	-2.97107411	-2.19975962
6	-2.54914269	-3.68117042	-0.99585422
6	-1.51316125	-3.58387266	-0.04828129
6	-0.37276470	-2.82352702	-0.30418609
1	-1.18796665	-1.64994154	-3.40473969
1	0.41925278	-2.73802266	0.43976411
1	-1.61429972	-4.09651254	0.90902489
6	-3.75154508	-4.54799650	-0.72141974
1	-3.22191298	-3.02409521	-2.94168413
8	-3.59886073	-3.15785823	2.58189276
8	-3.54968553	-1.52872512	4.58640451
6	-5.02878661	-0.91443298	2.47268104
6	-5.69650015	0.01679088	3.26905261
6	-6.79849494	0.69552382	2.74253618
6	-7.24104219	0.45707652	1.43342933
6	-6.54655351	-0.48497529	0.65351980
6	-5.44693994	-1.17227278	1.16304757
1	-5.36054441	0.18927042	4.29093666
1	-7.32547536	1.42192644	3.36372004
6	-8.44848401	1.16986796	0.87922858
1	-6.87796929	-0.68603131	-0.36696117
1	-4.92344027	-1.91212767	0.55728869
1	-3.51801878	-5.60487383	-0.92439514
1	-4.05485154	-4.48018661	0.33212393
1	-4.60134598	-4.27124498	-1.35931515
1	-9.33112996	0.51191299	0.89731336
1	-8.69052397	2.06518338	1.46567759
1	-8.29137489	1.47091784	-0.16557498
1	-2.11968123	-1.29722052	1.49381292

Energy = -8524.624762 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 31

Atomic N.	X	Y	Z
8	3.12931482	1.02998945	-0.33097956
8	3.70093657	-1.09055439	-0.74624820
6	4.38361657	-2.31675845	-0.40869883
1	3.65210731	-3.11488905	-0.57394660
1	4.69112290	-2.31431625	0.64233014
1	5.25270905	-2.45749275	-1.06770300
8	4.73042791	-0.01455147	0.99889733
6	4.23342205	0.22577898	-0.31174294
6	5.29544812	0.73996705	-1.30999708
1	5.22489693	1.83871737	-1.30525728
1	4.94641737	0.41979142	-2.30200443
6	6.75727111	0.32315392	-1.08460337
1	6.82804044	-0.74869778	-0.84353799
1	7.29602555	0.45825899	-2.03592024
6	7.47407943	1.14845242	-0.00496774
1	7.36534129	2.21830132	-0.25580718

1	8.55401842	0.93323578	-0.03989169
6	6.97000269	0.91289772	1.42315481
1	7.23967480	-0.10249837	1.75647569
1	7.47267629	1.61424777	2.11086759
6	5.46116016	1.07138683	1.59838895
1	5.10298653	2.03766855	1.20358586
1	5.20562240	1.03686806	2.66815143
50	1.43649078	-0.23244810	-0.52848983
7	0.25690622	1.78087358	0.92554670
6	1.22891662	2.89237594	1.02507246
1	0.84387945	3.68990067	1.68824153
1	2.18525651	2.52168871	1.40534095
1	1.41061647	3.30822444	0.02728354
7	1.36451219	-0.82119501	1.57058758
6	0.07446103	1.14903353	2.25965052
1	-0.02781288	1.93609263	3.03337536
1	-0.86056068	0.57359255	2.24197534
6	1.21571460	0.18971596	2.61244544
1	1.01260653	-0.27315393	3.59128142
1	2.16817545	0.73381664	2.71856743
16	1.01291264	-2.39566453	1.86654449
7	-1.90198076	0.81450777	-1.41883593
6	-1.03332841	2.34455414	0.44058102
1	-1.48719177	2.94070919	1.25799242
1	-0.81623434	3.04267064	-0.37757396
6	-2.07295025	1.32643303	-0.05277837
1	-3.05991581	1.80593170	-0.00205021
1	-2.12038373	0.45175056	0.61374409
16	-2.36351335	1.80226182	-2.72344430
8	-1.41644517	1.48099274	-3.80918920
8	-2.57421432	3.18898780	-2.24868235
6	-3.98502071	1.15219581	-3.17837271
6	-5.13331717	1.86484091	-2.83577822
6	-6.38141305	1.35697097	-3.20641010
6	-6.49321303	0.15398824	-3.91773656
6	-5.31528201	-0.53775238	-4.25392336
6	-4.06316638	-0.04724098	-3.89218814
1	-5.04264925	2.80920086	-2.30047679
1	-3.15176771	-0.57713189	-4.16768948
1	-5.38236358	-1.47258322	-4.81354149
6	-7.83967039	-0.37652975	-4.34143904
1	-7.28392467	1.91132363	-2.94284651
8	1.28016190	-3.06031722	0.55751967
8	1.65757831	-2.87248631	3.11056609
6	-0.77572093	-2.53041402	2.15728786
6	-1.26182760	-2.60853477	3.46351222
6	-2.64165706	-2.67049086	3.67726655
6	-3.54455569	-2.66660799	2.60399130
6	-3.02756089	-2.59775693	1.29810657
6	-1.65406135	-2.52940225	1.06887464
1	-0.55960930	-2.64055302	4.29609311
1	-3.02243371	-2.73239858	4.69861364
6	-5.03094736	-2.77178045	2.83821416
1	-3.71219840	-2.60231490	0.44753695
1	-1.25931585	-2.49262017	0.05287812
1	-8.65484883	0.11373451	-3.79441710
1	-8.00705539	-0.20273316	-5.41564041
1	-7.91304717	-1.46026319	-4.17554966

1	-5.37615500	-3.80788820	2.69718368
1	-5.29866211	-2.47112498	3.85936091
1	-5.59349422	-2.14534451	2.13253670
1	-0.97603712	0.41140522	-1.62126443

Energy = -8524.632184 Hartree
Number of imaginary frequencies = 0.

Compound I3a isomer 32

Atomic N.	X	Y	Z
8	3.06121427	1.18116383	-0.05967060
8	3.46405953	0.86209997	-2.21655941
6	4.28206716	0.63668562	-3.37878478
1	5.13367943	-0.01483346	-3.14569359
1	4.63538691	1.59619756	-3.78413832
1	3.61868946	0.15825705	-4.10840322
8	5.17035332	0.46443964	-0.76095258
6	4.06387981	1.35503103	-0.96659824
6	4.46768288	2.84527186	-1.07187412
1	4.24496870	3.29717349	-0.09309675
1	3.76279222	3.29985767	-1.78311404
6	5.91752651	3.17597513	-1.45917430
1	6.23793768	2.57998119	-2.32749317
1	5.94168985	4.22832177	-1.78493037
6	6.92633270	3.00351401	-0.31244616
1	6.55377285	3.55611240	0.56809027
1	7.87794870	3.48181787	-0.59447436
6	7.20662372	1.54963184	0.08398462
1	7.74204222	1.03596933	-0.73132367
1	7.87535701	1.52903599	0.96148873
6	5.96081605	0.73120282	0.41278469
1	5.33961667	1.21925336	1.18292881
1	6.25186536	-0.25573027	0.80270498
50	1.95463932	-0.50380024	-0.81306810
7	0.42800181	0.34012990	1.07567819
6	1.13265650	0.50558780	2.36272815
1	0.47154341	0.95846772	3.12420544
1	1.48057007	-0.46721338	2.73089792
1	2.00699265	1.14688987	2.20267136
7	-1.53472984	-2.89736722	1.29545439
6	-0.77443054	-0.51394249	1.21548488
1	-1.49126378	-0.03593644	1.90894654
1	-1.25363680	-0.56147685	0.22823898
6	-0.47144814	-1.95571508	1.65635409
1	-0.31222782	-2.04488245	2.73886688
1	0.45348002	-2.29912877	1.16309214
16	-2.79262203	-3.25179555	2.36644086
7	0.32159730	0.70240348	-1.66930892
6	0.04798823	1.67503695	0.53623630
1	-0.67824773	2.16881032	1.20953523
1	0.97148611	2.26811763	0.50927670
6	-0.53640267	1.58122820	-0.87578238
1	-0.57491436	2.59785940	-1.30010829
1	-1.57952901	1.21434505	-0.83856333
16	-0.20845725	0.20923133	-3.14335265
8	0.92709458	-0.57767174	-3.70016081
8	-0.81440550	1.32543278	-3.90318498
6	-1.55019629	-0.97916948	-2.82827771

6	-2.88172796	-0.56338290	-2.87163648
6	-3.89702178	-1.47884476	-2.57079682
6	-3.60511047	-2.80838430	-2.23360280
6	-2.25313960	-3.20495994	-2.20886630
6	-1.23062487	-2.30260492	-2.50098582
1	-3.11444825	0.46027081	-3.16435787
1	-0.18735301	-2.62125180	-2.50051858
1	-2.00307314	-4.24094713	-1.96998641
6	-4.69727130	-3.80039192	-1.92138416
1	-4.93869098	-1.15459639	-2.61500407
8	-3.64456352	-4.19724442	1.61985739
8	-2.15732322	-3.58955783	3.65296433
6	-3.76209737	-1.74734990	2.64083668
6	-3.63689218	-1.06131280	3.84917178
6	-4.37904281	0.10581156	4.04787635
6	-5.24467888	0.59396353	3.05821998
6	-5.35477735	-0.12333737	1.85317619
6	-4.62410882	-1.28984648	1.63892344
1	-2.97426098	-1.45010031	4.62161961
1	-4.28710330	0.64342037	4.99334419
6	-6.06042096	1.84188887	3.28303230
1	-6.02936766	0.23626918	1.07386467
1	-4.72765388	-1.84719117	0.70793527
1	-5.68934962	-3.33520522	-1.98284642
1	-4.67428672	-4.64404830	-2.62685736
1	-4.57297535	-4.22164192	-0.91235428
1	-7.12315874	1.59344700	3.42581303
1	-5.72254274	2.38775424	4.17273018
1	-6.00188301	2.51831700	2.41877393
1	-1.88489279	-2.82081320	0.33550277

Energy = -8524.637806 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 33

Atomic N.	X	Y	Z
8	3.11481930	1.09175674	-0.32434813
8	3.73908106	-1.01871462	-0.70499826
6	4.45931813	-2.22304421	-0.36857032
1	4.78545997	-2.20108058	0.67674680
1	5.31986973	-2.34754004	-1.04198175
1	3.74621718	-3.04177356	-0.51236604
8	4.72944650	0.10345165	1.03180747
6	4.23759925	0.31460096	-0.28628084
6	5.29603847	0.84056572	-1.28240087
1	5.19760684	1.93708734	-1.29490534
1	4.96510342	0.49692539	-2.27279754
6	6.76568518	0.46442660	-1.03681770
1	6.86104049	-0.60152885	-0.77878172
1	7.31020098	0.59916548	-1.98491431
6	7.45101014	1.32318918	0.03720817
1	7.31678642	2.38628586	-0.22945229
1	8.53643864	1.13571417	0.01461044
6	6.94033894	1.09401519	1.46398846
1	7.23316327	0.09057990	1.81361706
1	7.41817674	1.81745416	2.14651051
6	5.42632944	1.21553798	1.62340885
1	5.04728289	2.16703113	1.21244562

1	5.16172305	1.18865259	2.69121192
50	1.45427239	-0.21332646	-0.52105529
7	0.21552648	1.77841019	0.91565139
6	1.16323128	2.90974535	1.02483123
1	0.75465191	3.69952456	1.68319898
1	2.12289072	2.55926593	1.41575470
1	1.34722418	3.32859380	0.02873881
7	1.37890098	-0.79466321	1.58053553
6	0.03042374	1.14420680	2.24785439
1	-0.10194879	1.92807210	3.02053450
1	-0.88950222	0.54548489	2.21825749
6	1.18980838	0.21363945	2.61840385
1	0.98337477	-0.25332713	3.59458608
1	2.12693765	0.78098873	2.73818885
16	1.06109514	-2.37668361	1.87470137
7	-1.90133265	0.75444165	-1.44183059
6	-1.07985632	2.31510450	0.41398969
1	-1.55267807	2.90823640	1.22285581
1	-0.86728245	3.01135313	-0.40697766
6	-2.09608177	1.27507817	-0.08226094
1	-3.09150943	1.73844570	-0.04693015
1	-2.13724193	0.40566037	0.59144930
16	-2.37215083	1.72033893	-2.75925437
8	-1.42896424	1.38285041	-3.84330804
8	-2.58479036	3.11519471	-2.30968891
6	-3.99439353	1.05760290	-3.19293405
6	-5.14252295	1.77700729	-2.86407982
6	-6.39105644	1.25981172	-3.22004240
6	-6.50342257	0.04093679	-3.90366640
6	-5.32571914	-0.65780470	-4.22599306
6	-4.07318797	-0.15835811	-3.87817863
1	-5.05130472	2.73354116	-2.35101407
1	-3.16196288	-0.69392668	-4.14308545
1	-5.39333973	-1.60535209	-4.76374025
6	-7.85039771	-0.49889449	-4.31359855
1	-7.29342534	1.81932866	-2.96711557
8	1.36087649	-3.03617453	0.56992610
8	1.70082225	-2.83726728	3.12730603
6	-0.72741143	-2.55388591	2.14274961
6	-1.22791174	-2.64524681	3.44262595
6	-2.60856669	-2.73973881	3.63886298
6	-3.49765051	-2.75611899	2.55426583
6	-2.96596867	-2.67390675	1.25502166
6	-1.59172640	-2.57297263	1.04327063
1	-0.53568265	-2.66180756	4.28396074
1	-3.00064141	-2.81191784	4.65525685
6	-4.98409185	-2.89609600	2.76925550
1	-3.63946927	-2.69384440	0.39581756
1	-1.18521976	-2.52610225	0.03232224
1	-8.66426868	-0.00286963	-3.76979368
1	-8.02312420	-0.34003804	-5.38929680
1	-7.92055722	-1.58036856	-4.13258084
1	-5.30525669	-3.93741672	2.61100847
1	-5.27028764	-2.61394216	3.79063948
1	-5.55157852	-2.27293805	2.06454789
1	-0.96528700	0.36936697	-1.63288412

Energy = -8524.632175 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 34

Atomic N.	X	Y	Z
8	2.40006870	0.04602291	1.43069550
8	2.91120993	0.11865016	-0.72562905
6	3.71703164	0.39114086	-1.88607722
1	3.07556451	0.19277332	-2.75106502
1	4.59187609	-0.27255158	-1.89197723
1	4.03365723	1.44405912	-1.90862331
8	4.42488028	-0.83970940	0.68597140
6	3.48068532	0.24130857	0.64741083
6	4.12945319	1.63270151	0.87327337
1	3.93641077	1.88388151	1.92713590
1	3.53198467	2.34981681	0.28839303
6	5.62752400	1.81198192	0.57910020
1	5.89610742	1.37042479	-0.39248185
1	5.82208609	2.89293184	0.48970563
6	6.54742056	1.24699844	1.67240963
1	6.23053823	1.65947125	2.64627395
1	7.57397027	1.60985543	1.50399218
6	6.57297808	-0.28286743	1.75561741
1	7.04951718	-0.70093167	0.85365181
1	7.19252886	-0.59553791	2.61355911
6	5.19779837	-0.93000514	1.89912275
1	4.63157774	-0.49990634	2.74288353
1	5.31275699	-2.00712411	2.09583080
50	0.64052416	0.31673534	0.05242844
7	0.49253520	-2.15390955	0.82243554
6	1.67433766	-2.86574821	0.27808728
1	1.60148069	-3.94971725	0.48247868
1	1.74328079	-2.70441658	-0.80219498
1	2.57981435	-2.45515985	0.73805351
7	-0.21576070	-1.08364886	-1.55600764
6	-0.75013282	-2.65215938	0.18852002
1	-0.89611812	-3.72704279	0.40961217
1	-1.59561947	-2.09503355	0.61737728
6	-0.71836353	-2.43181301	-1.32827467
1	-1.74769524	-2.56375760	-1.70925378
1	-0.09413133	-3.19679556	-1.82061243
16	-0.09031889	-0.53265224	-3.08409225
7	-0.13131818	-0.05047186	2.92235475
6	0.48979253	-2.34487700	2.29322688
1	0.27358896	-3.40476636	2.52971675
1	1.51267571	-2.12967553	2.63226148
6	-0.47672428	-1.47233956	3.08818128
1	-0.42537924	-1.78672658	4.14310424
1	-1.51666664	-1.61603553	2.75923030
16	-0.98906432	1.05824209	3.92042048
8	-0.13822520	2.26142273	3.95731272
8	-1.43222896	0.38066265	5.15806021
6	-2.45606453	1.39361837	2.93034713
6	-3.66419506	0.77931470	3.26279503
6	-4.79530614	1.05117771	2.49016672
6	-4.73254234	1.92772811	1.39605868
6	-3.50416044	2.54272201	1.09807680
6	-2.36392126	2.28186274	1.85536385
1	-3.71361017	0.11696159	4.12638418

1	-1.41527384	2.76618530	1.62767753
1	-3.44055100	3.24011509	0.26086443
6	-5.94951801	2.19271414	0.54652683
1	-5.74516183	0.57957814	2.74782317
8	0.58824584	0.79070784	-2.93139977
8	0.47468042	-1.53402087	-4.02370134
6	-1.78197195	-0.19958766	-3.65487033
6	-2.31176976	-0.92579580	-4.71985689
6	-3.61688679	-0.65897760	-5.14670644
6	-4.39644858	0.32526036	-4.52507897
6	-3.83600756	1.04220855	-3.45151753
6	-2.53930395	0.78557536	-3.01306082
1	-1.69696553	-1.68131045	-5.20803766
1	-4.03345852	-1.22542196	-5.98183399
6	-5.79626961	0.62718551	-4.99988033
1	-4.42645331	1.81760602	-2.95813679
1	-2.10739126	1.34912846	-2.18486680
1	-6.87696295	2.00677954	1.10316375
1	-5.96489297	3.22766474	0.17975610
1	-5.95668223	1.53299535	-0.33558010
1	-5.84785546	1.62323255	-5.46547418
1	-6.13417095	-0.10708531	-5.74201943
1	-6.51167739	0.62497734	-4.16478510
1	0.87463794	0.14319934	3.04020264

Energy = -8524.626805 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 35

Atomic N.	X	Y	Z
8	2.52276273	0.25251262	1.64689567
8	3.36093035	0.71330932	-0.38074845
6	4.41363116	0.96301386	-1.31669210
1	3.92592502	1.07774713	-2.29208610
1	5.11938134	0.12046723	-1.35435842
1	4.95515786	1.89267755	-1.07833791
8	4.40105348	-0.86395119	0.87959921
6	3.71565097	0.39723107	0.98273049
6	4.57591353	1.50656006	1.65069764
1	4.24162887	1.56307739	2.69697406
1	4.26262967	2.45523270	1.18809926
6	6.10704733	1.37207992	1.61869236
1	6.46088443	1.09753570	0.61318667
1	6.53209818	2.36608697	1.83322509
6	6.66659632	0.37873647	2.64905364
1	6.25679623	0.63454908	3.64163601
1	7.75819536	0.51058034	2.72268126
6	6.36764683	-1.09283694	2.34321310
1	6.91687794	-1.40801098	1.44047971
1	6.73353939	-1.72357959	3.17155545
6	4.88887217	-1.40299520	2.12426308
1	4.26664221	-1.04421564	2.96068797
1	4.74533579	-2.49240018	2.05092157
50	0.78191404	0.91504435	0.68777096
7	0.40414311	-1.56005373	0.07819587
6	1.50161791	-2.12341460	-0.73698606
1	1.34933040	-3.20426445	-0.91542007
1	1.56994369	-1.60182580	-1.69780150

1	2.44689925	-1.97156246	-0.20133710
7	-0.61085423	-0.09025197	-2.34815807
6	-0.92921752	-1.76957404	-0.53568875
1	-1.23343980	-2.82853716	-0.41437628
1	-1.65379895	-1.15979993	0.02545910
6	-1.03773668	-1.45796827	-2.03067241
1	-2.08362141	-1.65666941	-2.32780432
1	-0.39657432	-2.13397976	-2.61022166
16	-0.25718631	0.28165423	-3.97177548
7	-0.45916386	-0.07932464	2.24773013
6	0.44302827	-2.17314146	1.43654089
1	0.25807032	-3.26249297	1.36495681
1	1.45967786	-2.00515511	1.81525868
6	-0.55472648	-1.52844411	2.40038536
1	-0.28714399	-1.84353105	3.42207991
1	-1.58229875	-1.88653749	2.20278834
16	-0.59720552	0.89497934	3.55649925
8	0.02877566	2.17209028	3.08386075
8	-0.14269338	0.25236443	4.81162938
6	-2.36421059	1.24079823	3.77587904
6	-3.06832189	0.61104710	4.80146907
6	-4.43460320	0.86872290	4.94962386
6	-5.10458116	1.75036165	4.09058554
6	-4.36633207	2.38010213	3.07198933
6	-3.00566697	2.13064002	2.90861509
1	-2.54077644	-0.05422025	5.48422665
1	-2.43171568	2.63709725	2.13231733
1	-4.86612892	3.08504124	2.40424573
6	-6.57979952	2.02397105	4.24863975
1	-4.98661184	0.38208137	5.75607521
8	0.08285394	1.71402956	-3.96333727
8	0.68393030	-0.76180476	-4.42089135
6	-1.78905335	0.07756695	-4.90856115
6	-2.06006627	-1.13949887	-5.53664622
6	-3.25743806	-1.28716405	-6.24025335
6	-4.18345082	-0.23676430	-6.32765102
6	-3.88029921	0.97806198	-5.68792746
6	-2.69090433	1.14405061	-4.98094119
1	-1.33003177	-1.94690178	-5.49109798
1	-3.47183830	-2.23470244	-6.73761103
6	-5.45936169	-0.39055924	-7.11585737
1	-4.58388814	1.81002558	-5.75357151
1	-2.44564138	2.09532061	-4.50876321
1	-6.97483764	1.57033559	5.16642478
1	-6.78319582	3.10388956	4.28515908
1	-7.15083086	1.61760457	3.39981372
1	-5.36915329	0.09510041	-8.09985478
1	-5.70013241	-1.44706446	-7.28872572
1	-6.30792014	0.07962333	-6.60044181
1	-1.19292897	0.65019654	-1.94821472

Energy = -8524.634822 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 36

Atomic N.	X	Y	Z
8	2.39662188	0.05086544	1.43657627
8	2.90075982	0.30025054	-0.70796876

6	3.69072100	0.69218596	-1.84486803
1	4.59612669	0.07295244	-1.89613422
1	3.95665342	1.75793753	-1.79255266
1	3.05794078	0.52500349	-2.72276041
8	4.46082491	-0.68161325	0.63556192
6	3.46565229	0.35273491	0.67122608
6	4.04670844	1.75432272	0.99639379
1	3.84358535	1.92049096	2.06507928
1	3.41408877	2.48122622	0.46280324
6	5.53382649	2.02637852	0.71816006
1	5.82198848	1.66780479	-0.28156497
1	5.67565519	3.11908802	0.70543761
6	6.48160429	1.43100877	1.77074766
1	6.14672656	1.75820436	2.77063185
1	7.48922296	1.85384827	1.63020017
6	6.58097978	-0.09789762	1.74615745
1	7.07594763	-0.42801305	0.81801998
1	7.21603502	-0.43993138	2.58125946
6	5.23886623	-0.81925556	1.84097112
1	4.65356726	-0.47732225	2.71161350
1	5.40646734	-1.90061573	1.96215888
50	0.62436454	0.33544525	0.07876580
7	0.59269698	-2.18752879	0.67219922
6	1.80706407	-2.80261737	0.08351758
1	1.78541217	-3.90060821	0.21002801
1	1.86897971	-2.56177129	-0.98229579
1	2.69187098	-2.38348866	0.57490747
7	-0.16431849	-0.98651804	-1.62748669
6	-0.62462099	-2.69794469	-0.00013191
1	-0.71941947	-3.79147365	0.14400529
1	-1.49584183	-2.21317084	0.46369898
6	-0.60255441	-2.36961414	-1.49743060
1	-1.62422845	-2.52300569	-1.89079982
1	0.05751690	-3.06759693	-2.04003443
16	-0.07227363	-0.32136945	-3.11205608
7	-0.12703868	-0.26727816	2.91225355
6	0.59786373	-2.48121595	2.12587263
1	0.43022114	-3.56380876	2.28686029
1	1.60961225	-2.24399891	2.48315957
6	-0.40808789	-1.71132354	2.97614669
1	-0.34410599	-2.09670422	4.00653084
1	-1.44004326	-1.87807243	2.63321109
16	-1.03669779	0.72997635	3.97971898
8	-0.23703537	1.96131865	4.11122050
8	-1.45888715	-0.05363372	5.16075199
6	-2.51025468	1.07600014	3.00320032
6	-3.69230911	0.38493441	3.27465734
6	-4.82851299	0.66493003	2.51320397
6	-4.79710543	1.62517651	1.48974262
6	-3.59588420	2.31497205	1.25318719
6	-2.45028228	2.04730780	2.00068869
1	-3.71829710	-0.34315139	4.08470676
1	-1.52285828	2.58940440	1.82099117
1	-3.55756328	3.07676310	0.47251620
6	-6.01937281	1.89798880	0.65030031
1	-5.75812996	0.13344439	2.72402602
8	0.54324814	1.01843502	-2.86512994
8	0.53538438	-1.22469377	-4.12178616

6	-1.78081209	-0.02897466	-3.65416948
6	-2.28222344	-0.70139494	-4.76714662
6	-3.60122407	-0.46727455	-5.16990863
6	-4.42278202	0.43132982	-4.47671262
6	-3.89023880	1.09525900	-3.35589861
6	-2.58003531	0.87018799	-2.94095178
1	-1.63546025	-1.38980212	-5.31021525
1	-3.99558438	-0.99168255	-6.04241587
6	-5.83824296	0.69956674	-4.92463620
1	-4.51381074	1.80375324	-2.80590902
1	-2.17035470	1.39259646	-2.07532781
1	-6.94341721	1.71911942	1.21538723
1	-6.03078386	2.93215959	0.28208756
1	-6.04018540	1.23510663	-0.22925329
1	-5.93697639	1.71890617	-5.32814108
1	-6.14983861	-0.00229454	-5.70847546
1	-6.54581853	0.61525032	-4.08716262
1	0.86870672	-0.03697442	3.04878264

Energy = -8524.626796 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 37

Atomic N.	X	Y	Z
8	2.51595387	0.30595500	1.64280124
8	3.31204835	0.88629801	-0.37081929
6	4.34163637	1.22693653	-1.30387166
1	5.08982033	0.42451668	-1.37953529
1	4.83619150	2.17372180	-1.03316784
1	3.83946535	1.35375764	-2.27038842
8	4.44316141	-0.68105432	0.82170303
6	3.69444584	0.53765795	0.97729966
6	4.50100394	1.66456263	1.68161061
1	4.17509353	1.66243010	2.73205164
1	4.13267549	2.61226583	1.25934753
6	6.03676313	1.61419013	1.63175155
1	6.39445894	1.39844223	0.61337848
1	6.41012272	2.62061346	1.88169955
6	6.65939290	0.61328132	2.61755350
1	6.24777740	0.80870682	3.62303165
1	7.74327130	0.80000562	2.68628618
6	6.43488859	-0.85930439	2.25765797
1	6.98934475	-1.11025905	1.33814913
1	6.84317591	-1.50081381	3.05743421
6	4.97208736	-1.23889415	2.04117941
1	4.34115118	-0.94439186	2.89596410
1	4.88491917	-2.33086239	1.92843774
50	0.73782341	0.91478660	0.71822120
7	0.48167186	-1.54618407	0.00718669
6	1.59881818	-2.02279085	-0.83625934
1	1.49684498	-3.10152274	-1.05778232
1	1.63518567	-1.46003371	-1.77524386
1	2.53952357	-1.84780796	-0.29956812
7	-0.59633068	-0.03486954	-2.36201744
6	-0.84518968	-1.78919634	-0.60879831
1	-1.10370315	-2.86392617	-0.52701787
1	-1.59161130	-1.23277731	-0.02139788
6	-0.97554835	-1.42643304	-2.09063477

1	-2.01660013	-1.64927089	-2.38770610
1	-0.31665943	-2.05905266	-2.69857989
16	-0.27333683	0.40568830	-3.97477661
7	-0.44090863	-0.20449486	2.24141627
6	0.55851283	-2.21456877	1.33756488
1	0.42613812	-3.30748915	1.21933835
1	1.56832155	-2.01399664	1.71875038
6	-0.46322179	-1.66163828	2.33269010
1	-0.17326640	-2.00619855	3.33867941
1	-1.47307650	-2.06178685	2.12476487
16	-0.61614771	0.70541795	3.59135966
8	-0.06719031	2.03350943	3.16588630
8	-0.11067468	0.03861684	4.81401142
6	-2.39693188	0.94065661	3.84313907
6	-3.05035041	0.23112321	4.85046275
6	-4.42673595	0.40311773	5.02374555
6	-5.15773083	1.27715981	4.20715074
6	-4.47019923	1.98927086	3.20798867
6	-3.09941605	1.82550418	3.01970417
1	-2.47606952	-0.42797694	5.50071679
1	-2.56559729	2.39541350	2.25892005
1	-5.01820920	2.69100995	2.57574523
6	-6.64587196	1.44826721	4.38618078
1	-4.93878082	-0.14521539	5.81687600
8	0.03433612	1.84430191	-3.91845464
8	0.68559563	-0.59801657	-4.47414259
6	-1.81270719	0.20183067	-4.89916368
6	-2.07046370	-1.00106001	-5.55971871
6	-3.27316557	-1.14866033	-6.25381271
6	-4.21769403	-0.11195430	-6.30013473
6	-3.92764648	1.08854851	-5.62854036
6	-2.73278233	1.25442092	-4.93046034
1	-1.32640849	-1.79676517	-5.54647746
1	-3.47742598	-2.08487248	-6.77628717
6	-5.49853415	-0.26458566	-7.08053581
1	-4.64596789	1.90974305	-5.66178272
1	-2.49801084	2.19532560	-4.43293862
1	-6.97914556	1.06311814	5.35836015
1	-6.93879657	2.50501738	4.31494762
1	-7.20144970	0.90572675	3.60535942
1	-5.40708241	0.20562819	-8.07200599
1	-5.74979658	-1.32113196	-7.23821869
1	-6.34019204	0.22100307	-6.56856890
1	-1.19499303	0.67230906	-1.92769558

Energy = -8524.634821 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 38

Atomic N.	X	Y	Z
8	1.89378977	-1.50261131	-0.28402016
8	2.90255135	0.24376577	-1.21186085
6	4.07566090	0.92095323	-1.68940020
1	3.73191191	1.56343028	-2.50741746
1	4.82188853	0.20662648	-2.06483572
1	4.51455212	1.54242941	-0.89325175
8	4.13810251	-1.64835436	-0.48995457
6	3.05246867	-0.80245849	-0.13161324

6	3.16825118	-0.10468389	1.22517026
1	3.96940834	0.65129177	1.19103086
1	2.22247851	0.43658980	1.35667808
6	3.39140021	-1.05269597	2.41558825
1	2.78612875	-1.96244135	2.27799653
1	2.99716185	-0.56298733	3.31716726
6	4.85985985	-1.42570206	2.65030659
1	5.43565033	-0.49961926	2.82622672
1	4.94060080	-2.01644993	3.57646876
6	5.51179214	-2.20121338	1.50112500
1	5.05416859	-3.19835571	1.39795276
1	6.57879142	-2.36434348	1.72929758
6	5.42651401	-1.50428187	0.14396923
1	5.71668059	-0.44339716	0.22937705
1	6.12042482	-1.97800466	-0.56546407
50	1.53280950	-1.44716154	-2.44055202
7	-0.57484299	-2.81717416	-1.75467833
6	-0.66186992	-3.74286912	-2.90434457
1	-1.57403647	-4.36415617	-2.84508050
1	-0.67513924	-3.18084749	-3.84690406
1	0.21781906	-4.40001867	-2.91549934
7	-0.25852803	-0.14201543	-2.58769969
6	-1.72860986	-1.87914492	-1.74161386
1	-2.67864520	-2.42169862	-1.90709309
1	-1.75341714	-1.40293527	-0.75651458
6	-1.57063354	-0.77608710	-2.78352965
1	-2.38844082	-0.05298859	-2.62499341
1	-1.69229225	-1.16013213	-3.81088666
16	0.00474641	1.25296547	-3.43057066
7	-0.46735947	-1.72455435	1.11025637
6	-0.43404691	-3.63258068	-0.50360799
1	-0.95441373	-4.59749133	-0.64584609
1	0.63692035	-3.85128566	-0.37986641
6	-0.99579711	-3.05353793	0.79806498
1	-0.76285705	-3.78661018	1.58898216
1	-2.09466873	-2.99352986	0.73565357
16	-0.83765683	-1.06624349	2.60847568
8	0.15828386	0.00421464	2.82978666
8	-1.05077351	-2.12880501	3.61743392
6	-2.44429775	-0.29082801	2.31408391
6	-3.56392983	-0.73227268	3.01659771
6	-4.79370930	-0.10358635	2.79725126
6	-4.91427470	0.95740860	1.88932105
6	-3.76529835	1.38068640	1.19512767
6	-2.53288147	0.76605415	1.40158287
1	-3.46277373	-1.55310718	3.72589352
1	-1.64839947	1.10175363	0.85969421
1	-3.83679022	2.20361611	0.48081722
6	-6.23826615	1.64431765	1.66569901
1	-5.67422959	-0.44542161	3.34426608
8	1.48489963	1.32347233	-3.60073191
8	-0.88001647	1.36880816	-4.61473458
6	-0.47156368	2.58301631	-2.29418474
6	-1.51253705	3.44437013	-2.63457135
6	-1.88370811	4.45222525	-1.73762352
6	-1.22701142	4.60822780	-0.50951597
6	-0.17712063	3.72439775	-0.19502731
6	0.20448658	2.71568051	-1.07596933

1	-2.01723574	3.32113395	-3.59230951
1	-2.69792171	5.13006325	-2.00154903
6	-1.62178668	5.69911586	0.45456070
1	0.34214537	3.82492968	0.76020984
1	1.01350098	2.02810386	-0.82438471
1	-7.05868833	1.10246265	2.15275998
1	-6.22241952	2.66725745	2.07158809
1	-6.46749410	1.72775094	0.59380148
1	-0.81421428	6.43832851	0.56612751
1	-2.51923872	6.23049561	0.11317524
1	-1.82248473	5.29202754	1.45620290
1	0.51647164	-1.54328715	0.81193239

Energy = -8524.635936 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 39

Atomic N.	X	Y	Z
8	2.73798146	-2.08746174	0.02526777
8	3.44911537	-1.14377455	1.91853476
6	4.45750093	-0.46951367	2.67985474
1	3.91492832	0.16679186	3.38897860
1	5.10037219	0.14744685	2.03563871
1	5.07038190	-1.19244428	3.24191789
8	4.89318415	-1.38674780	0.04987126
6	3.85942024	-2.04425616	0.78156651
6	4.22712681	-3.41193393	1.37416707
1	4.99774222	-3.29813605	2.15384513
1	3.31283258	-3.74223075	1.88437554
6	4.67387071	-4.45541105	0.33817157
1	4.05275819	-4.35213058	-0.56577719
1	4.46987641	-5.45892343	0.74300660
6	6.16273925	-4.37316744	-0.02208010
1	6.75477739	-4.53602295	0.89602694
1	6.42000818	-5.20086835	-0.70239186
6	6.59563971	-3.04776817	-0.65784893
1	6.13050746	-2.92284243	-1.64895230
1	7.68688625	-3.06517255	-0.81949800
6	6.26405581	-1.80585392	0.17186030
1	6.55242967	-1.95167881	1.22764509
1	6.83542754	-0.94534195	-0.20568558
50	1.67851310	-0.23970626	0.43776224
7	-0.09301420	-1.69306036	-0.90109954
6	0.52154117	-2.20492879	-2.14319401
1	-0.12026036	-2.97064632	-2.61899792
1	0.67989797	-1.38448330	-2.85337485
1	1.49820035	-2.63729109	-1.89803295
7	-0.99979186	1.33549877	-1.04898623
6	-1.41865479	-1.09521426	-1.17814163
1	-2.02323068	-1.81690358	-1.76399339
1	-1.93580927	-0.95431890	-0.21888797
6	-1.42306427	0.23800554	-1.92812142
1	-2.44431765	0.39005148	-2.32296898
1	-0.73798060	0.22067506	-2.78551961
16	-0.70921003	2.85489908	-1.75769636
7	0.22338575	-1.18703059	1.81326654
6	-0.24697582	-2.80901915	0.07331685
1	-0.99707053	-3.53906638	-0.28939537

1	0.73132814	-3.30247241	0.12845293
6	-0.63623319	-2.31550845	1.46979365
1	-0.50703948	-3.15358917	2.17484095
1	-1.70882683	-2.04033761	1.50446369
16	0.01393691	-0.44653089	3.25851196
8	1.14533790	0.51697970	3.35762550
8	-0.25722658	-1.41888493	4.34287278
6	-1.49407371	0.55605641	3.09008161
6	-2.72163180	0.05117406	3.52245203
6	-3.87985113	0.81329880	3.33825917
6	-3.82842524	2.08030736	2.73980872
6	-2.57732459	2.56934551	2.32123319
6	-1.41416052	1.81769105	2.48975288
1	-2.75806646	-0.91848328	4.01853321
1	-0.44749789	2.21211330	2.17430318
1	-2.50438840	3.56187490	1.87126101
6	-5.07341635	2.91891689	2.58761086
1	-4.83954990	0.41915878	3.67864747
8	-0.43698287	3.75194274	-0.62060647
8	0.25868510	2.61691764	-2.84291377
6	-2.26015681	3.38503654	-2.52514859
6	-2.48722777	3.11989233	-3.87711532
6	-3.69402435	3.52073348	-4.45444433
6	-4.67408517	4.18606901	-3.70247720
6	-4.41547822	4.44285498	-2.34474232
6	-3.21713202	4.04890062	-1.75182606
1	-1.71613048	2.62654328	-4.46789160
1	-3.87367083	3.31928807	-5.51200503
6	-5.95933150	4.64875969	-4.34051148
1	-5.16173403	4.96888850	-1.74632757
1	-3.00784408	4.27203951	-0.70590029
1	-5.97986902	2.30006672	2.60864308
1	-5.15387042	3.65075624	3.40649333
1	-5.06325724	3.48797335	1.64760153
1	-5.88995233	5.70955084	-4.62763044
1	-6.18626747	4.07581660	-5.24861319
1	-6.80723278	4.55515275	-3.64876851
1	-1.58904960	1.46168801	-0.21875047

Energy = -8524.634391 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 40

Atomic N.	X	Y	Z
8	1.99334675	-1.32223113	-0.44724031
8	2.82524978	0.55123342	-1.29902661
6	3.92164028	1.34769361	-1.77477580
1	4.34403205	1.95232245	-0.95701953
1	3.49556727	2.00957795	-2.53664313
1	4.70455569	0.71947640	-2.22252998
8	4.23142978	-1.27738881	-0.74594892
6	3.10034006	-0.54293322	-0.29401229
6	3.21969889	0.07782734	1.09935597
1	3.95819649	0.89568417	1.08353826
1	2.24162696	0.53352994	1.30054317
6	3.56518077	-0.92042140	2.21727602
1	3.02620511	-1.86513356	2.04424174
1	3.17309053	-0.51952019	3.16259731

6	5.06651448	-1.18974651	2.37249038
1	5.57667268	-0.23348852	2.58562032
1	5.23132639	-1.82753796	3.25528903
6	5.72674752	-1.83994415	1.15240987
1	5.34278572	-2.86197609	1.00283833
1	6.81179765	-1.93177446	1.32957640
6	5.53083971	-1.07049885	-0.15314367
1	5.74185161	0.00286988	-0.01051126
1	6.22835132	-1.44337535	-0.91711502
50	1.54253583	-1.16868007	-2.58190135
7	-0.42298174	-2.74023940	-1.90714933
6	-0.48546065	-3.59944907	-3.10887501
1	-1.34424457	-4.29318505	-3.05625722
1	-0.57988951	-2.98483234	-4.01318749
1	0.44072547	-4.18337253	-3.19269679
7	-0.34901517	-0.00477419	-2.58511367
6	-1.64441930	-1.89967365	-1.79335485
1	-2.55568408	-2.50554169	-1.95714559
1	-1.66486575	-1.48590694	-0.78031610
6	-1.61557377	-0.72815542	-2.77008590
1	-2.47900789	-0.08262098	-2.53614625
1	-1.75115632	-1.05921646	-3.81399623
16	-0.22985143	1.45380803	-3.34905459
7	-0.28363901	-1.81657350	1.01573093
6	-0.16850130	-3.61546632	-0.71586112
1	-0.61808902	-4.60846718	-0.89988697
1	0.92033161	-3.75512949	-0.64477193
6	-0.71973946	-3.16243108	0.63912297
1	-0.39843744	-3.92071090	1.37325451
1	-1.82158806	-3.18678917	0.62023638
16	-0.63725271	-1.28533295	2.56768133
8	0.27941101	-0.15248482	2.81910318
8	-0.71974840	-2.42257572	3.51231760
6	-2.31196410	-0.62755926	2.38898573
6	-3.35980283	-1.20047702	3.10702850
6	-4.64402148	-0.66162679	2.97925994
6	-4.88938897	0.43905700	2.14700384
6	-3.81031267	0.99611998	1.43518303
6	-2.52524656	0.47240158	1.55096391
1	-3.16209550	-2.05152748	3.75782751
1	-1.69557980	0.91161776	0.99654997
1	-3.97904859	1.85277813	0.77925504
6	-6.27268473	1.02654073	2.02002117
1	-5.46868726	-1.10623603	3.53927122
8	1.23246043	1.65518905	-3.56276604
8	-1.16462156	1.56579107	-4.49453033
6	-0.76893344	2.67111344	-2.11823635
6	-1.88661480	3.46346452	-2.37276301
6	-2.30464544	4.38220752	-1.40369919
6	-1.61992029	4.51711873	-0.18851959
6	-0.49295487	3.70436926	0.03866423
6	-0.06327431	2.78499791	-0.91498394
1	-2.41345717	3.35695810	-3.32050763
1	-3.17889247	5.00612316	-1.59992439
6	-2.06626173	5.51233349	0.85350726
1	0.04976002	3.78930882	0.98230532
1	0.80612081	2.15171592	-0.73147092
1	-7.01944197	0.40948593	2.53522779

1	-6.31146069	2.03685657	2.45461911
1	-6.57008154	1.11934369	0.96560938
1	-1.31622500	6.30640999	0.98743397
1	-3.01417611	5.98883877	0.57295760
1	-2.19937106	5.03049376	1.83301663
1	0.66991781	-1.53965240	0.69325342

Energy = -8524.635919 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 41

Atomic N.	X	Y	Z
8	2.81387629	-1.99829328	0.04685475
8	3.43011117	-1.08291288	1.98662270
6	4.39236894	-0.40636936	2.80343988
1	4.99722933	-1.12988792	3.37338721
1	3.80823446	0.20161820	3.50431186
1	5.04764684	0.23849558	2.20037738
8	4.95014960	-1.24961316	0.17170970
6	3.90438081	-1.94736944	0.84684328
6	4.28066607	-3.31962643	1.42325310
1	5.02255464	-3.20685926	2.23047132
1	3.35694652	-3.67902338	1.89538200
6	4.78309428	-4.33165769	0.38164862
1	4.19010870	-4.22161038	-0.54020240
1	4.58672426	-5.34740724	0.75880914
6	6.28087804	-4.21123921	0.07298914
1	6.84601578	-4.38299727	1.00629565
1	6.57767639	-5.01770494	-0.61670609
6	6.70619011	-2.86285299	-0.51803484
1	6.27004288	-2.72368310	-1.52037503
1	7.80209941	-2.85489614	-0.64517753
6	6.32360766	-1.64752443	0.32917686
1	6.57997767	-1.81360426	1.39027854
1	6.89077687	-0.76802472	-0.00882615
50	1.68923903	-0.19091085	0.46617866
7	0.00605970	-1.65746699	-0.96946009
6	0.67753939	-2.11820014	-2.20209943
1	0.07578490	-2.88995024	-2.71874322
1	0.83397895	-1.27507039	-2.88567128
1	1.65826827	-2.52745178	-1.93452517
7	-0.98782809	1.34661817	-1.06293059
6	-1.32643110	-1.09024714	-1.27634240
1	-1.88890352	-1.81206105	-1.90252693
1	-1.87969255	-0.99231731	-0.33196796
6	-1.34542771	0.26345871	-1.98832110
1	-2.35651339	0.39619765	-2.41513912
1	-0.63038666	0.29221876	-2.82057996
16	-0.74858699	2.90063109	-1.71449653
7	0.21350727	-1.21302006	1.76408010
6	-0.14813499	-2.80310368	-0.03018701
1	-0.86408606	-3.54393846	-0.43731038
1	0.84170891	-3.27002775	0.04569984
6	-0.59820250	-2.35824894	1.36447323
1	-0.46548774	-3.21002461	2.05227177
1	-1.67955487	-2.11723650	1.37021200
16	-0.05893900	-0.52156961	3.22300022
8	1.03715374	0.47495561	3.37860258

8	-0.32610519	-1.53197144	4.27298537
6	-1.59412785	0.43605606	3.04095221
6	-2.81611495	-0.12136323	3.42127081
6	-3.99306776	0.60940725	3.22825420
6	-3.96634458	1.89627144	2.67233997
6	-2.72065042	2.43807328	2.30567482
6	-1.53880408	1.71864706	2.48351111
1	-2.83512199	-1.10725438	3.88530660
1	-0.57707048	2.15357790	2.20894029
1	-2.66749429	3.44675395	1.89022215
6	-5.23314002	2.69957338	2.50997698
1	-4.94850356	0.17414818	3.52811604
8	-0.53926823	3.76936095	-0.54270003
8	0.25075623	2.74124200	-2.78546593
6	-2.30584764	3.38822365	-2.49730369
6	-2.49362515	3.15973428	-3.86195191
6	-3.70484657	3.52767605	-4.45182377
6	-4.72796560	4.12463303	-3.69983259
6	-4.50844486	4.34587167	-2.32900371
6	-3.30640059	3.98368839	-1.72346750
1	-1.68989005	2.72029599	-4.45177704
1	-3.85394583	3.35468824	-5.51911472
6	-6.01892115	4.55325830	-4.34998743
1	-5.28883860	4.81898961	-1.72994955
1	-3.12857145	4.17945760	-0.66631685
1	-6.12139950	2.05468650	2.51660336
1	-5.34416468	3.42461878	3.33125996
1	-5.22852944	3.27390898	1.57300022
1	-5.99006366	5.62514367	-4.60050478
1	-6.20219937	4.00219945	-5.28120129
1	-6.87576802	4.40004361	-3.68024711
1	-1.60194238	1.42016901	-0.24451249

Energy = -8524.634390 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 42

Atomic N.	X	Y	Z
8	4.54645876	2.26436462	0.00447609
8	4.38930371	1.54590606	2.12020133
6	4.11992321	1.71892340	3.51623046
1	4.00968127	0.71146610	3.93676821
1	3.19546076	2.29240547	3.67174077
1	4.96044496	2.22141382	4.02048908
8	3.18500158	3.38897303	1.50231676
6	4.44765454	2.76109622	1.26547802
6	5.67490137	3.61236591	1.64768813
1	5.48807729	4.14653449	2.59342868
1	6.48406153	2.89084147	1.83261221
6	6.12131781	4.58829160	0.54961355
1	6.19533974	4.02467102	-0.39170563
1	7.13514766	4.94356303	0.79242500
6	5.20386627	5.80094855	0.35941407
1	5.28029109	6.45749397	1.24465004
1	5.56953585	6.39372498	-0.49406960
6	3.72523682	5.45447702	0.14349583
1	3.59231124	4.79420757	-0.72682547
1	3.17429277	6.38405230	-0.07452503

6	3.05712631	4.81661018	1.36400229
1	3.41607432	5.31338481	2.28641636
1	1.96944526	4.96461218	1.31299374
50	4.09830957	0.21477295	-0.07974340
7	0.07737862	-1.30767698	1.90808074
6	0.45699257	-2.33884423	2.87438726
1	0.17520424	-2.07841453	3.91927297
1	-0.01314534	-3.29543828	2.61495807
1	1.54483338	-2.48178121	2.83722881
7	-1.86559644	-3.00962646	0.48365654
6	-1.36260500	-1.04926962	1.92754734
1	-1.68296706	-0.60802719	2.90185055
1	-1.58595016	-0.29646870	1.15576907
6	-2.25470718	-2.26970844	1.69531725
1	-3.29502093	-1.89915651	1.64260549
1	-2.20174413	-2.96757887	2.54065772
16	-2.93733068	-4.19835435	-0.06374580
7	1.83836531	0.43822666	-0.03557306
6	0.81704830	-0.06418900	2.16033664
1	0.39342854	0.48081867	3.03569207
1	1.84672540	-0.33960146	2.43468075
6	0.88998546	0.91239235	0.98203278
1	1.21601910	1.89228132	1.36703720
1	-0.10630564	1.06161153	0.53631174
16	1.61977946	0.85180511	-1.58704935
8	3.03925597	0.61071344	-2.12846652
8	0.99490670	2.16304949	-1.85810548
6	0.58937028	-0.38727514	-2.40910023
6	-0.25972213	0.01820336	-3.43950165
6	-1.00162056	-0.94715113	-4.12472319
6	-0.90881598	-2.30737325	-3.79263835
6	-0.06307948	-2.68163876	-2.73154919
6	0.68795737	-1.73208327	-2.04015322
1	-0.33027940	1.07468883	-3.69515967
1	1.33005308	-2.02496284	-1.20937973
1	-0.01056068	-3.72960946	-2.43434472
6	-1.67762183	-3.35460853	-4.55714879
1	-1.66144874	-0.63607009	-4.93696010
8	-2.35801908	-4.69785417	-1.32633653
8	-3.19532659	-5.08388720	1.08626316
6	-4.49493578	-3.36480893	-0.45972443
6	-5.58361810	-3.49426125	0.40243282
6	-6.77909203	-2.84009880	0.09091821
6	-6.89891627	-2.05791428	-1.06600212
6	-5.78317432	-1.94442469	-1.91578988
6	-4.58551296	-2.59189905	-1.62269483
1	-5.49168432	-4.11300157	1.29436843
1	-7.63483113	-2.94334997	0.76039033
6	-8.19208652	-1.36134942	-1.40648360
1	-5.85846827	-1.34326419	-2.82391344
1	-3.73062982	-2.50945362	-2.29442280
1	-1.01441020	-3.88386042	-5.25893042
1	-2.09742015	-4.10889104	-3.87768734
1	-2.49090527	-2.90814206	-5.14412660
1	-8.63072873	-1.77476067	-2.32708549
1	-8.93034002	-1.47048015	-0.60240444
1	-8.03068771	-0.28787671	-1.58157493
1	-1.55725885	-2.42440504	-0.29859153

Energy = -8524.623176 Hartree
 Number of imaginary frequencies = 0.

Compound I3a isomer 43

Atomic N.	X	Y	Z
8	3.02923946	0.82467087	2.24900097
8	2.61164090	1.90572218	0.28378183
6	2.62535340	1.87537485	-1.15069240
1	1.74373160	2.43329818	-1.48854594
1	2.56891585	0.84209322	-1.51582468
1	3.53340807	2.37773464	-1.52055398
8	3.88748198	-0.15169470	0.41875306
6	3.70280015	1.03197673	1.11471600
6	4.91353715	1.95958634	1.25006837
1	5.24840685	2.30968519	0.26024880
1	4.54156361	2.83800891	1.79223260
6	6.08682851	1.31739557	2.01057527
1	5.68764541	0.73160899	2.85348038
1	6.69691592	2.12099227	2.45110324
6	6.99134464	0.44773446	1.12783000
1	7.42584066	1.08422074	0.33636794
1	7.84088949	0.08216580	1.72652508
6	6.29070006	-0.74619885	0.46965638
1	5.96567537	-1.47471014	1.22924340
1	7.00827828	-1.26937564	-0.18460850
6	5.07029550	-0.38133266	-0.37468535
1	5.28390615	0.47609582	-1.03574610
1	4.78546031	-1.22976000	-1.01107592
50	1.03289279	1.55621278	1.89258103
7	-2.02012521	0.70740828	3.16805816
6	-1.79613245	1.26396242	4.49858256
1	-2.55969462	0.93167607	5.23487329
1	-0.80828772	0.96272138	4.87374852
1	-1.81139066	2.36158211	4.44926094
7	0.02129976	-0.48212823	1.46923565
6	-1.80033202	-0.74600393	3.13273019
1	-2.07654972	-1.22463539	4.09515760
1	-2.43778992	-1.19650636	2.36002829
6	-0.33939264	-1.06597374	2.78749725
1	-0.17913769	-2.15476227	2.80006503
1	0.32765959	-0.67160177	3.57761702
16	0.57217951	-1.58886120	0.34516526
7	-2.31594081	0.91669913	0.27921450
6	-3.28753252	1.17435082	2.60728467
1	-4.17113253	0.81116876	3.18208561
1	-3.28398057	2.27214924	2.68103776
6	-3.50036881	0.78271700	1.13366239
1	-4.31471485	1.39605293	0.72591951
1	-3.82252684	-0.26666169	1.04984481
16	-1.91172843	2.39348848	-0.38282379
8	-0.43410541	2.54343374	-0.19608125
8	-2.84295074	3.44185472	0.08356321
6	-2.15761759	2.18420835	-2.15694057
6	-3.15849780	2.91196696	-2.79758910
6	-3.33434046	2.74990380	-4.17474818
6	-2.52407974	1.87439679	-4.91092494
6	-1.52361208	1.15446399	-4.23206050

6	-1.32900685	1.30299397	-2.86080595
1	-3.78060738	3.59699246	-2.22284211
1	-0.55027685	0.73949861	-2.34239307
1	-0.88524985	0.46520210	-4.78812527
6	-2.70095260	1.71837290	-6.40043919
1	-4.11525068	3.31731336	-4.68415663
8	0.80547916	-0.79835654	-0.89202574
8	1.63272540	-2.47701339	0.87298974
6	-0.84555650	-2.68991187	0.02164307
6	-0.85523488	-3.96597388	0.58848274
6	-1.92940547	-4.82255131	0.33403552
6	-2.99256069	-4.42783836	-0.49097388
6	-2.95294127	-3.14246428	-1.05839965
6	-1.88974867	-2.27468429	-0.81005714
1	-0.01356853	-4.28266147	1.20375600
1	-1.93617520	-5.81952112	0.77906736
6	-4.13345095	-5.36770251	-0.79204830
1	-3.76643209	-2.81767895	-1.71059151
1	-1.86905922	-1.28255475	-1.25854868
1	-3.65244001	2.14732333	-6.73930270
1	-1.89139266	2.22776115	-6.94556449
1	-2.67205007	0.66066599	-6.69715478
1	-3.99702540	-5.84659483	-1.77424034
1	-4.20340581	-6.16657535	-0.04253628
1	-5.09440713	-4.83594624	-0.82275046
1	-1.46393493	0.44332938	0.66508636

Energy = -8524.615370 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 44

Atomic N.	X	Y	Z
8	4.57439893	2.28978490	0.09394388
8	4.42377098	1.44609977	2.16357876
6	4.16794741	1.53845958	3.56974595
1	5.01823230	2.00067735	4.09570096
1	4.04951701	0.50895374	3.93042699
1	3.25139245	2.11164022	3.76745741
8	3.24219349	3.34066392	1.66937869
6	4.49325758	2.71004628	1.38365274
6	5.73667635	3.51824312	1.80546969
1	5.56685538	3.99619403	2.78392201
1	6.53612780	2.77470908	1.93779624
6	6.18842707	4.55265664	0.76464292
1	6.24536441	4.04638224	-0.20977969
1	7.20971153	4.87730560	1.01887038
6	5.28816213	5.78813863	0.65769828
1	5.38232685	6.38803306	1.58059883
1	5.65551878	6.42666067	-0.16137581
6	3.80252623	5.47768558	0.43482499
1	3.65188198	4.87455697	-0.47326399
1	3.26417207	6.42709867	0.27976027
6	3.13476958	4.77586817	1.61994306
1	3.50862684	5.20978293	2.56778359
1	2.04905355	4.94239685	1.58767681
50	4.10611250	0.25355152	-0.11157731
7	0.08109656	-1.35500181	1.80091023
6	0.44023482	-2.44351751	2.71008947

8	2.47715362	0.77075054	1.76299419
8	4.23773423	1.74462881	0.75623098
6	5.64509030	1.89361411	0.54413788
1	5.75558149	2.49926909	-0.36437738
1	6.13150725	0.91905341	0.39246857
1	6.13042250	2.42393598	1.38082981
8	4.42093043	-0.43474554	1.41101715
6	3.83906034	0.82373958	1.82042802
6	4.30360721	1.34272163	3.19654143
1	5.39417111	1.22143589	3.29463380
1	4.10066765	2.42372800	3.17928426
6	3.57682890	0.71551490	4.39463264
1	2.49620217	0.74750787	4.19507546
1	3.75971877	1.34691266	5.27884175
6	4.00046337	-0.72059274	4.71957789
1	5.04539976	-0.71888653	5.07940239
1	3.38792079	-1.09068620	5.55689467
6	3.89550829	-1.69894261	3.54342389
1	2.86771837	-1.74786725	3.15335667
1	4.14435126	-2.71028834	3.90591886
6	4.85905312	-1.39132536	2.39451352
1	5.83986062	-1.07847400	2.80222248
1	5.02816607	-2.29779957	1.79623841
50	1.77092324	0.03243891	-0.07230755
7	0.71193658	2.41265901	-0.42108374
6	1.23104880	3.28028057	0.66105943
1	0.74098644	4.27089834	0.62519179
1	1.06352821	2.81157930	1.63477194
1	2.31511846	3.39525709	0.54354451
7	-0.31957832	0.04200322	0.68769362
6	-0.75010508	2.20565933	-0.27289860
1	-1.27069931	3.17457036	-0.14547485
1	-1.11742290	1.72786127	-1.18838248
6	-1.07845643	1.27452458	0.89618778
1	-2.16744045	1.08975081	0.87089624
1	-0.85015345	1.74106979	1.86846857
16	-0.46295926	-1.19156137	1.75496899
7	0.56124631	1.05937795	-3.13694787
6	1.08549517	3.04565288	-1.71539100
1	0.85325051	4.12817484	-1.67557833
1	2.18018497	2.96170984	-1.80007208
6	0.42222582	2.51555411	-2.98721628
1	0.85718339	3.06858884	-3.83669954
1	-0.65294511	2.74647133	-2.98163726
16	-0.16818462	0.39050093	-4.54034488
8	0.45481691	-0.93916933	-4.67958952
8	-0.15522443	1.35721101	-5.66093876
6	-1.87825691	0.21717702	-3.99508954
6	-2.89240240	0.80031614	-4.75466437
6	-4.21983001	0.62475169	-4.35649796
6	-4.54105079	-0.12094143	-3.21261165
6	-3.49492905	-0.69040834	-2.46422107
6	-2.16540915	-0.53105427	-2.84928829
1	-2.63540228	1.38113297	-5.63976879
1	-1.36063406	-0.96950630	-2.25928591
1	-3.72196606	-1.26735077	-1.56583917
6	-5.97665160	-0.32862131	-2.80059334
1	-5.01875993	1.07923391	-4.94491484

8	0.77329001	-1.99913001	1.47185301
8	-0.77316514	-0.75769784	3.13625301
6	-1.86518135	-2.19981975	1.20614740
6	-3.10514191	-2.05034059	1.82802906
6	-4.18704224	-2.81682666	1.38417656
6	-4.04383595	-3.73713151	0.33587234
6	-2.77787537	-3.87742236	-0.26147667
6	-1.69164511	-3.11481712	0.16295452
1	-3.20871566	-1.35969032	2.66435873
1	-5.15694700	-2.70626796	1.87282742
6	-5.21401941	-4.55681320	-0.14801544
1	-2.64125671	-4.59974622	-1.06863592
1	-0.70844129	-3.23746511	-0.29106188
1	-6.63632478	0.42766409	-3.24469934
1	-6.33548347	-1.31615654	-3.13027844
1	-6.08810981	-0.29187944	-1.70853395
1	-4.94712358	-5.61919148	-0.23783388
1	-6.07076852	-4.47409801	0.53259386
1	-5.54289406	-4.22444157	-1.14494259
1	1.53408054	0.73227434	-3.13932034

Energy = -8524.634429 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 46

Atomic N.	X	Y	Z
8	2.81099657	0.96303298	1.35305362
8	3.92777142	0.16791525	-0.40473786
6	4.93436243	-0.67463866	-0.97872650
1	5.88559468	-0.12823812	-1.07983120
1	4.56446602	-0.93640772	-1.97685554
1	5.08429629	-1.58389848	-0.37919643
8	4.52019718	-0.45561775	1.80397167
6	4.08517763	0.64706932	1.01501441
6	5.01103446	1.87068255	1.00091377
1	5.96924751	1.62113619	0.51709347
1	4.50516743	2.58858031	0.34219072
6	5.26251664	2.49193606	2.38391409
1	4.32590917	2.46791453	2.96318063
1	5.51741699	3.55437919	2.24742060
6	6.39532267	1.81892369	3.16917893
1	7.32913294	1.91119853	2.58655697
1	6.56545038	2.36947973	4.10827471
6	6.15986390	0.33916186	3.49024588
1	5.31560657	0.22292249	4.18863284
1	7.05089384	-0.06516226	3.99982678
6	5.87933765	-0.53975388	2.27007579
1	6.59961205	-0.32877505	1.46014743
1	5.99553674	-1.59877365	2.54217230
50	1.54508672	-0.22762365	0.09357933
7	-0.11659134	1.43225791	1.17200253
6	0.00337057	1.51515203	2.64251299
1	-0.65620205	2.30006900	3.05674775
1	-0.24874722	0.55077281	3.09723344
1	1.04637873	1.74704072	2.88487854
7	-1.54326361	-1.19482936	1.55746356
6	-1.50248241	1.15465806	0.72193262
1	-2.10996504	2.07884996	0.79241007

1	-1.45431764	0.88190872	-0.34370623
6	-2.26919834	0.07918168	1.49455214
1	-3.25626231	-0.01574478	1.00473936
1	-2.44664158	0.39626600	2.53002749
16	-2.19343488	-2.42446025	2.53983824
7	1.04798427	1.38066977	-1.33609773
6	0.36360294	2.70606747	0.56664369
1	-0.28556318	3.54534894	0.88313213
1	1.37488452	2.86753473	0.96103034
6	0.42144638	2.64434670	-0.96035922
1	1.00507547	3.51040412	-1.31486673
1	-0.59378983	2.73968505	-1.39184325
16	1.41399111	1.11222410	-2.91071715
8	2.10661182	-0.20753269	-2.91073919
8	2.04156988	2.29389021	-3.54721996
6	-0.17259948	0.86933190	-3.76215957
6	-0.74656830	1.92033186	-4.47860393
6	-1.98228831	1.72824140	-5.10320341
6	-2.64945617	0.49709172	-5.02999564
6	-2.04671534	-0.54607466	-4.30488361
6	-0.81761857	-0.36786485	-3.67157312
1	-0.21486603	2.86815932	-4.55771428
1	-0.34169647	-1.18452876	-3.12758576
1	-2.54566666	-1.51570298	-4.24543818
6	-3.96168387	0.28170737	-5.74246634
1	-2.43111955	2.54934014	-5.66571499
8	-1.28457312	-3.56912722	2.36722586
8	-2.44886735	-1.79284913	3.84794495
6	-3.79330775	-2.87493890	1.82835056
6	-4.95789259	-2.26328624	2.29684105
6	-6.18356316	-2.61094321	1.72488855
6	-6.26183199	-3.56257365	0.69666576
6	-5.07259778	-4.16368981	0.24879014
6	-3.84007348	-3.82902041	0.80717293
1	-4.90051387	-1.54373493	3.11290120
1	-7.09727124	-2.13900436	2.09055381
6	-7.59208567	-3.96091195	0.10938315
1	-5.11507803	-4.91365899	-0.54320829
1	-2.92232309	-4.31560788	0.47694018
1	-4.48518302	1.23101179	-5.91541893
1	-3.80000053	-0.18910137	-6.72482393
1	-4.62517326	-0.38172043	-5.17113969
1	-7.97219337	-4.87366372	0.59416023
1	-8.34538293	-3.17533246	0.25042630
1	-7.50857349	-4.17531188	-0.96444876
1	-1.27168964	-1.58577210	0.65044194

Energy = -8524.635440 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 47

Atomic N.	X	Y	Z
8	2.44139157	0.80564492	1.79317901
8	4.17809851	1.86075920	0.82779267
6	5.58152385	2.05988510	0.63176140
1	6.04240726	2.58760993	1.48381524
1	5.67980384	2.68815309	-0.26269306
1	6.10068835	1.10510149	0.46376117

8	4.42596226	-0.32733468	1.42940143
6	3.80038920	0.90098363	1.86490116
6	4.23523443	1.39986306	3.25786983
1	5.32862036	1.31553704	3.36309927
1	3.99425769	2.47316785	3.26606050
6	3.52108050	0.71764924	4.43334173
1	2.44159971	0.71763971	4.22511959
1	3.67498454	1.33232836	5.33468756
6	3.99109143	-0.71093487	4.72595687
1	5.03254408	-0.68298615	5.09467650
1	3.38507625	-1.12267634	5.54846568
6	3.92841008	-1.66212153	3.52483553
1	2.90590024	-1.73576809	3.12491733
1	4.20868212	-2.67338792	3.86386155
6	4.88942591	-1.29300948	2.39204667
1	5.85613652	-0.95782298	2.81535472
1	5.09319594	-2.17808715	1.77290470
50	1.77448365	0.09571314	-0.06747125
7	0.63786607	2.44916881	-0.35838933
6	1.12688395	3.30494458	0.74696762
1	0.60253507	4.27846135	0.73748815
1	0.97658599	2.80456271	1.70764690
1	2.20614785	3.46137056	0.63281189
7	-0.31975628	0.01446063	0.67900819
6	-0.81688102	2.19109649	-0.21833349
1	-1.36810116	3.13888524	-0.06365143
1	-1.16890626	1.72870411	-1.14760076
6	-1.11594337	1.21675983	0.92302045
1	-2.19880229	0.99964897	0.89228455
1	-0.90104962	1.66175726	1.90835579
16	-0.42512676	-1.25271878	1.71112247
7	0.53486539	1.16341464	-3.10953130
6	0.99167263	3.12776787	-1.63502043
1	0.72359533	4.20061153	-1.56747664
1	2.08863273	3.08253675	-1.71983541
6	0.34782867	2.60973755	-2.92169743
1	0.76549643	3.19891312	-3.75542659
1	-0.73424192	2.80534139	-2.91235633
16	-0.16834744	0.50736664	-4.53194946
8	0.50151045	-0.79527373	-4.70503860
8	-0.18771729	1.50310822	-5.62680633
6	-1.87256045	0.26069194	-3.99651936
6	-2.90473691	0.81152564	-4.75552686
6	-4.22652754	0.57832868	-4.36748476
6	-4.52427279	-0.19175938	-3.23380250
6	-3.46026594	-0.72805936	-2.48559919
6	-2.13624845	-0.51189051	-2.86100057
1	-2.66639762	1.41258025	-5.63228733
1	-1.31806225	-0.92480076	-2.27097708
1	-3.66868496	-1.32329662	-1.59463431
6	-5.95226092	-0.45696538	-2.82835493
1	-5.03963676	1.00665085	-4.95604697
8	0.83812904	-2.01074312	1.41023034
8	-0.75343165	-0.86821960	3.10278130
6	-1.79103389	-2.29163579	1.12890110
6	-3.03723038	-2.20095766	1.74939119
6	-4.09138076	-2.99070419	1.27985189
6	-3.91368721	-3.87669448	0.20770593

6	-2.64186585	-3.95737496	-0.38851467
6	-1.58344437	-3.17088604	0.06130126
1	-3.16699015	-1.53714831	2.60360915
1	-5.06632432	-2.92564397	1.76662161
6	-5.05198084	-4.72630505	-0.30012548
1	-2.47863360	-4.65130249	-1.21541733
1	-0.59546985	-3.24706312	-0.39250250
1	-6.64826970	0.21845413	-3.34154321
1	-6.24243456	-1.48901396	-3.07902432
1	-6.08734757	-0.33857949	-1.74439975
1	-4.76816153	-5.78756360	-0.34294630
1	-5.93800819	-4.63471746	0.34062786
1	-5.34031390	-4.43165040	-1.32086632
1	1.51779839	0.86821190	-3.11668617

Energy = -8524.634435 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 48

Atomic N.	X	Y	Z
8	2.21576774	-0.71009234	1.42007196
8	2.93173931	0.86506475	0.01269938
6	3.89614026	1.45361210	-0.86974953
1	3.32179798	2.02469467	-1.60787630
1	4.48459236	0.67322496	-1.37221280
1	4.56209580	2.13555366	-0.31731325
8	4.29781089	-0.99983249	0.58466184
6	3.36573335	-0.07700661	1.13558687
6	3.89476498	0.80028908	2.28188374
1	4.69847296	1.46712902	1.92939925
1	3.04543744	1.44286263	2.54978261
6	4.36669697	0.00950956	3.51235237
1	3.68145825	-0.83640809	3.67911871
1	4.27665527	0.65694103	4.39776976
6	5.81686839	-0.47943749	3.41401343
1	6.47817431	0.39946472	3.31388450
1	6.10192662	-0.96999579	4.35829560
6	6.09214742	-1.43515474	2.24834825
1	5.55890845	-2.38857117	2.39445674
1	7.16851735	-1.67585274	2.22526904
6	5.70575369	-0.88871038	0.87311753
1	6.06169610	0.14810259	0.74667040
1	6.17995269	-1.49331106	0.08643062
50	0.62948745	0.29237744	0.20243739
7	0.56728977	-2.23446596	-0.49599854
6	1.87390761	-2.58639337	-1.10128233
1	1.83915631	-3.60151460	-1.53875315
1	2.12950382	-1.86449250	-1.88362198
1	2.64723424	-2.53531972	-0.32822816
7	0.26346321	-0.03198681	-2.03623815
6	-0.50039505	-2.26286059	-1.52071942
1	-0.61395201	-3.28222431	-1.93856583
1	-1.44595103	-1.98445915	-1.03266345
6	-0.20222912	-1.26941631	-2.65037543
1	-1.13515414	-1.12348247	-3.22468766
1	0.54037319	-1.68912922	-3.35042868
16	0.42333035	1.29693611	-2.96668006
7	-0.48760775	-1.59057825	2.29607309

6	0.31313732	-3.19044084	0.60873446
1	0.10434520	-4.19458023	0.19067587
1	1.25053333	-3.25965111	1.17849985
6	-0.81112815	-2.83349054	1.57616138
1	-0.94273764	-3.68291095	2.26597400
1	-1.76776488	-2.69093696	1.05105198
16	-1.49128937	-1.19938185	3.63363209
8	-0.68631336	-0.26598396	4.44282067
8	-2.06575584	-2.43299498	4.21354477
6	-2.83630402	-0.29802694	2.84322042
6	-4.06323655	-0.93274304	2.64265007
6	-5.10120808	-0.22132589	2.03815097
6	-4.92788284	1.11216543	1.63531089
6	-3.68506389	1.72652768	1.86451661
6	-2.63600115	1.03159809	2.46423956
1	-4.20005895	-1.96042504	2.97735815
1	-1.67664529	1.51308379	2.64857331
1	-3.53718625	2.76758668	1.57204175
6	-6.04499416	1.86316586	0.95593960
1	-6.06561214	-0.70880457	1.88497647
8	0.92939651	2.33627381	-2.01896675
8	1.15904931	1.04199898	-4.23019214
6	-1.25519699	1.79482348	-3.45366408
6	-1.63280062	1.74899969	-4.79470967
6	-2.92866598	2.13384635	-5.15358402
6	-3.84946154	2.56763811	-4.19047885
6	-3.44160819	2.60170253	-2.84424844
6	-2.15577169	2.21763980	-2.47099742
1	-0.90871336	1.42384407	-5.54112086
1	-3.22608901	2.09911110	-6.20343756
6	-5.23718779	3.01061873	-4.58286918
1	-4.14378992	2.94093246	-2.07934184
1	-1.84397645	2.25262711	-1.42596403
1	-7.02852841	1.52386797	1.30651956
1	-5.96674521	2.94402875	1.13094586
1	-6.01368226	1.70229952	-0.13340648
1	-5.33008634	4.10621180	-4.52614514
1	-5.47842871	2.70932390	-5.61018094
1	-5.99803129	2.58751989	-3.91175547
1	0.48991923	-1.54080487	2.61859621

Energy = -8524.627643 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 49

Atomic N.	X	Y	Z
8	2.31337043	-0.70773251	2.04751696
8	3.53167211	1.24084100	2.44184935
6	3.34648317	1.34476859	3.86149089
1	3.13211999	2.40111048	4.06149719
1	4.25715650	1.05433167	4.41156625
1	2.49454954	0.73824560	4.20213453
8	3.76777647	0.05582534	0.52348632
6	3.54684316	-0.12091006	1.92715974
6	4.63836699	-0.97038157	2.61946574
1	5.44521253	-0.30378942	2.96254550
1	4.17377674	-1.39909941	3.51746491
6	5.24532966	-2.08395610	1.75201394

1	4.45294696	-2.58021204	1.16929684
1	5.66119025	-2.85278535	2.42237407
6	6.37378738	-1.60039039	0.82490163
1	7.12379827	-1.07647969	1.44321405
1	6.88943770	-2.47510064	0.39651987
6	5.93721676	-0.67826929	-0.32138125
1	5.36547697	-1.25259444	-1.06875169
1	6.83029186	-0.29110953	-0.84084674
6	5.07450358	0.50585756	0.10861720
1	5.54446489	1.09827083	0.90909699
1	4.89974352	1.17952339	-0.74274297
50	0.82829488	0.47194021	1.11512056
7	0.33781106	-1.70089125	-0.18086212
6	1.50977342	-2.16839155	-0.94833731
1	1.31899960	-3.15186788	-1.41615023
1	1.77507917	-1.43937874	-1.72156001
1	2.35673735	-2.25109034	-0.25819052
7	-0.07873975	0.40637845	-2.29860493
6	-0.88354577	-1.57329760	-1.01350294
1	-1.31155164	-2.57780926	-1.20329657
1	-1.62671053	-1.01262332	-0.42598010
6	-0.70559463	-0.91739862	-2.38483796
1	-1.70539064	-0.88636662	-2.85598129
1	-0.06067534	-1.53285769	-3.02486032
16	0.48916365	1.10970436	-3.74243781
7	-0.76384443	-0.71134573	2.14440580
6	0.08584420	-2.63814509	0.95073615
1	-0.18115308	-3.63946427	0.56027708
1	1.03089354	-2.70899006	1.50509138
6	-1.00636945	-2.12979304	1.89421529
1	-0.94943534	-2.71850193	2.82411241
1	-2.00970630	-2.29344138	1.45962911
16	-0.99766282	-0.08989493	3.63869697
8	-0.17826147	1.16841833	3.59555975
8	-0.79612420	-1.07521896	4.72656630
6	-2.73010338	0.43373948	3.74125734
6	-3.63178547	-0.31359440	4.49895068
6	-4.97086380	0.08287568	4.55158761
6	-5.41900177	1.21989905	3.86428606
6	-4.48657084	1.95628760	3.11219229
6	-3.14888371	1.57172352	3.04606415
1	-3.27701071	-1.18424549	5.04948072
1	-2.42558199	2.15511211	2.47598664
1	-4.81487233	2.84929104	2.57643164
6	-6.85716162	1.66593329	3.95531531
1	-5.67826344	-0.49948132	5.14516414
8	1.00014821	2.43095156	-3.34343090
8	1.33428304	0.08061657	-4.37701793
6	-0.95003653	1.36745909	-4.80519978
6	-1.29987759	0.39714978	-5.74558766
6	-2.42475587	0.60475595	-6.54764808
6	-3.20044550	1.76686092	-6.42466723
6	-2.81938448	2.72871690	-5.47194790
6	-1.70088338	2.53919720	-4.66318286
1	-0.68292160	-0.49351791	-5.85972432
1	-2.69916268	-0.14781351	-7.28888648
6	-4.39991263	1.99906479	-7.30818322
1	-3.40337890	3.64540348	-5.37063461

1	-1.39123920	3.29823820	-3.94482436
1	-7.51705456	0.83735884	4.24341958
1	-6.97336545	2.45855896	4.71091611
1	-7.21179453	2.07547602	2.99961174
1	-4.19556568	2.79239234	-8.04326191
1	-4.67296465	1.09196602	-7.86156685
1	-5.27125012	2.32161472	-6.72105407
1	-0.60368579	1.10237242	-1.76214383

Energy = -8524.637446 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 50

Atomic N.	X	Y	Z
8	2.20146201	-0.70935650	1.44924876
8	2.91720373	0.94507062	0.13578938
6	3.89028034	1.59410835	-0.69292853
1	4.50806821	0.85051541	-1.21561011
1	4.52724835	2.26280423	-0.09222391
1	3.32251614	2.18764508	-1.41836059
8	4.31026399	-0.91488179	0.65646250
6	3.34379545	-0.03968494	1.22543997
6	3.82377459	0.79447790	2.42413348
1	4.62373121	1.49120123	2.12496308
1	2.95496280	1.40861269	2.69627208
6	4.27652352	-0.04214995	3.63128153
1	3.60166944	-0.90539967	3.74190172
1	4.15147244	0.56429900	4.54112992
6	5.73708391	-0.50279074	3.55217998
1	6.38594327	0.39018711	3.51228161
1	6.00361169	-1.03241055	4.48066673
6	6.06204330	-1.39848148	2.35210153
1	5.54113427	-2.36594345	2.43779583
1	7.14258675	-1.62088440	2.34993765
6	5.70673584	-0.79424788	0.99277127
1	6.04748187	0.25320757	0.92577730
1	6.21464703	-1.35305858	0.19339826
50	0.62562569	0.31373608	0.23302708
7	0.65254304	-2.17273934	-0.59488350
6	1.98141838	-2.45625581	-1.18765236
1	1.98503016	-3.44762107	-1.67777578
1	2.23300658	-1.68754611	-1.92541469
1	2.73618858	-2.42500551	-0.39537513
7	0.32290690	0.09554378	-2.02844902
6	-0.39227684	-2.17706049	-1.64333400
1	-0.46937310	-3.17661878	-2.11397745
1	-1.35507380	-1.94838375	-1.16323871
6	-0.09704004	-1.12024936	-2.71468554
1	-1.02103317	-0.96895310	-3.30189467
1	0.67113438	-1.48470873	-3.41806019
16	0.47230369	1.47366850	-2.88575879
7	-0.49773867	-1.70655241	2.19399382
6	0.40406273	-3.19181711	0.45326418
1	0.24116414	-4.17965293	-0.02039669
1	1.32868866	-3.25795378	1.04384340
6	-0.75629253	-2.92345372	1.40637040
1	-0.87305967	-3.81010436	2.05053532
1	-1.70425566	-2.78985430	0.86356743

16	-1.55090160	-1.42017720	3.52009025
8	-0.80891868	-0.48975754	4.39054132
8	-2.08361818	-2.70212444	4.03114058
6	-2.91510242	-0.54476569	2.73312959
6	-4.11058385	-1.22022869	2.48353732
6	-5.16447889	-0.52907285	1.88246338
6	-5.03754865	0.82382843	1.53139468
6	-3.82547771	1.47882483	1.80954331
6	-2.76153291	0.80508107	2.40658492
1	-4.21166112	-2.26440850	2.77740874
1	-1.82634370	1.31740305	2.62854043
1	-3.71440357	2.53510433	1.55801391
6	-6.16912718	1.55503295	0.85443293
1	-6.10473356	-1.04892748	1.69066850
8	0.93376569	2.47308187	-1.87427039
8	1.24100848	1.30123007	-4.14351803
6	-1.20623879	1.96016499	-3.38453285
6	-1.54790898	1.99490944	-4.73528428
6	-2.84354104	2.37257877	-5.10328246
6	-3.79965025	2.71849038	-4.13930668
6	-3.42740662	2.67267673	-2.78294420
6	-2.14238480	2.29510673	-2.40103147
1	-0.79682963	1.73758014	-5.48148477
1	-3.11259899	2.40192424	-6.16090382
6	-5.18977659	3.14804330	-4.53814270
1	-4.15721727	2.94407819	-2.01678005
1	-1.85830228	2.26855933	-1.34784410
1	-7.14283868	1.12402295	1.12102161
1	-6.17499641	2.62017620	1.12068832
1	-6.07139519	1.49103414	-0.24097656
1	-5.34615449	4.21745533	-4.32953088
1	-5.36686729	2.98658841	-5.60897289
1	-5.95653870	2.59544131	-3.97617225
1	0.46813427	-1.64021178	2.54766403

Energy = -8524.627647 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 51

Atomic N.	X	Y	Z
8	2.29371426	-0.66867057	2.08093973
8	3.42996489	1.31596484	2.53458973
6	3.21859130	1.38312296	3.95278444
1	2.38406914	0.73901699	4.26648160
1	2.96251532	2.42653450	4.17090236
1	4.13042913	1.11419651	4.51173767
8	3.74226499	0.18023169	0.59721307
6	3.50583271	-0.03331401	1.99317267
6	4.61787358	-0.85469332	2.68665491
1	5.39355524	-0.16529721	3.05556824
1	4.15601297	-1.31849819	3.56847069
6	5.28005903	-1.92706830	1.80770699
1	4.51622996	-2.44080447	1.20244103
1	5.71409591	-2.69316883	2.46962013
6	6.40383913	-1.38304481	0.90880410
1	7.12409754	-0.84446210	1.54949587
1	6.95841192	-2.22913174	0.47163558
6	5.95090670	-0.45465077	-0.22601889

1	5.41308403	-1.03453784	-0.99397295
1	6.83677563	-0.02376910	-0.72289558
6	5.03737593	0.68733710	0.21298071
1	5.47190954	1.28058878	1.03262884
1	4.85067871	1.37105206	-0.62776037
50	0.78489201	0.47382348	1.13936603
7	0.39196124	-1.69806108	-0.19106383
6	1.59345544	-2.11863940	-0.93982207
1	1.44394281	-3.10240631	-1.42184322
1	1.85028963	-1.37275808	-1.69966098
1	2.42862464	-2.18217750	-0.23344896
7	-0.04485693	0.41980576	-2.29212553
6	-0.81590544	-1.59879100	-1.04688957
1	-1.20787663	-2.61382173	-1.25750202
1	-1.58827188	-1.06946807	-0.46802913
6	-0.63106494	-0.92039322	-2.40645057
1	-1.62219186	-0.91248215	-2.89650125
1	0.04374551	-1.50861235	-3.04119539
16	0.53318279	1.15565717	-3.71571044
7	-0.78609687	-0.77424230	2.12401400
6	0.14804014	-2.65694497	0.92402775
1	-0.07846516	-3.66141667	0.51642135
1	1.08380102	-2.70422455	1.49640340
6	-0.97841914	-2.19616731	1.85154626
1	-0.92090654	-2.79488548	2.77499433
1	-1.96721540	-2.38594750	1.39466900
16	-1.06873756	-0.17858107	3.62020993
8	-0.28745227	1.10447331	3.60835084
8	-0.85868958	-1.17064547	4.70036094
6	-2.81779082	0.29191639	3.69457861
6	-3.71264596	-0.49548048	4.41904713
6	-5.06353799	-0.13884525	4.45066576
6	-5.53043270	0.99786593	3.77544394
6	-4.60468793	1.77487399	3.05668111
6	-3.25528385	1.43028083	3.01159038
1	-3.34402706	-1.36554771	4.96134751
1	-2.53765633	2.04507422	2.46798016
1	-4.94774866	2.66823554	2.53083153
6	-6.98234384	1.40108217	3.84541697
1	-5.76562895	-0.75234950	5.01861917
8	1.00534016	2.48297614	-3.29020464
8	1.41417283	0.15471516	-4.34668088
6	-0.89105982	1.39394387	-4.80281293
6	-1.20759995	0.42178528	-5.75388602
6	-2.32216408	0.61270661	-6.57321010
6	-3.12033352	1.76112604	-6.45855918
6	-2.77377927	2.72384312	-5.49451896
6	-1.66538292	2.55043437	-4.66740595
1	-0.57330875	-0.45748912	-5.86115844
1	-2.57125114	-0.14180613	-7.32148146
6	-4.30098338	1.97796698	-7.37070300
1	-3.37709767	3.62830924	-5.39762599
1	-1.38303398	3.31023325	-3.93872701
1	-7.62253716	0.55084685	4.11407348
1	-7.13441553	2.18254830	4.60632992
1	-7.33257173	1.81013331	2.88782982
1	-4.02397206	2.62683149	-8.21613248
1	-4.66575335	1.03071599	-7.78790762

1 -5.13020683 2.46885667 -6.84388425
 1 -0.60035039 1.09418879 -1.75883805
 Energy = -8524.637446 Hartree
 Number of imaginary frequencies = 0.

Compound I3a isomer 52

Atomic N.	X	Y	Z
8	0.99903537	-0.86925062	-0.81206162
8	2.22328444	0.71799133	-1.73501916
6	3.36915725	1.54387942	-1.99071496
1	3.07681979	2.19349915	-2.82357400
1	4.24357064	0.94237058	-2.27983533
1	3.59919130	2.15036929	-1.10428007
8	2.05900922	0.72026443	0.52553742
6	2.16996490	-0.17585109	-0.56563374
6	3.38643559	-1.12921697	-0.49253567
1	3.03740264	-2.03726525	0.02218034
1	3.58936577	-1.43514398	-1.53144059
6	4.68039625	-0.63968812	0.18327554
1	4.94102777	0.37915514	-0.13922747
1	5.49883999	-1.28890627	-0.16659130
6	4.64320153	-0.69865032	1.71681411
1	4.37257623	-1.72263669	2.02355213
1	5.65501234	-0.50962119	2.10956022
6	3.66364622	0.28800930	2.35946343
1	3.99570569	1.32652808	2.19391961
1	3.64884213	0.13055138	3.45110615
6	2.23212645	0.15568827	1.84735043
1	1.91115033	-0.89758822	1.86167403
1	1.54782526	0.73035736	2.48888201
50	0.66010858	-0.70291339	-2.95631272
7	-1.60695306	-1.94532546	-2.53135331
6	-2.11333677	-2.00802260	-3.92110315
1	-3.18280311	-2.28557335	-3.94211953
1	-1.98550641	-1.04230637	-4.42456341
1	-1.54190799	-2.76369302	-4.47503970
7	-0.96701458	0.76691757	-2.68158031
6	-2.37981524	-0.97034309	-1.72421244
1	-3.43297353	-1.29573127	-1.61213882
1	-1.92221705	-0.93143420	-0.72754357
6	-2.34893778	0.43185787	-2.33405653
1	-2.75536422	1.12684485	-1.57727567
1	-3.01047606	0.49396450	-3.21391326
16	-0.71349276	2.11534616	-3.58372230
7	-0.07109795	-3.35097447	-0.06604322
6	-1.68064455	-3.33193425	-1.98333560
1	-2.68999390	-3.73211468	-2.20518730
1	-0.95350306	-3.94091350	-2.53994947
6	-1.46318509	-3.53116383	-0.48594327
1	-1.73190482	-4.57746115	-0.27919345
1	-2.16606478	-2.90357883	0.09082467
16	0.31411753	-3.92172338	1.46636198
8	1.68579447	-3.43787591	1.73184697
8	-0.01155007	-5.36065705	1.51460451
6	-0.81485834	-3.10156482	2.62872671
6	-1.50238545	-3.87489371	3.56452309
6	-2.35103738	-3.24465449	4.47760214

6	-2.52987823	-1.85342961	4.46345932
6	-1.83840178	-1.10165945	3.49785769
6	-0.98137830	-1.71392507	2.58401369
1	-1.37101621	-4.95636113	3.56543250
1	-0.45581715	-1.11593394	1.83777786
1	-1.97481455	-0.01908474	3.46045374
6	-3.42712932	-1.17546142	5.46817802
1	-2.88803218	-3.84783728	5.21198773
8	0.69684148	1.95455255	-4.05908948
8	-1.78584459	2.35998500	-4.57923280
6	-0.75372365	3.50974693	-2.42721718
6	-1.46502804	4.65983137	-2.77013222
6	-1.46746271	5.74455785	-1.88998142
6	-0.77040462	5.69285876	-0.67379299
6	-0.07429948	4.51495721	-0.35107096
6	-0.05827348	3.42244087	-1.21738845
1	-2.01107755	4.69166044	-3.71229132
1	-2.02411598	6.64607774	-2.15309198
6	-0.74930088	6.87895130	0.25804515
1	0.46385868	4.45002542	0.59675106
1	0.47806663	2.50973342	-0.95231246
1	-4.15366328	-1.87798178	5.89610885
1	-2.83676224	-0.76209632	6.30069794
1	-3.97717666	-0.33959934	5.01506527
1	0.15563926	7.48545678	0.09608245
1	-1.61624912	7.53273183	0.09648624
1	-0.74334966	6.56297549	1.31003224
1	0.35220987	-2.40809600	-0.22513304

Energy = -8524.639958 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 53

Atomic N.	X	Y	Z
8	2.69560935	-0.95791966	-2.00700619
8	4.56346152	-0.79762479	-0.63222929
6	5.15943106	0.40484013	-1.13070176
1	5.43484177	0.99726116	-0.24972568
1	4.45322433	0.98535442	-1.74724992
1	6.06620514	0.19567275	-1.72006043
8	3.48371719	-2.80351236	-0.96182075
6	3.85078511	-1.59171631	-1.62996714
6	4.68490803	-1.91737316	-2.88575109
1	4.03108820	-2.56529210	-3.48887750
1	4.81961898	-0.99095002	-3.46432942
6	6.04036903	-2.60379253	-2.67375104
1	6.75691656	-1.89237430	-2.22982920
1	6.43933864	-2.85126338	-3.67092828
6	6.03302584	-3.87262999	-1.80619264
1	5.27400575	-4.58132913	-2.17726617
1	7.00930241	-4.36976435	-1.92122354
6	5.80251883	-3.57538551	-0.31759988
1	6.39524878	-2.69102580	-0.03921954
1	6.17682314	-4.40976585	0.29780231
6	4.33289766	-3.35606089	0.06680469
1	3.85485606	-4.32456352	0.27459483
1	4.26330658	-2.74248186	0.97721734
50	1.71547901	0.09005274	-0.42071916

7	-0.26565361	-1.01524282	-1.57874919
6	-0.21615772	-0.78588587	-3.03974613
1	-0.99148086	-1.37745017	-3.55973510
1	-0.36424689	0.27729026	-3.26268569
1	0.77768438	-1.07796624	-3.39747757
7	-1.30017056	1.63446494	-0.31924302
6	-1.60746744	-0.71346587	-1.02323121
1	-2.35350283	-1.36588685	-1.51871847
1	-1.59720904	-0.98519513	0.04121589
6	-2.09640497	0.72864186	-1.15475732
1	-3.16636895	0.73650019	-0.87899178
1	-2.02203226	1.08344104	-2.19034354
16	-1.37566841	3.30297191	-0.64921160
7	1.03454746	-1.62335345	0.77548897
6	0.06886640	-2.44289429	-1.29002907
1	-0.71159241	-3.10634403	-1.70756671
1	1.02157030	-2.64480910	-1.79462453
6	0.23698362	-2.70944020	0.20880208
1	0.74102005	-3.68210880	0.32421903
1	-0.74635433	-2.79646303	0.70875028
16	1.21415455	-1.53640036	2.40545026
8	2.27610158	-0.52115002	2.62314359
8	1.29877480	-2.88736051	3.00558752
6	-0.32885511	-0.79733207	3.02438676
6	-1.38880723	-1.61442231	3.42381439
6	-2.59170608	-1.02842587	3.83026975
6	-2.74881213	0.36512497	3.85973490
6	-1.66076945	1.16572715	3.46681828
6	-0.45638819	0.59606817	3.05038014
1	-1.25768540	-2.69626530	3.43704822
1	0.39074371	1.22107946	2.76460342
1	-1.74967768	2.25367625	3.50805647
6	-4.03163577	0.99135133	4.34769646
1	-3.41929198	-1.66797143	4.14386803
8	-0.54759534	3.92794388	0.39578382
8	-1.09000171	3.43579687	-2.08976939
6	-3.08867525	3.81810855	-0.38434463
6	-3.98426431	3.82164564	-1.45578946
6	-5.30827638	4.20469367	-1.23220540
6	-5.74824652	4.58940508	0.04360492
6	-4.82211728	4.58171923	1.10112788
6	-3.49687005	4.20069919	0.89691429
1	-3.63760582	3.55039512	-2.45238156
1	-6.01068279	4.21313537	-2.06750167
6	-7.16971495	5.03734018	0.27051428
1	-5.14308911	4.88988551	2.09797614
1	-2.77280848	4.22318807	1.71111811
1	-4.89294592	0.33403023	4.16994227
1	-3.98408527	1.18353734	5.43101866
1	-4.22165195	1.95490016	3.85574844
1	-7.23974213	6.13580705	0.23890127
1	-7.84354121	4.64203587	-0.50021664
1	-7.53927507	4.71722322	1.25387825
1	-1.40829701	1.47965028	0.68948637

Energy = -8524.628119 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 54

Atomic N.	X	Y	Z
8	1.45121664	-0.73008843	-0.85664144
8	3.13411357	0.42420657	-1.85316417
6	3.58756649	1.78943705	-1.91888317
1	4.43505528	1.95764590	-1.24140471
1	2.78153144	2.49697757	-1.69437975
1	3.91397679	1.92801496	-2.95709822
8	2.50906362	0.96166750	0.30626896
6	2.67595597	-0.13942131	-0.56079648
6	3.70049404	-1.19608264	-0.11950829
1	3.24221383	-1.81039380	0.66979083
1	3.81616974	-1.85008789	-0.99576503
6	5.07484335	-0.68561100	0.33888232
1	5.42777362	0.11798909	-0.32683800
1	5.79674223	-1.50886450	0.22168606
6	5.10623264	-0.22768916	1.80339534
1	4.80090758	-1.07677503	2.43760202
1	6.14198999	0.01794588	2.08778563
6	4.20218580	0.96852482	2.11995289
1	4.57558608	1.88107025	1.62610931
1	4.23133573	1.16533130	3.20505596
6	2.73925336	0.77579922	1.72359990
1	2.35796675	-0.20227965	2.05475416
1	2.12222159	1.55523613	2.19403300
50	1.08459592	-0.64806731	-2.95685248
7	-0.90259802	-2.53290923	-2.59903753
6	-1.12211016	-2.80508997	-4.03293895
1	-2.04567600	-3.39319783	-4.19430883
1	-1.19617444	-1.86823785	-4.59897792
1	-0.26881474	-3.37092399	-4.42895572
7	-0.93002058	0.26597258	-2.56624250
6	-2.05011950	-1.79851368	-2.01974354
1	-2.99087531	-2.37467640	-2.13530406
1	-1.85751652	-1.66852283	-0.94813193
6	-2.22295330	-0.40871650	-2.63299395
1	-2.98674737	0.11936568	-2.03485498
1	-2.61099648	-0.46551644	-3.66420433
16	-0.79656070	1.80844195	-3.07528328
7	0.45702410	-3.23043504	0.22346974
6	-0.67280526	-3.84483235	-1.93245266
1	-1.45917623	-4.55295829	-2.26578862
1	0.29015752	-4.23280073	-2.29714471
6	-0.69823253	-3.88479805	-0.40804192
1	-0.67063248	-4.94570260	-0.12298127
1	-1.66048195	-3.48880498	-0.03687466
16	0.39391060	-3.17172674	1.90584989
8	1.62831074	-2.48512373	2.33886460
8	0.06715364	-4.53083234	2.38006694
6	-1.01197621	-2.10611735	2.33082193
6	-2.03780898	-2.61321087	3.12785898
6	-3.11156140	-1.78336199	3.46259270
6	-3.17617115	-0.45983440	3.00407037
6	-2.13353399	0.01932582	2.19043813
6	-1.05020662	-0.79092417	1.85355158
1	-1.98614624	-3.64443313	3.47567383
1	-0.25352813	-0.41026129	1.21086401
1	-2.17174184	1.04145186	1.80768542

6	-4.32660218	0.43878342	3.38333893
1	-3.91586793	-2.17577114	4.08762244
8	0.70134412	1.92623806	-3.24635799
8	-1.68366410	2.17040598	-4.20476489
6	-1.24634702	2.88308701	-1.68997267
6	-2.31490332	3.76814955	-1.82671289
6	-2.65886287	4.59035476	-0.74979393
6	-1.94464111	4.54116580	0.45545924
6	-0.87260654	3.63582571	0.56231982
6	-0.51760210	2.80430486	-0.49823176
1	-2.85836963	3.80991832	-2.76997465
1	-3.49463329	5.28501603	-0.85212630
6	-2.29584111	5.45230394	1.60496943
1	-0.30515935	3.58345350	1.49400475
1	0.31605079	2.10587281	-0.39973199
1	-5.18294893	-0.13949102	3.75304234
1	-4.02890613	1.13832562	4.17978180
1	-4.65867727	1.04441839	2.52893456
1	-1.58543598	6.29099007	1.66993389
1	-3.30070680	5.87773126	1.48781067
1	-2.25382973	4.92058485	2.56578024
1	0.75782799	-2.30824846	-0.16046247

Energy = -8524.639106 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 55

Atomic N.	X	Y	Z
8	3.11603041	-0.84064063	-1.14635885
8	3.92150953	-0.12838629	0.80475470
6	4.55884214	-0.30679082	2.08576483
1	5.58907940	0.07769926	2.05323718
1	4.54875548	-1.36222327	2.37978580
1	3.96150865	0.27600914	2.79516166
8	4.13704383	-2.35192743	0.30245930
6	4.17237929	-1.06391883	-0.31005155
6	5.50736800	-0.73866727	-1.01907351
1	5.38424086	-1.03056541	-2.07355785
1	5.58066360	0.35823417	-1.01699837
6	6.79183540	-1.37149479	-0.45999598
1	6.81020373	-1.30250843	0.63757462
1	7.64539468	-0.77337702	-0.81715105
6	7.00677306	-2.82706000	-0.90133501
1	6.95983781	-2.86570827	-2.00395022
1	8.02557064	-3.14395335	-0.62662072
6	6.00389778	-3.82996506	-0.32063239
1	6.16709907	-3.94407169	0.76340961
1	6.17410064	-4.82270675	-0.77126212
6	4.53814622	-3.45454149	-0.52990436
1	4.32119802	-3.23490040	-1.58971338
1	3.89376116	-4.29472190	-0.22917823
50	1.67498836	0.32564292	-0.08831193
7	0.14672852	-1.15371456	-1.55921570
6	0.54673110	-1.19539717	-2.98033263
1	-0.06205329	-1.92146043	-3.55007434
1	0.44176366	-0.20118054	-3.42902131
1	1.60214293	-1.48707075	-3.02778431
7	-0.98955075	1.58497462	-2.07091489

6	-1.27951101	-0.79052564	-1.37104761
1	-1.92060720	-1.66217801	-1.60968070
1	-1.42365321	-0.56745715	-0.30290506
6	-1.80961974	0.37402709	-2.20889103
1	-2.85599812	0.53122062	-1.88647831
1	-1.83312478	0.11630798	-3.27532210
16	-1.54344829	2.99627833	-2.84367821
7	0.80331019	-1.28693218	1.13975422
6	0.41672181	-2.47744786	-0.93194283
1	-0.20421314	-3.25880327	-1.41105997
1	1.47513565	-2.69505862	-1.12375129
6	0.16775339	-2.47546090	0.57709289
1	0.59488852	-3.40149069	0.99633372
1	-0.91854064	-2.49536530	0.78915541
16	0.59566822	-0.96087785	2.73279208
8	1.40572653	0.26912228	2.96475176
8	0.78827141	-2.16483906	3.57259474
6	-1.14555623	-0.47999817	2.93067449
6	-2.08439935	-1.41916239	3.36143156
6	-3.42831463	-1.04742725	3.46001145
6	-3.84797901	0.25270594	3.14273040
6	-2.88111701	1.18063300	2.71737036
6	-1.53759295	0.82339667	2.60937241
1	-1.75438384	-2.42128802	3.63381470
1	-0.78567773	1.55035215	2.29960303
1	-3.18618018	2.20100659	2.47523687
6	-5.29323254	0.65880008	3.29198836
1	-4.16285149	-1.78107077	3.79808435
8	-0.53562441	4.02379702	-2.53612036
8	-1.88199982	2.59079187	-4.22045697
6	-3.08042979	3.46375944	-2.01301452
6	-4.30672727	3.05960148	-2.54229089
6	-5.48329256	3.41465708	-1.87648310
6	-5.44989078	4.16672402	-0.69361796
6	-4.19891779	4.56800500	-0.18995854
6	-3.01585772	4.22295031	-0.83936444
1	-4.33389316	2.49856386	-3.47583769
1	-6.44538441	3.10876877	-2.29109060
6	-6.72001815	4.54689253	0.02476508
1	-4.15377776	5.17221662	0.71831170
1	-2.04947431	4.55887077	-0.46306994
1	-5.96632900	-0.20091675	3.17694548
1	-5.47702917	1.08878090	4.28910900
1	-5.57362299	1.42136426	2.55268108
1	-6.76877059	5.63168597	0.19656635
1	-7.60836970	4.25060671	-0.54656688
1	-6.77505987	4.06275998	1.01162985
1	-0.70299534	1.80604500	-1.11088135

Energy = -8524.634744 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 56

Atomic N.	X	Y	Z
8	3.41025466	1.55945112	0.33873803
8	4.29577577	1.06711430	2.42281923
6	4.83699210	2.37882827	2.60517530
1	4.68530910	2.62699985	3.66316997

1	4.32108533	3.11760905	1.97338938
1	5.91891631	2.41404365	2.38844603
8	3.40648414	-0.56501375	1.15755478
6	4.17700198	0.65481444	1.03680947
6	5.56472129	0.49617322	0.38248874
1	5.42245712	0.03436681	-0.60774461
1	5.89579254	1.52354305	0.17477740
6	6.64055264	-0.24010534	1.19324019
1	6.62447328	0.13297275	2.22887604
1	7.62628758	0.02475554	0.77891338
6	6.50842225	-1.76616373	1.20143630
1	6.65714882	-2.14697462	0.17563205
1	7.32109454	-2.19569433	1.80897961
6	5.16036711	-2.27894168	1.71785168
1	4.98355390	-1.95180222	2.75470543
1	5.17939153	-3.38133340	1.73214950
6	3.96816352	-1.85919859	0.85895790
1	4.22539783	-1.92527590	-0.21384057
1	3.11943104	-2.53514314	1.03214089
50	1.78624064	0.72526747	-0.70723372
7	0.34713834	1.38144213	1.30441595
6	0.77732123	0.71330133	2.55263855
1	0.18176368	1.06982414	3.41346631
1	0.67031366	-0.37300063	2.45930139
1	1.83859584	0.92848943	2.72533232
7	-1.08782285	-0.95614395	-0.07331562
6	-1.11150764	1.23405449	1.07626043
1	-1.65784867	1.77465648	1.87483169
1	-1.35624427	1.72753585	0.12540829
6	-1.65269120	-0.19516466	1.04745714
1	-2.75410231	-0.12639793	0.99462658
1	-1.39943307	-0.73201247	1.96995832
16	-1.18558276	-2.65473053	-0.01950813
7	1.00276729	2.77446531	-1.02203314
6	0.68780677	2.83204115	1.37747013
1	0.12579540	3.31278923	2.20034153
1	1.76103932	2.88272673	1.60221337
6	0.41743377	3.56339251	0.06162549
1	0.87533191	4.56385559	0.12544449
1	-0.66828702	3.72269797	-0.08021894
16	0.61617156	3.17431445	-2.56871293
8	1.50463942	2.33943608	-3.41640378
8	0.53879295	4.64343300	-2.73458598
6	-1.07233484	2.54465516	-2.83314925
6	-2.17488034	3.37332950	-2.61156909
6	-3.46507587	2.85124773	-2.74700713
6	-3.67421426	1.51406137	-3.11595679
6	-2.54759424	0.70415983	-3.34740155
6	-1.25351396	1.20886992	-3.20908063
1	-2.01555338	4.42188332	-2.36017416
1	-0.38210340	0.58482284	-3.41240443
1	-2.68730231	-0.33236227	-3.66337899
6	-5.06890136	0.97187442	-3.30831942
1	-4.32579724	3.50079888	-2.57508583
8	-0.60186973	-3.10485688	-1.29400887
8	-0.63826508	-3.04348201	1.29411715
6	-2.94216060	-3.08128068	-0.02955628
6	-3.61461778	-3.27936950	1.17786995

6	-4.97657859	-3.58719855	1.15288350
6	-5.67353444	-3.70351825	-0.05934770
6	-4.96809325	-3.50285145	-1.25890871
6	-3.60888223	-3.19443577	-1.25358155
1	-3.06890249	-3.21453863	2.11858506
1	-5.50562275	-3.74794128	2.09383792
6	-7.13571506	-4.07002384	-0.08123596
1	-5.49108600	-3.60019816	-2.21214827
1	-3.05717122	-3.06760286	-2.18506475
1	-5.78733548	1.46397796	-2.63928515
1	-5.41444663	1.14164880	-4.34009344
1	-5.10864567	-0.11051481	-3.12622308
1	-7.26339175	-5.14515333	-0.28167459
1	-7.61871210	-3.85373990	0.88006727
1	-7.67304891	-3.52759986	-0.87081893
1	-1.39135540	-0.62596017	-0.99533214

Energy = -8524.632575 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 57

Atomic N.	X	Y	Z
8	2.73047393	-0.48455406	1.41870850
8	3.10176931	-1.84488711	-0.28966428
6	3.87142167	-2.47142180	-1.33102924
1	3.13192136	-2.87180979	-2.03321130
1	4.45994868	-3.30184794	-0.91473541
1	4.52917822	-1.74646970	-1.82733104
8	4.60453797	-0.17402645	0.06099716
6	3.77138138	-1.09263082	0.77979475
6	4.54231538	-2.02541466	1.74395321
1	4.40519846	-1.60844000	2.75337470
1	4.00143507	-2.98294607	1.73585542
6	6.04193022	-2.24519030	1.49115096
1	6.23229375	-2.47482448	0.43143152
1	6.34432021	-3.14099562	2.05709886
6	6.93151834	-1.07242421	1.93356178
1	6.67937177	-0.81539895	2.97752994
1	7.98295950	-1.40175648	1.94425484
6	6.81965647	0.18388101	1.06241211
1	7.23450444	-0.01674092	0.06093015
1	7.43066645	0.99182064	1.50005671
6	5.39629985	0.70495410	0.88312651
1	4.89347835	0.86936242	1.85107346
1	5.41155326	1.66882259	0.35301723
50	1.23295636	-0.25042399	-0.08900380
7	-0.11556484	0.67076335	2.04246106
6	0.85819359	0.95427294	3.12290442
1	0.33451297	1.29679657	4.03451672
1	1.44362985	0.05677789	3.34269332
1	1.55483140	1.73298641	2.79153157
7	-0.05759319	-1.83570058	0.69746192
6	-0.98394592	-0.47341226	2.44316897
1	-1.23370369	-0.38879771	3.51801021
1	-1.91983881	-0.41095711	1.87235432
6	-0.34219073	-1.82432761	2.13317614
1	-1.05898956	-2.61655247	2.40671595
1	0.56871471	-1.98700335	2.73355717

16	-0.00245322	-3.27226253	-0.10414321
7	-1.08025056	2.44500560	-0.66207224
6	-0.94291118	1.89380475	1.83726394
1	-1.63373068	1.99584405	2.69723100
1	-0.27954402	2.76681860	1.86033692
6	-1.76143773	1.93522972	0.53478756
1	-2.64378788	2.56695313	0.70483567
1	-2.14110124	0.93378496	0.27989326
16	-0.83144882	4.12011618	-0.80783144
8	0.42743898	4.25946032	-1.56566664
8	-1.03136309	4.77234664	0.50687894
6	-2.19438215	4.64652194	-1.86684988
6	-3.27364689	5.33148585	-1.31013508
6	-4.31550562	5.74594395	-2.14425691
6	-4.28703635	5.49030596	-3.52240915
6	-3.18080549	4.80273875	-4.05402557
6	-2.13415710	4.38121060	-3.23816491
1	-3.28376855	5.54615766	-0.24225984
1	-1.27193980	3.86132796	-3.65474265
1	-3.13852747	4.60001103	-5.12577411
6	-5.39947543	5.96286729	-4.42402229
1	-5.16256526	6.28383038	-1.71480512
8	0.50813219	-2.90772562	-1.45678506
8	0.64922376	-4.35255024	0.67410947
6	-1.73635625	-3.76836790	-0.30033433
6	-2.23735332	-4.84211406	0.43527513
6	-3.57675880	-5.21094179	0.27832571
6	-4.41827237	-4.52700160	-0.61004656
6	-3.88468040	-3.45057631	-1.34173775
6	-2.55363748	-3.06729857	-1.19224005
1	-1.57446263	-5.38418211	1.10901025
1	-3.97160583	-6.05085291	0.85326139
6	-5.85231410	-4.95246578	-0.80479740
1	-4.52333670	-2.90947519	-2.04285641
1	-2.13983434	-2.24151463	-1.77115516
1	-6.28811447	6.25079678	-3.84829477
1	-5.08192772	6.83983482	-5.00899326
1	-5.68946604	5.18423838	-5.14311734
1	-5.95397071	-5.58309020	-1.70185720
1	-6.21761384	-5.53512410	0.05072558
1	-6.51345965	-4.08594869	-0.94230368
1	-0.21093795	1.95337348	-0.91216129

Energy = -8524.633296 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 58

Atomic N.	X	Y	Z
8	2.67178574	1.05329125	0.87833089
8	2.82899149	-0.70144093	2.26183872
6	3.52777018	-1.78580763	2.88492073
1	4.20081986	-1.42407095	3.68028438
1	4.09988208	-2.37060799	2.15144017
1	2.75501541	-2.42012293	3.33571078
8	4.16899682	-0.66702269	0.42688092
6	3.59421211	0.19952808	1.42526553
6	4.64378267	1.01119844	2.23169775
1	4.64971839	2.02487016	1.80420541

1	4.23793729	1.11038619	3.24968975
6	6.08617360	0.48161493	2.28471529
1	6.10173865	-0.59366367	2.51970187
1	6.59161836	0.98637310	3.12432040
6	6.89950660	0.74079520	1.00693514
1	6.81438368	1.81029800	0.74658578
1	7.96593726	0.55829384	1.21680194
6	6.48121137	-0.10715188	-0.19907606
1	6.71899608	-1.16757894	-0.01239685
1	7.06728838	0.19650367	-1.08319001
6	5.00164484	-0.00908549	-0.55568903
1	4.67393858	1.03467515	-0.68460567
1	4.80172171	-0.53030302	-1.50243502
50	1.13979776	-0.04784571	-0.07252821
7	-0.36221706	1.34045834	1.48494858
6	-0.02876463	1.13930209	2.91032007
1	-0.61767044	1.81322167	3.55940683
1	-0.20897828	0.09892224	3.20097060
1	1.03902324	1.34696412	3.04186236
7	-1.69864892	-1.35744126	1.53570495
6	-1.79807197	1.11091980	1.18991564
1	-2.39324508	1.98060811	1.53272987
1	-1.90628126	1.05862549	0.09561778
6	-2.43472685	-0.12384692	1.83316907
1	-3.48405303	-0.15845649	1.48607949
1	-2.45463388	-0.02150369	2.92556741
16	-2.08228004	-2.74924809	2.43864927
7	0.44466969	1.80340329	-1.11803907
6	0.02602428	2.72304600	1.08331849
1	-0.57634811	3.46257160	1.64603766
1	1.08237849	2.83515023	1.36038748
6	-0.11910878	2.95699649	-0.42190039
1	0.42373653	3.88302869	-0.67173915
1	-1.17881205	3.10998292	-0.69708432
16	1.36537102	2.01766512	-2.45219657
8	2.13756508	0.73072688	-2.52014807
8	2.07671816	3.31722716	-2.47833347
6	0.25256703	2.01847485	-3.88326168
6	-0.02895109	3.21835414	-4.53640879
6	-0.90822007	3.21330384	-5.62267076
6	-1.50311020	2.02497819	-6.06983129
6	-1.19724434	0.82996124	-5.39473995
6	-0.32603434	0.81883884	-4.30729338
1	0.45134439	4.13702584	-4.20122027
1	-0.07810547	-0.11210479	-3.79711292
1	-1.64476033	-0.10691685	-5.73283928
6	-2.42148230	2.01839323	-7.26655400
1	-1.12890881	4.15089942	-6.13659148
8	-1.21325516	-3.80512610	1.89422183
8	-2.04110851	-2.32636036	3.85117999
6	-3.79313211	-3.17905322	2.04497734
6	-4.82950397	-2.70786564	2.85256331
6	-6.14728838	-3.03611186	2.52462415
6	-6.44174334	-3.82906856	1.40581208
6	-5.37563045	-4.29327281	0.61458044
6	-4.05517356	-3.97614285	0.92562960
1	-4.60000930	-2.11409597	3.73670418
1	-6.96104147	-2.67583398	3.15636144

6	-7.86310351	-4.20199283	1.06837271
1	-5.58442608	-4.92219248	-0.25288115
1	-3.22874946	-4.35950118	0.32724658
1	-2.84161355	3.01472871	-7.45559020
1	-1.87861186	1.71102701	-8.17408135
1	-3.25173247	1.31165128	-7.13171274
1	-8.04343302	-5.27003459	1.26382820
1	-8.58196544	-3.62624587	1.66446760
1	-8.07899007	-4.02926246	0.00459366
1	-1.63109775	-1.59790417	0.54297700

Energy = -8524.637065 Hartree
Number of imaginary frequencies = 0.

Compound I3a isomer 59

Atomic N.	X	Y	Z
8	0.99857777	-0.62268229	0.81579196
8	2.44801654	1.10145461	0.70961132
6	3.70755264	1.70520085	0.36491363
1	3.78418340	1.87728437	-0.71999693
1	4.54628320	1.08758434	0.71117296
1	3.72171038	2.67711509	0.87161447
8	3.29443048	-0.99205392	0.92409558
6	2.21736634	-0.28011748	0.29170464
6	2.18007925	-0.42466696	-1.25339507
1	1.42500241	-1.19341809	-1.47597556
1	1.77118158	0.51992642	-1.64161680
6	3.48335473	-0.78194822	-1.98771473
1	4.31831723	-0.15643074	-1.63856070
1	3.33877259	-0.53240420	-3.05143940
6	3.87718982	-2.26323428	-1.88838966
1	3.01062892	-2.87972673	-2.18563555
1	4.67159475	-2.47418889	-2.62217702
6	4.35570655	-2.70148999	-0.50067073
1	5.31270813	-2.20998375	-0.25969963
1	4.55226548	-3.78697728	-0.50439603
6	3.37342775	-2.40634112	0.62737025
1	2.36757546	-2.80101195	0.41297605
1	3.71122952	-2.87714976	1.56098246
50	0.99253970	-0.51298867	2.94054744
7	-1.11378381	1.06935403	3.05168737
6	-1.10722672	1.46019142	4.47666280
1	-1.99738398	2.06457905	4.72843238
1	-1.09095911	0.56863185	5.11633675
1	-0.20619324	2.04957379	4.68823435
7	-0.88964633	-1.67948713	2.92991847
6	-2.31040505	0.24435453	2.74725328
1	-3.22623522	0.74330240	3.11940757
1	-2.38815098	0.15658563	1.65676521
6	-2.19519936	-1.16647087	3.32908110
1	-3.01790064	-1.77238701	2.91158108
1	-2.32642121	-1.16486282	4.42488264
16	-0.49146274	-3.24374951	3.16997042
7	0.10754740	2.65918598	-0.02074375
6	-1.07150994	2.30330193	2.21938864
1	-1.94259934	2.93840474	2.46369396
1	-0.18044504	2.86597967	2.52396965
6	-1.00598651	2.03230322	0.69446660

1	-1.94605415	2.33088575	0.21053999
1	-0.86929648	0.95582273	0.51799560
16	0.16752076	4.33627198	-0.16029206
8	1.60192784	4.66829897	-0.29693631
8	-0.68101953	4.96992705	0.87667555
6	-0.63587350	4.65248402	-1.74742229
6	-1.92631349	5.17960583	-1.77455609
6	-2.53144070	5.43097834	-3.00924121
6	-1.86109422	5.16952663	-4.21224789
6	-0.55747653	4.64427126	-4.15198741
6	0.05935099	4.38593310	-2.93066843
1	-2.43725508	5.40009148	-0.83814180
1	1.07450673	3.99247941	-2.88709239
1	-0.01776637	4.43976253	-5.07861965
6	-2.50499407	5.46863723	-5.54275334
1	-3.54139044	5.84411990	-3.03568012
8	1.00747686	-3.19483366	3.01126789
8	-1.06991915	-3.85219238	4.38973859
6	-1.14910720	-4.16931790	1.75965172
6	-1.87092673	-5.34121595	1.98082942
6	-2.36051174	-6.05335229	0.88236841
6	-2.13705601	-5.60824650	-0.42823524
6	-1.41248993	-4.41722500	-0.61734365
6	-0.91602580	-3.69370541	0.46509379
1	-2.04447099	-5.67997029	3.00161542
1	-2.92823922	-6.97064868	1.04916811
6	-2.64378070	-6.39349185	-1.61212023
1	-1.23767166	-4.05147237	-1.63134760
1	-0.36133751	-2.76405334	0.31883718
1	-3.58785755	5.61429843	-5.44092345
1	-2.08500979	6.38655297	-5.98236673
1	-2.33053962	4.65725822	-6.26292004
1	-1.82904053	-6.97216593	-2.07456274
1	-3.42785758	-7.10273628	-1.31774506
1	-3.04960111	-5.73054437	-2.38875017
1	1.03490146	2.26742412	0.22607076

Energy = -8524.640101 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 60

Atomic N.	X	Y	Z
8	3.36688621	0.45132514	-0.28132743
8	3.32795365	-0.62921677	-2.22931388
6	3.47527968	-0.71880173	-3.66048326
1	2.60602756	-1.28637455	-4.00982908
1	4.40282694	-1.25333335	-3.91444014
1	3.46792729	0.27843431	-4.11423273
8	3.98320325	1.56554156	-2.23151252
6	4.07316654	0.37617414	-1.44802456
6	5.52212302	-0.09265271	-1.17764289
1	5.81298623	0.33038118	-0.20363921
1	5.45572945	-1.17947716	-1.02583247
6	6.59848262	0.24741652	-2.22073113
1	6.23097827	0.05825398	-3.24097640
1	7.44449865	-0.44159762	-2.06833071
6	7.12598504	1.68655698	-2.11670739
1	7.46276807	1.85985377	-1.07942428

1	8.02010146	1.79317638	-2.75160342
6	6.11328840	2.76962383	-2.50428611
1	5.90726704	2.72479562	-3.58617026
1	6.54570663	3.76543221	-2.30676372
6	4.77457248	2.67665527	-1.77462484
1	4.90979794	2.62718752	-0.68020895
1	4.17158070	3.57164222	-1.99160142
50	1.52348210	-0.58999529	-0.55048788
7	0.80697358	1.32416107	1.03477844
6	1.70845050	1.50130116	2.19122662
1	1.43254427	2.39181718	2.78568544
1	1.67746102	0.61279182	2.83184778
1	2.72962708	1.61732983	1.81084360
7	-0.36156986	-1.08225923	2.42025798
6	-0.61644802	1.18969218	1.42961580
1	-1.02263905	2.18383342	1.70298524
1	-1.17367564	0.84694343	0.54453411
6	-0.91771377	0.26388463	2.60890000
1	-2.01798657	0.25727622	2.72245167
1	-0.49589596	0.66088801	3.54089334
16	-0.65514585	-2.22737383	3.64593028
7	0.44369284	0.95547208	-1.70360551
6	0.96393337	2.47739677	0.10519604
1	0.65038847	3.41411897	0.60512875
1	2.03474482	2.53805458	-0.12745352
6	0.17587898	2.29775968	-1.19275941
1	0.50313153	3.07439629	-1.90350392
1	-0.90457792	2.45922489	-1.01393906
16	-0.39448525	0.43317534	-3.01262877
8	0.16380915	-0.91952406	-3.29481417
8	-0.45758620	1.46565286	-4.07190197
6	-2.10492262	0.17797132	-2.45270054
6	-3.06315851	1.17201662	-2.65731647
6	-4.36054465	0.98283133	-2.17092949
6	-4.71779546	-0.18967655	-1.49017728
6	-3.73522805	-1.17870572	-1.30438439
6	-2.43636207	-1.00253912	-1.77893498
1	-2.79375564	2.07117421	-3.21083676
1	-1.68132989	-1.77976796	-1.65344961
1	-3.99723481	-2.10483019	-0.78801409
6	-6.12853534	-0.40623904	-1.00134132
1	-5.11077915	1.75942854	-2.33225100
8	-0.01453400	-3.46568724	3.17427438
8	-0.28504360	-1.56330214	4.90943700
6	-2.44215448	-2.50349743	3.67178246
6	-3.24242052	-1.78655168	4.56229797
6	-4.62382673	-1.99797965	4.55418249
6	-5.21339425	-2.91410166	3.67120791
6	-4.37919741	-3.63054951	2.79379368
6	-3.00022304	-3.43241077	2.78683786
1	-2.78174187	-1.09426290	5.26624757
1	-5.25321139	-1.44656749	5.25481682
6	-6.70527349	-3.13267222	3.65685614
1	-4.81739319	-4.36518119	2.11539459
1	-2.35249604	-4.00921100	2.12647143
1	-6.67016916	0.54348182	-0.90407806
1	-6.69304563	-1.03896613	-1.70390995
1	-6.14133409	-0.91459621	-0.02715239

1	-6.95104053	-4.20317578	3.69767389
1	-7.19204953	-2.63536232	4.50491586
1	-7.15117877	-2.73521679	2.73218269
1	-0.55615685	-1.50286791	1.50562956

Energy = -8524.634755 Hartree
Number of imaginary frequencies = 0.

Compound I3a isomer 61

Atomic N.	X	Y	Z
8	2.94867023	0.23690008	0.04430377
8	3.63813938	0.77896909	-2.03077057
6	4.64471685	0.99908565	-3.02248502
1	4.11514911	1.31588781	-3.92999365
1	5.20565159	0.07738604	-3.24740569
1	5.34233552	1.79068324	-2.71171133
8	4.73755191	1.66653658	-0.25360947
6	4.08838806	0.46562989	-0.68493099
6	5.01965438	-0.78176252	-0.64903132
1	4.75606746	-1.32875161	0.26792405
1	4.70334407	-1.42934587	-1.48220095
6	6.54161843	-0.56789490	-0.68255708
1	6.82572200	0.14838070	-1.46863892
1	7.00553723	-1.52857678	-0.95971630
6	7.13690153	-0.11757432	0.66090167
1	6.79247166	-0.81092412	1.44766693
1	8.23366170	-0.21688109	0.62059349
6	6.78654861	1.31881403	1.06433934
1	7.27172833	2.03066919	0.37586882
1	7.19001155	1.52793031	2.06995385
6	5.29071455	1.62299548	1.07781219
1	4.72972261	0.90341110	1.69586208
1	5.11829993	2.62453488	1.50088905
50	1.23561629	-0.42871560	-0.94632727
7	0.35401641	2.02515821	-0.86571784
6	1.45935884	2.85610161	-0.33379203
1	1.10695666	3.88819074	-0.15271344
1	1.84892488	2.42151122	0.59074129
1	2.28724331	2.86664561	-1.05196477
7	-0.01268139	-0.15781729	0.86375791
6	-0.78073827	1.98738828	0.09063463
1	-1.07362001	3.01320877	0.38667559
1	-1.63042140	1.51087165	-0.41202491
6	-0.45170997	1.15543853	1.33216077
1	-1.37703760	1.08387179	1.93162837
1	0.30777677	1.64499898	1.96337074
16	0.38204685	-1.32170120	1.95002801
7	-1.38625039	0.61813726	-2.91960390
6	-0.02102264	2.57959104	-2.19499806
1	-0.11340802	3.68083268	-2.11992945
1	0.82786777	2.38012735	-2.86735470
6	-1.32023646	2.08483293	-2.83148757
1	-1.40664929	2.56935381	-3.81857702
1	-2.18567010	2.42018727	-2.24194818
16	-2.83136214	-0.01359574	-3.60305634
8	-2.48744508	-1.40117016	-3.96609763
8	-3.39779632	0.91604776	-4.60565466
6	-3.92788179	-0.00005423	-2.17213196

6	-5.14424157	0.67654969	-2.25925902
6	-6.01170171	0.64898815	-1.16431489
6	-5.67547970	-0.04052421	0.00976565
6	-4.43836510	-0.70827246	0.06819065
6	-3.56359366	-0.69723733	-1.01578310
1	-5.39740806	1.21295889	-3.17300943
1	-2.60478392	-1.21248919	-0.95983116
1	-4.15230007	-1.24426947	0.97504078
6	-6.62163933	-0.08404527	1.18307148
1	-6.96507913	1.17665246	-1.22457619
8	1.18374098	-2.27804345	1.11711145
8	0.92296158	-0.78705739	3.21987600
6	-1.15873891	-2.17923181	2.37120215
6	-1.83805284	-1.84025037	3.54179219
6	-3.03637218	-2.49247063	3.84835465
6	-3.55852963	-3.48583279	3.00765579
6	-2.84392344	-3.81735488	1.84197490
6	-1.65327374	-3.17025545	1.51738995
1	-1.41531520	-1.09317700	4.21292737
1	-3.56682702	-2.23297958	4.76652415
6	-4.85361986	-4.18581851	3.33676656
1	-3.22514179	-4.59874713	1.18158199
1	-1.09295834	-3.44105448	0.62261923
1	-7.40701104	0.67717450	1.09535588
1	-7.11447988	-1.06639082	1.24854067
1	-6.08822610	0.07265495	2.13075706
1	-4.73843393	-5.27819985	3.29357873
1	-5.21080438	-3.91843700	4.33924812
1	-5.64137294	-3.91927692	2.61526018
1	-0.61751268	0.20089319	-3.45649333

Energy = -8524.632506 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 62

Atomic N.	X	Y	Z
8	2.48500919	0.52610256	0.26238532
8	2.71348782	1.61924804	-1.69677169
6	3.48001376	2.08622865	-2.80955897
1	2.79072653	2.66913257	-3.43415096
1	3.87824379	1.25267948	-3.41114388
1	4.30721732	2.73207918	-2.48014639
8	4.28684161	1.92766035	-0.08895277
6	3.43382707	0.91788040	-0.64285040
6	4.21798840	-0.31344098	-1.18597993
1	4.12053098	-1.09409845	-0.41749270
1	3.65327720	-0.68206053	-2.05721223
6	5.70446657	-0.14596253	-1.54022961
1	5.86949517	0.75637364	-2.14878026
1	5.99310495	-1.00104002	-2.17326973
6	6.63646306	-0.11773019	-0.31827326
1	6.41302986	-0.99419103	0.31442811
1	7.67820011	-0.23894536	-0.65671282
6	6.53885511	1.15497117	0.52989801
1	6.92183386	2.01673134	-0.04186202
1	7.18394607	1.05505128	1.41962558
6	5.12631636	1.49257182	1.00006484
1	4.65361794	0.64711252	1.52559688

1	5.16004014	2.33893785	1.70309104
50	0.51918189	0.23383551	-0.39698809
7	-0.00180176	2.62739413	0.48381871
6	1.25136655	3.15556647	1.07320853
1	1.04757989	4.09369394	1.62157780
1	1.69765886	2.41585719	1.74304588
1	1.97932946	3.34102021	0.27548002
7	-0.29184270	0.10860842	1.66105525
6	-1.02023672	2.39700120	1.53891276
1	-1.20330505	3.32727382	2.11071503
1	-1.95567616	2.09931686	1.04799766
6	-0.60423743	1.27143889	2.48737136
1	-1.46025477	1.07442989	3.15753817
1	0.24567576	1.56980241	3.12289944
16	0.20375241	-1.28467762	2.36733588
7	-2.00349247	2.07616907	-1.75151885
6	-0.45182384	3.60485748	-0.54180398
1	-0.44037363	4.62302934	-0.10472662
1	0.30886202	3.59368933	-1.33775383
6	-1.84453771	3.41106250	-1.13884740
1	-1.99936529	4.22902942	-1.86423733
1	-2.62277041	3.51054982	-0.37212203
16	-3.62082797	1.77309425	-2.28432506
8	-3.90476704	2.49458017	-3.54536842
8	-4.46590002	1.99378294	-1.09337340
6	-3.51631066	0.01672037	-2.65333753
6	-3.45639871	-0.90489463	-1.60406352
6	-3.40253643	-2.26227373	-1.90909371
6	-3.40345919	-2.71186599	-3.24169563
6	-3.47297200	-1.76061553	-4.26992831
6	-3.53056849	-0.39458428	-3.98593420
1	-3.45710027	-0.56211071	-0.56989330
1	-3.59947589	0.34850503	-4.77949649
1	-3.48605718	-2.09191928	-5.30949764
6	-3.30971818	-4.18398270	-3.55091462
1	-3.35645738	-2.99071903	-1.09772768
8	0.70979964	-2.07370239	1.19725582
8	1.05949206	-1.07380248	3.55709976
6	-1.29416372	-2.11521959	2.95839160
6	-1.63723321	-2.04184551	4.30858895
6	-2.81023032	-2.66171742	4.74866043
6	-3.64109603	-3.35850136	3.86010203
6	-3.26033781	-3.43121405	2.50812593
6	-2.09785176	-2.81296725	2.05234656
1	-0.97681227	-1.52423193	5.00359740
1	-3.07864551	-2.60988006	5.80551024
6	-4.91701850	-4.00784133	4.33464962
1	-3.88374671	-3.99011291	1.80674752
1	-1.78979371	-2.88559349	1.00916951
1	-2.27884328	-4.54331216	-3.40820373
1	-3.95280130	-4.77445213	-2.88408034
1	-3.59706767	-4.39640955	-4.58822344
1	-5.05771779	-4.99693736	3.87723269
1	-4.92392044	-4.12777358	5.42550431
1	-5.79209071	-3.39768905	4.06181499
1	-1.39759331	1.97524667	-2.57430085

Energy = -8524.631130 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 63

Atomic N.	X	Y	Z
8	2.42240179	0.57974946	0.12932875
8	2.98497379	1.57998948	-1.80944928
6	3.91777147	1.94922393	-2.82720487
1	3.35936798	2.56689686	-3.54225414
1	4.31413532	1.06842401	-3.35894520
1	4.75080076	2.53527962	-2.41153446
8	4.36779562	1.81475420	-0.02221491
6	3.50585431	0.86304728	-0.66193502
6	4.23920091	-0.44949197	-1.06857511
1	3.98946997	-1.18839323	-0.29322424
1	3.74729716	-0.80489953	-1.98793694
6	5.76510831	-0.41737526	-1.25346547
1	6.07439162	0.44773237	-1.85968666
1	6.04881911	-1.31362923	-1.82909279
6	6.55243841	-0.42584396	0.06627949
1	6.18804671	-1.26240402	0.68731678
1	7.61247604	-0.63840407	-0.14724460
6	6.46244148	0.87612956	0.86952988
1	6.97807694	1.68721951	0.32880301
1	6.98972776	0.75304213	1.83111072
6	5.03715744	1.33822998	1.16268627
1	4.43923197	0.54545353	1.64116053
1	5.05958286	2.19544329	1.85336319
50	0.50363632	0.42879935	-0.70587822
7	-0.03229779	2.74771942	0.36781744
6	1.27218964	3.43937727	0.50398327
1	1.13850019	4.42224898	0.99108861
1	1.96268808	2.82032067	1.08414244
1	1.72236468	3.57378364	-0.48699042
7	-0.23644208	0.12089286	1.34887778
6	-0.59788810	2.45736402	1.71600027
1	-0.44456500	3.32639510	2.38290106
1	-1.67527052	2.28620524	1.61021503
6	0.00626299	1.19004852	2.31982168
1	-0.50691472	0.99132892	3.27591790
1	1.07985388	1.31115613	2.53826884
16	-0.08549321	-1.44281112	1.82055723
7	-2.33113249	1.83767025	-1.48291237
6	-0.92443201	3.61738501	-0.44214330
1	-1.03257505	4.60066601	0.05798160
1	-0.40153565	3.80604432	-1.39264144
6	-2.33819291	3.10815192	-0.72832086
1	-2.86843911	3.91154292	-1.26824821
1	-2.89394654	2.92939124	0.20068211
16	-3.89948087	1.10113121	-1.56169891
8	-4.80978848	1.88883908	-2.42372109
8	-4.26869772	0.84041058	-0.15411764
6	-3.49478590	-0.43055607	-2.40898859
6	-2.72573042	-1.40234793	-1.76154193
6	-2.43865098	-2.58876152	-2.43096763
6	-2.91241703	-2.81913296	-3.73478931
6	-3.68908653	-1.82762233	-4.35371552
6	-3.98329868	-0.62862127	-3.70129058
1	-2.35181498	-1.24908915	-0.75047393

1	-4.59068061	0.14245517	-4.17373711
1	-4.07112775	-1.99439525	-5.36218992
6	-2.57297559	-4.09976776	-4.45355369
1	-1.82730941	-3.33920671	-1.92752980
8	-0.08482682	-2.18596889	0.51750426
8	1.00997659	-1.69558043	2.78544718
6	-1.62492894	-1.84554125	2.69548848
6	-1.56815400	-2.74787515	3.76086771
6	-2.74759350	-3.10329656	4.41569012
6	-3.98568855	-2.56653927	4.02618076
6	-4.01032149	-1.64955601	2.96393540
6	-2.83996102	-1.28624164	2.29487349
1	-0.60449830	-3.14934859	4.07244061
1	-2.70469106	-3.80564633	5.25061237
6	-5.25771033	-2.97784623	4.72503579
1	-4.95710055	-1.20416915	2.65311801
1	-2.87967052	-0.55748248	1.48482090
1	-1.51473161	-4.10428735	-4.75683448
1	-2.72323577	-4.97239495	-3.80316568
1	-3.18272143	-4.22923957	-5.35647760
1	-5.62787305	-3.93672854	4.32960229
1	-5.09759414	-3.11269283	5.80349272
1	-6.05216026	-2.23414853	4.58181590
1	-2.03360863	1.98739402	-2.45406799

Energy = -8524.631976 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 64

Atomic N.	X	Y	Z
8	3.34904596	0.55630556	-0.24235107
8	3.36483874	-0.54466813	-2.17829793
6	3.54768453	-0.65796603	-3.60358328
1	4.48393232	-1.19199538	-3.82418815
1	3.54656933	0.33170607	-4.07378961
1	2.69023423	-1.23604407	-3.96493995
8	3.95921991	1.66623718	-2.19707368
6	4.07223452	0.48842682	-1.39909707
6	5.53028450	0.06325909	-1.10579206
1	5.79694686	0.50432210	-0.13285440
1	5.49235226	-1.02340216	-0.94312650
6	6.60988888	0.42232471	-2.13916228
1	6.26104141	0.21159106	-3.16170303
1	7.47301692	-0.24055751	-1.96807893
6	7.09545365	1.87686350	-2.04493723
1	7.41391981	2.07097274	-1.00555218
1	7.99434078	2.00152090	-2.66974115
6	6.05787651	2.92663139	-2.45739950
1	5.86668711	2.86370993	-3.54109572
1	6.45973428	3.93640820	-2.26638270
6	4.71339393	2.80404727	-1.74294534
1	4.83665502	2.76977609	-0.64651742
1	4.08819390	3.67933379	-1.97671541
50	1.53946800	-0.53998606	-0.52339466
7	0.75066969	1.36134489	1.04074015
6	1.63117567	1.57064583	2.20805623
1	1.32262869	2.45695530	2.79263918
1	1.61624717	0.68558151	2.85394619

1	2.65371180	1.71292167	1.84036271
7	-0.35994336	-1.06858910	2.42896951
6	-0.67346560	1.18694927	1.41733170
1	-1.11301120	2.17004765	1.67873061
1	-1.20791700	0.82237001	0.52694480
6	-0.96266285	0.25986824	2.59875978
1	-2.06372305	0.21825973	2.69607927
1	-0.56783843	0.67690312	3.53378678
16	-0.62788626	-2.21195254	3.66212058
7	0.43101729	0.96758772	-1.69859570
6	0.88669455	2.51377435	0.10701150
1	0.54019237	3.44369390	0.59777580
1	1.95830200	2.60365092	-0.11211938
6	0.12090570	2.30527082	-1.19996645
1	0.43694471	3.08610307	-1.91125484
1	-0.96569929	2.43919421	-1.03616923
16	-0.37167136	0.41565712	-3.01751187
8	0.22794869	-0.92275062	-3.28285365
8	-0.44627189	1.44008886	-4.08377607
6	-2.08302581	0.11679354	-2.48263839
6	-3.06394083	1.08505344	-2.70440163
6	-4.36247691	0.86376315	-2.23571829
6	-4.69887900	-0.31584412	-1.55600807
6	-3.69393094	-1.27826594	-1.35315495
6	-2.39324355	-1.06983251	-1.81004510
1	-2.81010483	1.98939016	-3.25680727
1	-1.61998199	-1.82646814	-1.67065442
1	-3.93899345	-2.20903569	-0.83690066
6	-6.11116355	-0.56693254	-1.08855076
1	-5.13012639	1.62035047	-2.40980557
8	0.06837718	-3.42871399	3.21404580
8	-0.30381265	-1.52099442	4.92390565
6	-2.40273168	-2.55812645	3.66318304
6	-3.24587513	-1.86083918	4.52984782
6	-4.61708206	-2.12830507	4.50352676
6	-5.15490284	-3.08038854	3.62523878
6	-4.27841705	-3.77561704	2.77269094
6	-2.90840957	-3.52190093	2.78431077
1	-2.82475002	-1.14120770	5.23114739
1	-5.27932758	-1.59328831	5.18639697
6	-6.63714909	-3.35433090	3.58776269
1	-4.67546457	-4.53798572	2.09965831
1	-2.22721782	-4.08234444	2.14387829
1	-6.65684195	0.37320398	-0.93507954
1	-6.67053953	-1.15463753	-1.83319195
1	-6.12699583	-1.13566285	-0.14866829
1	-6.84279091	-4.43307173	3.55240430
1	-7.14553340	-2.93440830	4.46463518
1	-7.09481052	-2.90901751	2.69074509
1	-0.52921907	-1.50372819	1.51595871

Energy = -8524.634806 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 65

Atomic N.	X	Y	Z
8	2.59802060	-0.35250651	-1.51276631
8	3.73073049	1.59566910	-0.90422168

6	4.05079860	1.98061081	-2.24912855
1	3.95368743	3.07214979	-2.27956685
1	3.35188179	1.53129383	-2.96903141
1	5.08540097	1.70506258	-2.51342337
8	3.12279512	0.02801066	0.65273836
6	3.58279865	0.17641024	-0.71467728
6	4.88432613	-0.61868364	-0.93084629
1	4.64465795	-1.65411056	-0.64569214
1	5.09222464	-0.63649658	-2.01102610
6	6.12027990	-0.13557391	-0.16579083
1	6.44420634	0.84078861	-0.56297294
1	6.93861305	-0.84120869	-0.38220912
6	5.95774339	-0.00652064	1.35729544
1	5.55297685	-0.94298074	1.77685666
1	6.95805420	0.12534933	1.79918915
6	5.08240461	1.18660115	1.76847876
1	5.35617702	2.05110265	1.14629946
1	5.29657909	1.46703786	2.81270809
6	3.57080946	0.94710465	1.68255331
1	3.20898858	0.46830229	2.60312423
1	3.04177225	1.90496890	1.57139562
50	0.71223399	0.31026504	-0.90139542
7	0.23411231	-2.14251285	-0.02589026
6	1.52262850	-2.87261791	-0.07133665
1	1.36939618	-3.94097073	0.16901974
1	1.97585726	-2.77494409	-1.06282736
1	2.21261203	-2.42505650	0.65287529
7	-0.26459758	-0.86607763	-2.49814042
6	-0.70552258	-2.70955771	-1.03100607
1	-0.74029829	-3.81141011	-0.92754585
1	-1.70859925	-2.31610118	-0.81695464
6	-0.34503468	-2.32269060	-2.46511336
1	-1.14687199	-2.70172073	-3.12306945
1	0.59505289	-2.79877804	-2.78944874
16	0.01700796	-0.08098153	-3.90781366
7	-1.11845360	0.00676886	2.16740875
6	-0.33222689	-2.29079317	1.34484941
1	-0.68585593	-3.33424485	1.46483104
1	0.48095177	-2.14470722	2.06590367
6	-1.48411135	-1.33974757	1.71206520
1	-2.06349824	-1.81267908	2.51671931
1	-2.17926820	-1.21157599	0.86832347
16	-0.53098023	0.20619214	3.74874400
8	0.42617849	1.32764861	3.67060784
8	-0.15201790	-1.11100347	4.30931491
6	-1.98381878	0.76605460	4.66112258
6	-2.65035087	-0.12101867	5.50583490
6	-3.76803083	0.32845082	6.21361320
6	-4.22044505	1.65015979	6.09232448
6	-3.52223793	2.52171222	5.23725367
6	-2.40698522	2.09104975	4.52292665
1	-2.28503422	-1.14152524	5.61384143
1	-1.85967327	2.77243814	3.87223939
1	-3.85664781	3.55569126	5.13456510
6	-5.40827309	2.13977018	6.88162268
1	-4.29343117	-0.36082421	6.87705350
8	0.48561018	1.26236757	-3.41210782
8	0.83523263	-0.84142210	-4.87814206

6	-1.59448505	0.18428243	-4.68892352
6	-1.90534831	-0.49396307	-5.86707253
6	-3.15754658	-0.29615630	-6.45590159
6	-4.09763324	0.57426024	-5.88700100
6	-3.75459700	1.24630634	-4.69971948
6	-2.51297140	1.05701713	-4.09785445
1	-1.16534405	-1.15590012	-6.31545121
1	-3.40430625	-0.82517910	-7.37834651
6	-5.43442852	0.81138142	-6.54392526
1	-4.47228543	1.93139542	-4.24411241
1	-2.24741118	1.58887611	-3.18427436
1	-6.02805222	1.30541224	7.23384586
1	-5.08083851	2.70697867	7.76679128
1	-6.03777783	2.81148767	6.28220591
1	-5.43023541	1.75739929	-7.10751583
1	-5.68313173	0.00775895	-7.24885056
1	-6.24000667	0.88247233	-5.80022824
1	-0.53413696	0.54818134	1.51477922

Energy = -8524.635470 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 66

Atomic N.	X	Y	Z
8	3.21726443	-0.98745356	-0.39708712
8	5.01533810	0.49203759	-0.64394925
6	5.44684627	-0.07679567	-1.88189576
1	5.84080294	0.75498191	-2.47756954
1	4.60687169	-0.54496478	-2.41629401
1	6.24849311	-0.82121634	-1.73448943
8	3.73125211	0.42343260	1.26153624
6	4.30117206	-0.42181247	0.20508925
6	5.19759453	-1.49683831	0.84346922
1	4.54796536	-2.03001958	1.55344718
1	5.46342167	-2.21937247	0.05627748
6	6.46401600	-1.00659773	1.55233122
1	7.16653408	-0.59016381	0.81136241
1	6.96100714	-1.88883665	1.98688301
6	6.24555750	0.03874712	2.65895433
1	5.47520926	-0.31067377	3.36561697
1	7.18025921	0.12804805	3.23444755
6	5.88100163	1.42828647	2.11304727
1	6.51511785	1.63973808	1.23989177
1	6.11181275	2.19802853	2.86732843
6	4.40903189	1.61939679	1.73794826
1	3.80865765	1.88528329	2.61829811
1	4.30738568	2.41592820	0.98608666
50	1.55872594	0.29017731	0.07457897
7	0.41416546	-1.83140933	-0.85954042
6	0.97403210	-2.29378836	-2.14662743
1	0.51608719	-3.24842947	-2.46544772
1	0.81458123	-1.53748462	-2.92317888
1	2.05279718	-2.43264399	-2.01506069
7	-0.98008591	0.35206584	-2.38807173
6	-1.05795704	-1.65079332	-0.90534325
1	-1.55759408	-2.63877694	-0.85682753
1	-1.35040903	-1.09743793	0.00047110
6	-1.61775384	-0.94678216	-2.14343130

1	-2.71043662	-0.86484703	-1.99466391
1	-1.45412048	-1.55516057	-3.04201576
16	-1.31536116	1.13342773	-3.86343414
7	0.78307835	-0.93736781	1.73591633
6	0.77018758	-2.80924164	0.20716123
1	0.29873274	-3.78863113	-0.00329055
1	1.86121225	-2.92032862	0.16442707
6	0.36670399	-2.32982818	1.60152526
1	0.86497904	-2.97736239	2.34229280
1	-0.72409158	-2.44557804	1.75229868
16	0.61939895	-0.19678018	3.18942131
8	1.19892749	1.15985749	2.97988256
8	1.08587436	-1.05333507	4.30456847
6	-1.16564756	0.02827732	3.44215261
6	-1.87142754	-0.85699393	4.25703811
6	-3.24936206	-0.68452913	4.42221783
6	-3.93123182	0.36335625	3.78849945
6	-3.19290283	1.24837596	2.98179343
6	-1.82044876	1.08617972	2.80294369
1	-1.33596011	-1.65319751	4.77339848
1	-1.24522948	1.78805702	2.19801779
1	-3.70183941	2.08523590	2.49864586
6	-5.41913685	0.54299092	3.96191108
1	-3.80132420	-1.37174624	5.06638444
8	-0.57966823	2.40627061	-3.79295779
8	-1.07121237	0.12319843	-4.91017954
6	-3.08274441	1.51217298	-3.87047349
6	-3.97926265	0.62441384	-4.46817638
6	-5.34326190	0.92395949	-4.45055108
6	-5.82177522	2.09772969	-3.84890138
6	-4.89410881	2.97365741	-3.25827515
6	-3.52930192	2.69133343	-3.26560579
1	-3.60559069	-0.27433265	-4.95764463
1	-6.04796772	0.23583044	-4.92076068
6	-7.29150691	2.43345548	-3.86517726
1	-5.24681126	3.89673883	-2.79459549
1	-2.80940952	3.38506667	-2.83132833
1	-5.80366538	-0.07358277	4.78423340
1	-5.67279951	1.59191753	4.17045280
1	-5.96085911	0.25568811	3.04740101
1	-7.51959751	3.13721284	-4.68075569
1	-7.90673093	1.53804062	-4.02024401
1	-7.60389332	2.91281843	-2.92766895
1	-1.04960901	1.02371921	-1.61813503

Energy = -8524.635955 Hartree

Number of imaginary frequencies = 0.

Compound I3a isomer 67

Atomic N.	X	Y	Z
8	2.56737797	-0.87355860	0.45928865
8	2.84776601	0.55238756	-1.21330687
6	3.40687402	1.71531746	-1.86207722
1	3.56929826	2.52449448	-1.13978963
1	2.66760616	2.02013614	-2.61026130
1	4.35257837	1.44368891	-2.35394136
8	3.50872418	1.21797243	0.86755857
6	3.46708438	0.04261451	0.04219530

6	4.85955816	-0.57882512	-0.22930900
1	4.93377980	-1.46236481	0.42336109
1	4.83263408	-0.96243020	-1.26019767
6	6.09890123	0.30512564	-0.01857630
1	5.97054808	1.28136690	-0.51081962
1	6.94507245	-0.18579724	-0.52610979
6	6.47791509	0.51379392	1.45680977
1	6.52581617	-0.47305934	1.95006578
1	7.49574826	0.93238561	1.50967320
6	5.53047523	1.42734366	2.24308496
1	5.60928904	2.46015986	1.86554747
1	5.83891081	1.45451037	3.30198726
6	4.06232471	1.01676549	2.18412363
1	3.91426570	-0.02921033	2.49964088
1	3.46247493	1.64520288	2.85786482
50	0.65066178	0.07631434	-0.21816881
7	0.47301697	-2.52852587	-0.66679298
6	1.57865449	-2.91444523	-1.57469747
1	1.45234517	-3.95467899	-1.92845095
1	1.60764618	-2.23897875	-2.43599152
1	2.52295279	-2.81413778	-1.03111805
7	-0.30185456	-0.45196955	-2.22566832
6	-0.82758313	-2.64435448	-1.36383247
1	-1.01908475	-3.69421371	-1.66064633
1	-1.61608101	-2.33725407	-0.66112263
6	-0.86964474	-1.74070504	-2.60098036
1	-1.92474693	-1.65340015	-2.91810773
1	-0.32334875	-2.20541193	-3.43966043
16	-0.46209985	0.80551281	-3.25221897
7	0.32341448	-1.65289288	2.24990347
6	0.53823466	-3.39811554	0.53272347
1	0.19200740	-4.41811662	0.27535362
1	1.59959311	-3.47391657	0.80855434
6	-0.23728952	-2.92195871	1.75719858
1	-0.17880540	-3.71450079	2.52067698
1	-1.30285457	-2.76808351	1.52692166
16	-0.10835844	-1.17952625	3.84009004
8	0.95720623	-0.24576824	4.25127395
8	-0.44946317	-2.37127196	4.64728481
6	-1.63269560	-0.25999772	3.56515200
6	-2.85623867	-0.84752257	3.88972194
6	-4.03050548	-0.12107103	3.68246940
6	-3.99515092	1.18002569	3.15747793
6	-2.74592589	1.74761198	2.85295979
6	-1.56328462	1.03745067	3.05101611
1	-2.87722114	-1.84978995	4.31612058
1	-0.59646711	1.48394837	2.82256685
1	-2.69819397	2.76339893	2.45666299
6	-5.26929867	1.94677468	2.90819707
1	-4.99052382	-0.57102842	3.94139556
8	0.23380976	1.92641920	-2.54903143
8	-0.08873240	0.47381636	-4.64899148
6	-2.23103277	1.22006194	-3.28815866
6	-2.95712857	1.06784879	-4.46842994
6	-4.31794997	1.38985964	-4.48002331
6	-4.96069324	1.86526261	-3.32892916
6	-4.20383510	2.00628524	-2.15138173
6	-2.84825838	1.68667818	-2.12355972

1	-2.44971180	0.70986609	-5.36372977
1	-4.88827681	1.27155782	-5.40339083
6	-6.42106167	2.24283681	-3.35263424
1	-4.68672846	2.37772622	-1.24479808
1	-2.26566781	1.80522718	-1.20858373
1	-6.06921154	1.62945440	3.58968637
1	-5.11745782	3.02740755	3.02839553
1	-5.62860276	1.77881017	1.88046953
1	-6.54207677	3.33622435	-3.40095398
1	-6.93182673	1.81451430	-4.22453098
1	-6.93903739	1.90055162	-2.44584716
1	1.34944458	-1.58782984	2.17134603

Energy = -8524.628162 Hartree
Number of imaginary frequencies = 0.

Compound I3a isomer 68

Atomic N.	X	Y	Z
8	2.77373768	-0.96777945	0.62323264
8	3.55490641	0.48768946	-0.88994745
6	4.47314801	1.48229132	-1.35898557
1	4.66868074	2.24383993	-0.59147466
1	3.98994839	1.95124216	-2.22462303
1	5.42394237	1.02778705	-1.68439170
8	3.93832903	0.92458452	1.30693710
6	3.85511987	-0.16518575	0.36723499
6	5.14179426	-1.03112363	0.29449130
1	4.94302506	-1.93580204	0.88809074
1	5.22820916	-1.36359060	-0.75093032
6	6.46552195	-0.40537135	0.76323889
1	6.59916614	0.59962310	0.33453000
1	7.28360405	-1.02294281	0.35756061
6	6.62460025	-0.33852287	2.29022725
1	6.41986435	-1.33910422	2.70954051
1	7.67562330	-0.11178742	2.53223328
6	5.72510752	0.69184550	2.98151101
1	6.03448068	1.71106956	2.69621646
1	5.85397387	0.61766997	4.07478524
6	4.23984551	0.54270238	2.66883756
1	3.87589324	-0.47933305	2.85974131
1	3.64687847	1.22020891	3.29916461
50	0.99286648	0.16640035	0.54819588
7	0.32617064	-1.62822053	-1.17062507
6	1.26477401	-1.68402927	-2.31036442
1	1.02079745	-2.52049000	-2.99092425
1	1.24631962	-0.74060113	-2.86632734
1	2.27594312	-1.82117879	-1.91125178
7	-0.82747004	0.88169142	-2.37443210
6	-1.08701732	-1.47281362	-1.59469854
1	-1.47242725	-2.44160962	-1.97032813
1	-1.67486808	-1.21838952	-0.69936675
6	-1.35593986	-0.44777739	-2.69930765
1	-2.44835301	-0.44293950	-2.87065277
1	-0.87832703	-0.75854677	-3.63712912
16	-0.76431480	2.03812945	-3.62263191
7	-0.11881789	-1.49390836	1.55473443
6	0.47878872	-2.86461085	-0.35111229
1	0.18294814	-3.75064210	-0.94598098

1	1.54633460	-2.93724890	-0.10565395
6	-0.32581772	-2.80692614	0.94932395
1	0.03764301	-3.61458912	1.60522989
1	-1.39860491	-2.99319903	0.75834912
16	0.11229339	-1.35910814	3.16773774
8	0.79170817	-0.02393473	3.28391186
8	0.72129277	-2.56212149	3.78203202
6	-1.51894590	-1.16704803	3.93481053
6	-2.07157125	-2.22712935	4.65320852
6	-3.34057415	-2.07861135	5.21975469
6	-4.06066481	-0.88323516	5.08478576
6	-3.47644301	0.16995769	4.35874487
6	-2.21412216	0.03628843	3.78427340
1	-1.50126613	-3.14737079	4.77518819
1	-1.75746985	0.86091214	3.23662725
1	-4.01846569	1.11151384	4.24908539
6	-5.41397234	-0.71396258	5.72937558
1	-3.77458037	-2.90619521	5.78423673
8	-0.23501950	3.25450486	-2.98485177
8	-0.09134133	1.36638012	-4.75033861
6	-2.46975053	2.36930974	-4.12146588
6	-3.03005972	1.66239055	-5.18657946
6	-4.35496321	1.91883874	-5.54825136
6	-5.12372286	2.87147345	-4.86367798
6	-4.52941841	3.57157794	-3.79839938
6	-3.20976366	3.32944224	-3.42320030
1	-2.42553969	0.94113251	-5.73547540
1	-4.79598370	1.37358037	-6.38448801
6	-6.54604256	3.16238013	-5.27071338
1	-5.10800611	4.32599713	-3.26199352
1	-2.74256115	3.89243008	-2.61523645
1	-5.87439712	-1.68408252	5.95674254
1	-5.32930357	-0.15774727	6.67603940
1	-6.09873870	-0.14821948	5.08269051
1	-6.62453816	4.15887264	-5.73134773
1	-6.91448083	2.42716239	-5.99684158
1	-7.21858178	3.15645175	-4.40135070
1	-1.21103428	1.30965810	-1.52730041

Energy = -8524.637067 Hartree

Number of imaginary frequencies = 0.

Intermediate 3b (I3b)

Compound I3b isomer 1

Atomic N.	X	Y	Z
8	-0.08121442	-1.16213254	-0.11091672
8	0.43419539	-0.91572810	2.05623842
6	0.22894004	-1.22668565	3.43429272
1	0.53281341	-0.33558051	3.99711116
1	0.85529835	-2.07737002	3.75435528
1	-0.82803908	-1.44042083	3.64614988
8	-1.33303522	-2.34236197	1.35828644
6	-0.01044803	-1.89204441	1.02632564
6	1.04540112	-3.01059093	0.94411903
1	1.22437814	-3.44894682	1.93936253
1	1.97079026	-2.48839480	0.66520693
6	0.72804604	-4.12372183	-0.06687260

1	0.26197968	-3.67743150	-0.95984215
1	1.67536059	-4.57393210	-0.40287015
6	-0.16192426	-5.23898088	0.49648493
1	0.35362404	-5.69674678	1.35930309
1	-0.26741749	-6.03738393	-0.25556260
6	-1.55386867	-4.77932143	0.94164834
1	-2.15128778	-4.45777853	0.07303357
1	-2.08832281	-5.63127642	1.39531485
6	-1.54778624	-3.63279700	1.95469375
1	-0.82573520	-3.83306726	2.76532999
1	-2.54099477	-3.54669147	2.42083102
50	0.05223676	0.99093541	0.26784141
7	-1.51008804	0.94156254	-1.66697005
6	-1.67728449	2.30846560	-2.19740416
1	-2.46530493	2.33889622	-2.97171283
1	-0.73509770	2.66191974	-2.63021235
1	-1.95327486	2.98430458	-1.38036071
7	1.29200180	0.08755902	-2.52513466
6	-1.17294227	-0.02092082	-2.74819659
1	-1.97577906	-0.00283687	-3.51079078
1	-1.16746973	-1.01601098	-2.28216092
6	0.16148060	0.20892935	-3.45395208
1	0.21451752	-0.53203392	-4.27722907
1	0.19097517	1.19688058	-3.93370371
6	2.59763635	0.20506606	-3.08660734
6	3.08953334	1.47078006	-3.47894271
6	4.37816639	1.56453993	-4.02017403
6	5.21054034	0.45022748	-4.16383624
6	4.71513963	-0.79005532	-3.74463230
6	3.42838961	-0.93422954	-3.21495465
7	-1.90597738	1.45888462	1.07517425
6	-2.75745043	0.47550477	-0.99433495
1	-2.57122228	-0.56579758	-0.69592990
1	-3.60163795	0.50279807	-1.70976096
6	-3.08929949	1.29656417	0.24644425
1	-3.52118295	2.27910620	-0.04519802
1	-3.91034145	0.76013337	0.75734907
6	-2.10550372	1.97876334	2.37975074
6	-2.83904641	1.25257463	3.36231325
6	-2.99049427	1.77807812	4.65086953
6	-2.44032688	3.00768859	5.02781000
6	-1.72158726	3.71424255	4.05984050
6	-1.55186272	3.23440885	2.75392277
6	2.27675039	2.72496620	-3.27636738
1	4.74840327	2.54957527	-4.31571502
6	6.61171594	0.58476742	-4.71001349
1	5.34530117	-1.67808208	-3.84023161
6	2.94662735	-2.29742129	-2.77899063
6	-3.42758461	-0.10429573	3.06201353
1	-3.54450528	1.19276914	5.39075736
6	-2.64215670	3.56204179	6.41784012
1	-1.28637947	4.68282484	4.32116894
6	-0.79147354	4.09173989	1.76940688
1	2.93099905	3.60544822	-3.23666580
1	1.70941253	2.66740774	-2.33601295
1	1.55664167	2.89501111	-4.09375128
1	2.81090298	-2.35324425	-1.68731206
1	3.67434284	-3.06972956	-3.05813009

1	1.98129727	-2.56350714	-3.23594738
1	6.70464930	1.46249244	-5.36356009
1	6.90461561	-0.30429375	-5.28564720
1	7.34560325	0.70172920	-3.89678013
1	-3.49352010	-0.70325437	3.98147176
1	-2.82097245	-0.64765868	2.32459439
1	-4.45179609	-0.02760882	2.66051346
1	-1.23032608	4.02998801	0.76407100
1	0.26066925	3.78081446	1.67152666
1	-0.79429905	5.14163119	2.09302522
1	-2.64261237	2.76269390	7.17248662
1	-3.60705881	4.08730808	6.50314159
1	-1.85420001	4.28075051	6.68098584
1	1.19075640	-0.77240691	-1.97901837

Energy = -7584.962712 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 2

Atomic N.	X	Y	Z
8	0.89492010	-0.67203707	0.48785229
8	1.27783043	0.29272262	2.48120459
6	1.00299411	0.35115121	3.88224067
1	1.10975002	1.40326050	4.17443843
1	1.73189374	-0.24706008	4.45522389
1	-0.01917628	0.01404956	4.10179472
8	-0.00595802	-1.69778627	2.27905442
6	1.13678272	-1.02974510	1.77584156
6	2.47337064	-1.77399332	1.94461638
1	2.73453986	-1.86283642	3.01224167
1	3.21781245	-1.10444242	1.49327427
6	2.52711069	-3.15399632	1.27113738
1	2.00796645	-3.09939380	0.30158758
1	3.57837209	-3.39015580	1.04483506
6	1.94994282	-4.28637628	2.12974479
1	2.53331098	-4.35104548	3.06553255
1	2.09590552	-5.24827063	1.61239605
6	0.46824628	-4.12613015	2.48551088
1	-0.15780525	-4.20195052	1.58169873
1	0.16462752	-4.95190143	3.15122118
6	0.12228477	-2.80946543	3.18309743
1	0.84151642	-2.59405622	3.99263319
1	-0.87360862	-2.88259126	3.64361775
50	0.96325595	1.44018808	0.24024359
7	-2.31986388	2.91697606	-2.66324901
6	-1.90569046	4.14180770	-3.32509392
1	-0.91521841	4.53888859	-3.01469801
1	-2.64834658	4.93038657	-3.13306242
1	-1.86444911	3.97216767	-4.41294000
7	0.51009305	0.60562678	-2.19979501
6	-1.61339893	1.72384034	-3.09670766
1	-1.88610248	1.53937227	-4.15098444
1	-2.00859384	0.87719279	-2.51535463
6	-0.05350612	1.72587487	-3.01408138
1	0.36727340	1.65805357	-4.02661414
1	0.28954936	2.68113689	-2.58988543
6	1.56296103	-0.17155722	-2.80024516
6	2.77171761	0.43562048	-3.20492265

6	3.77170082	-0.36886395	-3.76941402
6	3.62136389	-1.74794405	-3.93608445
6	2.42238175	-2.32685131	-3.50497362
6	1.39042897	-1.56826902	-2.94418594
7	-1.14354540	1.85508498	0.39423218
6	-2.66912583	3.05116934	-1.24944282
1	-3.31998011	2.20619186	-0.97241268
1	-3.29030932	3.96030231	-1.17973854
6	-1.54527316	3.14893856	-0.17639013
1	-0.66141167	3.64715764	-0.62029981
1	-1.90773011	3.83851632	0.60625184
6	-1.95528313	1.40620935	1.47845693
6	-2.68310384	0.19117708	1.37284402
6	-3.49855206	-0.22938782	2.42949253
6	-3.62541896	0.50420461	3.61392199
6	-2.87433770	1.67674929	3.72767065
6	-2.04129603	2.13591247	2.69799358
6	3.04416579	1.91185762	-3.02893324
1	4.70744896	0.10706065	-4.07279780
6	4.70617559	-2.58302827	-4.57199139
1	2.28023168	-3.40527715	-3.60843840
6	0.12341554	-2.25134365	-2.48941622
6	-2.58249251	-0.66907055	0.14036258
1	-4.05435633	-1.16440264	2.31886356
6	-4.54588790	0.05025252	4.72140886
1	-2.91989262	2.25029397	4.65805777
6	-1.22031071	3.37760977	2.95448479
1	4.12529492	2.09975371	-3.04675045
1	2.65334275	2.28806198	-2.07227354
1	2.59262711	2.51686279	-3.83029229
1	-0.01147846	-2.15250569	-1.40073154
1	0.16031344	-3.32130066	-2.72809651
1	-0.77330753	-1.83848226	-2.98019183
1	4.51292918	-2.73382044	-5.64594457
1	4.76908834	-3.57840302	-4.11097206
1	5.68798694	-2.09953017	-4.48060196
1	-3.24789365	-1.53889864	0.22161458
1	-1.55287646	-1.03184666	0.01376685
1	-2.85939651	-0.10938250	-0.76499126
1	-1.75383281	4.29941160	2.67132628
1	-0.27868889	3.36637579	2.38688131
1	-0.98210774	3.46269304	4.02378105
1	-4.55332981	-1.04491631	4.81546861
1	-5.58452348	0.36533589	4.53173837
1	-4.24744901	0.47568441	5.68945445
1	-0.24801399	-0.02286813	-1.92611291

Energy = -7584.938911 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 3

Atomic N.	X	Y	Z
8	2.02992755	-1.68857923	-0.20388263
8	0.68655695	-0.39049671	1.05720375
6	-0.50020978	-0.24702869	1.84327348
1	-0.27159291	-0.33517972	2.91818765
1	-1.25215262	-0.99646974	1.55840111
1	-0.88677904	0.75942536	1.64094010

8	0.31057354	-2.72667724	0.83428213
6	1.34574190	-1.77392845	0.95483752
6	2.25793075	-1.91572093	2.18329386
1	1.68083516	-1.79598926	3.11495437
1	2.93989083	-1.05759869	2.11802428
6	3.06086701	-3.22587087	2.21764363
1	3.40293727	-3.45646313	1.19665942
1	3.96723655	-3.06392911	2.82163842
6	2.28833846	-4.41098600	2.80923493
1	2.02406269	-4.17314671	3.85519032
1	2.94921916	-5.29151536	2.85358087
6	1.00861744	-4.77978918	2.05144933
1	1.24659553	-5.14828757	1.04090881
1	0.50304145	-5.60593014	2.57969623
6	0.00430142	-3.63499386	1.90701172
1	-0.12265992	-3.10083598	2.86584214
1	-0.97837362	-4.03907381	1.62436743
50	1.61346192	0.18084118	-1.15082854
7	0.18337755	2.46932994	-2.64445038
6	1.20101032	2.71146282	-3.66974851
1	0.78249630	3.20314413	-4.57275332
1	1.66975953	1.76771923	-3.97750556
1	1.98915079	3.35351604	-3.25448264
7	0.15799701	-0.61266112	-2.47121679
6	-0.89348940	1.59669356	-3.13251707
1	-1.40346335	2.05956368	-4.00817698
1	-1.63413753	1.49580504	-2.32710514
6	-0.44465185	0.19209281	-3.54232713
1	-1.34942796	-0.31893731	-3.91034464
1	0.22280678	0.25677765	-4.42518115
6	-0.18953911	-1.99861426	-2.54436780
6	0.73408626	-2.95733054	-3.02590127
6	0.35007301	-4.30112353	-3.10941173
6	-0.92267272	-4.73705823	-2.72531897
6	-1.81955339	-3.78089281	-2.23966542
6	-1.47829779	-2.42638700	-2.14160873
7	-0.47688781	3.08181782	0.22272898
6	-0.33621314	3.76015826	-2.16251469
1	-0.92864796	4.26651058	-2.95740959
1	0.53387221	4.40278015	-1.95440761
6	-1.19959136	3.69219482	-0.90321308
1	-1.48597265	4.72913241	-0.65999672
1	-2.13601335	3.15079478	-1.11233403
6	-0.55690565	3.65088892	1.51203813
6	-1.80950108	3.86087103	2.13859807
6	-1.84297818	4.41179741	3.42629703
6	-0.68225722	4.73452201	4.13605796
6	0.54641100	4.46778684	3.51977855
6	0.63306317	3.93839004	2.22880938
6	2.13290027	-2.56911679	-3.43693444
1	1.07234935	-5.02976549	-3.48709189
6	-1.31935329	-6.18860867	-2.85380899
1	-2.81404734	-4.09748993	-1.91325043
6	-2.48079426	-1.44986762	-1.58033568
6	-3.10117957	3.42202492	1.48972826
1	-2.81689094	4.56508434	3.89858683
6	-0.74998374	5.35449298	5.51101434
1	1.47316444	4.68614931	4.05657954

6	1.98550503	3.67003803	1.61462486
1	2.57199653	-3.33680993	-4.08808779
1	2.78325968	-2.47273887	-2.55338672
1	2.15250071	-1.60822336	-3.96986459
1	-1.98902138	-0.71792284	-0.92530595
1	-3.25740283	-1.97608188	-1.00965629
1	-2.99064815	-0.87784252	-2.37312454
1	-1.59614700	-6.43612550	-3.89108434
1	-2.18375959	-6.42411795	-2.21824449
1	-0.49378818	-6.85730029	-2.57166121
1	-3.90282105	3.36911596	2.23762857
1	-2.99089546	2.42718962	1.03198262
1	-3.43912814	4.10480713	0.69545593
1	2.12432926	4.21094451	0.66411353
1	2.14064977	2.59971636	1.39826828
1	2.78662785	3.98495487	2.29474211
1	0.08057672	5.01639248	6.14620518
1	-1.69192627	5.10248752	6.01713710
1	-0.69150190	6.45352496	5.45770421
1	0.48315938	2.87256730	-0.04619345

Energy = -7584.947052 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 4

Atomic N.	X	Y	Z
8	0.62688943	-0.31614369	0.56274519
8	1.99783251	-0.27643698	-1.21746471
6	3.15534580	0.25813635	-1.86103442
1	2.92752841	0.27332720	-2.93408524
1	4.03799860	-0.38393448	-1.69751161
1	3.36843574	1.28248608	-1.52576622
8	2.53073066	0.87526544	0.80604224
6	1.95291109	-0.32009035	0.27567492
6	2.66161132	-1.61365729	0.71728608
1	3.65213085	-1.68417608	0.23859526
1	2.05430668	-2.42134815	0.28638104
6	2.80392165	-1.78945780	2.23812512
1	1.89663219	-1.40977081	2.73396430
1	2.85365687	-2.86614203	2.46341465
6	4.04881108	-1.11790312	2.83169378
1	4.94363747	-1.53706875	2.33841040
1	4.13342960	-1.38413994	3.89745926
6	4.07348619	0.40642440	2.68899827
1	3.28194142	0.86524370	3.30338063
1	5.03421039	0.79326025	3.06903185
6	3.89957072	0.90214216	1.25381689
1	4.56334860	0.35010750	0.56735061
1	4.18001635	1.96436762	1.19054872
50	-0.55235189	0.22777967	-1.19460492
7	-2.19813322	1.16877269	0.50425519
6	-3.56970022	1.01984298	-0.02274091
1	-4.31483570	1.46884150	0.65945341
1	-3.80356888	-0.03806627	-0.17085702
1	-3.63317631	1.52376545	-0.99468369
7	-1.88021118	-1.84336367	1.05812214
6	-2.05934471	0.53581528	1.84652832
1	-2.62797723	1.13317669	2.58527358

8	0.49934323	-0.82664325	-0.13209893
8	1.51399295	-0.03668490	-1.97669934
6	2.64829932	0.11531828	-2.82863557
1	2.41875931	0.95400076	-3.49804151
1	2.83170117	-0.78500614	-3.44029590
1	3.55170580	0.35720254	-2.24787783
8	2.72974385	-0.36080239	-0.04537311
6	1.66299821	-0.92861497	-0.83877031
6	1.91992274	-2.37338504	-1.32828015
1	2.91495615	-2.45531096	-1.79499298
1	1.18219604	-2.52343860	-2.13164834
6	1.73141117	-3.46425979	-0.26470949
1	0.80587483	-3.25196856	0.28967951
1	1.58028310	-4.42729030	-0.77789705
6	2.90356803	-3.61015170	0.71051838
1	3.79197998	-3.97015994	0.16064860
1	2.66160889	-4.39154761	1.44874274
6	3.28135410	-2.31806413	1.44251833
1	2.43701239	-1.94894281	2.04519173
1	4.10413693	-2.53477542	2.14473194
6	3.75406155	-1.19360239	0.51497433
1	4.39621435	-1.61177245	-0.28422336
1	4.37027835	-0.48039383	1.08229315
50	-1.33430798	-0.32317052	-1.08509407
7	-3.31990134	1.54359926	-0.35961238
6	-4.31603073	1.60801068	-1.43535333
1	-5.15626403	2.28426556	-1.18242942
1	-4.72403695	0.60598638	-1.62188894
1	-3.84391872	1.95629884	-2.36299066
7	-2.28596230	-0.92342417	0.76326618
6	-3.88926128	0.91670009	0.85209226
1	-4.95894798	1.18766369	0.95630928
1	-3.35750888	1.30179241	1.73211419
6	-3.71038424	-0.60317868	0.82093080
1	-4.15883453	-1.01924935	1.73849582
1	-4.30717163	-1.01605530	-0.02168729
6	-1.86886975	-2.05774455	1.51515862
6	-2.32777663	-3.36684007	1.21513150
6	-1.89190265	-4.45300797	1.98762933
6	-1.00296827	-4.29619671	3.05426387
6	-0.55924099	-2.99992691	3.34363067
6	-0.97294340	-1.88734521	2.60268722
7	-0.34256404	2.05568526	-0.32371148
6	-2.71287370	2.85584685	-0.08994385
1	-3.36164980	3.47185532	0.56581319
1	-2.61906800	3.39578545	-1.04111100
6	-1.33454512	2.72662224	0.56000199
1	-0.98546980	3.73040424	0.85433502
1	-1.41755406	2.12242492	1.47488657
6	0.51758473	2.96483797	-1.06480001
6	1.70232401	3.42190240	-0.43330005
6	2.53917397	4.31130637	-1.11061506
6	2.24388072	4.76672955	-2.40270343
6	1.08286583	4.28878400	-3.00944797
6	0.21303729	3.38725002	-2.37153882
6	-3.25508852	-3.62335431	0.05247976
1	-2.25045052	-5.45442440	1.73361444
6	-0.51146681	-5.48350857	3.84744230

1	0.12642382	-2.84604135	4.18156547
6	-0.46965291	-0.51781687	2.97989375
6	2.08764278	2.93890201	0.94459094
1	3.45125059	4.65393723	-0.61578476
6	3.16912887	5.72227835	-3.11641461
1	0.84144064	4.60943796	-4.02601382
6	-0.98826318	2.90247998	-3.14655635
1	-3.22645072	-4.68100960	-0.24066177
1	-2.97775369	-3.01330308	-0.82095390
1	-4.30136040	-3.37627559	0.29263411
1	0.17730503	-0.11858479	2.18525971
1	0.11016450	-0.56093769	3.91193075
1	-1.30180054	0.18768962	3.12040556
1	-0.39445704	-5.23503827	4.91185602
1	0.47141446	-5.82596413	3.48533344
1	-1.20361019	-6.33273526	3.76820036
1	3.00098089	3.44394818	1.28287697
1	2.28646304	1.85434290	0.94322295
1	1.30308076	3.13418451	1.69128889
1	-1.80166919	3.64577736	-3.13967245
1	-1.38003856	1.95737433	-2.75005894
1	-0.71733645	2.73727531	-4.19831387
1	4.14730493	5.25685592	-3.31124363
1	3.35675107	6.62269486	-2.51311895
1	2.74985706	6.03964440	-4.07985799
1	0.26987806	1.47085256	0.25578203

Energy = -7584.953285 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 6

Atomic N.	X	Y	Z
8	0.58284230	0.13865758	-0.23445182
8	1.43954119	2.20581983	-0.37799536
6	2.49309878	3.12768530	-0.10213219
1	2.03631724	4.12569135	-0.09887119
1	3.26797064	3.10251413	-0.88740412
1	2.95523270	2.93380029	0.87751130
8	2.59633578	0.49623109	0.77079224
6	1.77702709	0.74524525	-0.38911928
6	2.42094417	0.40432799	-1.74112869
1	3.30697441	1.03583901	-1.91821327
1	1.66780759	0.70330758	-2.48200084
6	2.78204967	-1.07882771	-1.91877474
1	1.98474987	-1.69346506	-1.47297114
1	2.78980423	-1.30868945	-2.99591724
6	4.14474195	-1.46443707	-1.33083868
1	4.92903647	-0.87672307	-1.84112763
1	4.35586934	-2.52105200	-1.56273127
6	4.27197677	-1.24618561	0.18044744
1	3.59043528	-1.91608954	0.72866300
1	5.29748936	-1.50535144	0.49579434
6	3.99139717	0.18745588	0.63915883
1	4.50854045	0.91264015	-0.01559337
1	4.38802090	0.33178407	1.65559826
50	-0.63809185	1.32489636	1.06550506
7	-3.21440946	0.73781959	2.08706581
6	-3.58758546	1.88510160	2.92187977

1	-4.63495805	1.81645830	3.27840002
1	-3.47687530	2.81656481	2.35331356
1	-2.91678931	1.94124524	3.78969881
7	-2.09202548	1.56425962	-0.50429527
6	-3.98109947	0.71218161	0.82911679
1	-5.06551770	0.84704359	1.02885700
1	-3.83807608	-0.27240802	0.36331773
6	-3.49544179	1.77118087	-0.16195392
1	-4.11790283	1.67232082	-1.06949112
1	-3.72236639	2.78279890	0.23911526
6	-1.71302229	2.09033113	-1.77883452
6	-1.57420478	3.48436802	-1.99746406
6	-1.21156897	3.95618923	-3.26690929
6	-0.97671004	3.09241498	-4.33996633
6	-1.12699414	1.71924007	-4.11458890
6	-1.48845401	1.20553099	-2.86334743
7	-1.07972057	-1.33400400	2.25826355
6	-3.33006403	-0.51407839	2.85305562
1	-4.38960560	-0.83235624	2.94462822
1	-2.97774775	-0.30544628	3.87659928
6	-2.51686976	-1.67544240	2.28558710
1	-2.70965630	-2.56416574	2.91460694
1	-2.85623482	-1.92250943	1.27278033
6	-0.12307425	-2.38877460	2.13824901
6	-0.13105704	-3.28283744	1.04637770
6	0.84653171	-4.28616477	0.98880213
6	1.84708045	-4.42077831	1.95408186
6	1.85882689	-3.49672538	3.00591919
6	0.89978018	-2.48660563	3.11412454
6	-1.80589591	4.48441274	-0.89087149
1	-1.10237203	5.03413941	-3.41538799
6	-0.54756832	3.61822414	-5.68899479
1	-0.96171276	1.02140800	-4.94014670
6	-1.63629154	-0.28294105	-2.68422813
6	-1.11270944	-3.15606510	-0.09150856
1	0.83291845	-4.96975839	0.13620107
6	2.90899229	-5.48812028	1.84322845
1	2.64035169	-3.55942719	3.76733338
6	0.98311298	-1.49906239	4.25465840
1	-1.28912296	5.42908426	-1.10614261
1	-1.44779470	4.10488211	0.07771433
1	-2.87602119	4.71747213	-0.76897814
1	-0.84625638	-0.66099496	-2.01987510
1	-1.56622980	-0.79898890	-3.65135389
1	-2.59879650	-0.53929466	-2.21863668
1	-0.96704882	3.01546455	-6.50682069
1	0.54876849	3.59079634	-5.79573163
1	-0.86469959	4.66007969	-5.83283618
1	-0.72194489	-3.66095255	-0.98436871
1	-1.27947543	-2.10137928	-0.34685171
1	-2.08837994	-3.61259337	0.13880807
1	0.07400839	-1.49718901	4.87971413
1	1.14037991	-0.47005249	3.89163398
1	1.82554837	-1.74531784	4.91259862
1	3.86171042	-5.06564015	1.48616714
1	2.61179020	-6.27517476	1.13774758
1	3.10946197	-5.95953137	2.81600593
1	-0.86902204	-0.81130726	3.10973289

Energy = -7584.952434 Hartree
 Number of imaginary frequencies = 0.

Compound I3b isomer 7

Atomic N.	X	Y	Z
8	0.58128018	0.19490941	-0.18843725
8	1.70421266	2.10131630	0.19043352
6	2.85948416	2.77367957	0.68807506
1	2.54327262	3.79704557	0.92904052
1	3.65661492	2.82820322	-0.07328567
1	3.25068585	2.29036685	1.59602857
8	2.57604804	0.02302674	0.90048825
6	1.84786914	0.65364975	-0.17317914
6	2.50179011	0.56347353	-1.56047355
1	3.46475866	1.09984068	-1.57170640
1	1.82081658	1.12265103	-2.21558193
6	2.68618488	-0.86861631	-2.08654219
1	1.80152324	-1.46339904	-1.81112771
1	2.71054800	-0.83462091	-3.18719025
6	3.96577548	-1.55553866	-1.59446434
1	4.83641519	-0.96779826	-1.93725729
1	4.05667562	-2.54371259	-2.07403545
6	4.05444464	-1.72486107	-0.07421778
1	3.27550246	-2.41549179	0.28608373
1	5.02735772	-2.17972834	0.18047823
6	3.92848729	-0.41966972	0.71610507
1	4.55675829	0.36960280	0.26400001
1	4.29543742	-0.57502933	1.74212031
50	-0.56222223	1.16265901	1.34485089
7	-3.19326253	0.59662366	2.09522336
6	-3.55029351	1.62733469	3.07751474
1	-4.61993764	1.57539199	3.36264776
1	-3.34869884	2.62443676	2.66802795
1	-2.93385129	1.50313222	3.97789398
7	-1.89259354	1.88499426	-0.17306740
6	-3.88337677	0.80786030	0.81116663
1	-4.97639460	0.93025465	0.96681786
1	-3.72232901	-0.08477813	0.19139777
6	-3.32653631	2.01129361	0.04980852
1	-3.85842083	2.04980087	-0.91876396
1	-3.61705777	2.95005636	0.57271758
6	-1.41678611	2.62950644	-1.29863566
6	-1.01805118	3.98121040	-1.16667142
6	-0.57984323	4.68926909	-2.29389133
6	-0.51725667	4.09928130	-3.56029505
6	-0.90281265	2.75896243	-3.67511071
6	-1.34913907	2.01778701	-2.57371487
7	-1.25132683	-1.67247884	1.94782488
6	-3.42751184	-0.74323570	2.65960823
1	-4.51246674	-0.97545203	2.69812875
1	-3.07604613	-0.72030155	3.70426734
6	-2.71289616	-1.87906953	1.93065712
1	-2.99527360	-2.82605959	2.42781058
1	-3.06027529	-1.95245125	0.89343665
6	-0.41010739	-2.77410178	1.59997830
6	-0.47137570	-3.37736830	0.32558231
6	0.38781969	-4.44853775	0.04367843

6	1.32177823	-4.92781162	0.96547940
6	1.39879189	-4.27992810	2.20440437
6	0.55556703	-3.21669465	2.53733325
6	-1.02809670	4.66960986	0.17726875
1	-0.27585229	5.73289058	-2.17545153
6	-0.07510143	4.88957301	-4.76895129
1	-0.84916599	2.26924024	-4.65136720
6	-1.71492103	0.56626168	-2.74560008
6	-1.37934996	-2.86122703	-0.76195705
1	0.33720949	-4.90263745	-0.94913244
6	2.22156334	-6.09525377	0.63926599
1	2.14064120	-4.60810110	2.93675126
6	0.70671070	-2.53580573	3.87776308
1	-0.85234036	5.74738704	0.06110763
1	-0.23899702	4.27164306	0.83462378
1	-1.98075744	4.53219703	0.70757023
1	-1.02625871	-0.05986022	-2.16056742
1	-1.65393472	0.27281928	-3.80218223
1	-2.73291384	0.35176585	-2.38841830
1	-0.93845753	5.32061162	-5.30078758
1	0.46437356	4.25606802	-5.48685797
1	0.58227629	5.72245178	-4.48440391
1	-0.99593942	-3.15782485	-1.74680919
1	-1.43166109	-1.76471456	-0.73588711
1	-2.40388312	-3.25845098	-0.68081856
1	-0.22160541	-2.56566276	4.47263554
1	0.99793822	-1.47830405	3.76722425
1	1.48662982	-3.02847457	4.47128416
1	3.25368968	-5.91214478	0.97096685
1	2.24047605	-6.29354523	-0.44059912
1	1.87991268	-7.01571357	1.13850145
1	-0.99194156	-1.35568406	2.88336745

Energy = -7584.952274 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 8

Atomic N.	X	Y	Z
8	1.88461040	-0.94981943	1.42533145
8	1.31207388	0.24789005	-0.39784306
6	1.61779224	1.32929497	-1.28422498
1	0.66150286	1.71665562	-1.65678965
1	2.21461057	0.97640174	-2.14189306
1	2.15674562	2.13413822	-0.76479346
8	3.35310306	0.64600787	0.76307186
6	2.48128733	-0.41008654	0.35497169
6	3.09110775	-1.46082275	-0.58230911
1	3.38706484	-1.00360508	-1.54102118
1	2.26386888	-2.14930051	-0.79740856
6	4.27327725	-2.23149139	0.02665602
1	4.05493443	-2.43481163	1.08652735
1	4.34204851	-3.21206066	-0.46945100
6	5.62278598	-1.51757504	-0.11851745
1	5.83893232	-1.38630073	-1.19401764
1	6.42262647	-2.16412525	0.27724922
6	5.69852269	-0.14899924	0.56677987
1	5.62143171	-0.25822319	1.66053084
1	6.68348067	0.30377748	0.36081199

6	4.62384060	0.84523103	0.12105293
1	4.52810130	0.84895199	-0.97941506
1	4.91261458	1.86209003	0.42570562
50	0.10222918	0.17965695	1.85223808
7	-2.78731734	0.62139946	2.52136405
6	-2.89695744	1.58490308	3.61530836
1	-3.87034756	1.51194991	4.14569802
1	-2.78499845	2.60931835	3.23910413
1	-2.08880551	1.40973561	4.33871559
7	-2.24477083	1.85877616	-0.24654589
6	-3.76701479	0.88778520	1.46379435
1	-4.78337798	1.03616805	1.89260766
1	-3.82859146	-0.00375270	0.82136358
6	-3.44076333	2.09464607	0.58297078
1	-4.33356700	2.30813933	-0.03825163
1	-3.27318868	2.98796037	1.19816331
6	-1.89007792	2.90295129	-1.15152365
6	-1.30960241	4.09673343	-0.66281001
6	-0.93132763	5.09071578	-1.57379217
6	-1.08970544	4.94036901	-2.95577888
6	-1.64113564	3.74092065	-3.41992609
6	-2.05150532	2.72647913	-2.54722704
7	-0.99942169	-1.61992628	1.60709672
6	-2.87179445	-0.75378271	3.03237695
1	-3.90767495	-1.01084816	3.34778122
1	-2.23754079	-0.80030747	3.93232612
6	-2.37978432	-1.81409979	2.05050881
1	-2.47314523	-2.78518518	2.57345637
1	-3.07888112	-1.89042076	1.19087542
6	-0.47653706	-2.78776396	0.96342397
6	-0.67513941	-3.00034269	-0.42008662
6	-0.18494907	-4.16986689	-1.01736806
6	0.50389129	-5.14188257	-0.28474213
6	0.69587538	-4.91426535	1.08281022
6	0.22597690	-3.75773670	1.71673468
6	-1.04244294	4.29664594	0.80826401
1	-0.47375570	6.00427714	-1.18548052
6	-0.69642892	6.04117952	-3.91117876
1	-1.76597772	3.58973625	-4.49510439
6	-2.64253856	1.45324876	-3.10755891
6	-1.37013746	-1.96682963	-1.27210159
1	-0.34373638	-4.32011147	-2.08865127
6	1.05227816	-6.38068281	-0.95212015
1	1.23571951	-5.65639720	1.67693799
6	0.50900382	-3.54156261	3.18143841
1	-0.21513522	5.00303221	0.95591835
1	-0.78280283	3.34577069	1.29592109
1	-1.91765776	4.71190559	1.33437109
1	-1.98013700	0.58476202	-2.95794156
1	-2.80607055	1.55024960	-4.18805963
1	-3.61140627	1.20649603	-2.64633212
1	-1.53547805	6.73322550	-4.08652638
1	-0.39724448	5.63765377	-4.88804876
1	0.13782842	6.63608348	-3.51495666
1	-1.44160995	-2.30878919	-2.31315738
1	-0.80819319	-1.02088059	-1.25623212
1	-2.38981198	-1.75356940	-0.91689036
1	-0.38731530	-3.23417414	3.73798029

1	1.25728330	-2.74450182	3.30715238
1	0.90467513	-4.45789999	3.63903863
1	2.10724598	-6.24340068	-1.23883659
1	0.49394428	-6.62448736	-1.86616397
1	1.00985973	-7.25008449	-0.28137274
1	-2.37637195	0.98746069	-0.76197921

Energy = -7584.950514 Hartree
Number of imaginary frequencies = 0.

Compound I3b isomer 9

Atomic N.	X	Y	Z
8	0.21492835	-0.01168685	-0.77329991
8	0.20933935	2.14172932	-1.38106065
6	0.91113608	3.34171200	-1.71625754
1	0.23898566	4.16993069	-1.45982084
1	1.12758889	3.38757947	-2.79630984
1	1.84615721	3.43578401	-1.14477437
8	2.24451381	0.96030736	-1.06837944
6	0.90924157	0.82672778	-1.57611948
6	0.80821692	0.43833051	-3.05835046
1	1.19711421	1.24938349	-3.69540661
1	-0.27007017	0.37677587	-3.25332368
6	1.49103479	-0.89077274	-3.41967407
1	1.32453767	-1.61585084	-2.60739171
1	0.99425555	-1.30444538	-4.31105290
6	2.98937550	-0.75841563	-3.71938821
1	3.11866950	-0.06920458	-4.57296776
1	3.38206816	-1.73288071	-4.05059456
6	3.83312674	-0.25164040	-2.54527143
1	3.84616666	-0.99354100	-1.73081143
1	4.87791601	-0.12887408	-2.87766448
6	3.36886726	1.08309306	-1.96024282
1	3.16999872	1.81454731	-2.76275722
1	4.16146749	1.50561780	-1.32500917
50	-0.54846617	1.17001674	0.88580521
7	-1.69877489	-0.94419753	1.59331224
6	-2.25936092	-0.59089587	2.91870871
1	-2.96857601	-1.36321006	3.26550820
1	-2.77849909	0.37303050	2.86358951
1	-1.44076783	-0.50672275	3.64398696
7	-2.56632256	1.37441372	0.20040753
6	-2.78771180	-1.04157021	0.57971304
1	-3.50750797	-1.82571172	0.88529522
1	-2.31925360	-1.34203449	-0.36607453
6	-3.51336925	0.28516997	0.37216567
1	-4.16141577	0.15429009	-0.51402674
1	-4.21287148	0.46789300	1.21750744
6	-3.05128548	2.55829589	-0.41389716
6	-3.17990171	3.76273278	0.32614079
6	-3.62350332	4.92888144	-0.31217160
6	-3.96179927	4.95203836	-1.66893680
6	-3.82989140	3.76062635	-2.39086832
6	-3.38157868	2.57524870	-1.79681737
7	1.27539924	-2.45153290	0.58842910
6	-0.99818474	-2.25963473	1.73475791
1	-1.77564129	-3.01330542	1.97025268
1	-0.34394336	-2.19206494	2.61582726

6	-0.15658091	-2.74479139	0.53290019
1	-0.30737753	-3.82785750	0.44720210
1	-0.52468739	-2.29871996	-0.39934616
6	2.08302092	-2.96427316	1.62732694
6	2.21395505	-4.36324044	1.82679675
6	3.03869806	-4.83645095	2.85571857
6	3.77771356	-3.98330436	3.67997379
6	3.68774527	-2.60961168	3.42706748
6	2.86015853	-2.08541679	2.42882504
6	-2.85679043	3.81543894	1.80094923
1	-3.71922026	5.84523226	0.27676902
6	-4.47762097	6.20996639	-2.32609422
1	-4.06469461	3.75552640	-3.45914808
6	-3.21311593	1.34206475	-2.64788977
6	1.56240128	-5.36492747	0.90444191
1	3.12889495	-5.91782388	2.99015029
6	4.63765364	-4.52027889	4.79863990
1	4.27524314	-1.91446984	4.03268995
6	2.80631432	-0.59381542	2.21575608
1	-3.32681404	4.69182061	2.26726445
1	-1.77304255	3.88672182	1.98747772
1	-3.20380623	2.91116088	2.31927897
1	-2.39237620	0.72152236	-2.26345350
1	-3.00001544	1.61574906	-3.69004850
1	-4.12328780	0.71984438	-2.65850450
1	-4.16555090	6.26979102	-3.37819705
1	-4.11706832	7.10977411	-1.80932255
1	-5.57885413	6.24392052	-2.31232143
1	2.10763952	-6.31752093	0.93578082
1	1.55884035	-4.99931425	-0.13275420
1	0.51725246	-5.58484247	1.17830990
1	1.80023367	-0.18393797	2.40910870
1	3.05926049	-0.29780133	1.18569003
1	3.50394977	-0.08271840	2.89140542
1	5.54710492	-3.91781068	4.93171325
1	4.94074525	-5.55872974	4.60665130
1	4.09821070	-4.50962569	5.75950946
1	1.43445921	-1.46721370	0.36699632

Energy = -7584.958823 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 10

Atomic N.	X	Y	Z
8	0.29828106	0.45577945	-0.32975147
8	0.98942031	2.52570447	0.20089681
6	2.05185847	3.45982601	0.38201111
1	1.67901499	4.22330018	1.07736360
1	2.32136235	3.95722884	-0.56571443
1	2.94432088	2.98092094	0.81231696
8	2.54747348	0.82188620	-0.29950964
6	1.25532289	1.33911395	-0.67588600
6	1.11703497	1.77950092	-2.14138441
1	1.79057346	2.62484237	-2.35790446
1	0.09175887	2.16628742	-2.20990089
6	1.32825886	0.65649303	-3.16869834
1	0.86376712	-0.26510041	-2.78520857
1	0.78495335	0.92072603	-4.08967448

6	2.79762251	0.40488505	-3.52761936
1	3.21738046	1.32832359	-3.96580633
1	2.85370090	-0.36081401	-4.31851677
6	3.67739659	-0.02438368	-2.34885845
1	3.36490121	-1.01001873	-1.96896640
1	4.71891917	-0.13169854	-2.69830117
6	3.67926404	0.95421909	-1.17136189
1	3.79649816	1.99298059	-1.53103172
1	4.53906513	0.74062489	-0.51832432
50	-0.11764569	0.59628757	1.76633161
7	-1.79058075	-1.09019988	3.25221691
6	-1.86189336	-0.49451984	4.59208129
1	-2.59593285	-1.01527189	5.23875531
1	-2.15111182	0.56083373	4.52020052
1	-0.87218013	-0.54020284	5.06583816
7	-2.15873567	1.01144337	1.26333599
6	-3.05427583	-0.91833848	2.51484688
1	-3.91595557	-1.26047418	3.12670575
1	-3.00460975	-1.54208992	1.61178163
6	-3.27062702	0.52871776	2.07051764
1	-4.20375819	0.54467363	1.47794180
1	-3.48569703	1.16418653	2.95887702
6	-2.51366901	2.06167087	0.35924314
6	-2.43652295	3.42037022	0.74886229
6	-2.81237970	4.42396405	-0.15397342
6	-3.26393632	4.12778193	-1.44411439
6	-3.32501908	2.78151539	-1.82077180
6	-2.96019938	1.74907022	-0.94736921
7	0.36101102	-2.33989587	1.59289206
6	-1.37162342	-2.49938375	3.34492828
1	-2.20461786	-3.13945033	3.70362658
1	-0.58302539	-2.55407440	4.11330941
6	-0.82671163	-3.09021245	2.04634414
1	-0.58768852	-4.15343421	2.23592565
1	-1.59325684	-3.07350836	1.26246853
6	1.20993976	-2.93659339	0.61092494
6	0.73262763	-3.27670191	-0.67345671
6	1.62039193	-3.85141558	-1.59306108
6	2.96854546	-4.07501704	-1.30041001
6	3.42784688	-3.69181883	-0.03498047
6	2.57858492	-3.12774459	0.92108032
6	-1.92857496	3.81214857	2.11585876
1	-2.74772642	5.46859237	0.16253812
6	-3.69836117	5.22265732	-2.38928136
1	-3.65935284	2.52358157	-2.82944216
6	-3.00466448	0.31822440	-1.41736094
6	-0.68111108	-2.98122646	-1.10668959
1	1.24057151	-4.10636145	-2.58565941
6	3.90958947	-4.65243022	-2.33003332
1	4.48097672	-3.83473705	0.21956065
6	3.13776074	-2.71159124	2.26186033
1	-2.14186081	4.87003576	2.31954177
1	-0.83851035	3.67209207	2.18993090
1	-2.38068835	3.20836292	2.91463113
1	-1.99185925	-0.10842971	-1.39679439
1	-3.39611248	0.25764633	-2.44165615
1	-3.63682361	-0.31013375	-0.77246416
1	-3.53262480	4.93633849	-3.43705154

1	-3.15304344	6.15717151	-2.19822389
1	-4.77220150	5.44278930	-2.27743204
1	-0.74073108	-2.94445523	-2.20210854
1	-1.00909273	-2.00824040	-0.71689226
1	-1.39622712	-3.74810743	-0.76872379
1	2.63905456	-3.22143435	3.10323337
1	3.04089587	-1.62570171	2.42559190
1	4.20538677	-2.95592621	2.32316836
1	4.43048316	-3.85407511	-2.88273856
1	3.37156717	-5.26349089	-3.06712411
1	4.68115267	-5.27980050	-1.86245619
1	0.92668475	-2.12429409	2.41514895

Energy = -7584.952326 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 11

Atomic N.	X	Y	Z
8	2.79825513	-0.39165218	0.24278595
8	0.93240784	0.40291608	-0.73411060
6	0.24527491	1.47235879	-1.39440540
1	-0.81374924	1.37987238	-1.12289453
1	0.34118078	1.37534562	-2.48775495
1	0.62502352	2.45304092	-1.07401015
8	2.94926858	1.66899103	-0.68822816
6	2.47225443	0.33691777	-0.83753746
6	2.80689550	-0.36118411	-2.15975770
1	2.33683596	0.16506818	-3.00681536
1	2.32260118	-1.34288295	-2.08415352
6	4.31397992	-0.53006580	-2.41066581
1	4.80578131	-0.79134412	-1.46075600
1	4.45906415	-1.39074805	-3.08164988
6	4.98026297	0.69817284	-3.04247118
1	4.50631893	0.89240604	-4.02131769
1	6.03748245	0.47196398	-3.25502240
6	4.89989968	1.97396756	-2.19731883
1	5.47974919	1.86072623	-1.26722225
1	5.35719417	2.80736324	-2.75734113
6	3.47971811	2.39377014	-1.81346155
1	2.80498992	2.33770179	-2.68587817
1	3.48231111	3.43834552	-1.46961185
50	1.17791025	-0.19388357	1.62822623
7	-1.43009238	-0.82155608	3.24457233
6	-1.51469068	-0.12883379	4.53097892
1	-2.12883244	-0.68550493	5.27075295
1	-1.95255992	0.86952865	4.40836671
1	-0.50369599	-0.00288065	4.94210226
7	-2.46070529	1.16273064	1.32223838
6	-2.74194391	-0.94102656	2.59304158
1	-3.46371516	-1.48060449	3.24753177
1	-2.60893518	-1.53757224	1.68115985
6	-3.36368427	0.39838842	2.19667820
1	-4.29483212	0.17823507	1.65845348
1	-3.65538681	0.97851149	3.09410989
6	-2.92651545	2.40951184	0.82180082
6	-2.30939634	3.62041022	1.22347388
6	-2.74663729	4.83019861	0.67371188
6	-3.78961008	4.88956418	-0.25839001

6	-4.37012921	3.68209968	-0.65906339
6	-3.95359666	2.44484047	-0.15110275
7	0.56692199	-2.18972763	1.32452300
6	-0.79210772	-2.13385955	3.44250882
1	-1.44669153	-2.80175364	4.04607873
1	0.12122120	-1.95966368	4.03591559
6	-0.40243026	-2.88451343	2.17107110
1	0.01971532	-3.85122025	2.50922967
1	-1.31152301	-3.15434264	1.59899179
6	0.99800558	-2.97901378	0.21233725
6	0.18417197	-3.12180913	-0.93770211
6	0.63405854	-3.91304288	-2.00475924
6	1.86634227	-4.57174856	-1.97326437
6	2.65684110	-4.42319752	-0.82719461
6	2.25071905	-3.63957984	0.25889810
6	-1.18092757	3.61949417	2.22781192
1	-2.26015128	5.75567486	0.99228936
6	-4.27640680	6.21127817	-0.80193493
1	-5.15972059	3.69443494	-1.41498728
6	-4.56127479	1.17692790	-0.69914544
6	-1.15484463	-2.43528307	-1.04894714
1	0.00076335	-4.00607458	-2.89123006
6	2.34671806	-5.39109862	-3.14742987
1	3.62424968	-4.92971601	-0.77609084
6	3.16293293	-3.49451890	1.45082278
1	-0.86659098	4.64620141	2.45318348
1	-0.29128366	3.07927579	1.86355295
1	-1.47321883	3.14510993	3.17778793
1	-3.81101704	0.37477443	-0.75204355
1	-4.96416473	1.34964219	-1.70579749
1	-5.39350590	0.80667627	-0.07901276
1	-5.01674729	6.67099450	-0.12784814
1	-4.75903581	6.08758756	-1.78090729
1	-3.45151165	6.92844637	-0.91440269
1	-1.40590697	-2.24501152	-2.10107625
1	-1.15781808	-1.47993992	-0.50876354
1	-1.96467129	-3.05612961	-0.63148640
1	2.61419170	-3.56453492	2.39980000
1	3.65913091	-2.51210948	1.43334597
1	3.94252025	-4.26772782	1.43715718
1	3.05360265	-4.81835150	-3.76882318
1	1.51163991	-5.69390291	-3.79324487
1	2.87113731	-6.29845829	-2.81605261
1	-1.56928491	1.27660335	1.80779470

Energy = -7584.952539 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 12

Atomic N.	X	Y	Z
8	2.52523252	-0.13929978	0.34210658
8	0.81729764	0.77648050	-0.81072012
6	0.28980877	1.91246668	-1.50349864
1	-0.79899075	1.88964236	-1.37181025
1	0.51725388	1.85465023	-2.58109694
1	0.68434184	2.85212122	-1.09192821
8	2.87310525	1.93699574	-0.50075576
6	2.34720316	0.63004946	-0.73923545

6	2.79971301	-0.05034389	-2.03801281
1	2.45524344	0.51879677	-2.91732586
1	2.26442989	-1.00845642	-2.04645582
6	4.31510532	-0.29288918	-2.12187756
1	4.67927111	-0.60265014	-1.13003509
1	4.49450006	-1.14338276	-2.79777298
6	5.11096777	0.91294171	-2.63604505
1	4.76373283	1.15628470	-3.65627607
1	6.17305362	0.63540550	-2.73280693
6	4.99782879	2.17036273	-1.76749149
1	5.45917426	2.00316339	-0.78090034
1	5.55881470	2.99118532	-2.24615205
6	3.56502057	2.65563777	-1.53580853
1	2.99542485	2.65545520	-2.48229790
1	3.58139308	3.69166676	-1.16630036
50	0.84472447	0.13659927	1.65927922
7	-1.40241133	-0.68009760	3.47321315
6	-1.35814880	0.10864213	4.70326169
1	-1.89902907	-0.38355135	5.53953709
1	-1.80056249	1.09940931	4.54188411
1	-0.31188432	0.25987605	5.00257928
7	-2.61918038	0.78146291	1.05101712
6	-2.76937081	-0.80705243	2.95885413
1	-3.47032546	-1.11573354	3.76653130
1	-2.78044024	-1.61565239	2.21234822
6	-3.32392472	0.45956302	2.30526478
1	-4.40824211	0.30304294	2.13656908
1	-3.23916211	1.31530376	2.98716292
6	-3.09303561	1.92060288	0.33510161
6	-2.82052148	3.22273833	0.81567886
6	-3.25947596	4.32635125	0.07372064
6	-3.94434493	4.19000201	-1.13858012
6	-4.18018226	2.89349137	-1.60962647
6	-3.77741593	1.75992301	-0.89427983
7	0.46635303	-1.94602596	1.48192318
6	-0.75452372	-1.98385820	3.67204365
1	-1.37602241	-2.65819114	4.30269348
1	0.18118573	-1.79568296	4.22290825
6	-0.40385472	-2.70977626	2.37579515
1	0.09796617	-3.64985255	2.67541242
1	-1.33111858	-3.03905809	1.86089234
6	1.02319977	-2.76871181	0.45013732
6	0.31864434	-2.99166684	-0.75504732
6	0.86820439	-3.83385010	-1.73172830
6	2.10454725	-4.46317419	-1.55504682
6	2.79202301	-4.22736308	-0.35882658
6	2.27959594	-3.39119395	0.64028139
6	-2.02362332	3.44498937	2.07697534
1	-3.03361336	5.32775805	0.44909482
6	-4.42784650	5.39877103	-1.90302280
1	-4.70229749	2.75565846	-2.55983760
6	-4.06178728	0.38444965	-1.45253420
6	-0.99797777	-2.30483080	-1.02314147
1	0.31292911	-3.99643050	-2.65945014
6	2.69528899	-5.34255061	-2.63137086
1	3.76304509	-4.70332501	-0.19827185
6	3.08815092	-3.13380107	1.88612579
1	-1.52404116	4.42214790	2.04851205

1	-1.25961827	2.66435429	2.20455434
1	-2.66150321	3.43601106	2.97602974
1	-3.14194356	-0.13823989	-1.76269397
1	-4.70468574	0.45621281	-2.33862384
1	-4.57316499	-0.26273646	-0.72318251
1	-5.45105630	5.67545293	-1.60272269
1	-4.44620044	5.20930758	-2.98493249
1	-3.78733156	6.27184140	-1.71797722
1	-1.39789681	-2.60430572	-2.00098910
1	-0.86398741	-1.21269529	-1.02354726
1	-1.75494840	-2.54647711	-0.26154498
1	2.49014175	-3.24673201	2.80115609
1	3.47616155	-2.10404823	1.87809347
1	3.94234031	-3.82138938	1.94254084
1	3.40747107	-4.78094515	-3.25689835
1	1.91684676	-5.73955932	-3.29690921
1	3.24389044	-6.19136627	-2.19981377
1	-2.64493468	-0.04032140	0.44592457

Energy = -7584.950521 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 13

Atomic N.	X	Y	Z
8	2.51855401	1.07950149	0.71400323
8	2.85508466	-0.76769663	-0.53311087
6	3.32150389	-1.34317647	-1.75559765
1	2.66352047	-2.19503289	-1.96691935
1	4.35694545	-1.71112236	-1.65294843
1	3.25690446	-0.62688290	-2.58574203
8	3.73180680	1.35487064	-1.16816010
6	3.48197744	0.51211901	-0.04461930
6	4.72789962	0.12047632	0.77004084
1	5.40138135	-0.51317578	0.16958575
1	4.33580418	-0.51368624	1.57621056
6	5.50336390	1.30953038	1.35828098
1	4.78281433	2.07037979	1.69779913
1	6.04075885	0.96737144	2.25650663
6	6.52224883	1.92429679	0.39036855
1	7.25841996	1.14783859	0.11604647
1	7.08996188	2.71378790	0.90868716
6	5.91638716	2.50151218	-0.89322927
1	5.29097230	3.37983171	-0.66535287
1	6.72989097	2.85408490	-1.54993204
6	5.06210124	1.51510077	-1.69186560
1	5.57742239	0.54444373	-1.79580597
1	4.89812691	1.90497839	-2.70750544
50	0.71266265	-0.09313240	0.66250118
7	-0.40783203	2.07683267	1.35876490
6	0.62951573	3.12427211	1.52057230
1	0.15413315	4.10755049	1.68853166
1	1.27561789	3.15860446	0.63979760
1	1.26496252	2.87490311	2.37859585
7	-0.15449896	0.67436114	-1.15726666
6	-1.27202444	2.37240766	0.18504048
1	-1.61141350	3.42634475	0.22060591
1	-2.14394354	1.70998035	0.23768560
6	-0.54190141	2.07973017	-1.12634328

1	-1.24792161	2.29757996	-1.94641436
1	0.29944609	2.78949552	-1.24644920
6	-0.15391536	-0.00500582	-2.39314597
6	0.43584559	0.54091302	-3.57032930
6	0.37436483	-0.17317401	-4.77476273
6	-0.22525854	-1.43136329	-4.87664163
6	-0.77495196	-1.97297929	-3.70984064
6	-0.75976967	-1.29254856	-2.48723195
7	-2.32100450	-0.18208415	2.28843826
6	-1.16546351	2.00955793	2.64435081
1	-1.41169702	3.04079737	2.96311323
1	-0.46850992	1.60324621	3.39499050
6	-2.47496604	1.22305751	2.67958103
1	-2.85520167	1.32417415	3.71598115
1	-3.22074409	1.70984174	2.03585930
6	-3.36346231	-1.09050095	2.61978492
6	-4.64145449	-0.97604753	2.02620827
6	-5.63446596	-1.90488841	2.36469076
6	-5.40179432	-2.96188462	3.24945514
6	-4.11649237	-3.08279862	3.79162314
6	-3.09890829	-2.16947349	3.49971532
6	1.21496821	1.83550332	-3.54679587
1	0.84192798	0.26605827	-5.66084161
6	-0.29909175	-2.16512506	-6.19430035
1	-1.25664472	-2.95395736	-3.75202118
6	-1.41839890	-1.93911548	-1.29342995
6	-4.93965262	0.07667555	0.98730817
1	-6.61618733	-1.80941600	1.89366255
6	-6.49742281	-3.93416742	3.61461154
1	-3.89717744	-3.91110853	4.47011391
6	-1.73016662	-2.34959325	4.11393022
1	1.84905758	1.90632374	-4.44119417
1	1.86114227	1.88955335	-2.65914206
1	0.56731192	2.72610199	-3.53925590
1	-0.68902209	-2.43358940	-0.62895162
1	-2.12928409	-2.71175535	-1.61607588
1	-1.94800046	-1.19950847	-0.67644361
1	-1.27430028	-2.01315805	-6.68470095
1	-0.17084137	-3.24877277	-6.06085689
1	0.47432157	-1.81297615	-6.89084029
1	-5.79758793	-0.22495075	0.37279958
1	-4.07558398	0.22561864	0.32339252
1	-5.18813178	1.05324934	1.43296750
1	-1.41863781	-1.46793349	4.69710545
1	-0.95123855	-2.52466755	3.35362421
1	-1.72419680	-3.21263145	4.79115440
1	-6.10358720	-4.95079090	3.75182386
1	-7.27462182	-3.96985351	2.83931565
1	-6.98834939	-3.64602473	4.55792735
1	-1.42340778	-0.53710846	2.62091147

Energy = -7584.955823 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 14

Atomic N.	X	Y	Z
8	1.63015249	0.26631765	1.87567357
8	3.12116128	-1.43490970	1.26013557

6	2.90292459	-2.31478984	2.36279996
1	2.89891999	-3.33070841	1.94855925
1	1.93294085	-2.12328008	2.85074118
1	3.70491722	-2.24364083	3.11803045
8	3.19640581	0.62044660	0.30073066
6	2.92542261	-0.01682306	1.55747983
6	3.88694835	0.43520993	2.68663731
1	4.78362852	-0.20481105	2.67355927
1	3.36567938	0.23626911	3.63265914
6	4.32208229	1.90743721	2.62476817
1	3.46711112	2.53905650	2.33473337
1	4.60931552	2.22685895	3.63918941
6	5.51879365	2.15795398	1.69150960
1	6.33842216	1.48423883	1.99733742
1	5.89236671	3.18305809	1.84712733
6	5.23980576	1.95685890	0.19611319
1	4.59289739	2.76814234	-0.17715303
1	6.18682333	2.02711943	-0.36602209
6	4.56407622	0.63104064	-0.15051999
1	5.10966926	-0.23395933	0.25801463
1	4.52070416	0.50286098	-1.24290710
50	0.17547917	-0.39994542	0.42065035
7	-0.44853106	2.00299168	0.39664641
6	0.69662391	2.88359801	0.08195587
1	0.42790552	3.94415227	0.23821873
1	1.01580498	2.74102121	-0.95551574
1	1.53455265	2.60915048	0.73112717
7	-1.34985139	0.71746325	-2.30942026
6	-1.63051335	2.33149191	-0.44390380
1	-1.90803056	3.38783072	-0.26185305
1	-2.46422882	1.70988665	-0.08640064
6	-1.47423926	2.13719260	-1.95098938
1	-2.35659966	2.61123190	-2.42680218
1	-0.59846013	2.67913237	-2.32931863
6	-1.20617919	0.41319255	-3.69697808
6	0.01878227	0.66192204	-4.35608422
6	0.13826154	0.33331657	-5.71241769
6	-0.90453257	-0.25577321	-6.43453169
6	-2.09565942	-0.52892093	-5.75202208
6	-2.26830601	-0.20068322	-4.40317472
7	-1.45421370	-0.18975749	1.80348425
6	-0.80207599	2.16843818	1.84035722
1	-1.18973432	3.19054836	2.01226533
1	0.13749108	2.04319921	2.39430531
6	-1.80896427	1.12384452	2.31860234
1	-1.80550445	1.17347679	3.42360233
1	-2.84078551	1.41079040	2.01811694
6	-2.05193779	-1.31371927	2.43369976
6	-2.96364958	-2.12861974	1.71257588
6	-3.53695929	-3.24877035	2.32542102
6	-3.24384398	-3.60131171	3.64767640
6	-2.34167028	-2.79568323	4.34935992
6	-1.73717954	-1.67072035	3.77274164
6	1.21219993	1.21562686	-3.61844784
1	1.09259678	0.52142269	-6.21078468
6	-0.75528948	-0.57765232	-7.90184742
1	-2.92085016	-1.00712350	-6.28562803
6	-3.57499164	-0.52362506	-3.71556135

6	-3.33225699	-1.79670941	0.28643474
1	-4.24185628	-3.85902147	1.75405326
6	-3.85108769	-4.83125403	4.27921456
1	-2.08096238	-3.05940814	5.37831351
6	-0.72788062	-0.88652112	4.57582718
1	2.14093831	0.95121081	-4.14022652
1	1.26219320	0.81413543	-2.59617703
1	1.18650815	2.31553045	-3.54679235
1	-3.45705070	-1.30264141	-2.94421657
1	-4.30696098	-0.89948373	-4.44109526
1	-4.01742397	0.35733284	-3.22478629
1	-1.14074061	0.24156109	-8.52953630
1	-1.31285239	-1.48462863	-8.17304379
1	0.29832557	-0.72880146	-8.17272601
1	-4.19955173	-2.38778940	-0.03733328
1	-2.50279585	-2.01203116	-0.40681897
1	-3.57162130	-0.72890568	0.17731218
1	-1.19514135	-0.05169381	5.12383968
1	0.04877850	-0.45888360	3.92556357
1	-0.24973903	-1.53139314	5.32562592
1	-3.26227777	-5.73214020	4.04311941
1	-4.87244910	-5.00714375	3.91346250
1	-3.88916199	-4.74296950	5.37342622
1	-2.15301808	0.21308673	-1.93176281

Energy = -7584.960637 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 15

Atomic N.	X	Y	Z
8	2.49930746	0.78849925	1.05015365
8	2.75617130	0.32810969	-1.14120343
6	3.04032145	0.80072252	-2.46005032
1	2.42603806	0.20057369	-3.14247263
1	4.10369829	0.65239412	-2.71557494
1	2.77002093	1.85928152	-2.57267670
8	3.32165084	2.45501495	-0.22989689
6	3.35241656	1.05376024	0.03645443
6	4.75422752	0.46144823	0.26738803
1	5.35874090	0.52463157	-0.65251286
1	4.57051295	-0.60559592	0.45034092
6	5.51962813	1.07924535	1.44791181
1	4.81064273	1.27227687	2.26852892
1	6.23881974	0.33620346	1.82648922
6	6.28887968	2.35628724	1.08707023
1	7.02709349	2.11156533	0.30270329
1	6.87112384	2.69242356	1.96013855
6	5.41238755	3.51174077	0.59256701
1	4.76442412	3.88112898	1.40386580
1	6.05958356	4.35463266	0.29587288
6	4.51701683	3.16525894	-0.59863530
1	5.08746120	2.62524950	-1.37429608
1	4.13952341	4.09025093	-1.05938688
50	0.81773113	-0.36334909	0.35511365
7	-0.33735271	0.55807158	2.42013080
6	0.61746242	1.41512823	3.16394333
1	0.09780450	1.93714641	3.98764821
1	1.08513262	2.13714147	2.48988338

1	1.41904352	0.79069287	3.57584896
7	-0.42760613	1.23265785	-0.38910522
6	-1.42669531	1.37890902	1.82742879
1	-1.84665288	2.06044941	2.59319923
1	-2.21083553	0.69413679	1.48366843
6	-0.92830144	2.16478539	0.61400019
1	-1.79064450	2.72635505	0.21455119
1	-0.19165234	2.92324559	0.94294007
6	-0.58941339	1.54779707	-1.75426323
6	-0.26731399	2.82888615	-2.29086420
6	-0.47560441	3.08515896	-3.65238317
6	-0.97068145	2.12054953	-4.53493906
6	-1.25707486	0.85820167	-4.00582383
6	-1.08729308	0.55647593	-2.64948582
7	-1.84781219	-2.06407232	1.72960741
6	-0.83435596	-0.47524782	3.37751356
1	-1.10322049	0.02496568	4.32787038
1	0.02164415	-1.13371181	3.59648789
6	-2.04367390	-1.31913342	2.97776134
1	-2.23196626	-1.99466235	3.83624987
1	-2.93396654	-0.68012635	2.89574787
6	-2.72235508	-3.14951623	1.44985638
6	-4.09768116	-2.92944961	1.20766308
6	-4.92108859	-4.02542101	0.91711376
6	-4.42844247	-5.33060331	0.82893981
6	-3.05545798	-5.52029865	1.02794718
6	-2.19753972	-4.46149162	1.34031746
6	0.38464541	3.90402745	-1.45282109
1	-0.21140674	4.07382608	-4.03899686
6	-1.21182417	2.43705729	-5.99152878
1	-1.65061093	0.07979850	-4.66554482
6	-1.46810009	-0.82064960	-2.16394737
6	-4.68435004	-1.53953648	1.18528304
1	-5.98135613	-3.84117704	0.72567211
6	-5.34306081	-6.49607528	0.53859771
1	-2.63616368	-6.52619358	0.94487085
6	-0.72403330	-4.72536226	1.54579089
1	0.83946249	4.66219632	-2.10498351
1	1.17167120	3.48056623	-0.81271501
1	-0.32853731	4.42794003	-0.79743711
1	-0.59444094	-1.48800224	-2.06736643
1	-2.15873382	-1.30137919	-2.86992475
1	-1.93946613	-0.78123973	-1.17177265
1	-2.23586969	2.80919851	-6.15760949
1	-1.08397447	1.54697409	-6.62326469
1	-0.52279915	3.21388958	-6.35185212
1	-5.62032597	-1.52897227	0.61212706
1	-3.98631817	-0.82894759	0.71888859
1	-4.91760626	-1.16191472	2.19373908
1	-0.38010253	-4.40049615	2.54112378
1	-0.09874116	-4.20329085	0.80292593
1	-0.51015422	-5.79760792	1.45601169
1	-4.85048167	-7.24595775	-0.09588896
1	-6.26005173	-6.16748334	0.03117800
1	-5.64611588	-7.00541431	1.46734658
1	-0.87498066	-2.36454829	1.65475193

Energy = -7584.955828 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 16

Atomic N.	X	Y	Z
8	1.95028701	-0.71850040	1.39053717
8	3.41294825	-1.26280454	-0.35907768
6	3.49289507	-2.67004016	-0.13325991
1	3.48655603	-3.14062031	-1.12432650
1	2.62928588	-3.03953460	0.44412609
1	4.42261502	-2.95640894	0.38851321
8	3.12517992	0.87999135	0.33131626
6	3.17062071	-0.46109751	0.83954044
6	4.30567476	-0.68076496	1.87251688
1	5.22804286	-0.96205068	1.33959998
1	4.00843168	-1.54883098	2.47621921
6	4.60232989	0.51794892	2.78663730
1	3.65952313	0.99655725	3.09639452
1	5.07395491	0.14057452	3.70788978
6	5.55334497	1.55195628	2.15999159
1	6.47033563	1.02486619	1.84289310
1	5.86727456	2.27140678	2.93362044
6	4.98712613	2.32951506	0.96461063
1	4.21228120	3.03474720	1.30848165
1	5.78777396	2.93914830	0.51176844
6	4.36492528	1.45505503	-0.12289648
1	5.05153779	0.66542061	-0.46620605
1	4.10786742	2.06793022	-1.00035667
50	0.28741480	-0.53400671	0.01942842
7	-0.51569546	1.11213701	1.69641299
6	0.46911235	2.18327657	1.95827390
1	0.15381934	2.80110520	2.81864140
1	0.58324251	2.82266028	1.07695387
1	1.43958845	1.72006045	2.16425925
7	-1.84019395	1.77387537	-1.05911150
6	-1.86492082	1.67351658	1.42093602
1	-2.18302421	2.26966073	2.29810303
1	-2.55766843	0.82358740	1.33718246
6	-2.00041830	2.55098881	0.17786395
1	-2.99480069	3.03808840	0.23803150
1	-1.26377902	3.36407569	0.18704631
6	-1.95481080	2.48861272	-2.28980290
6	-0.90970505	3.33777000	-2.71876739
6	-1.03903211	4.00798188	-3.94166745
6	-2.15648732	3.84928083	-4.76785725
6	-3.16197865	2.97416681	-4.34147387
6	-3.08585681	2.29796451	-3.11898154
7	-1.03970316	-1.60602447	1.32389679
6	-0.58289500	0.21604175	2.89194355
1	-1.00758884	0.77259590	3.74893940
1	0.45599094	-0.05591806	3.12024221
6	-1.38687151	-1.05513677	2.62486759
1	-1.16579161	-1.74347970	3.46202302
1	-2.47747258	-0.84899549	2.69878488
6	-1.40838125	-2.95491523	1.07439477
6	-2.37948413	-3.25264308	0.08311182
6	-2.72750314	-4.58324389	-0.17832994
6	-2.14751132	-5.65094065	0.51534769
6	-1.18848776	-5.34896205	1.48764811

6	-0.80291762	-4.03327085	1.77529710
6	0.36046704	3.48935276	-1.91959647
1	-0.22128748	4.65513557	-4.26881708
6	-2.27872382	4.60350265	-6.06980654
1	-4.03781938	2.81493402	-4.97541545
6	-4.19919015	1.36019843	-2.71196885
6	-3.05306824	-2.14662457	-0.69333260
1	-3.48287081	-4.79018625	-0.94140237
6	-2.51570141	-7.08049250	0.19722987
1	-0.70600321	-6.16590164	2.03183714
6	0.28252894	-3.79193580	2.79619465
1	1.18296032	3.81940412	-2.56710392
1	0.64685807	2.53556765	-1.45370192
1	0.26288393	4.23926836	-1.11731754
1	-3.86973808	0.30812541	-2.69247134
1	-5.03160068	1.42205762	-3.42381927
1	-4.59929759	1.59547717	-1.71335751
1	-2.80874602	5.55874789	-5.92740008
1	-2.84158880	4.02713736	-6.81659689
1	-1.29139512	4.83806573	-6.49017183
1	-3.92164949	-2.53272755	-1.24370277
1	-2.36772877	-1.69112670	-1.42670819
1	-3.38806687	-1.34044641	-0.02460482
1	-0.12900820	-3.63229193	3.80648875
1	0.87663651	-2.90318947	2.53916033
1	0.95073214	-4.66159113	2.85845371
1	-1.86281180	-7.49493979	-0.58764778
1	-3.54970949	-7.15614012	-0.16673451
1	-2.41449409	-7.72695636	1.07975004
1	-2.50956832	1.00320088	-1.04960836

Energy = -7584.960628 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 17

Atomic N.	X	Y	Z
8	2.42436424	-0.89577883	-1.16997274
8	4.36522373	0.38137470	-1.41712179
6	4.82984906	-0.23175914	-2.61750792
1	5.25799268	0.57283669	-3.22832744
1	4.00382423	-0.70556922	-3.17282922
1	5.61517228	-0.98457709	-2.42791776
8	3.14604695	0.40431645	0.49791365
6	3.57179030	-0.48284661	-0.56448412
6	4.43055724	-1.66469883	-0.05409265
1	5.47768418	-1.33842569	0.05011862
1	4.40864719	-2.41778048	-0.85389497
6	3.95295728	-2.29005287	1.26521488
1	2.85059310	-2.31933069	1.28547273
1	4.28791690	-3.33863283	1.29699221
6	4.49633265	-1.57769453	2.51493208
1	5.59742040	-1.54156309	2.44041528
1	4.27006221	-2.18510096	3.40586743
6	3.96406056	-0.15713654	2.74268644
1	2.90131805	-0.19467001	3.03315139
1	4.50340378	0.30571511	3.58641483
6	4.07899972	0.77128029	1.53629843
1	5.09788310	0.79596037	1.11965370

1	3.80894964	1.79932853	1.81747428
50	0.67343368	-0.18404434	-0.13135807
7	-0.32206819	-0.66264094	-2.35045661
6	0.14656082	-1.94628455	-2.91983649
1	-0.18228161	-2.05025437	-3.96952618
1	-0.24989835	-2.78788693	-2.34070891
1	1.23999105	-1.97296827	-2.86242405
7	-2.69415732	-1.39856486	-0.25702151
6	-1.80759560	-0.54325588	-2.44168368
1	-2.07595538	-0.57895719	-3.51564133
1	-2.08366304	0.44674639	-2.05635002
6	-2.64721109	-1.59322977	-1.71310802
1	-3.66795301	-1.48037432	-2.10136655
1	-2.33365583	-2.61735901	-1.99437469
6	-3.66500610	-2.15989855	0.45626576
6	-3.26412868	-3.19489217	1.33519381
6	-4.23536999	-3.89674049	2.05747137
6	-5.60104634	-3.61651489	1.93175770
6	-5.97455036	-2.57475241	1.07646448
6	-5.03715959	-1.83302172	0.34668469
7	0.41348643	1.72880790	-1.01771662
6	0.30770893	0.46336932	-3.11083198
1	-0.09260482	0.48115561	-4.14202729
1	1.38199231	0.23918583	-3.14569312
6	0.10595235	1.81826586	-2.43691658
1	0.76357365	2.52833320	-2.97293133
1	-0.92818566	2.18829151	-2.60716877
6	0.51766399	2.94586756	-0.29177508
6	-0.44226439	3.27424247	0.70218508
6	-0.31164852	4.46532321	1.42860717
6	0.73889081	5.36092133	1.20639936
6	1.67583070	5.03017135	0.22167211
6	1.59251205	3.84733749	-0.52364210
6	-1.80361407	-3.53782035	1.51362268
1	-3.91222486	-4.69169587	2.73436893
6	-6.63521829	-4.41799612	2.68508237
1	-7.03091772	-2.30694068	0.99074505
6	-5.50205915	-0.66398063	-0.48674975
6	-1.61704788	2.37009830	0.99152561
1	-1.06559983	4.70405708	2.18377731
6	0.87536838	6.62400268	2.02286457
1	2.51426954	5.70694333	0.03397289
6	2.67085020	3.53964888	-1.53232715
1	-1.69088889	-4.41261969	2.16628636
1	-1.23407089	-2.71183454	1.96960873
1	-1.31190600	-3.77011978	0.55577684
1	-4.75691230	0.14394145	-0.47447642
1	-6.45286288	-0.27300721	-0.10153356
1	-5.67255354	-0.93861475	-1.54069378
1	-6.95099412	-5.30203218	2.10830154
1	-7.53577182	-3.82160573	2.88560700
1	-6.24225486	-4.77942077	3.64518025
1	-2.41855845	2.92885963	1.49331242
1	-1.34121847	1.53304645	1.65312720
1	-2.01909333	1.91833429	0.07524161
1	2.39127434	3.87292555	-2.54585350
1	2.87826235	2.46223287	-1.57972101
1	3.60075694	4.06251295	-1.27105697

1	1.49780244	6.45574526	2.91647111
1	-0.10287377	6.98317664	2.37116013
1	1.34988712	7.42780830	1.44325324
1	-1.76407256	-1.53721846	0.14652640

Energy = -7584.959404 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 18

Atomic N.	X	Y	Z
8	2.22162871	-0.20629228	-1.30773681
8	3.59308589	1.40135245	-2.30066444
6	4.10188659	0.57831473	-3.34763030
1	4.17132313	1.21818630	-4.23627300
1	3.42441637	-0.26445505	-3.56206468
1	5.10767896	0.18316139	-3.12027437
8	2.65329524	1.71993656	-0.25884329
6	3.22731825	0.68630493	-1.09202966
6	4.47815523	0.02774541	-0.46195452
1	5.36463118	0.64650637	-0.67468342
1	4.61631953	-0.92298423	-0.99503998
6	4.38280301	-0.23136051	1.04920192
1	3.36199109	-0.55889905	1.30809332
1	5.04663465	-1.07274847	1.30232989
6	4.79547883	0.97640593	1.90651282
1	5.80842618	1.28934219	1.59764060
1	4.88011658	0.66200001	2.95907949
6	3.85429461	2.18526000	1.83045143
1	2.90147114	1.95326927	2.33386359
1	4.30043223	3.03265221	2.37819790
6	3.52458236	2.65236179	0.41476171
1	4.42680113	2.81690319	-0.19473671
1	2.96623911	3.59914188	0.44563641
50	0.46533653	0.23508164	-0.14492037
7	-0.51532461	-1.20423105	-1.89999845
6	0.27381718	-2.41823988	-2.19678614
1	-0.14724289	-2.96497959	-3.05961238
1	0.28647652	-3.07221839	-1.31764880
1	1.30204407	-2.11155480	-2.41670035
7	-1.61136078	-2.58400621	0.61186749
6	-1.94754417	-1.51400761	-1.62567961
1	-2.45734707	-1.71824404	-2.58651236
1	-2.39786851	-0.60124813	-1.20682786
6	-2.23703621	-2.70468007	-0.71175125
1	-3.34094058	-2.77382518	-0.64236438
1	-1.90163889	-3.63335000	-1.19363143
6	-2.08219769	-3.43734819	1.64857182
6	-1.86913929	-4.83392869	1.59055856
6	-2.33065567	-5.63786212	2.64125362
6	-2.97369978	-5.10749912	3.76360284
6	-3.13514915	-3.71802416	3.82199325
6	-2.70938207	-2.87709624	2.78913245
7	-0.60124430	1.56904748	-1.43253322
6	-0.41917537	-0.25516200	-3.05142064
1	-0.90121668	-0.70371929	-3.94052839
1	0.65357352	-0.12767465	-3.24746333
6	-1.03762854	1.10535380	-2.74077995
1	-0.73221797	1.78025295	-3.56210132

1	-2.14628338	1.04736865	-2.80155638
6	-0.83291841	2.93403470	-1.11265827
6	-1.75332356	3.28180935	-0.08894389
6	-1.95308383	4.62795880	0.24399537
6	-1.27585323	5.66247023	-0.40871769
6	-0.37700515	5.31058129	-1.42127402
6	-0.13771817	3.97865417	-1.78216776
6	-1.09411733	-5.46869156	0.46255322
1	-2.15343616	-6.71512502	2.58712881
6	-3.48351103	-5.99988200	4.86937307
1	-3.61496725	-3.27044879	4.69594252
6	-2.90915047	-1.38420830	2.90796686
6	-2.54357156	2.22422336	0.64513646
1	-2.67149343	4.87373793	1.03086507
6	-1.48323344	7.10545021	-0.01476962
1	0.17445081	6.09847932	-1.94223770
6	0.88157435	3.68359623	-2.85390501
1	-0.70180870	-6.44641151	0.77075482
1	-0.24664135	-4.83237654	0.16838470
1	-1.71039936	-5.63524850	-0.43534657
1	-1.95178130	-0.83815797	2.93867420
1	-3.45067002	-1.14173344	3.83071439
1	-3.48912862	-0.97451185	2.06568223
1	-4.54628049	-6.25010969	4.72183354
1	-3.39848077	-5.51260059	5.85048833
1	-2.92756592	-6.94646325	4.90765164
1	-3.38354565	2.67858935	1.18766142
1	-1.92668173	1.68579378	1.38219496
1	-2.93954718	1.46851761	-0.04789904
1	0.41321503	3.58400077	-3.84739474
1	1.42582589	2.75297885	-2.64600812
1	1.60984799	4.50252212	-2.92638280
1	-0.70773288	7.44123168	0.69231480
1	-2.45616801	7.25048695	0.47432857
1	-1.43522980	7.77156931	-0.88754868
1	-1.64583350	-1.61102711	0.91960760

Energy = -7584.959365 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 19

Atomic N.	X	Y	Z
8	1.32804939	-0.45903698	1.46907146
8	2.54017329	-1.26394707	-0.25565502
6	3.70531908	-1.15882595	-1.07665564
1	3.41873701	-1.50615978	-2.07828730
1	4.51104823	-1.80966906	-0.69885125
1	4.06448077	-0.12149873	-1.13803841
8	3.35093892	0.50338742	1.11906847
6	2.61551371	-0.71320072	1.18680912
6	3.21266156	-1.82212567	2.05960722
1	4.19492012	-2.13623029	1.66919409
1	2.53042473	-2.67183250	1.92957897
6	3.32541733	-1.45374971	3.54743055
1	2.42665077	-0.89041023	3.84268705
1	3.31568962	-2.38373357	4.13640028
6	4.59403753	-0.66725228	3.89870953
1	5.47409167	-1.28887803	3.65460768

1	4.63052791	-0.50004214	4.98715955
6	4.73093357	0.67901144	3.17945800
1	3.93831095	1.37381701	3.50031641
1	5.69209998	1.14196655	3.46059803
6	4.68506894	0.59180485	1.65268168
1	5.32273856	-0.23335947	1.28856254
1	5.07515922	1.52302481	1.21674732
50	0.30002025	-0.14907635	-0.38188358
7	-1.82342303	-0.54477649	-2.65553836
6	-1.23323203	-1.52398182	-3.56883102
1	-1.99980199	-2.10669123	-4.12340519
1	-0.59430534	-2.22464697	-3.01704529
1	-0.60657266	-0.99871791	-4.30257355
7	-0.82963269	-1.90910850	-0.08899814
6	-2.68749618	-1.16780177	-1.64395158
1	-3.60172447	-1.59797839	-2.11366129
1	-3.01115249	-0.37670562	-0.95030639
6	-2.03597593	-2.28557695	-0.83207310
1	-2.81078452	-2.62814244	-0.12012948
1	-1.84484777	-3.15602181	-1.48979564
6	-0.44607136	-2.92010293	0.85232882
6	0.29139810	-4.05561319	0.43963428
6	0.63447618	-5.03358955	1.38422540
6	0.26540254	-4.92885744	2.72864050
6	-0.45845410	-3.79670467	3.12026913
6	-0.81675818	-2.79268580	2.21292745
7	-2.15327904	2.31579423	-1.81838702
6	-2.54808183	0.46836326	-3.43979718
1	-3.37464418	-0.00409121	-4.01852589
1	-1.83617677	0.88026614	-4.17311316
6	-3.15421729	1.61919831	-2.63692971
1	-3.60514933	2.31129506	-3.36883026
1	-3.98358038	1.24491398	-2.01483502
6	-2.17104179	3.72464826	-1.73298927
6	-3.32086682	4.40404840	-1.26371497
6	-3.30396563	5.80261373	-1.18672293
6	-2.17825856	6.55854575	-1.52772652
6	-1.03465738	5.86443939	-1.94140417
6	-1.00884077	4.47114173	-2.05458910
6	0.73688985	-4.22917668	-0.99129612
1	1.21602807	-5.89898125	1.05537169
6	0.61703329	-6.01003216	3.72262474
1	-0.74973546	-3.68483587	4.16789382
6	-1.56397885	-1.57930373	2.70532145
6	-4.52663508	3.64775581	-0.76029357
1	-4.19735058	6.31256922	-0.81665152
6	-2.19595638	8.06686627	-1.46114595
1	-0.13102846	6.42485775	-2.19505583
6	0.25217120	3.77835316	-2.51161247
1	1.53806090	-4.97669289	-1.05872383
1	1.10735688	-3.28159458	-1.40421453
1	-0.08579761	-4.57283806	-1.63862220
1	-0.88658240	-0.71394683	2.76511192
1	-1.97480802	-1.75887781	3.70758725
1	-2.38688150	-1.30049930	2.03341802
1	-0.22717733	-6.70131680	3.87394119
1	0.86744988	-5.58604890	4.70516532
1	1.47209673	-6.60727801	3.37817051

1	-5.15923374	4.30319450	-0.14785258
1	-4.21565523	2.79045191	-0.14429522
1	-5.15504614	3.25055277	-1.57233106
1	0.07869325	3.14974180	-3.40044467
1	0.67174994	3.12033099	-1.73282396
1	1.02331044	4.51489037	-2.76999175
1	-1.22258133	8.46726823	-1.14485291
1	-2.95836710	8.42656322	-0.75671577
1	-2.42462599	8.50860087	-2.44444894
1	-1.22069664	1.94196888	-1.98670111

Energy = -7584.947809 Hartree
Number of imaginary frequencies = 0.

Compound I3b isomer 20

Atomic N.	X	Y	Z
8	2.12965700	0.25694424	-0.97689458
8	2.50162122	1.74842000	0.65365321
6	3.14184457	2.10834722	1.87923568
1	2.49731128	2.86026367	2.35129274
1	4.13221046	2.55969384	1.69862017
1	3.24621376	1.24300904	2.55024411
8	3.53305042	-0.38434688	0.68903755
6	3.13984042	0.68185327	-0.18654267
6	4.27805600	1.32048262	-0.99804409
1	4.98316092	1.84048547	-0.32931889
1	3.78518240	2.09603359	-1.59872256
6	5.03815214	0.34531063	-1.91091437
1	4.31942753	-0.36086409	-2.35574402
1	5.47142500	0.91594476	-2.74719697
6	6.16959640	-0.41348838	-1.20632609
1	6.89785266	0.32150749	-0.81952672
1	6.71460330	-1.02377860	-1.94437530
6	5.71483316	-1.30993577	-0.05002880
1	5.09867731	-2.14321562	-0.42454817
1	6.60170969	-1.76044596	0.42732441
6	4.91276306	-0.58837038	1.03519026
1	5.40654557	0.35779903	1.31965705
1	4.86714563	-1.21485832	1.93829904
50	0.29015335	0.36825332	0.15279997
7	-0.55037746	-0.55881464	-1.98368723
6	0.23374854	-1.70754719	-2.48397438
1	-0.10758519	-2.01620656	-3.48844746
1	0.13705638	-2.54815210	-1.78744726
1	1.28708505	-1.40955287	-2.52518518
7	-1.92596949	-2.46488409	-0.00644210
6	-2.01110241	-0.85099197	-1.91863643
1	-2.43276817	-0.78229598	-2.93959485
1	-2.47189182	-0.04883935	-1.32218446
6	-2.42341895	-2.21473171	-1.36514488
1	-3.53045392	-2.23729484	-1.41056873
1	-2.07305928	-3.00896005	-2.03899107
6	-2.54029603	-3.49737470	0.75305337
6	-2.43231500	-4.85113346	0.35995836
6	-3.03701502	-5.83989045	1.14774483
6	-3.72330959	-5.54180535	2.32826012
6	-3.78040738	-4.19956613	2.72324972
6	-3.21031107	-3.17620072	1.96037512

7	-0.60713032	2.02193019	-0.87084110
6	-0.31606352	0.62761349	-2.86161451
1	-0.72530298	0.42761666	-3.87016000
1	0.77353179	0.74206061	-2.93189984
6	-0.92257985	1.90569132	-2.28654722
1	-0.51873631	2.74137345	-2.88885466
1	-2.02064253	1.92120187	-2.46081186
6	-0.79092679	3.29297538	-0.26530931
6	-1.80301655	3.48008732	0.71358293
6	-1.95985629	4.72940410	1.32557153
6	-1.14812688	5.82274110	1.00179425
6	-0.15603065	5.63022837	0.03567514
6	0.04199106	4.39532608	-0.59584101
6	-1.62163901	-5.26322518	-0.84401647
1	-2.94030541	-6.88296649	0.83549401
6	-4.38504873	-6.62448476	3.14622537
1	-4.29219135	-3.93583920	3.65228866
6	-3.30331081	-1.74539451	2.43635550
6	-2.73026797	2.35173573	1.09828917
1	-2.75042178	4.85424849	2.07073084
6	-1.31926974	7.15262056	1.69662135
1	0.50116743	6.46397786	-0.22740923
6	1.16447867	4.25070351	-1.59264478
1	-1.33025282	-6.31858292	-0.76507526
1	-0.70733376	-4.65712180	-0.92370984
1	-2.17713000	-5.14999723	-1.78868334
1	-2.31185952	-1.31351837	2.65111910
1	-3.89144236	-1.68592690	3.36052488
1	-3.78664970	-1.09188392	1.69248319
1	-5.46405794	-6.68394781	2.93177761
1	-4.27970887	-6.43572703	4.22377513
1	-3.95277182	-7.61025603	2.92785588
1	-3.58514755	2.73358423	1.67239907
1	-2.22259572	1.59720778	1.71985942
1	-3.10907446	1.82519696	0.21089688
1	0.83251282	4.46798492	-2.62139225
1	1.56021042	3.22674378	-1.57846025
1	1.97883004	4.95108772	-1.36309816
1	-0.79343006	7.16786963	2.66477468
1	-2.37818603	7.36500591	1.90121823
1	-0.91552343	7.97556740	1.09152782
1	-1.91533316	-1.59371428	0.52601999

Energy = -7584.958500 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 21

Atomic N.	X	Y	Z
8	0.54918957	-0.15724539	0.27785644
8	2.03613449	-1.56424478	-0.63596946
6	3.37457473	-1.86235593	-1.03023587
1	3.30064229	-2.60455625	-1.83543285
1	3.95067758	-2.30609674	-0.20027202
1	3.89606050	-0.96826230	-1.40384009
8	2.69740121	0.58143602	0.09990033
6	1.83677764	-0.52752637	0.42839838
6	2.08832433	-1.17750707	1.79695885
1	3.09590072	-1.62304776	1.83540256

1	1.37404177	-2.01038357	1.83641265
6	1.87713085	-0.23783629	2.99460538
1	1.00457127	0.40264587	2.79313245
1	1.62158650	-0.84791083	3.87530326
6	3.10087594	0.62013809	3.33785653
1	3.94162139	-0.04962246	3.59366598
1	2.89089489	1.20733183	4.24662067
6	3.54908994	1.56719326	2.21977598
1	2.78193890	2.33495129	2.03059479
1	4.46092716	2.09869611	2.54283403
6	3.85903867	0.87516954	0.88958141
1	4.47655889	-0.02645684	1.05585576
1	4.44499269	1.55338495	0.25083731
50	0.04781992	-0.20857249	-1.80402505
7	-2.38099724	0.55635212	-3.04619763
6	-2.18671749	0.33161592	-4.48293559
1	-3.12198492	0.48522928	-5.05780942
1	-1.83696686	-0.69279749	-4.66013115
1	-1.41704268	1.01782726	-4.86101919
7	-1.44459404	-1.71402694	-1.42542633
6	-3.28746732	-0.44631313	-2.45960998
1	-4.20731768	-0.54909440	-3.07390678
1	-3.57998738	-0.09742511	-1.45984642
6	-2.61037806	-1.80827862	-2.29832934
1	-3.35633080	-2.48854035	-1.84929345
1	-2.39459040	-2.23327895	-3.30257243
6	-1.09990358	-2.93707581	-0.76974659
6	-0.50696473	-4.01692442	-1.47170406
6	-0.19537389	-5.20178619	-0.79005712
6	-0.44907027	-5.36074737	0.57488932
6	-1.04434612	-4.29182345	1.25470501
6	-1.37247796	-3.09167907	0.61275753
7	-1.13098742	2.38418103	-1.05470640
6	-2.82008014	1.93936993	-2.79742098
1	-3.89625817	2.06835539	-3.03724005
1	-2.26554936	2.58930021	-3.49410855
6	-2.57312440	2.42977355	-1.37250426
1	-2.97284023	3.45762853	-1.29260779
1	-3.12827107	1.81544158	-0.65399585
6	-0.64450712	3.14370931	0.05370765
6	-1.14118750	2.95906714	1.36151844
6	-0.60606459	3.73220800	2.40181256
6	0.41936995	4.65909307	2.20241993
6	0.92445603	4.79440799	0.90340519
6	0.41715340	4.05600367	-0.16826153
6	-0.19637336	-3.92505238	-2.94596379
1	0.26790862	-6.02164517	-1.34610203
6	-0.06889968	-6.62993994	1.29952438
1	-1.26568930	-4.39414717	2.32073269
6	-2.01383413	-1.97792495	1.39882181
6	-2.17794538	1.91417863	1.69025191
1	-0.99538600	3.57699649	3.41113207
6	0.99842123	5.45288321	3.34869569
1	1.74283278	5.49394165	0.71525025
6	1.02605088	4.22100650	-1.54119680
1	0.58725985	-4.64238978	-3.22374434
1	0.14100266	-2.91578131	-3.22524683
1	-1.08031541	-4.15100994	-3.56401659

1	-1.32222278	-1.12702131	1.47752637
1	-2.27734410	-2.31810439	2.40946735
1	-2.92390574	-1.60835982	0.90469920
1	-0.79643904	-6.87681037	2.08557189
1	0.91387242	-6.52979486	1.78761101
1	-0.00664462	-7.48247634	0.60957314
1	-2.13680002	1.66598062	2.75866969
1	-1.99556232	0.99193691	1.12317966
1	-3.20363335	2.25338527	1.47502494
1	0.28926105	4.54808054	-2.29448054
1	1.47745047	3.28210562	-1.90184930
1	1.82024051	4.97729485	-1.51853884
1	2.00450727	5.09163547	3.61421748
1	0.37001428	5.37497028	4.24550882
1	1.09625434	6.51785896	3.09246412
1	-0.62045089	2.67910817	-1.88838558

Energy = -7584.952423 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 22

Atomic N.	X	Y	Z
8	0.22771405	-0.32233227	0.11757326
8	2.26684500	-0.35737113	-0.77193817
6	3.34180630	-0.91538446	-1.54216009
1	4.03873545	-0.08843423	-1.72397344
1	2.98164073	-1.32463875	-2.49550995
1	3.86366841	-1.69644038	-0.96802772
8	0.67436842	-1.60273322	-1.79506943
6	1.09758462	-1.18727889	-0.48008499
6	1.44765129	-2.36914051	0.46032575
1	0.59536795	-2.48985222	1.14620773
1	2.28530641	-2.02459866	1.08447295
6	1.77947886	-3.73094072	-0.17121810
1	2.51034780	-3.61714083	-0.98631179
1	2.27627530	-4.33877428	0.60250964
6	0.55717778	-4.50969821	-0.68295420
1	-0.19703349	-4.55211424	0.12268940
1	0.85312901	-5.55283039	-0.87925923
6	-0.08629521	-3.93488228	-1.94970627
1	0.60416112	-4.04432276	-2.80227266
1	-0.99109384	-4.51437203	-2.19999361
6	-0.47562215	-2.46303182	-1.84501087
1	-1.12445061	-2.27861254	-0.97371722
1	-1.03868485	-2.15494187	-2.73859951
50	0.52102027	1.56213939	-0.97479392
7	-1.08546048	2.75388569	0.58595758
6	-2.09419659	3.47750955	-0.21402091
1	-2.73041872	4.11892721	0.42247124
1	-2.71934563	2.76190641	-0.75772651
1	-1.57639327	4.10899532	-0.94672371
7	-2.70076448	0.15061242	0.15551204
6	-1.71953243	1.90643071	1.64083543
1	-2.02225412	2.56210028	2.48003968
1	-0.94950934	1.21890672	2.01852243
6	-2.95710901	1.10892850	1.23404412
1	-3.31095859	0.61920692	2.16575683
1	-3.76978909	1.78748223	0.93026692

6	-3.77622217	-0.76836145	-0.08062515
6	-4.78373951	-0.42919174	-1.01026074
6	-5.82753855	-1.33186670	-1.25104569
6	-5.90073490	-2.57056161	-0.60484919
6	-4.88965678	-2.89332866	0.30773244
6	-3.83796596	-2.01262833	0.59009969
7	1.79659948	2.53329507	0.47806243
6	-0.15999025	3.73430111	1.22869064
1	-0.66976620	4.21671134	2.08464148
1	0.06923838	4.50372412	0.47803844
6	1.14836310	3.08396588	1.65852764
1	1.77604568	3.87239866	2.11243517
1	0.94736250	2.35306977	2.46882494
6	3.19802683	2.35445711	0.49743697
6	3.86450537	1.62027314	1.51501776
6	5.26010239	1.49313402	1.48140319
6	6.03811915	2.04392326	0.45909712
6	5.37077418	2.74662684	-0.55136273
6	3.98136791	2.91307752	-0.55156374
6	-4.72755394	0.87324485	-1.76785860
1	-6.59507392	-1.06359931	-1.98144749
6	-7.04710384	-3.51836871	-0.86425615
1	-4.92343784	-3.85541327	0.82555064
6	-2.79232897	-2.40121631	1.60923410
6	3.09649497	0.90493630	2.59892036
1	5.75010103	0.92018481	2.27392556
6	7.53715587	1.86308202	0.42535507
1	5.95188283	3.19885440	-1.36002884
6	3.33801053	3.71145050	-1.65928293
1	-5.41622820	0.85710043	-2.62245381
1	-3.70845324	1.06468523	-2.13124572
1	-5.01277575	1.72904625	-1.13462098
1	-1.79102793	-2.49564077	1.16288528
1	-3.04283706	-3.36542052	2.06937664
1	-2.70695877	-1.65573568	2.41365249
1	-7.87142515	-3.34673940	-0.15388051
1	-6.73514712	-4.56580174	-0.75390554
1	-7.45524757	-3.38575800	-1.87537885
1	3.71334136	0.11314192	3.04496176
1	2.18296381	0.45013459	2.18917673
1	2.79062421	1.57815603	3.41583260
1	2.57399160	4.39511807	-1.26313596
1	2.82552675	3.06841403	-2.39428765
1	4.09261773	4.29215393	-2.20679917
1	7.83036956	1.06290571	-0.27322328
1	7.92963382	1.59487710	1.41549477
1	8.04504065	2.78044427	0.09430144
1	-1.81041294	-0.33442076	0.32472464

Energy = -7584.958588 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 23

Atomic N.	X	Y	Z
8	0.50297627	-0.35102131	0.21342565
8	2.10339025	-1.12437416	-1.13897565
6	3.13085756	-2.04533813	-1.51703987
1	3.31708374	-1.87510033	-2.58530662

1	2.81690026	-3.08651258	-1.36000247
1	4.06221299	-1.84567072	-0.96242882
8	1.06519187	-2.62072140	0.22312741
6	1.51997211	-1.24766744	0.19735026
6	2.55409319	-0.92472407	1.30989318
1	2.00612383	-0.37957878	2.09346159
1	3.25553712	-0.19793690	0.87462010
6	3.31924877	-2.08987372	1.95816395
1	3.72457678	-2.76908754	1.19251931
1	4.19104839	-1.66212763	2.48028755
6	2.49823834	-2.89745004	2.97637229
1	2.03904112	-2.19399064	3.69344290
1	3.17874131	-3.53528462	3.56381039
6	1.40287805	-3.77710334	2.36329108
1	1.86142398	-4.59257483	1.77955883
1	0.81956443	-4.25553145	3.16908057
6	0.43584336	-3.02827755	1.44900708
1	-0.00798881	-2.15525899	1.95456765
1	-0.39351271	-3.69008008	1.15555684
50	-0.39516682	-0.25459995	-1.75917277
7	-2.41164906	1.42565335	-2.63969792
6	-3.43948910	0.78441081	-3.46269114
1	-4.09137435	1.52909156	-3.96264166
1	-4.06826894	0.12339662	-2.85560682
1	-2.95431061	0.16868660	-4.23200481
7	-2.38876561	0.34384922	0.13811685
6	-2.97515845	2.13567461	-1.48557168
1	-3.80879289	2.80496020	-1.78687657
1	-2.18449342	2.77324411	-1.06571726
6	-3.47877976	1.19311466	-0.39133949
1	-3.93933698	1.80398169	0.40737057
1	-4.26967752	0.53689511	-0.77426326
6	-2.80501688	-0.64672953	1.09739998
6	-3.50072749	-1.80102935	0.67850648
6	-3.88042739	-2.74837042	1.63917974
6	-3.58590296	-2.59728562	2.99707125
6	-2.87346734	-1.45662331	3.38448131
6	-2.48212861	-0.47871950	2.46409002
7	0.36262130	1.75279024	-1.97231043
6	-1.54534074	2.27004109	-3.47899307
1	-2.10737640	3.12823906	-3.90531819
1	-1.21990456	1.63697364	-4.31984304
6	-0.31178075	2.78722694	-2.74385845
1	0.35177445	3.22073695	-3.51827762
1	-0.59369530	3.65409031	-2.10411175
6	1.66954318	2.15703447	-1.55761820
6	1.87322047	2.80047925	-0.31529679
6	3.16024224	3.21797739	0.04928912
6	4.26734221	3.01601414	-0.78109774
6	4.05278842	2.38395420	-2.01124988
6	2.78187984	1.95324065	-2.41146793
6	-3.81879039	-2.06835396	-0.77206403
1	-4.40751817	-3.64486547	1.30336161
6	-4.03014241	-3.62166417	4.01286581
1	-2.61072150	-1.32023564	4.43631149
6	-1.68797358	0.71476828	2.93796212
6	0.72215434	3.02009340	0.63250769
1	3.29951679	3.71336548	1.01414968

6	5.65263443	3.43842962	-0.35297477
1	4.90072315	2.21867104	-2.68169006
6	2.61507568	1.26755510	-3.74478170
1	-3.91735151	-3.14739303	-0.94748237
1	-3.02915463	-1.68611391	-1.43492374
1	-4.77157209	-1.60492129	-1.07730450
1	-0.66518609	0.69587365	2.52874980
1	-1.60922682	0.71299892	4.03208027
1	-2.14631143	1.67170951	2.64258476
1	-4.99186156	-3.33705699	4.46838251
1	-3.30103866	-3.72036933	4.82871556
1	-4.16601010	-4.60912475	3.55177332
1	1.04510996	3.58802358	1.51515664
1	0.33443413	2.04648296	0.96445990
1	-0.10496243	3.56931916	0.15845491
1	1.91843159	1.80764094	-4.40369041
1	2.20565796	0.25426597	-3.62248561
1	3.57941929	1.19011477	-4.26424804
1	6.18034217	2.61435943	0.15359585
1	5.61549160	4.28218207	0.34967002
1	6.26648668	3.73565502	-1.21458285
1	-1.68947880	0.94547672	0.58118413

Energy = -7584.957895 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 24

Atomic N.	X	Y	Z
8	-0.48456379	-2.49689793	0.18120450
8	0.67886744	-0.67600865	0.73301542
6	1.87563937	0.02610757	1.10963849
1	1.70652455	1.07747982	0.84959170
1	2.75063389	-0.35507309	0.56844414
1	2.03816274	-0.05657284	2.19539748
8	1.84790132	-2.51626482	0.05633740
6	0.66404396	-2.16056408	0.80359655
6	0.68308564	-2.65814423	2.26996119
1	-0.00768493	-3.51354921	2.31016764
1	0.21081711	-1.86760852	2.87127196
6	2.03195569	-3.06778738	2.88091977
1	2.79694925	-2.29660191	2.69981173
1	1.89695319	-3.11614798	3.97378956
6	2.55236483	-4.43231976	2.40022103
1	1.74265353	-5.17489091	2.51007819
1	3.36561846	-4.76324754	3.06626497
6	3.06491451	-4.45104290	0.95562744
1	3.98038032	-3.84138486	0.87746180
1	3.34720160	-5.48100126	0.67704046
6	2.06619499	-3.93246234	-0.07583674
1	1.10239294	-4.46615279	-0.02074532
1	2.46468131	-4.07986752	-1.09144637
50	-0.80156251	-0.97444382	-1.30633655
7	-2.05473299	1.39266732	-2.77482282
6	-2.83860325	0.72294054	-3.81357574
1	-3.63836596	1.37296983	-4.22710630
1	-3.30586483	-0.18680273	-3.41524355
1	-2.17317762	0.42453663	-4.63494747
7	-2.57405105	-0.36283103	-0.33323292

6	-2.87731475	1.78658753	-1.62513583
1	-3.68785416	2.48474903	-1.93661551
1	-2.22781426	2.31825659	-0.91596289
6	-3.52059130	0.61576621	-0.88128280
1	-4.10056062	1.06117701	-0.05541074
1	-4.27710995	0.12808026	-1.52898897
6	-3.02088988	-0.93974685	0.89910469
6	-3.61867745	-2.22034924	0.92726313
6	-4.07119883	-2.74140236	2.14654563
6	-3.94079588	-2.03952460	3.34897659
6	-3.32946062	-0.78138148	3.30770978
6	-2.87148276	-0.21922455	2.10993682
7	0.69369270	2.25320304	-1.96528467
6	-1.33687411	2.53325541	-3.36352720
1	-2.04973857	3.31598068	-3.70828274
1	-0.81930623	2.15953615	-4.26205338
6	-0.31193073	3.20911905	-2.45381533
1	0.15947677	4.01478566	-3.04590489
1	-0.82092894	3.70110062	-1.61209457
6	2.01347645	2.68988124	-1.70679386
6	2.27209802	3.73396637	-0.78659988
6	3.59843528	4.11655936	-0.54593102
6	4.68567653	3.48659196	-1.15876667
6	4.41001400	2.42317244	-2.02692794
6	3.10400220	2.01621859	-2.31463998
6	-3.74911701	-3.05252015	-0.32408214
1	-4.53501648	-3.73124844	2.15438939
6	-4.46215562	-2.60919503	4.64674325
1	-3.19551516	-0.22062204	4.23685978
6	-2.20256276	1.13255788	2.12958997
6	1.16401512	4.38475560	0.00644195
1	3.78271470	4.92109833	0.17081970
6	6.10251347	3.94031545	-0.90215842
1	5.23813241	1.89362333	-2.50476963
6	2.86868843	0.85924802	-3.25598021
1	-4.49803997	-3.84399302	-0.18758256
1	-2.78969890	-3.53803366	-0.56218203
1	-4.03553622	-2.44668194	-1.19442605
1	-1.29034555	1.12499171	1.51769875
1	-1.94142747	1.42068109	3.15637896
1	-2.85682841	1.92145365	1.72402905
1	-5.47686225	-2.23959003	4.86502555
1	-3.82424657	-2.32357197	5.49491314
1	-4.51406583	-3.70575036	4.61033897
1	1.57867497	4.90825498	0.87757240
1	0.44516598	3.63280051	0.36599999
1	0.59536670	5.12374502	-0.57875546
1	2.23428130	1.14300772	-4.11176234
1	2.37535852	0.00881179	-2.75622305
1	3.82077084	0.49211912	-3.65867667
1	6.80476527	3.09530120	-0.91877577
1	6.19187885	4.44025404	0.07194714
1	6.43783668	4.65665969	-1.66925076
1	0.68758233	1.41613580	-2.54618834

Energy = -7584.950328 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 25

Atomic N.	X	Y	Z
8	0.37053107	0.06879942	0.30103782
8	1.82808961	1.29433106	-0.85050389
6	3.08144261	1.56053772	-1.49734595
1	2.90722928	2.43548003	-2.13501030
1	3.40799248	0.70712254	-2.10665704
1	3.85409938	1.81279848	-0.75460632
8	2.05865477	-0.95523066	-0.96485020
6	1.69336789	0.08816925	-0.03725142
6	2.58910813	0.13404139	1.22742379
1	2.01126024	-0.33324546	2.03940736
1	2.67881072	1.19626482	1.49889995
6	3.97997378	-0.51769826	1.16262885
1	4.51960566	-0.20096938	0.25715831
1	4.56234662	-0.13334325	2.01586960
6	3.96721337	-2.05249343	1.24213560
1	3.36323078	-2.35547877	2.11576295
1	4.99063336	-2.41000080	1.43973745
6	3.43393594	-2.75596197	-0.01076564
1	4.12654583	-2.59540378	-0.85341993
1	3.39712567	-3.84459480	0.16427788
6	2.04605219	-2.29551264	-0.44770220
1	1.31787962	-2.37698002	0.37514384
1	1.67775524	-2.92755832	-1.26947588
50	-0.66010650	0.77576051	-1.50348522
7	-2.87492943	0.76497735	-0.25851011
6	-3.88602039	0.08233631	-1.09140619
1	-4.89442391	0.15816924	-0.64556466
1	-3.61637663	-0.97156512	-1.21417500
1	-3.90124272	0.55130513	-2.08303487
7	-1.74492900	-1.97808017	0.60806018
6	-2.83790532	0.20811985	1.12729937
1	-3.70973742	0.60086932	1.68526702
1	-1.93094007	0.59504022	1.61341808
6	-2.87613949	-1.31288636	1.25972016
1	-2.92012387	-1.51296573	2.35118222
1	-3.81618667	-1.71356491	0.84896037
6	-1.63957659	-3.37834969	0.90249816
6	-2.27882630	-4.31120552	0.05672064
6	-2.16663477	-5.67948846	0.33537742
6	-1.43052554	-6.15624899	1.42540647
6	-0.79769466	-5.21775460	2.24882251
6	-0.89747596	-3.84049469	2.01490375
7	-0.94716645	2.82761136	-0.87738330
6	-3.18013480	2.22657426	-0.19409265
1	-4.00179707	2.40044468	0.52671873
1	-3.51913599	2.53309714	-1.19319776
6	-1.94545028	3.04641267	0.15844250
1	-2.24731521	4.10874007	0.18644777
1	-1.61663679	2.79490683	1.18774415
6	-0.01459397	3.85090463	-1.14885604
6	0.76031082	4.47598365	-0.13287924
6	1.64974370	5.50512373	-0.46905878
6	1.83664409	5.93543814	-1.78605287
6	1.09912144	5.28843778	-2.78395649
6	0.18381896	4.26968573	-2.49510298
6	-3.04920777	-3.85205318	-1.15544635

1	-2.65545791	-6.39287327	-0.33296721
6	-1.34242579	-7.63465914	1.71912037
1	-0.21564968	-5.56495992	3.10644342
6	-0.21797104	-2.87327516	2.95636826
6	0.71573869	3.99792111	1.29791961
1	2.23890341	5.96505096	0.32970614
6	2.77996065	7.06734223	-2.11625677
1	1.22397787	5.59808512	-3.82531718
6	-0.59597422	3.64607651	-3.62682206
1	-3.23875263	-4.69094740	-1.83753449
1	-2.49514926	-3.06989921	-1.69240004
1	-4.02836357	-3.42677082	-0.88115824
1	0.56770232	-2.28720664	2.45621725
1	0.25054040	-3.41223645	3.78954447
1	-0.92700217	-2.14755174	3.38131127
1	-2.15498246	-7.95409138	2.39086190
1	-0.39389679	-7.89058181	2.21033553
1	-1.42598049	-8.23086588	0.80034307
1	1.61379183	4.32786901	1.83722086
1	0.66517342	2.90040271	1.33691092
1	-0.15620719	4.38491885	1.84918016
1	-1.65133246	3.50811934	-3.35166525
1	-0.21369163	2.64789811	-3.89876711
1	-0.53793727	4.27138213	-4.52794513
1	3.24879837	6.92717540	-3.10035294
1	3.57830177	7.15430830	-1.36612801
1	2.25203556	8.03436647	-2.14319093
1	-0.87543942	-1.47335179	0.82234050

Energy = -7584.958629 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 26

Atomic N.	X	Y	Z
8	0.88919562	-0.34709124	-0.49726365
8	2.44911863	1.10026578	-1.15504900
6	3.78565371	1.51251573	-1.47545837
1	3.68161083	2.43220801	-2.06367791
1	4.31230819	0.74803999	-2.06215234
1	4.35093342	1.74098226	-0.55846265
8	2.91131472	-1.11451054	-1.38992885
6	2.24094385	-0.19486697	-0.50130114
6	2.80968972	-0.21088476	0.94175967
1	2.10349032	-0.79602282	1.55012392
1	2.73890366	0.82280916	1.31092424
6	4.22871354	-0.75943029	1.16226136
1	4.93381278	-0.32744359	0.43584747
1	4.56348726	-0.41714576	2.15499369
6	4.32614108	-2.29274897	1.12428800
1	3.56205420	-2.71137476	1.80302091
1	5.30157205	-2.60159046	1.53314226
6	4.15827211	-2.91083640	-0.26780617
1	5.01344682	-2.63365179	-0.90598397
1	4.16827126	-4.01120137	-0.18704113
6	2.87932746	-2.49505035	-0.98988779
1	1.98471403	-2.69301428	-0.37502089
1	2.76884609	-3.07196312	-1.92082896
50	0.22322575	0.51145752	-2.39649011

7	-2.10210919	-0.11110590	-1.62545274
6	-2.85472997	-0.77446977	-2.71139613
1	-3.90013860	-0.96646856	-2.40941677
1	-2.37964928	-1.72493748	-2.97918388
1	-2.85093124	-0.12931201	-3.59864014
7	-1.03689654	-2.96386760	0.66116856
6	-2.09200472	-0.94948712	-0.39519748
1	-3.12535078	-1.03398836	-0.00832928
1	-1.49004042	-0.41768768	0.35157476
6	-1.48424583	-2.34998439	-0.59564150
1	-2.19654720	-3.01655617	-1.09458420
1	-0.59646898	-2.26836985	-1.23860839
6	-1.96950295	-3.21289006	1.70134874
6	-3.05204278	-4.10740275	1.51364119
6	-3.93165903	-4.34751350	2.57677289
6	-3.76768054	-3.76251982	3.83628240
6	-2.65735104	-2.93079832	4.02012251
6	-1.76188992	-2.64470953	2.98461910
7	-0.58048997	2.33252378	-1.58367839
6	-2.71079626	1.22208321	-1.32886303
1	-3.60781670	1.08435770	-0.69669495
1	-3.01941419	1.66026515	-2.28809049
6	-1.70541568	2.16415714	-0.67415660
1	-2.21281872	3.13043903	-0.50574586
1	-1.43956848	1.77692237	0.33013135
6	0.15603543	3.53869930	-1.55804540
6	0.66643819	4.10702314	-0.35928139
6	1.36329886	5.32212526	-0.40782959
6	1.61237946	5.99668187	-1.60631603
6	1.13018431	5.41500629	-2.78463126
6	0.41165573	4.21454650	-2.78475454
6	-3.23883696	-4.87088411	0.22481700
1	-4.75913879	-5.04372211	2.41602003
6	-4.75110338	-4.01689844	4.95308721
1	-2.48127953	-2.48182402	5.00099706
6	-0.57053497	-1.75621392	3.25608464
6	0.53794913	3.39805640	0.96718086
1	1.74620413	5.73941948	0.52790135
6	2.40084129	7.28439060	-1.63558240
1	1.29968040	5.92249663	-3.73839921
6	-0.10864380	3.67192648	-4.09328956
1	-3.81455596	-5.78785765	0.40720954
1	-2.26889722	-5.14983451	-0.21137585
1	-3.78782698	-4.29354238	-0.53716006
1	0.38245126	-2.30111075	3.14686464
1	-0.60557023	-1.37091707	4.28265633
1	-0.52345498	-0.89027415	2.57706962
1	-5.57501760	-3.28550322	4.93506692
1	-4.26931347	-3.94004317	5.93738960
1	-5.20204552	-5.01546993	4.86991843
1	1.28329190	3.78154016	1.67682948
1	0.69350245	2.31711515	0.84503254
1	-0.45273394	3.53655555	1.42881094
1	-1.14491842	3.31909660	-3.99216604
1	0.47832248	2.80935247	-4.45068608
1	-0.06486881	4.44122411	-4.87587239
1	3.46271624	7.10047585	-1.86585971
1	2.36085134	7.80029392	-0.66663283

1 2.01890107 7.97124430 -2.40427393
 1 -0.24545121 -2.42130507 1.00722981
 Energy = -7584.961239 Hartree
 Number of imaginary frequencies = 0.

Compound I3b isomer 27

Atomic N.	X	Y	Z
8	0.92619054	-3.24933416	-0.70970349
8	0.77427198	0.12286866	-0.07322148
6	1.84152253	0.60545221	-0.87344156
1	1.98280701	1.68917952	-0.71865878
1	1.68862417	0.44260801	-1.95964598
1	2.79021403	0.10284880	-0.60461038
8	3.10456934	-3.44581402	-1.01934852
6	2.02595879	-3.35329575	-0.18844733
6	2.24431461	-3.37066868	1.31085635
1	2.79296394	-4.28472542	1.59593779
1	1.24546136	-3.42986897	1.75701530
6	2.98392017	-2.12605317	1.84702676
1	2.55038336	-1.22676930	1.38223520
1	2.76059444	-2.04697708	2.92102645
6	4.50409321	-2.17235542	1.66228698
1	4.90854103	-3.01359348	2.25299730
1	4.94782280	-1.25841362	2.08727941
6	4.97393193	-2.33025732	0.21188964
1	4.69127643	-1.45283031	-0.39207286
1	6.07522993	-2.37911985	0.19293876
6	4.45247278	-3.58047766	-0.49020227
1	4.50710608	-4.46432439	0.16622733
1	5.04634500	-3.79020921	-1.38859566
50	-0.80181419	-0.80902092	-1.05163505
7	-3.50478109	0.08905885	-1.45976847
6	-4.10578111	-0.95679181	-2.29591360
1	-5.20618662	-0.84587217	-2.37452133
1	-3.88760788	-1.94788160	-1.87952694
1	-3.66934459	-0.91675659	-3.30278740
7	-1.90433951	-1.07513573	0.78185746
6	-3.96801250	-0.00318221	-0.06413501
1	-5.07718156	-0.06820505	-0.02803892
1	-3.66141567	0.91378292	0.45785377
6	-3.35921664	-1.19354674	0.67826113
1	-3.79826060	-1.19765633	1.69088804
1	-3.70861188	-2.13369500	0.20395403
6	-1.35253221	-1.65784362	1.96175446
6	-1.43255129	-3.05283418	2.21120568
6	-0.91843112	-3.57517636	3.40826720
6	-0.31257061	-2.76595768	4.37299122
6	-0.23757955	-1.39157233	4.11305606
6	-0.74505115	-0.82432248	2.93839610
7	-1.41370340	2.17198405	-2.12511721
6	-3.76386594	1.41847009	-2.04148121
1	-4.78837316	1.76472854	-1.79144792
1	-3.73156461	1.31299434	-3.13819317
6	-2.76562152	2.49764790	-1.63106137
1	-3.12402553	3.45993996	-2.04230681
1	-2.74709759	2.60512516	-0.53816792
6	-0.47975203	3.23248816	-2.29241777

6	-0.05187682	4.01031973	-1.19255787
6	0.88478357	5.02946423	-1.40838839
6	1.43625817	5.29105687	-2.66631813
6	1.03214825	4.47857545	-3.73206289
6	0.08589690	3.46189257	-3.57110901
6	-2.02535214	-4.00229908	1.19972157
1	-0.98441613	-4.65326872	3.57963833
6	0.25707310	-3.34974321	5.64431162
1	0.21586853	-0.73131534	4.85766376
6	-0.66558276	0.66629893	2.73825495
6	-0.51573621	3.71560411	0.21204640
1	1.21447641	5.61831869	-0.54860753
6	2.42625658	6.41237241	-2.87055814
1	1.46157977	4.64168268	-4.72374696
6	-0.30878211	2.61338540	-4.75777633
1	-1.67700648	-5.02733473	1.38306858
1	-1.73653376	-3.71885632	0.17773867
1	-3.12595310	-4.01869656	1.24139301
1	0.00579187	0.90229053	1.89942439
1	-0.29595992	1.15919906	3.64758053
1	-1.65131519	1.08360991	2.48554199
1	-0.08471135	-4.38200509	5.79788006
1	-0.03650424	-2.75898651	6.52431327
1	1.35858869	-3.36436529	5.62146545
1	0.18563603	4.14180951	0.94093347
1	-0.57078706	2.63107874	0.38283266
1	-1.50772763	4.14315454	0.42778391
1	-1.39034245	2.66522410	-4.96557527
1	-0.05265263	1.55047911	-4.61322713
1	0.21333183	2.95143165	-5.66136002
1	3.17357236	6.15470560	-3.63382002
1	2.95673223	6.65126443	-1.93883377
1	1.92302673	7.33331757	-3.20605324
1	-1.50312295	1.66169650	-3.00333192

Energy = -7584.961372 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 28

Atomic N.	X	Y	Z
8	0.68781519	-2.41796689	-0.48469501
8	1.08261611	-0.37871051	0.32704294
6	1.91935060	0.75026877	0.63149278
1	1.24607318	1.60922071	0.73363756
1	2.64434520	0.93890763	-0.17008528
1	2.44483012	0.58646802	1.58492497
8	2.62670706	-1.26944536	-1.09899001
6	1.72064839	-1.66809623	-0.04762320
6	2.42653639	-2.32392184	1.16448062
1	2.22272353	-3.40249180	1.08844383
1	1.88552826	-1.98291536	2.05920136
6	3.93815626	-2.10490910	1.33100730
1	4.19474199	-1.03852615	1.23244469
1	4.20046283	-2.39002962	2.36289126
6	4.80428168	-2.93411423	0.36871454
1	4.47613932	-3.98708938	0.42074370
1	5.84872302	-2.91973534	0.72007332
6	4.77215046	-2.46466592	-1.09020108

1	5.25714320	-1.47801003	-1.17476193
1	5.35962592	-3.15943108	-1.71492010
6	3.37152154	-2.35146014	-1.68659141
1	2.80447455	-3.29253153	-1.58856528
1	3.43819654	-2.11965195	-2.76071151
50	-0.71431156	-1.02494893	-1.33596146
7	-3.24415252	0.65568020	-1.69941512
6	-3.98084316	-0.11923208	-2.69895292
1	-5.06524672	0.11988593	-2.70598572
1	-3.86639827	-1.19466897	-2.51194965
1	-3.57138737	0.09194830	-3.69602277
7	-2.14275700	-1.52159117	0.13907732
6	-3.71853018	0.39533799	-0.33511261
1	-4.79738902	0.65452849	-0.23342884
1	-3.15002479	1.04367400	0.34596532
6	-3.53231578	-1.04902211	0.13136713
1	-3.93538745	-1.09246195	1.15710585
1	-4.18556374	-1.72250450	-0.45958274
6	-1.86715916	-2.43293378	1.20866748
6	-1.82213941	-3.82895063	0.98015129
6	-1.57896570	-4.69387143	2.05317159
6	-1.36452264	-4.22305401	3.35400078
6	-1.39634300	-2.84094762	3.56071327
6	-1.64466721	-1.93953521	2.51642795
7	-0.99952490	2.59305773	-1.28474800
6	-3.30546252	2.08347277	-2.04724311
1	-4.34793342	2.46662412	-1.96917114
1	-3.01553720	2.16976781	-3.10709394
6	-2.41043743	3.00385654	-1.21864287
1	-2.54540920	4.02558192	-1.61794369
1	-2.75931797	3.03051480	-0.17579180
6	0.02200374	3.56827429	-1.21974413
6	0.12188791	4.45080384	-0.11737268
6	1.16486626	5.38599232	-0.08612263
6	2.13416796	5.46489415	-1.09052531
6	2.04569937	4.54941181	-2.14628073
6	1.01382545	3.61039519	-2.23315063
6	-2.00207859	-4.40199474	-0.40357514
1	-1.55157152	-5.77024163	1.86344003
6	-1.11756512	-5.18118574	4.49502615
1	-1.21487963	-2.44593332	4.56393486
6	-1.64677414	-0.45777279	2.79827308
6	-0.81214605	4.35043424	1.06493301
1	1.23196949	6.05751520	0.77382808
6	3.23005404	6.50227029	-1.04419419
1	2.80088385	4.56846293	-2.93613965
6	0.97320062	2.64498405	-3.39342573
1	-2.25020640	-5.47046776	-0.35151430
1	-1.07060621	-4.30332473	-0.98275016
1	-2.79358481	-3.88608831	-0.96395011
1	-1.08249354	0.08605640	2.02847023
1	-1.20238451	-0.24959154	3.78046178
1	-2.66709440	-0.04084636	2.80545996
1	-2.02891258	-5.74559549	4.74727092
1	-0.79523193	-4.64874549	5.39967349
1	-0.34313846	-5.91912839	4.23945823
1	-0.38359480	4.86879458	1.93239379
1	-0.98238660	3.29874579	1.34152714

1	-1.79886287	4.79827720	0.87089036
1	0.02805573	2.71268900	-3.95687338
1	1.08021941	1.59680265	-3.06747859
1	1.79091149	2.85273225	-4.09455526
1	4.16622372	6.11757938	-1.47207330
1	3.43212053	6.82458475	-0.01359833
1	2.95484827	7.40077330	-1.61952618
1	-0.85848969	1.95907179	-2.06974636

Energy = -7584.950300 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 29

Atomic N.	X	Y	Z
8	0.82912769	0.51749332	-0.05087054
8	2.76490603	1.17128697	1.09258054
6	2.86194329	2.55304331	0.70518726
1	3.08369373	3.10301783	1.62858457
1	1.91925801	2.92201688	0.27425376
1	3.67293457	2.70400837	-0.02069376
8	2.85504884	0.63418946	-1.12152091
6	2.19468044	0.30279461	0.10086515
6	2.51049222	-1.12862207	0.58819230
1	1.76641382	-1.80591418	0.14503964
1	2.32893347	-1.11904776	1.67474198
6	3.92605496	-1.64059232	0.28524821
1	4.65523300	-0.82979640	0.43707529
1	4.17870418	-2.42739302	1.01433927
6	4.06259473	-2.23635849	-1.12644034
1	3.28581139	-3.01175186	-1.24748735
1	5.03221656	-2.75366085	-1.21222133
6	3.94132228	-1.22449564	-2.27379042
1	4.83260037	-0.57626732	-2.29788315
1	3.91470230	-1.76218252	-3.23757809
6	2.71700472	-0.31209282	-2.19063407
1	1.78197496	-0.88633486	-2.08140638
1	2.63112506	0.28283575	-3.11344369
50	-0.35410376	0.71377556	1.67290942
7	-3.02585159	0.17527079	2.30477819
6	-3.21396404	0.76260831	3.63758056
1	-4.27594263	0.74278844	3.95271107
1	-2.87068142	1.80418538	3.64416173
1	-2.61338745	0.20664247	4.36981972
7	-1.60795517	2.08931908	0.60632266
6	-3.70196735	0.96679164	1.26181251
1	-4.76333699	1.14896759	1.53275191
1	-3.68028007	0.38623959	0.32957485
6	-2.99640891	2.29636902	1.00277554
1	-3.54600772	2.79813977	0.18558224
1	-3.11783431	2.95843061	1.88625139
6	-1.03382975	3.20255270	-0.08932358
6	-0.68622939	4.39882127	0.58741275
6	-0.13147655	5.46665866	-0.13423158
6	0.09045754	5.39526492	-1.51115090
6	-0.26848275	4.21200283	-2.16826514
6	-0.82178354	3.12164830	-1.48906610
7	-1.44347679	-2.10000107	1.15454380
6	-3.45134206	-1.23441085	2.31020887

1	-4.55837486	-1.31453190	2.32639962
1	-3.09280898	-1.67933554	3.25294392
6	-2.92021264	-2.06773927	1.14711986
1	-3.34766372	-3.08352976	1.24230715
1	-3.26971497	-1.66779424	0.18744682
6	-0.80781412	-3.08587562	0.33580276
6	-0.89600990	-3.02837575	-1.07208623
6	-0.23010248	-4.00137439	-1.82960520
6	0.53772237	-5.01333809	-1.24605646
6	0.63004556	-5.03488009	0.15065328
6	-0.02821082	-4.09568754	0.95031645
6	-0.88628401	4.56165779	2.07533409
1	0.14250709	6.37779549	0.40448701
6	0.72077433	6.54154617	-2.26510379
1	-0.10964985	4.13105873	-3.24684030
6	-1.17817612	1.87266378	-2.25099289
6	-1.63894652	-1.92320508	-1.77893762
1	-0.29889295	-3.94466132	-2.91875417
6	1.28273638	-6.01800733	-2.09108347
1	1.23085543	-5.80758788	0.63630574
6	0.11628248	-4.16267846	2.45329925
1	-0.18990052	5.30745997	2.48078815
1	-0.72765344	3.61473700	2.61237098
1	-1.90601224	4.90365377	2.31503091
1	-0.50065713	1.05639327	-1.96315858
1	-1.09304275	2.04191266	-3.33275315
1	-2.20229308	1.54149644	-2.02637169
1	0.20425805	6.72793556	-3.21769827
1	1.77360511	6.32600701	-2.50613979
1	0.69849497	7.46829018	-1.67641430
1	-1.25454723	-1.79731424	-2.79914919
1	-1.51791546	-0.96734336	-1.25185876
1	-2.71746686	-2.13278782	-1.86355028
1	-0.85614705	-4.25698861	2.96352584
1	0.61883026	-3.27011914	2.86185360
1	0.72086818	-5.03129072	2.74131468
1	2.32499645	-5.70076663	-2.25437418
1	0.81676940	-6.13531746	-3.07841017
1	1.31583125	-7.00393978	-1.60720196
1	-1.13897155	-2.23637921	2.11994247

Energy = -7584.952252 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 30

Atomic N.	X	Y	Z
8	0.72752202	-0.16444899	0.12739897
8	1.55000547	1.91137926	-0.15268522
6	2.54135289	2.83906008	-0.59056414
1	2.09678345	3.83538081	-0.47057163
1	2.79911191	2.68361531	-1.64884810
1	3.45706259	2.78545515	0.02427530
8	1.85202350	0.38004864	-1.81168032
6	1.80446689	0.51307939	-0.37892420
6	3.12463479	0.03642450	0.30507328
1	2.93342401	-0.98876586	0.65616717
1	3.23883035	0.65501983	1.20998775
6	4.42774355	0.03663379	-0.51186547

1	4.54059239	0.97313204	-1.07844427
1	5.26989674	0.00269316	0.19910149
6	4.55807789	-1.15990901	-1.46748736
1	4.38104508	-2.08650744	-0.89372803
1	5.59473751	-1.21684943	-1.83779185
6	3.60487944	-1.12107186	-2.66685846
1	3.88497259	-0.29493207	-3.34159220
1	3.70674571	-2.05317832	-3.24930164
6	2.13356778	-0.94561352	-2.29437632
1	1.80633485	-1.69609369	-1.55603441
1	1.50840247	-1.07638431	-3.19234589
50	-0.26810746	0.47406547	1.88445430
7	-2.88270377	0.40632874	2.66176416
6	-3.27829119	1.51526891	3.53456599
1	-4.27939158	1.35033709	3.98041987
1	-3.29503687	2.45952406	2.97825926
1	-2.54388209	1.61808800	4.34452400
7	-2.02398974	1.34502481	-0.02029785
6	-3.72867314	0.30341427	1.46541369
1	-4.80657915	0.34454966	1.72728697
1	-3.54593639	-0.67874921	1.00798442
6	-3.43388325	1.39199592	0.43412566
1	-4.13117760	1.26739483	-0.41425250
1	-3.62518754	2.38819790	0.85047996
6	-1.66868563	2.39262440	-0.94974270
6	-1.50406836	3.71977675	-0.50726061
6	-1.16623433	4.70470605	-1.44595631
6	-0.96938476	4.41200759	-2.79795801
6	-1.10861710	3.07971114	-3.20449056
6	-1.45546604	2.06571688	-2.30754211
7	-0.94598248	-1.57558674	1.97053991
6	-2.80705084	-0.84950943	3.42893623
1	-3.80897648	-1.16256063	3.79065250
1	-2.18636056	-0.63473674	4.31305705
6	-2.16975149	-1.99023245	2.63850072
1	-1.97713393	-2.80426116	3.36490241
1	-2.91744643	-2.41272184	1.93149795
6	-0.17325269	-2.66118877	1.46508528
6	-0.56033641	-3.36703189	0.29920789
6	0.22218535	-4.43397250	-0.16236378
6	1.39106332	-4.83518865	0.49052786
6	1.76146752	-4.13617684	1.64533952
6	1.00654275	-3.06648096	2.14089084
6	-1.63968866	4.11036399	0.94414226
1	-1.03154338	5.73142602	-1.09633252
6	-0.62326434	5.49496905	-3.79102111
1	-0.93400860	2.81622348	-4.25024536
6	-1.56313357	0.63888595	-2.78932195
6	-1.78754022	-2.96848594	-0.48017928
1	-0.08648581	-4.95588401	-1.07251615
6	2.24387597	-5.95954158	-0.04700908
1	2.66556081	-4.43532013	2.18284868
6	1.46618743	-2.35954721	3.39299642
1	-1.04765685	5.01102617	1.15226427
1	-1.28531749	3.31083500	1.61068753
1	-2.68260527	4.34268210	1.21702839
1	-0.80581515	0.00259145	-2.30443552
1	-1.39178192	0.58747532	-3.87151920

1	-2.55696568	0.20395239	-2.59348409
1	-1.50776695	5.79774290	-4.37347326
1	0.13500402	5.15293515	-4.50921137
1	-0.23832548	6.39116654	-3.28658566
1	-1.70367153	-3.27991914	-1.52972635
1	-1.91887806	-1.87826227	-0.44567367
1	-2.70508360	-3.42442321	-0.07413561
1	0.63280624	-2.16997860	4.08312794
1	1.91346977	-1.37751989	3.16640927
1	2.23025690	-2.95237317	3.91360269
1	3.07326077	-5.57143988	-0.65999103
1	1.65846529	-6.63942267	-0.68066583
1	2.69148913	-6.54840097	0.76600527
1	-1.86272925	0.44974104	-0.49104212

Energy = -7584.954616 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 31

Atomic N.	X	Y	Z
8	0.67353839	-0.31907706	0.15461842
8	1.77475727	1.56622615	0.69961164
6	2.92971071	2.40318282	0.72527988
1	2.59469502	3.36846680	1.12614598
1	3.34017866	2.55425209	-0.28431202
1	3.71648960	2.00095114	1.38749955
8	2.16352018	0.61953960	-1.33534569
6	1.89347955	0.29240793	0.04038622
6	3.01357273	-0.59464383	0.66998458
1	2.64523622	-1.63046093	0.62250599
1	3.04667018	-0.32900212	1.73904151
6	4.42625111	-0.55150077	0.06328711
1	4.74384702	0.48416139	-0.12974046
1	5.12650160	-0.95422372	0.81383485
6	4.57193103	-1.38082697	-1.22236295
1	4.19285721	-2.39914135	-1.02625416
1	5.64177406	-1.48875583	-1.46483774
6	3.84424265	-0.79900526	-2.43907192
1	4.32889023	0.14102628	-2.75159538
1	3.93128361	-1.49739034	-3.28943245
6	2.36262970	-0.50880454	-2.20534803
1	1.83004858	-1.39038616	-1.81211194
1	1.88533997	-0.23792032	-3.16089495
50	-0.52067553	-0.11296814	1.89149169
7	-3.21763724	0.02240072	2.28777029
6	-3.61446168	0.84584799	3.43329649
1	-4.68829690	0.72077213	3.67710836
1	-3.42303369	1.90639321	3.23321246
1	-3.01790453	0.55863946	4.30943034
7	-1.81539926	1.60299780	0.20269089
6	-3.85862256	0.45144878	1.03784599
1	-4.95173987	0.59132485	1.17088022
1	-3.72446323	-0.35034469	0.29868913
6	-3.26465610	1.74395287	0.47898660
1	-3.82066093	2.01643451	-0.43648030
1	-3.39868219	2.57317138	1.18376880
6	-1.18303868	2.81328122	-0.26904126
6	-0.93560969	3.88432930	0.61125470

6	-0.32535507	5.04199196	0.10766451
6	0.06326084	5.16039532	-1.22892743
6	-0.16724912	4.06879755	-2.07502813
6	-0.78351753	2.89967765	-1.62173852
7	-1.44802632	-1.93500740	1.19282799
6	-3.42272107	-1.40605111	2.58560653
1	-4.50108567	-1.64367392	2.70131207
1	-2.93513621	-1.59271698	3.55540005
6	-2.80704333	-2.32602010	1.53356075
1	-2.83844099	-3.34952284	1.95652465
1	-3.47289188	-2.36699152	0.64342040
6	-0.74278704	-2.91639867	0.43738437
6	-1.01705718	-3.13284191	-0.93565565
6	-0.30826832	-4.11328101	-1.64271694
6	0.67789348	-4.89809891	-1.03843111
6	0.93720503	-4.68125897	0.31997754
6	0.25006702	-3.71381854	1.06274698
6	-1.26641298	3.81501718	2.08208051
1	-0.12864021	5.86735601	0.79654458
6	0.71091138	6.42093577	-1.74905673
1	0.14934186	4.12242009	-3.11929948
6	-0.98216885	1.73837270	-2.56586984
6	-2.03980074	-2.30027704	-1.66575782
1	-0.52538523	-4.25404979	-2.70530910
6	1.46093252	-5.91977510	-1.82799645
1	1.69627139	-5.28799565	0.82144520
6	0.58147519	-3.53589664	2.52466788
1	-0.61117456	4.48745493	2.65083158
1	-1.13199811	2.79770683	2.47719165
1	-2.30350098	4.12632788	2.29104670
1	-0.40284047	0.86120149	-2.23655139
1	-0.63627073	2.00171429	-3.57292974
1	-2.04070832	1.44216730	-2.64955970
1	0.01465287	6.99554179	-2.37977039
1	1.59162682	6.19268493	-2.36614023
1	1.02991210	7.07444484	-0.92649530
1	-1.81934743	-2.26240530	-2.74073920
1	-2.04341030	-1.27514183	-1.27072163
1	-3.06050782	-2.70057791	-1.55344920
1	-0.32419335	-3.43974878	3.13892280
1	1.17581300	-2.62390051	2.70007135
1	1.17210116	-4.38512891	2.89375225
1	2.41633171	-5.50088213	-2.18298500
1	0.90299712	-6.25746268	-2.71184487
1	1.70193752	-6.80104495	-1.21701936
1	-1.68935439	0.88900424	-0.52077954

Energy = -7584.954605 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 32

Atomic N.	X	Y	Z
8	0.78551183	-0.34920432	0.39943637
8	2.73829018	-1.42180853	1.09419502
6	3.03891843	-2.30179180	-0.00345469
1	4.11536533	-2.19012677	-0.18143872
1	2.48805521	-2.02287167	-0.91440168
1	2.80845900	-3.34456477	0.25250240

8	0.72134055	-2.48817161	1.24470022
6	1.33674001	-1.21405619	1.35944114
6	1.28635352	-0.60799069	2.77564941
1	0.31205191	-0.11152406	2.90114454
1	2.04444882	0.19151705	2.77536150
6	1.55164909	-1.58407686	3.93135909
1	2.35666719	-2.27930033	3.64641828
1	1.92897399	-1.00998639	4.79253683
6	0.30241997	-2.35723384	4.37995467
1	-0.48235304	-1.62696231	4.64422090
1	0.52972442	-2.91367476	5.30359746
6	-0.25883419	-3.33080560	3.33700696
1	0.42894085	-4.18125875	3.20035887
1	-1.21256429	-3.74847329	3.70188789
6	-0.50570217	-2.70813003	1.96353077
1	-1.08696766	-1.77609242	2.04553688
1	-1.08489330	-3.40208636	1.33622783
50	2.04325297	1.28033173	-0.08445656
7	0.34767775	3.16008075	-0.35257944
6	1.28205088	4.31088693	-0.35080504
1	0.76359200	5.23507123	-0.66206473
1	2.12143856	4.12890314	-1.03247348
1	1.68577602	4.44711546	0.66052531
7	1.48005328	1.25962034	-2.16087488
6	-0.21026712	2.94673793	-1.71428145
1	-0.68582464	3.87700623	-2.08106623
1	-0.97486095	2.16448831	-1.63886967
6	0.85905926	2.46305089	-2.69096237
1	0.34825637	2.24185288	-3.64673461
1	1.56385066	3.29264142	-2.92117708
6	2.21590486	0.46366780	-3.09154438
6	3.46651391	0.86988436	-3.62274561
6	4.14396895	0.03072181	-4.51958957
6	3.62638200	-1.20596152	-4.91381094
6	2.38537282	-1.59105385	-4.39130053
6	1.67360091	-0.78421556	-3.49644547
7	-1.70341550	1.23193656	1.27953290
6	-0.70488474	3.46104603	0.66882329
1	-1.06323895	4.49231279	0.48081049
1	-0.20675007	3.45351884	1.64980540
6	-1.94174229	2.56890362	0.73489949
1	-2.63112465	3.09111976	1.41508321
1	-2.45921466	2.55386259	-0.24561416
6	-2.88590977	0.49650415	1.60141109
6	-3.36355187	-0.53320967	0.75516568
6	-4.49536784	-1.26255290	1.13812407
6	-5.18776222	-0.99238480	2.32481795
6	-4.70031226	0.02890429	3.14681635
6	-3.56062762	0.77226613	2.81349802
6	4.09526436	2.18999457	-3.24687382
1	5.11090161	0.35517830	-4.91364999
6	4.39031263	-2.11174966	-5.84960717
1	1.95238740	-2.54835640	-4.69361307
6	0.32950890	-1.23562176	-2.98281906
6	-2.66925890	-0.85097539	-0.54725008
1	-4.85129732	-2.06018116	0.48097525
6	-6.43082184	-1.76591429	2.69412619
1	-5.20612152	0.24171067	4.09219024

6	-3.04504740	1.81942115	3.76915325
1	5.17677721	2.17330268	-3.43465241
1	3.93519376	2.42569208	-2.18401525
1	3.67355333	3.02332114	-3.83138628
1	0.31239100	-1.27351864	-1.88471832
1	0.07830428	-2.22820197	-3.37978591
1	-0.46507203	-0.53518255	-3.28196084
1	3.71577159	-2.62846298	-6.54677430
1	4.93594579	-2.88920234	-5.29161529
1	5.12819541	-1.54999325	-6.43787175
1	-3.20447989	-1.64362500	-1.08522347
1	-1.63090393	-1.18315577	-0.39828171
1	-2.62507000	0.02912437	-1.20735159
1	-3.39691853	2.83117093	3.50831648
1	-1.94647223	1.84606287	3.75689503
1	-3.38917810	1.61403642	4.79126568
1	-6.59730474	-1.76106100	3.77984661
1	-6.36774976	-2.81090334	2.36073383
1	-7.32548205	-1.32787616	2.22357724
1	-1.05782073	0.68058310	0.70268152

Energy = -7584.952871 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 33

Atomic N.	X	Y	Z
8	0.74111380	-0.18554364	0.57472490
8	1.98078938	0.52818834	2.42810225
6	3.32685661	0.30998377	1.97053835
1	3.88097773	1.21739844	2.24240684
1	3.36813848	0.16612370	0.88065885
1	3.77620212	-0.56170491	2.46619486
8	1.60067620	-1.69291855	2.07580360
6	1.00951796	-0.40159917	1.92136269
6	-0.24027332	-0.20106805	2.80703042
1	-1.11502165	-0.54367912	2.23579815
1	-0.34410136	0.88889522	2.92936008
6	-0.20674670	-0.89413276	4.17658145
1	0.80199270	-0.81253860	4.61009168
1	-0.88393294	-0.35649456	4.85989281
6	-0.65541564	-2.36437010	4.11828095
1	-1.64996630	-2.40012729	3.63974679
1	-0.79162043	-2.74593815	5.14344301
6	0.29503818	-3.30457465	3.36486455
1	1.21763900	-3.45279582	3.94963033
1	-0.17631070	-4.29732064	3.25983041
6	0.70962253	-2.81254960	1.97751549
1	-0.16304873	-2.56005017	1.35247005
1	1.27122747	-3.60205304	1.45388104
50	0.45908167	1.78932069	-0.08461394
7	-0.96990513	2.98108780	-2.16423959
6	-0.53166670	4.38276987	-2.15562618
1	-0.92411841	4.94447349	-3.02618215
1	0.56350883	4.43707016	-2.17396748
1	-0.87655221	4.86744603	-1.23252963
7	1.37838273	1.25674030	-1.94948198
6	-0.41795127	2.24575177	-3.31576349
1	-0.62091708	2.78831107	-4.26308968

1	-0.91910427	1.26955880	-3.36497588
6	1.08178152	1.99647112	-3.17085725
1	1.39605887	1.40529281	-4.05056885
1	1.62787313	2.95986550	-3.25682578
6	2.65695618	0.61008482	-1.96215216
6	3.86102633	1.34754844	-1.83115269
6	5.09143814	0.67382787	-1.85078074
6	5.17567591	-0.71238177	-1.99975397
6	3.97954718	-1.42604650	-2.14153288
6	2.73041215	-0.79643271	-2.12529700
7	-2.52015240	1.17826500	-0.33597070
6	-2.43917416	2.91208421	-2.09862177
1	-2.89372238	3.19846009	-3.07002540
1	-2.76785068	3.66723925	-1.36583903
6	-2.99881942	1.55466993	-1.68160245
1	-4.10232854	1.62499730	-1.71393496
1	-2.71241208	0.77573094	-2.39867091
6	-3.18669141	0.08963552	0.31088479
6	-3.08578835	-1.22559283	-0.19191148
6	-3.73323382	-2.26130620	0.49524069
6	-4.45596534	-2.04607036	1.67231074
6	-4.52140165	-0.73698191	2.16417678
6	-3.90524795	0.33199586	1.50662002
6	3.86465410	2.84819721	-1.66040032
1	6.01004395	1.25562536	-1.73598679
6	6.50724610	-1.42377672	-1.97786365
1	4.01703487	-2.51152828	-2.26549736
6	1.47909879	-1.62079461	-2.27384435
6	-2.26173949	-1.55059312	-1.41177854
1	-3.64404357	-3.27706601	0.10222933
6	-5.10170186	-3.19008224	2.41580084
1	-5.07066238	-0.53808297	3.08758107
6	-4.00070232	1.72280577	2.09055657
1	4.77698221	3.17752390	-1.14586466
1	2.99757503	3.19277814	-1.07762995
1	3.83145851	3.36919055	-2.63081410
1	0.92229285	-1.62460108	-1.32612740
1	1.72753389	-2.65544938	-2.54568452
1	0.81160586	-1.20582373	-3.04270008
1	6.54291809	-2.23252220	-2.72159187
1	6.69511074	-1.88163232	-0.99377662
1	7.33481836	-0.73168974	-2.18345641
1	-1.95204196	-2.60329106	-1.39347465
1	-1.35483915	-0.93252898	-1.45084232
1	-2.82259381	-1.39507435	-2.34757290
1	-4.44403852	2.44379340	1.38457798
1	-3.01447157	2.11585189	2.38890650
1	-4.62940360	1.71827064	2.98927970
1	-4.44609654	-3.55740319	3.22130418
1	-5.30725904	-4.03692008	1.74776963
1	-6.04782551	-2.88284483	2.88251906
1	-2.59304781	2.00265105	0.26290710

Energy = -7584.952260 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 34

Atomic N. X Y Z

8	-0.93695273	0.70371514	2.39294703
8	1.09664770	0.48757370	1.28383340
6	2.02347530	1.40028516	1.88193930
1	2.47482604	1.95658091	1.05037618
1	2.81477556	0.86593478	2.42959861
1	1.52506020	2.11526314	2.55850768
8	-0.23241359	-1.26023167	1.34816047
6	0.10190435	-0.14731938	2.19079198
6	0.71163256	-0.57942021	3.53728271
1	-0.13635792	-0.76437521	4.21298777
1	1.22654845	0.29340294	3.96071974
6	1.63510429	-1.80607284	3.50065516
1	2.24339303	-1.79368076	2.58206624
1	2.34097698	-1.74199316	4.34403002
6	0.86937974	-3.13424249	3.61142667
1	0.25475731	-3.10023777	4.52799921
1	1.58566341	-3.95955648	3.75304322
6	-0.03197809	-3.45833519	2.41353613
1	0.58703648	-3.72679222	1.54168240
1	-0.64778769	-4.34371232	2.64736979
6	-0.96367702	-2.32563354	1.97999293
1	-1.56943454	-1.93885854	2.81589432
1	-1.66862864	-2.69604754	1.22288817
50	-1.11012024	2.18637341	0.86260368
7	-0.81694825	2.60633533	-1.85716693
6	-0.08982463	3.85351866	-2.11233019
1	-0.25188586	4.23036647	-3.14174130
1	0.98198964	3.70009599	-1.94665761
1	-0.43675579	4.61712168	-1.40278087
7	1.81220550	1.06241708	-1.70838358
6	-0.41878420	1.50756748	-2.75950506
1	-0.85784469	1.67046908	-3.76743448
1	-0.86052241	0.58212179	-2.36164705
6	1.08275649	1.30269724	-2.96124552
1	1.18215325	0.45511776	-3.66942621
1	1.51814362	2.17506968	-3.47095272
6	3.14991410	0.58220339	-1.85776328
6	4.18645751	1.47501157	-2.21099521
6	5.49586560	0.99048094	-2.33178930
6	5.81778633	-0.34947682	-2.09622886
6	4.78013722	-1.21375145	-1.72563049
6	3.45502382	-0.77907388	-1.61151584
7	-2.70136036	1.18711180	-0.13006637
6	-2.27082726	2.84646065	-1.93020619
1	-2.57412457	3.10544628	-2.96616495
1	-2.48102270	3.72580672	-1.29850171
6	-3.11894856	1.67047132	-1.44592105
1	-4.16676549	2.02731240	-1.42133530
1	-3.09954672	0.86561493	-2.20443443
6	-3.55099510	0.18294412	0.41746071
6	-3.62663110	-1.11104869	-0.15840480
6	-4.52569712	-2.05049028	0.36483102
6	-5.34750171	-1.76762301	1.45883607
6	-5.24083400	-0.49795575	2.03717227
6	-4.36272705	0.47406072	1.54456383
6	3.91696542	2.94532434	-2.40961822
1	6.29027122	1.69287238	-2.59714081
6	7.23221261	-0.85397999	-2.25391091

1	5.00439760	-2.26539287	-1.52903212
6	2.37074231	-1.75976700	-1.23239342
6	-2.70977950	-1.52981110	-1.28052142
1	-4.56767333	-3.04315271	-0.09210843
6	-6.28739509	-2.80519427	2.02451498
1	-5.86593450	-0.25027979	2.89916108
6	-4.29714605	1.81335733	2.23613301
1	4.84500493	3.52493733	-2.32107930
1	3.19928397	3.31037213	-1.66072345
1	3.49124243	3.16346816	-3.40240457
1	1.89307530	-1.50860483	-0.27242841
1	2.78572668	-2.77204394	-1.14516295
1	1.56916414	-1.79133911	-1.98720921
1	7.37892463	-1.32539709	-3.23878197
1	7.47682450	-1.60941869	-1.49420493
1	7.96012177	-0.03570980	-2.17065106
1	-2.64046188	-2.62462516	-1.33119608
1	-1.70068992	-1.12576201	-1.11564068
1	-3.05617710	-1.18389542	-2.26758215
1	-4.26442660	2.64566042	1.51878981
1	-3.39869096	1.88697002	2.87113853
1	-5.16596772	1.95306924	2.89294810
1	-5.84888843	-3.30212631	2.90458745
1	-6.51445485	-3.58511589	1.28539611
1	-7.23564362	-2.35344867	2.34855273
1	1.28265559	0.43001023	-1.10439914

Energy = -7584.947154 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 35

Atomic N.	X	Y	Z
8	2.34425595	1.46396840	0.33031818
8	2.28965321	0.74217459	-1.77786130
6	2.86526855	0.20384405	-2.97585615
1	2.01998191	-0.11950648	-3.59521499
1	3.52083438	-0.65045971	-2.75900836
1	3.42645584	0.97977568	-3.52032146
8	3.96155897	-0.03859452	-0.44268810
6	3.18205347	1.15496258	-0.69083568
6	4.05034622	2.37935154	-1.08734836
1	4.08635649	3.03151389	-0.20162919
1	3.47669841	2.93226035	-1.84599256
6	5.48274385	2.12828608	-1.58438688
1	5.49812323	1.34382889	-2.35669130
1	5.82641557	3.05192085	-2.07819915
6	6.48519029	1.77612720	-0.47344023
1	6.39624399	2.52672174	0.33171405
1	7.50917804	1.87067706	-0.86957382
6	6.31712883	0.37340939	0.12057585
1	6.57432158	-0.38640081	-0.63604886
1	7.02589308	0.23830309	0.95581175
6	4.91055396	0.06970042	0.63045525
1	4.56894381	0.82422139	1.35979146
1	4.89996962	-0.90693481	1.13928398
50	0.71733772	0.02917367	0.22114662
7	-0.16779461	1.24259474	2.25837602
6	0.83830384	2.24597711	2.68399528

1	0.42967743	2.87455730	3.49555198
1	1.13621880	2.86887060	1.83684831
1	1.73683769	1.72898810	3.04126156
7	-0.75025662	1.39110105	-0.55332818
6	-1.38551521	1.91612474	1.72841857
1	-1.71113595	2.71108956	2.42725556
1	-2.17464446	1.15977779	1.64696748
6	-1.13562321	2.48254134	0.33040047
1	-2.08082308	2.93821082	-0.01488038
1	-0.40271674	3.31153063	0.39506780
6	-1.03380152	1.49126117	-1.93410496
6	-0.68307471	2.62954625	-2.71114179
6	-1.02386436	2.67623734	-4.06945436
6	-1.67738421	1.62243582	-4.71504984
6	-1.97913949	0.48870063	-3.95216962
6	-1.67783437	0.40314800	-2.58823342
7	-1.56411741	-1.52734645	2.26738036
6	-0.44523533	0.37596376	3.44351049
1	-0.60863242	1.02616708	4.32453176
1	0.47914123	-0.19226972	3.63539036
6	-1.63421693	-0.58159015	3.38547730
1	-1.64734623	-1.09947489	4.36571595
1	-2.57173482	-0.01103118	3.33374819
6	-2.40061382	-2.67645839	2.30288296
6	-3.80748749	-2.55430557	2.23535271
6	-4.59260470	-3.71479810	2.25325773
6	-4.03600469	-4.99594013	2.30719519
6	-2.63955091	-5.09563151	2.32766329
6	-1.81484387	-3.96670819	2.33147331
6	0.12802037	3.76092856	-2.12759384
1	-0.73923160	3.56040470	-4.64726725
6	-2.06073432	1.71133876	-6.17290878
1	-2.48531699	-0.35580969	-4.42813146
6	-2.05800931	-0.84470365	-1.82988194
6	-4.47951724	-1.21307498	2.07374810
1	-5.67867512	-3.60686289	2.19379696
6	-4.90718037	-6.22813468	2.34981577
1	-2.17339980	-6.08395282	2.34763841
6	-0.31338714	-4.13490871	2.35299693
1	0.61072813	4.33542518	-2.92964663
1	0.90706679	3.37196635	-1.45683040
1	-0.48402058	4.46753844	-1.54437641
1	-1.19746967	-1.51966085	-1.68443229
1	-2.82390236	-1.41241160	-2.37508639
1	-2.43022843	-0.60289703	-0.82513444
1	-3.10049801	2.05615096	-6.29358219
1	-1.98472396	0.73406188	-6.67017341
1	-1.41806486	2.42074704	-6.71248141
1	-5.48294335	-1.33773512	1.64682027
1	-3.89833639	-0.56332719	1.40320986
1	-4.59900479	-0.68091129	3.03116101
1	0.14739930	-3.63300271	3.21925006
1	0.16576717	-3.72349992	1.44934028
1	-0.04729209	-5.19777261	2.40744223
1	-4.45202575	-7.06151741	1.79696417
1	-5.89814283	-6.03193545	1.91861569
1	-5.06237384	-6.57105937	3.38526524
1	-0.59419179	-1.80297799	2.10810107

Energy = -7584.957096 Hartree
 Number of imaginary frequencies = 0.

Compound I3b isomer 36

Atomic N.	X	Y	Z
8	1.97676908	0.24967112	1.41594790
8	2.82789511	1.52674266	-0.22856457
6	3.86553790	1.90402804	-1.13681630
1	3.40690865	2.60308515	-1.84826547
1	4.26068044	1.03607674	-1.68350933
1	4.69055366	2.42210113	-0.61830388
8	3.48558121	-0.64743638	-0.12590632
6	3.12809525	0.47120123	0.71994312
6	4.26357193	0.87767504	1.70522055
1	3.98065534	0.47215098	2.68814608
1	4.21008669	1.97285213	1.80183550
6	5.70399566	0.44610343	1.38459506
1	5.95742753	0.66710367	0.33655096
1	6.37841832	1.06345500	2.00068955
6	6.00049417	-1.03234081	1.68192081
1	5.66854315	-1.25807874	2.71061550
1	7.09108600	-1.19065745	1.66868613
6	5.34723263	-2.02126571	0.71078342
1	5.79692618	-1.91472414	-0.29029552
1	5.55359783	-3.05396819	1.04069803
6	3.83628324	-1.85733339	0.56852268
1	3.33011939	-1.88990562	1.54828272
1	3.42629345	-2.67833298	-0.03978155
50	0.26025225	-0.15926920	0.16764956
7	-0.64215324	1.83166786	1.35414848
6	0.23682084	3.01547079	1.24020791
1	-0.11907784	3.82885427	1.89837599
1	0.26642797	3.37327457	0.20605875
1	1.25305216	2.72214834	1.52270336
7	-2.12294458	1.55204496	-1.38728076
6	-2.04989357	2.16986045	1.01573563
1	-2.39638475	2.96375453	1.70548750
1	-2.65581033	1.27507703	1.21992041
6	-2.31650780	2.63635916	-0.41412608
1	-3.35195823	3.03268304	-0.43305694
1	-1.66492775	3.47761786	-0.68183097
6	-2.35922803	1.86825228	-2.75935372
6	-1.42503988	2.64503504	-3.48059107
6	-1.67225035	2.92273721	-4.83112131
6	-2.80016802	2.43762287	-5.50056589
6	-3.69262860	1.63780289	-4.77713614
6	-3.49784676	1.35026858	-3.42208580
7	-0.89886305	-0.91292249	1.81223521
6	-0.57693992	1.31953286	2.75829988
1	-1.02589616	2.06258629	3.44455427
1	0.49141640	1.21793682	2.98910797
6	-1.25649976	-0.03898774	2.91858563
1	-0.93864751	-0.43038210	3.90329835
1	-2.35936216	0.08345232	2.99728420
6	-1.14284166	-2.30196305	1.98040297
6	-2.11505950	-2.95425159	1.17728258
6	-2.33890738	-4.32777585	1.32660691

6	-1.63140829	-5.09716280	2.25730306
6	-0.67338237	-4.44762662	3.04180677
6	-0.41012842	-3.07683098	2.91946872
6	-0.14629465	3.12961615	-2.84445017
1	-0.93950530	3.51754286	-5.38231835
6	-3.05318118	2.77219504	-6.95072637
1	-4.57290571	1.22839834	-5.27903183
6	-4.49197689	0.47697606	-2.69158481
6	-2.92182192	-2.18009363	0.16249157
1	-3.09697638	-4.80901862	0.70248926
6	-1.86823078	-6.58345623	2.38056299
1	-0.09349252	-5.02896909	3.76433960
6	0.68151858	-2.46003717	3.75966123
1	0.61271113	3.32567168	-3.61285593
1	0.25154444	2.38093693	-2.14445719
1	-0.28717863	4.06951645	-2.28563211
1	-4.05529923	-0.49113167	-2.39527632
1	-5.35331634	0.25683487	-3.33430264
1	-4.87496370	0.95578189	-1.77685193
1	-3.72895942	3.63691485	-7.04691928
1	-3.52331647	1.93256377	-7.48100436
1	-2.11992353	3.02693466	-7.47063617
1	-3.76380343	-2.78246962	-0.20441050
1	-2.30952353	-1.89474637	-0.70850876
1	-3.31576669	-1.24934790	0.59603524
1	0.29221888	-2.05001965	4.70609877
1	1.17455079	-1.63679121	3.22304054
1	1.43440999	-3.21464967	4.02499958
1	-1.27308182	-7.14423290	1.64207577
1	-2.92317278	-6.83747081	2.20577319
1	-1.58693520	-6.95303071	3.37594694
1	-2.70729421	0.76051121	-1.11491845

Energy = -7584.959992 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 37

Atomic N.	X	Y	Z
8	0.83968925	0.00217456	-0.48478558
8	0.76473137	1.03662758	-2.45367788
6	1.30897189	1.51902486	-3.69190699
1	0.44741031	1.72460471	-4.33854434
1	1.96390733	0.77169802	-4.15897561
1	1.86088849	2.45747337	-3.52916196
8	2.43851135	-0.47068392	-2.12902726
6	1.67529065	0.52673575	-1.41734672
6	2.55028267	1.65746524	-0.81657525
1	2.64025228	1.44235278	0.25905847
1	1.95298382	2.57825273	-0.88985978
6	3.95418409	1.88316444	-1.40056456
1	3.92162696	1.91619619	-2.50034321
1	4.29081854	2.88053959	-1.07391128
6	4.99954971	0.85135609	-0.94762002
1	4.96645967	0.77798297	0.15382713
1	6.00550069	1.22341847	-1.20018030
6	4.82610946	-0.54580250	-1.55321873
1	5.02732989	-0.51187341	-2.63662386
1	5.57022509	-1.23325767	-1.11565110

6	3.43832802	-1.14970507	-1.35272206
1	3.15152406	-1.15439886	-0.28721416
1	3.42864640	-2.19423656	-1.70012561
50	-0.84916241	-0.78549426	-1.63140999
7	-1.86458255	-1.03048589	0.63121906
6	-1.25427277	-0.15119517	1.65636377
1	-1.91657725	-0.08430391	2.53774832
1	-1.08484805	0.84501458	1.23862279
1	-0.29212411	-0.55755765	1.96635660
7	-2.31131373	0.78766975	-1.49868615
6	-3.23874079	-0.54121856	0.31831659
1	-3.84498567	-0.50525301	1.24281694
1	-3.69298367	-1.26779727	-0.37243384
6	-3.20326015	0.83000102	-0.35223392
1	-4.23999814	1.06162396	-0.66428157
1	-2.94155776	1.60115048	0.40242056
6	-2.37147619	1.86553657	-2.41723881
6	-1.96862364	3.17934716	-2.05754423
6	-2.03952070	4.21206053	-3.00090985
6	-2.48375685	3.99655381	-4.30975852
6	-2.85514094	2.69441828	-4.66223339
6	-2.81185989	1.63412730	-3.74764471
7	0.55658224	-2.94757412	1.74495154
6	-1.91526163	-2.43993373	1.10941209
1	-2.68010020	-2.95620826	0.50875170
1	-2.25734208	-2.45373787	2.16056463
6	-0.62523370	-3.27016573	0.94553420
1	-0.91818528	-4.31613930	1.10813371
1	-0.30870089	-3.20909204	-0.10747907
6	0.56756333	-2.80892187	3.14545930
6	-0.15502179	-3.66038170	4.02103337
6	-0.09457536	-3.42347023	5.40217487
6	0.68471268	-2.41230830	5.96856529
6	1.46488595	-1.64619465	5.09477100
6	1.42888694	-1.82544378	3.71034192
6	-1.40445597	3.46778744	-0.68975450
1	-1.71590438	5.21435114	-2.70586898
6	-2.58352568	5.13338454	-5.29869021
1	-3.20397285	2.49592933	-5.67941031
6	-3.24533356	0.25858059	-4.19472594
6	-0.90770756	-4.88399681	3.54929503
1	-0.66337517	-4.08635516	6.05954348
6	0.69600430	-2.16360025	7.45721691
1	2.13066211	-0.88047344	5.50119310
6	2.35000384	-1.01164619	2.83242601
1	-0.79184464	4.37907060	-0.70720733
1	-0.78123003	2.62812028	-0.34974925
1	-2.19402285	3.62059147	0.06373026
1	-2.38588095	-0.40699996	-4.37829080
1	-3.81775370	0.31810956	-5.13017669
1	-3.85899773	-0.23531768	-3.42905866
1	-3.57562310	5.61111982	-5.25751041
1	-2.43367799	4.78431562	-6.32966915
1	-1.83894327	5.91375411	-5.08868747
1	-1.15773704	-5.51748812	4.41002472
1	-0.29983107	-5.48604418	2.85784560
1	-1.85387028	-4.65047478	3.03556622
1	1.82305079	-0.44114556	2.04891990

1	3.08150387	-1.65549157	2.31513913
1	2.91677616	-0.29315702	3.43742327
1	1.69647364	-1.87540434	7.80955551
1	0.38299268	-3.05740351	8.01392859
1	0.00827945	-1.34821625	7.73359522
1	1.12129407	-2.23563513	1.28684321

Energy = -7584.956043 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 38

Atomic N.	X	Y	Z
8	2.16864467	1.19148246	1.26896444
8	2.16125361	1.89904614	-0.84481403
6	2.77498955	2.25751413	-2.09029881
1	1.96064192	2.30259887	-2.82341817
1	3.51995658	1.51256282	-2.40124772
1	3.24417891	3.25175156	-2.02084913
8	3.92828088	0.63222803	-0.16718680
6	3.01951501	1.64904478	0.31662276
6	3.74238289	2.93860050	0.79119765
1	3.71601684	2.91939446	1.89120266
1	3.10249583	3.78083899	0.48866595
6	5.18799181	3.17832609	0.32820368
1	5.28113944	3.03199647	-0.75901979
1	5.42198967	4.23895518	0.51630897
6	6.23550054	2.31908112	1.05456547
1	6.07169279	2.40984886	2.14292181
1	7.23815385	2.73267261	0.85952393
6	6.23164427	0.83752848	0.66258078
1	6.56057651	0.72851362	-0.38410911
1	6.96258889	0.28907063	1.28154410
6	4.87423750	0.15299191	0.80198057
1	4.46167137	0.26833391	1.81904944
1	4.97822265	-0.92649805	0.61035604
50	0.70764276	-0.03116590	0.22651214
7	-0.27434955	-0.39010170	2.53174841
6	0.62092351	0.24443654	3.52982087
1	0.15905246	0.20828386	4.53284982
1	0.83217508	1.27897333	3.24789315
1	1.57782248	-0.29049094	3.55005215
7	-0.91386440	1.36978274	0.35056460
6	-1.56773806	0.34303576	2.44896174
1	-1.96860505	0.51680856	3.46654477
1	-2.26911026	-0.28298199	1.88529414
6	-1.40494735	1.66053856	1.69028719
1	-2.40064286	2.13596227	1.63736740
1	-0.76875637	2.34937170	2.28135457
6	-1.22891199	2.25525284	-0.70486162
6	-1.01683795	3.65896269	-0.62059050
6	-1.38093107	4.48298473	-1.69372935
6	-1.92478297	3.97560758	-2.87749532
6	-2.08952517	2.58886023	-2.96737524
6	-1.76030768	1.72685336	-1.91518156
7	-1.35204426	-2.72806025	0.79642545
6	-0.43410153	-1.81879178	2.93923265
1	-0.65441384	-1.85274383	4.02364814
1	0.55089942	-2.29282194	2.80052334

6	-1.50956646	-2.65870779	2.25261979
1	-1.44950353	-3.66068053	2.72336326
1	-2.50566449	-2.26790632	2.50246736
6	-2.04620351	-3.75067574	0.09343264
6	-3.45908799	-3.76123297	0.03447551
6	-4.10223834	-4.77632899	-0.68538763
6	-3.39793718	-5.76906019	-1.37367041
6	-1.99970244	-5.71362555	-1.33967128
6	-1.31283629	-4.73141611	-0.61904532
6	-0.32630765	4.27994015	0.56932647
1	-1.20352464	5.55893801	-1.60725528
6	-2.33717665	4.88901078	-4.00703697
1	-2.50746596	2.15909434	-3.88201680
6	-1.99036744	0.24489632	-2.08171657
6	-4.28592015	-2.66969182	0.66818005
1	-5.19440492	-4.76896230	-0.72905397
6	-4.11886759	-6.86673032	-2.11777516
1	-1.42074970	-6.46250169	-1.88593215
6	0.19811668	-4.72029373	-0.61914872
1	0.07796738	5.26565221	0.30235638
1	0.50091721	3.64244420	0.91199586
1	-1.00351045	4.42720681	1.42591081
1	-1.05959672	-0.29392627	-2.32774956
1	-2.69979315	0.05121195	-2.89740572
1	-2.36916639	-0.20650789	-1.15476093
1	-3.40882267	5.13958062	-3.94895934
1	-2.16754665	4.42055457	-4.98676074
1	-1.77989940	5.83564988	-3.97926594
1	-5.27556253	-2.61744572	0.19642734
1	-3.79665454	-1.69162576	0.55182050
1	-4.44908053	-2.83365406	1.74548647
1	0.61287873	-4.78530071	0.39985372
1	0.60869711	-3.80500780	-1.07642634
1	0.58807234	-5.57251317	-1.18932880
1	-3.53125514	-7.22557916	-2.97384701
1	-5.09532705	-6.52636482	-2.48911625
1	-4.30540545	-7.73519246	-1.46571328
1	-0.35991516	-2.74768794	0.55673638

Energy = -7584.957137 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 39

Atomic N.	X	Y	Z
8	1.96658579	-0.52047604	1.35485297
8	2.66456343	1.55969539	0.86073056
6	3.64429954	2.49895533	0.41123585
1	3.10757161	3.44250321	0.24738196
1	4.11088315	2.17797607	-0.53087203
1	4.42491790	2.66720778	1.17293260
8	3.52470863	-0.16321730	-0.34861412
6	3.07972298	0.17538494	0.98610241
6	4.18956772	-0.00587590	2.06311859
1	3.96731078	-0.95078745	2.58121644
1	4.03136678	0.79165982	2.80505395
6	5.65851966	-0.02042333	1.60913459
1	5.86770141	0.81580128	0.92475363
1	6.28180265	0.15031851	2.50238150

6	6.10469381	-1.33890815	0.95769586
1	5.82086817	-2.17372688	1.62242966
1	7.20492485	-1.35550092	0.89553987
6	5.52834377	-1.58695189	-0.44026565
1	5.94165899	-0.85249053	-1.15119038
1	5.84196752	-2.58284522	-0.79764635
6	4.00561162	-1.50880209	-0.51475592
1	3.52763610	-2.17419515	0.22415681
1	3.66255589	-1.82583861	-1.51171218
50	0.27598429	-0.22152785	0.04239936
7	-0.78739427	0.55389425	2.15298965
6	-0.02283241	1.62829630	2.82214355
1	-0.44474419	1.84199204	3.82104447
1	-0.03737875	2.54205898	2.21959042
1	1.01904072	1.30557097	2.91674869
7	-2.25777362	1.91224464	-0.24741961
6	-2.22485622	0.91177197	2.02437453
1	-2.63829732	1.07781029	3.03806032
1	-2.73904982	0.03562297	1.60307082
6	-2.55222669	2.13814828	1.17451723
1	-3.62330811	2.36810524	1.34637576
1	-1.99388559	3.01702605	1.52057770
6	-2.54378094	2.98472925	-1.14482768
6	-1.71049495	4.12533681	-1.17814227
6	-2.00242028	5.15293034	-2.08423859
6	-3.07665620	5.08108632	-2.97665923
6	-3.86612411	3.92533697	-2.95306310
6	-3.62512678	2.88222839	-2.05279784
7	-0.78766206	-1.91106081	0.83678116
6	-0.65719881	-0.69996677	2.95790877
1	-1.16253408	-0.56795391	3.93352949
1	0.41900362	-0.83514454	3.12704665
6	-1.20827984	-1.92397147	2.22913453
1	-0.84334292	-2.80725542	2.78643712
1	-2.31655628	-1.96339256	2.31637374
6	-0.90853130	-3.12860655	0.11548142
6	-1.83204454	-3.23072096	-0.95704619
6	-1.93528147	-4.42531045	-1.68028354
6	-1.15195344	-5.54441795	-1.37894609
6	-0.24080518	-5.43382691	-0.32320777
6	-0.09756833	-4.25578914	0.42059181
6	-0.48551164	4.23069183	-0.30456328
1	-1.34697087	6.02721791	-2.10772612
6	-3.38183866	6.21397259	-3.92658253
1	-4.70099228	3.83239244	-3.65218191
6	-4.50703419	1.65500134	-2.07558537
6	-2.71612711	-2.06425280	-1.32806545
1	-2.65793097	-4.48486502	-2.49875925
6	-1.25754161	-6.81380642	-2.19003798
1	0.39754720	-6.28764477	-0.07848166
6	0.94938917	-4.19389066	1.50603767
1	0.23687341	4.93201313	-0.74192942
1	0.00176578	3.25129862	-0.19437096
1	-0.72270455	4.60289795	0.70574736
1	-3.96141010	0.75795618	-2.41218875
1	-5.34566685	1.79863858	-2.76805501
1	-4.93056066	1.42678731	-1.08502911
1	-4.15586612	6.88069751	-3.51428662

1	-3.75493506	5.84105547	-4.89042479
1	-2.49031915	6.82621999	-4.11762427
1	-3.51145817	-2.38359562	-2.01497545
1	-2.14315494	-1.26585443	-1.82733152
1	-3.17823708	-1.61717615	-0.43593731
1	0.53970268	-4.47262431	2.49085441
1	1.36282071	-3.17929638	1.59777063
1	1.76733000	-4.89487405	1.29102945
1	-0.51444857	-6.82964422	-3.00344045
1	-2.24922644	-6.91165537	-2.65262099
1	-1.07898291	-7.70319558	-1.56993241
1	-2.74821388	1.07082736	-0.55351478

Energy = -7584.959976 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 40

Atomic N.	X	Y	Z
8	2.33066052	-0.12898646	-0.36679534
8	2.63114541	-0.41666990	-2.59717800
6	3.46148245	-0.68345195	-3.72912525
1	2.78629616	-0.74331541	-4.59256751
1	4.00128145	-1.63616287	-3.62301912
1	4.18361814	0.13105675	-3.90745685
8	3.68880358	-1.83140328	-1.16891033
6	3.26344782	-0.44641900	-1.30349762
6	4.45832455	0.55366010	-1.21242590
1	4.43056774	0.96669572	-0.19372628
1	4.20854793	1.39085723	-1.88188958
6	5.88071241	0.04715151	-1.50347318
1	5.90797063	-0.55450529	-2.42449666
1	6.51300722	0.92994213	-1.69488523
6	6.51019618	-0.75254743	-0.35227831
1	6.41639668	-0.16479253	0.57775685
1	7.59082082	-0.86402512	-0.53814246
6	5.90170781	-2.14189896	-0.13586127
1	6.13911185	-2.79241597	-0.99404054
1	6.35907033	-2.61143538	0.75217990
6	4.38570831	-2.14295421	0.04903836
1	4.07038703	-1.45284029	0.84981155
1	4.05197874	-3.15335079	0.33683720
50	0.32810732	0.42555950	0.08393153
7	-0.40864365	-1.83847027	-0.64533444
6	0.53162138	-2.90019853	-0.22075160
1	0.24396027	-3.87065970	-0.66423865
1	0.53096782	-2.99426808	0.87124382
1	1.54270313	-2.63056975	-0.54977304
7	-2.06880238	-0.94903906	1.84024275
6	-1.80847057	-2.18835901	-0.28794315
1	-2.05474812	-3.16370045	-0.75008388
1	-2.46221380	-1.43771429	-0.75518457
6	-2.13421796	-2.27143021	1.20170036
1	-3.14264937	-2.72378245	1.28582800
1	-1.44795550	-2.95512790	1.71647806
6	-2.39990516	-0.86742270	3.22490156
6	-1.52981025	-1.39944979	4.20296152
6	-1.87531170	-1.28037846	5.55505275
6	-3.03998494	-0.63048528	5.97598925

6	-3.86507467	-0.07258102	4.99246040
6	-3.57093402	-0.18234529	3.62951421
7	-0.74550811	0.72293853	-1.74906810
6	-0.30010133	-1.65549165	-2.12458134
1	-0.68547727	-2.55576802	-2.64013173
1	0.77028656	-1.55043994	-2.34543911
6	-1.03555105	-0.40927120	-2.61846235
1	-0.68367035	-0.22635336	-3.65307459
1	-2.12239086	-0.61354606	-2.70587272
6	-1.22303382	1.99630999	-2.15940503
6	-2.61337693	2.28908779	-2.21593714
6	-3.04480498	3.55859315	-2.62126568
6	-2.14904084	4.57429930	-2.96722180
6	-0.78285602	4.28659499	-2.88114408
6	-0.30496622	3.02975626	-2.49076369
6	-0.21250345	-2.03113313	3.82708026
1	-1.19182870	-1.68873234	6.30383694
6	-3.39982416	-0.54076995	7.43926169
1	-4.76994868	0.46187002	5.29219890
6	-4.49157292	0.44820928	2.60994171
6	-3.64761768	1.27913229	-1.78655775
1	-4.11894223	3.76292858	-2.64711790
6	-2.63647868	5.92544460	-3.43214725
1	-0.05750022	5.06353670	-3.13780781
6	1.18507278	2.79546904	-2.43639333
1	0.48970815	-1.98231296	4.66919213
1	0.23830035	-1.51049182	2.96979247
1	-0.31761842	-3.09483937	3.55752887
1	-4.00174144	1.26881449	2.05958386
1	-5.37434935	0.87462561	3.10207789
1	-4.84908254	-0.27927291	1.86396353
1	-4.04807743	-1.37881748	7.74116633
1	-3.94291568	0.38752075	7.66322740
1	-2.50425764	-0.57606549	8.07425587
1	-4.57356003	1.78050385	-1.47502980
1	-3.26984578	0.68126507	-0.94360252
1	-3.91189204	0.57443322	-2.59121101
1	1.45345390	1.78718035	-2.77718122
1	1.57676333	2.89201477	-1.40954083
1	1.71278735	3.53993392	-3.04826171
1	-1.97753802	6.73260015	-3.08285402
1	-3.65258764	6.13085767	-3.06847324
1	-2.66449544	5.98282792	-4.53213175
1	-2.66129810	-0.30520842	1.31472039

Energy = -7584.950693 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 41

Atomic N.	X	Y	Z
8	2.02715616	-1.24931922	0.66241251
8	3.05818142	-0.54299778	-1.21428509
6	4.21914342	-0.27249077	-2.00168869
1	3.85283935	0.07573248	-2.97617742
1	4.82624767	-1.17884693	-2.14440382
1	4.84033078	0.52277055	-1.55731634
8	3.79202828	-2.45268651	-0.22962588
6	3.26450377	-1.15222125	0.08785293

6	4.22396440	-0.31261340	0.98386206
1	3.83127497	-0.39732812	2.00794281
1	4.07328918	0.73941972	0.69400573
6	5.72199435	-0.65857279	0.99805509
1	6.10845111	-0.79352825	-0.02353937
1	6.25954185	0.20721785	1.41844623
6	6.06818484	-1.89469485	1.84319314
1	5.62214893	-1.77107307	2.84558116
1	7.15905085	-1.93456225	1.99450587
6	5.60400080	-3.22698808	1.24470069
1	6.17159118	-3.44224708	0.32408309
1	5.82607820	-4.04570700	1.95069348
6	4.11663352	-3.28000562	0.90198839
1	3.48968561	-3.00331407	1.76596700
1	3.83902554	-4.30504109	0.61092801
50	0.49024478	0.10524557	0.09272488
7	-0.43238092	-1.62854544	-1.45488152
6	0.53139883	-2.75742574	-1.50774188
1	0.08812812	-3.60364718	-2.06176484
1	0.80568128	-3.06783946	-0.49659443
1	1.45214765	-2.42666433	-2.00112823
7	-0.96792965	-0.93073518	1.27050388
6	-1.68212962	-2.04586573	-0.75982044
1	-2.05687354	-2.98941630	-1.20085740
1	-2.42798773	-1.25648603	-0.91132591
6	-1.45494909	-2.19769140	0.74444514
1	-2.42909463	-2.45372662	1.19978650
1	-0.79338746	-3.06695245	0.93187921
6	-1.15043492	-0.64513349	2.64769289
6	-0.69556955	-1.51216090	3.67781470
6	-0.92980156	-1.17775212	5.01851830
6	-1.57812899	0.00245488	5.39370800
6	-1.98879065	0.86669416	4.37252512
6	-1.79549729	0.56679833	3.01944656
7	-1.50925903	1.11263779	-2.42517878
6	-0.66874959	-1.19450043	-2.86377613
1	-0.92622868	-2.08611172	-3.46689840
1	0.30023334	-0.82794793	-3.23805718
6	-1.75208586	-0.15158734	-3.12922538
1	-1.77787768	-0.01612665	-4.22945191
1	-2.73787209	-0.54611796	-2.85048887
6	-2.29028176	2.24462631	-2.79370634
6	-3.68120994	2.28113459	-2.54614490
6	-4.40571895	3.42551858	-2.90558501
6	-3.79991912	4.54801816	-3.47719749
6	-2.41405464	4.50773937	-3.67333538
6	-1.65199814	3.38163997	-3.34880231
6	0.10789314	-2.75119029	3.36507458
1	-0.56499406	-1.85565425	5.79551470
6	-1.84137133	0.32583032	6.84501193
1	-2.49295287	1.80108592	4.63411215
6	-2.28963910	1.53350796	1.97195307
6	-4.39190167	1.14945206	-1.84617142
1	-5.47960230	3.44393386	-2.70299179
6	-4.60894552	5.75873714	-3.87531345
1	-1.90739589	5.37823008	-4.09755884
6	-0.15818909	3.39622340	-3.57817667
1	0.66705564	-3.07475361	4.25326788

1	0.82134644	-2.55623105	2.55068537
1	-0.52616475	-3.59728765	3.05486607
1	-1.46632388	2.10420861	1.51126062
1	-2.98532883	2.26004615	2.41230887
1	-2.79047199	1.00342590	1.15059798
1	-2.85652001	0.01968452	7.14520884
1	-1.75824083	1.40452221	7.03876972
1	-1.13488170	-0.19605052	7.50501377
1	-5.31476658	1.51079655	-1.37456433
1	-3.75350161	0.71268635	-1.06472197
1	-4.67784253	0.33893623	-2.53592654
1	0.16850057	2.57754946	-4.23971709
1	0.40812831	3.30065394	-2.63695387
1	0.14848233	4.33960642	-4.04646509
1	-4.06241235	6.69096955	-3.67570522
1	-5.56256271	5.79798189	-3.33202931
1	-4.84406803	5.74464181	-4.95151010
1	-0.51829791	1.34748127	-2.49010392

Energy = -7584.956438 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 42

Atomic N.	X	Y	Z
8	2.31436526	0.57718928	-0.10040840
8	2.78543666	0.58473575	-2.32152672
6	3.70431753	0.48244339	-3.41195162
1	3.09671643	0.53168376	-4.32475921
1	4.25534591	-0.46944055	-3.39271026
1	4.41891132	1.32233516	-3.42346893
8	3.75942015	-0.99224384	-1.01546034
6	3.32192499	0.38960007	-1.00324923
6	4.48338283	1.38111753	-0.68461122
1	4.36847192	1.65496057	0.37414079
1	4.27100767	2.29732999	-1.25603636
6	5.93322758	0.92860197	-0.92486066
1	6.04340004	0.45494369	-1.91204058
1	6.56142853	1.83435467	-0.94741791
6	6.48592000	-0.01142777	0.15772967
1	6.30943649	0.44736899	1.14644286
1	7.57951792	-0.08817520	0.04518937
6	5.88870401	-1.42229700	0.14092715
1	6.20402072	-1.95170482	-0.77350302
1	6.28434638	-2.00148021	0.99297152
6	4.36365743	-1.45974887	0.20364596
1	3.97406186	-0.88485975	1.06033818
1	4.02417392	-2.50080099	0.32586208
50	0.25156593	0.85474642	0.19083956
7	-0.37482706	-1.15841712	-1.05836135
6	0.56683794	-2.28682240	-0.82974101
1	0.38213775	-3.08242233	-1.57249677
1	0.40492742	-2.70604675	0.16887122
1	1.59775123	-1.92442761	-0.93031549
7	-1.56828341	-2.27021138	1.60888746
6	-1.78617609	-1.59586342	-0.82827851
1	-1.88514588	-2.63581729	-1.18678879
1	-2.43426040	-0.96489241	-1.45255388
6	-2.30935750	-1.48374547	0.60608529

1	-2.34663445	-0.41537035	0.89435960
1	-3.35087856	-1.82986181	0.59078579
6	-2.31023446	-2.77320173	2.71706215
6	-3.24484089	-3.81672486	2.52467739
6	-3.94238244	-4.31679806	3.63164613
6	-3.72928784	-3.83765678	4.92821748
6	-2.76752599	-2.83502696	5.10142168
6	-2.05940113	-2.29162990	4.02442240
7	-0.60866817	1.59766633	-1.60396534
6	-0.19556790	-0.66227578	-2.45861469
1	-0.57018168	-1.42064003	-3.17098220
1	0.88663079	-0.54277642	-2.60198574
6	-0.88441262	0.67965585	-2.70128149
1	-0.48964159	1.06749652	-3.66125314
1	-1.97098662	0.53025153	-2.86573912
6	-1.08267753	2.93229473	-1.73365885
6	-2.47163478	3.23225476	-1.74044677
6	-2.89458464	4.56078529	-1.87697037
6	-1.99200864	5.62229373	-1.99020125
6	-0.62699104	5.31806145	-1.95858949
6	-0.15733491	4.00497714	-1.83333359
6	-3.45426851	-4.44308912	1.16742155
1	-4.65800725	-5.12765930	3.47314843
6	-4.51529104	-4.37458056	6.10004787
1	-2.56547917	-2.45477041	6.10591770
6	-1.02938401	-1.21318143	4.26855554
6	-3.51128675	2.15623389	-1.54894642
1	-3.96784967	4.77059352	-1.87547247
6	-2.47146972	7.04983376	-2.10019632
1	0.10222559	6.12806397	-2.04663451
6	1.32962001	3.75005564	-1.81410740
1	-3.86146029	-5.45707250	1.27233696
1	-2.50505738	-4.49997602	0.61522350
1	-4.16066711	-3.87583266	0.54027332
1	-0.00664052	-1.55292736	4.03438509
1	-1.03277666	-0.91069207	5.32304499
1	-1.21374191	-0.31204925	3.66298890
1	-5.38681799	-3.73761409	6.32002807
1	-3.90307248	-4.41202511	7.01169712
1	-4.89245952	-5.38632521	5.89862680
1	-4.43584636	2.58162284	-1.13688190
1	-3.14404043	1.38225194	-0.85927124
1	-3.77633256	1.65491591	-2.49381862
1	1.59445119	2.83724096	-2.36242727
1	1.70480551	3.60914211	-0.78653293
1	1.87202635	4.60536278	-2.23963073
1	-2.52650350	7.52844655	-1.10927681
1	-3.47428934	7.10360362	-2.54519584
1	-1.79021564	7.65497814	-2.71445024
1	-0.78729125	-1.70889126	1.95218542

Energy = -7584.949923 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 43

Atomic N.	X	Y	Z
8	2.33783831	-0.31265010	-0.00603339
8	3.04091448	-0.07120624	-2.14962778

6	4.05551059	-0.13528248	-3.15378763
1	3.55486328	0.08777352	-4.10487748
1	4.51180385	-1.13478685	-3.20877919
1	4.84227800	0.62007996	-2.98876870
8	3.73150625	-1.89133574	-0.98017775
6	3.41375533	-0.48063723	-0.81999549
6	4.62056848	0.34296007	-0.27047537
1	4.41937533	0.49709878	0.79952188
1	4.54914136	1.33820005	-0.73518454
6	6.04341096	-0.21703012	-0.43113306
1	6.21673561	-0.57531666	-1.45716059
1	6.74648963	0.61785699	-0.27482535
6	6.39459928	-1.33257168	0.56555530
1	6.15145492	-0.98433349	1.58476569
1	7.48355301	-1.50183690	0.54971207
6	5.68547451	-2.66504040	0.30326424
1	6.05133381	-3.10392935	-0.63991702
1	5.93771267	-3.38203884	1.10362446
6	4.16405635	-2.56321721	0.21413100
1	3.73326263	-2.06878772	1.10118830
1	3.73303624	-3.57647595	0.16195049
50	0.33166347	0.34738144	0.23774435
7	-0.39838704	-1.58523012	-1.15248439
6	0.37652315	-2.81245597	-0.86101779
1	0.11789480	-3.61217468	-1.57847065
1	0.16454560	-3.16386236	0.15531173
1	1.44611673	-2.58147887	-0.93650375
7	-2.43042754	-1.13402117	1.16579396
6	-1.85964866	-1.85661630	-1.13280185
1	-2.07623486	-2.66356162	-1.85905455
1	-2.36506862	-0.95120749	-1.49868740
6	-2.46342705	-2.25263857	0.21287770
1	-3.49773961	-2.59721200	0.01268216
1	-1.93267453	-3.11029064	0.64411117
6	-3.00726059	-1.34274144	2.45283359
6	-2.37922780	-2.19052743	3.39257006
6	-2.96311193	-2.35361557	4.65545633
6	-4.13289584	-1.68630102	5.03170206
6	-4.71312485	-0.81620315	4.10096009
6	-4.17792584	-0.63644414	2.82163851
7	-0.36247554	1.18567145	-1.61051939
6	-0.00233735	-1.06827279	-2.49754263
1	-0.33931766	-1.77325733	-3.28127507
1	1.09496149	-1.02927162	-2.50314797
6	-0.55241591	0.33115342	-2.77496747
1	-0.00071272	0.71640876	-3.65522423
1	-1.61374744	0.27118884	-3.09205835
6	-0.67330595	2.56406194	-1.75700419
6	-2.00628353	3.00997770	-1.97061370
6	-2.27203837	4.37822982	-2.11137775
6	-1.26515056	5.34428846	-2.03268772
6	0.04050699	4.89826339	-1.80193723
6	0.35529406	3.54110394	-1.66423281
6	-1.06570704	-2.86811186	3.09063419
1	-2.46556902	-3.00617990	5.37737733
6	-4.75332588	-1.89998915	6.39115254
1	-5.61441930	-0.26212982	4.37480708
6	-4.84003568	0.32260986	1.85910209

6	-3.16443575	2.04441103	-1.99578292
1	-3.30613646	4.69671976	-2.27051165
6	-1.57738617	6.81659096	-2.15386065
1	0.85028766	5.63054099	-1.74010217
6	1.79202923	3.14055050	-1.43329857
1	-0.53340044	-3.10285214	4.02133483
1	-0.42342804	-2.21760334	2.47944124
1	-1.19694196	-3.81819319	2.54720033
1	-4.19272177	1.18235931	1.61820115
1	-5.76174570	0.72779924	2.29448474
1	-5.11005808	-0.16152171	0.90710242
1	-5.54934359	-2.66042706	6.34964995
1	-5.20698012	-0.97607965	6.77561917
1	-4.00842975	-2.24548316	7.12051337
1	-4.10022065	2.55392783	-1.73028917
1	-2.99414214	1.22595920	-1.28041882
1	-3.31188353	1.58423659	-2.98591453
1	2.05024926	2.21576221	-1.96505153
1	1.99653784	2.95385991	-0.36533583
1	2.46992198	3.94510463	-1.74994009
1	-1.68978240	7.28334984	-1.16216812
1	-2.51341834	6.98432317	-2.70352926
1	-0.77267925	7.35467546	-2.67445266
1	-2.86807624	-0.32204680	0.72899261

Energy = -7584.950668 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 44

Atomic N.	X	Y	Z
8	1.77906588	-1.59083461	0.64565298
8	3.20871971	-0.59246643	-0.78377206
6	4.51897851	-0.27874688	-1.25900332
1	4.37875739	0.31926508	-2.16881709
1	5.08393611	-1.18977353	-1.50652049
1	5.08716989	0.32232543	-0.52981593
8	3.60680190	-2.74512679	-0.18020786
6	3.11057122	-1.50116431	0.34463850
6	3.92189471	-0.99816395	1.57640451
1	3.32794222	-1.27215456	2.46086022
1	3.89797080	0.10225276	1.53171874
6	5.36239434	-1.49860579	1.77346736
1	5.93596239	-1.43871254	0.83588063
1	5.85849001	-0.81503478	2.48187127
6	5.45465794	-2.92491115	2.33839093
1	4.82708173	-2.98514983	3.24478627
1	6.48891926	-3.11684693	2.66693123
6	5.03528875	-4.02709711	1.35962569
1	5.75993447	-4.08788402	0.53064107
1	5.05998991	-5.00420839	1.87215460
6	3.64568485	-3.83804241	0.75501090
1	2.87808349	-3.69770730	1.53419901
1	3.36676671	-4.73351633	0.17815695
50	0.47902468	0.02525156	0.18135016
7	-0.24108080	-1.17617463	-1.88991528
6	0.64259818	-2.35683707	-2.06685350
1	0.25785732	-2.99476195	-2.88200020
1	0.70434206	-2.92593286	-1.13601596

1	1.65794063	-2.01881364	-2.30239107
7	-1.24387254	-1.09050485	0.79269161
6	-1.62363044	-1.60987719	-1.54392313
1	-1.96580061	-2.37564062	-2.26623872
1	-2.27639355	-0.73164477	-1.61372410
6	-1.69604694	-2.13826118	-0.11120683
1	-2.75239871	-2.39191398	0.09268049
1	-1.13464921	-3.09118718	-0.04078911
6	-1.66889447	-1.12076802	2.14528539
6	-1.48228478	-2.25316902	2.98381939
6	-1.94776245	-2.22085528	4.30526439
6	-2.57365098	-1.09668982	4.85182509
6	-2.71905557	0.02554326	4.02868974
6	-2.28896741	0.03429306	2.69706333
7	-0.94634777	1.81446476	-2.29083453
6	-0.17935618	-0.39394253	-3.16027367
1	-0.37288002	-1.08178155	-4.00550645
1	0.86365883	-0.05421508	-3.26059625
6	-1.12666110	0.79202498	-3.32762664
1	-0.93391733	1.19197175	-4.34368287
1	-2.16942452	0.44905631	-3.33089649
6	-1.57324082	3.07885091	-2.47816200
6	-2.98029768	3.20250613	-2.47537273
6	-3.55151119	4.47197863	-2.64350279
6	-2.78090478	5.62843828	-2.78502298
6	-1.38747244	5.48854127	-2.74391608
6	-0.77211350	4.24280335	-2.59825095
6	-0.71885277	-3.46599100	2.50958404
1	-1.78694150	-3.10038825	4.93528166
6	-3.08821967	-1.09809320	6.27141166
1	-3.19896631	0.92287673	4.42884503
6	-2.50342277	1.27176745	1.86123074
6	-3.88141323	2.01717392	-2.23276635
1	-4.64125176	4.55494891	-2.63593925
6	-3.41989695	6.98493057	-2.96115606
1	-0.75691542	6.37664641	-2.83425742
6	0.73598761	4.15196393	-2.55788157
1	-0.36822853	-4.05351794	3.36871371
1	0.15231085	-3.16576171	1.90857605
1	-1.33496450	-4.13568192	1.88832795
1	-1.57031684	1.84031421	1.71294700
1	-3.22383012	1.94559285	2.34368166
1	-2.86526095	1.01211839	0.85720055
1	-4.15542570	-1.37007771	6.31059580
1	-2.98973920	-0.10701878	6.73611253
1	-2.54446258	-1.82299731	6.89277608
1	-4.85565325	2.34936960	-1.85173076
1	-3.43721966	1.33488284	-1.49371614
1	-4.07417261	1.43732591	-3.14987008
1	1.13400050	3.49362752	-3.34706210
1	1.10356305	3.76414151	-1.59339781
1	1.18338036	5.14338973	-2.70023993
1	-3.08909192	7.68893945	-2.18307760
1	-4.51454824	6.91821869	-2.91252885
1	-3.15342804	7.43024959	-3.93194182
1	0.05111202	1.95060096	-2.12394010

Energy = -7584.956395 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 45

Atomic N.	X	Y	Z
8	0.48207415	0.17939501	0.15951781
8	2.00774139	0.28157797	-1.46955137
6	3.23180670	-0.15625320	-2.06618031
1	3.13631275	0.04679575	-3.13985205
1	3.39549386	-1.23199737	-1.90628208
1	4.09075176	0.41452037	-1.67695957
8	2.24825290	-1.24036996	0.32660214
6	1.82811533	0.08898763	0.00275674
6	2.57406622	1.21078300	0.74014918
1	3.63201857	1.23467530	0.43243594
1	2.11927987	2.13688506	0.36591493
6	2.47028277	1.14907498	2.27271396
1	1.45249555	0.83544602	2.55454450
1	2.60151732	2.16759237	2.66989133
6	3.51268353	0.23591685	2.92972850
1	4.52020339	0.61171403	2.67687356
1	3.42397681	0.31116982	4.02511948
6	3.41933866	-1.23729884	2.51976065
1	2.48383521	-1.68426276	2.89238910
1	4.24531392	-1.79625798	2.99126760
6	3.49204866	-1.48224490	1.01187016
1	4.31962163	-0.90793472	0.56025683
1	3.69146227	-2.54651957	0.81865321
50	-0.45462562	-0.49892666	-1.68225919
7	-2.56067773	0.29885196	-0.53787471
6	-3.55544750	-0.78562738	-0.39518578
1	-4.54078454	-0.39095465	-0.09041661
1	-3.21709417	-1.51761068	0.34588239
1	-3.66265224	-1.29481363	-1.36139330
7	-1.38731103	-0.74827119	2.24397496
6	-2.34448150	1.04713320	0.74651577
1	-3.12554406	1.82691919	0.82084883
1	-1.37111689	1.54868002	0.67510098
6	-2.41872441	0.26224979	2.05884439
1	-2.37657051	1.04825959	2.83701092
1	-3.41341795	-0.20288409	2.16252524
6	-1.62549264	-1.92023676	2.97934260
6	-2.22370537	-1.86840250	4.26603326
6	-2.48495022	-3.06252989	4.95173913
6	-2.13498760	-4.31475196	4.44025727
6	-1.48124490	-4.34175466	3.20238419
6	-1.22527442	-3.18302204	2.46306407
7	-0.83676774	1.41136282	-2.59703387
6	-3.03382184	1.25306650	-1.58642902
1	-3.90286090	1.81900790	-1.20023851
1	-3.36241436	0.65173759	-2.44678348
6	-1.93177544	2.19838981	-2.04932855
1	-2.36613339	2.85105050	-2.82875340
1	-1.65264126	2.86995117	-1.21228299
6	0.04731602	2.02087634	-3.51658298
6	0.74992808	3.22044280	-3.21826639
6	1.60400643	3.78538864	-4.17391167
6	1.81916372	3.19929526	-5.42485754
6	1.14658701	2.00355222	-5.69957542

6	0.26914686	1.41153743	-4.78318865
6	-2.47809818	-0.55719633	4.97345313
1	-2.94429666	-3.00040358	5.94204195
6	-2.45040300	-5.58752019	5.18856140
1	-1.16983177	-5.30224320	2.78306753
6	-0.53900607	-3.28985252	1.12621417
6	0.65278229	3.86644224	-1.85871541
1	2.13922300	4.70392394	-3.91650665
6	2.72076890	3.84530601	-6.44943892
1	1.29218258	1.52057142	-6.66980301
6	-0.44492802	0.14059913	-5.17478804
1	-2.61438328	-0.73150234	6.04873077
1	-3.37404176	-0.02857990	4.61327892
1	-1.62561984	0.12605571	4.84235274
1	-1.17220060	-2.90575039	0.30865365
1	-0.30571993	-4.33729996	0.89550468
1	0.39937805	-2.71675175	1.07792232
1	-1.65476077	-6.33564923	5.06456519
1	-3.38471435	-6.04540058	4.82537820
1	-2.57647384	-5.39817071	6.26345153
1	1.52617051	4.50627473	-1.67477094
1	0.60446133	3.10073191	-1.07171729
1	-0.24315830	4.49928736	-1.75478095
1	-1.49670791	0.16159945	-4.85637281
1	0.00269249	-0.75308209	-4.70849376
1	-0.40216690	-0.00756819	-6.26221842
1	3.21080670	3.09474609	-7.08509198
1	3.50215179	4.45116129	-5.96996202
1	2.15288832	4.51472696	-7.11561756
1	-0.65131795	-0.75381679	1.53431938

Energy = -7584.957701 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 46

Atomic N.	X	Y	Z
8	0.63166826	-0.10286723	-0.19100863
8	1.47215291	-0.03737914	-2.27595168
6	2.16566829	-0.69916450	-3.33127077
1	1.80998952	-0.24888245	-4.26758671
1	1.95150950	-1.77822366	-3.34428761
1	3.25588060	-0.53963658	-3.26297941
8	1.74399322	-1.94995405	-0.89983030
6	1.72045548	-0.51304843	-0.87168361
6	3.01066912	0.16221204	-0.37823031
1	3.83475594	-0.02645717	-1.08598162
1	2.79045561	1.23641685	-0.42989711
6	3.44461558	-0.22218137	1.04414347
1	2.55143679	-0.29250760	1.68423355
1	4.05494955	0.59757735	1.45473798
6	4.25833358	-1.51961892	1.12323426
1	5.17556351	-1.39608331	0.51982270
1	4.59480415	-1.67765948	2.16088825
6	3.51636403	-2.76934773	0.63834687
1	2.66741578	-2.99982492	1.30201576
1	4.20011377	-3.63442963	0.68428680
6	2.97986579	-2.67161081	-0.79208027
1	3.75301320	-2.26269953	-1.46748988

1	2.72910389	-3.67820861	-1.15929555
50	-1.09858116	-0.06423452	-1.49685731
7	-3.69243799	0.71682003	-0.89935794
6	-4.74808162	-0.11828581	-1.47592714
1	-5.74622459	0.35609205	-1.38407014
1	-4.78192717	-1.09737600	-0.98485396
1	-4.53521722	-0.28666558	-2.54023749
7	-2.01008049	-0.80095997	1.04292969
6	-3.80996014	0.84850616	0.55739793
1	-4.84047206	1.13284400	0.85924079
1	-3.14377359	1.66287787	0.87528042
6	-3.41796690	-0.42718224	1.30549363
1	-3.59773604	-0.26577177	2.38468209
1	-4.05698589	-1.26705844	1.00720416
6	-1.59557426	-2.05414114	1.62200584
6	-2.02330245	-3.27819130	1.06709521
6	-1.59023537	-4.47495811	1.65507388
6	-0.73883560	-4.50023362	2.76230059
6	-0.30965292	-3.27285290	3.28074738
6	-0.72494883	-2.05390916	2.73638765
7	-1.17514715	2.06977670	-1.20276707
6	-3.62731943	2.00802963	-1.60322944
1	-4.54874214	2.60650268	-1.43829551
1	-3.57587243	1.76980806	-2.67761510
6	-2.40756114	2.84420317	-1.22387935
1	-2.35890262	3.67218509	-1.95922252
1	-2.59095767	3.34953032	-0.24863613
6	-0.01388100	2.90048151	-1.14362986
6	0.52047591	3.32073128	0.09688102
6	1.64019319	4.16288220	0.12299541
6	2.26161577	4.60552640	-1.04948191
6	1.72240469	4.18629880	-2.27071444
6	0.60276401	3.34759231	-2.33826751
6	-2.90447003	-3.34637314	-0.15584649
1	-1.91727785	-5.41854778	1.21122974
6	-0.30210665	-5.80372925	3.38597796
1	0.37115375	-3.25969493	4.13547362
6	-0.21844652	-0.76092972	3.32810959
6	-0.08110290	2.84331702	1.39363182
1	2.04096670	4.47604591	1.09101858
6	3.49138168	5.48066573	-0.99966218
1	2.18632908	4.52142634	-3.20241013
6	0.07424026	2.92035765	-3.68502805
1	-2.74099768	-4.29131949	-0.68991338
1	-2.69310494	-2.52183690	-0.85171616
1	-3.97526849	-3.30550750	0.10458088
1	0.41219603	-0.21576079	2.60793748
1	0.39073182	-0.95878808	4.21869126
1	-1.03681856	-0.08864522	3.63113225
1	-0.89353636	-6.03163599	4.28682513
1	0.75284929	-5.76842724	3.69197941
1	-0.42888032	-6.64206158	2.68822928
1	0.42436900	3.30450524	2.25243362
1	0.03313029	1.75236421	1.46641801
1	-1.15380353	3.07634753	1.46581763
1	-0.99492225	3.15007064	-3.80137893
1	0.17948753	1.83417626	-3.82293596
1	0.62300713	3.42237052	-4.49296687

1	4.41132480	4.87460867	-1.02432866
1	3.52040047	6.07999214	-0.07938069
1	3.53163252	6.16619996	-1.85753018
1	-1.40231807	-0.06447902	1.41080241

Energy = -7584.956338 Hartree
Number of imaginary frequencies = 0.

Compound I3b isomer 47

Atomic N.	X	Y	Z
8	0.51084288	-0.02565015	0.02321990
8	2.19305086	0.07641437	-1.46762527
6	3.27163900	-0.53464607	-2.17190381
1	3.47312633	0.11143493	-3.03540292
1	2.99998447	-1.53829062	-2.53436228
1	4.19260171	-0.60109057	-1.56531475
8	1.48777461	-1.98240971	-0.54425750
6	1.72794248	-0.56573442	-0.24468844
6	2.73315341	-0.33118816	0.89339648
1	3.74942453	-0.60028188	0.56298402
1	2.73239774	0.75701424	1.03782682
6	2.40449471	-1.03809366	2.21641040
1	1.31635486	-1.00563581	2.37415744
1	2.85634587	-0.46071190	3.03832896
6	2.91733390	-2.48151404	2.30264638
1	4.01268238	-2.47594210	2.15637875
1	2.74770861	-2.86565155	3.32128617
6	2.28387724	-3.44976317	1.29863286
1	1.21641176	-3.59517442	1.52254546
1	2.76501885	-4.43792697	1.39716787
6	2.41300934	-3.02101365	-0.16030997
1	3.44819915	-2.72057512	-0.39539963
1	2.15813151	-3.86182727	-0.82261154
50	-0.93959058	-1.03085091	-1.23602466
7	-2.79879538	0.60057941	-0.82006652
6	-3.83983622	0.11601743	-1.75747060
1	-4.79518597	0.64396054	-1.58946376
1	-4.00138207	-0.96006897	-1.62535253
1	-3.50605660	0.29270917	-2.78705999
7	-2.01805794	-1.83648197	0.46247014
6	-3.19891538	0.31750079	0.58442293
1	-4.18186402	0.78442183	0.78993999
1	-2.44761998	0.78071369	1.23811665
6	-3.25163602	-1.17891247	0.87026955
1	-3.43419296	-1.29056264	1.95188940
1	-4.14758572	-1.62205542	0.38274940
6	-1.68807231	-3.02443004	1.15763405
6	-1.61256030	-4.27362387	0.48407796
6	-1.27130082	-5.43217286	1.19480421
6	-1.01022212	-5.41725316	2.56829723
6	-1.07399273	-4.18196795	3.22222510
6	-1.39757230	-2.99579443	2.55302481
7	-0.21122713	2.74804764	-1.32093078
6	-2.63521775	2.06742705	-1.04627607
1	-3.54969416	2.56135010	-0.66194142
1	-2.60449303	2.22214403	-2.13132480
6	-1.39315415	2.73828018	-0.43971321
1	-1.66535763	3.77696597	-0.20314800

1	-1.13368004	2.26237213	0.52027619
6	0.39763793	4.00753713	-1.57992375
6	1.68671748	4.31096592	-1.07463614
6	2.27081792	5.54723834	-1.37148181
6	1.61746606	6.51615543	-2.14176542
6	0.35187269	6.19671998	-2.64188114
6	-0.26341162	4.96387481	-2.38847921
6	-1.90859846	-4.39008010	-0.99177078
1	-1.22569846	-6.38179650	0.65475882
6	-0.68639770	-6.68561197	3.32065871
1	-0.83882069	-4.13150687	4.28927164
6	-1.36070100	-1.69676463	3.32066048
6	2.43175764	3.32123761	-0.21531182
1	3.26513142	5.76291316	-0.97152974
6	2.24844967	7.86228308	-2.40527763
1	-0.17058265	6.91918330	-3.27448450
6	-1.58652928	4.65601247	-3.04312637
1	-2.14273671	-5.42975693	-1.25793918
1	-1.05343876	-4.08133328	-1.61555609
1	-2.75427523	-3.75143554	-1.28254079
1	-1.04034204	-0.87243721	2.66788508
1	-0.66325750	-1.77072256	4.16591507
1	-2.34307626	-1.42571483	3.74112169
1	-1.58795091	-7.11776511	3.78365138
1	0.03385501	-6.49913739	4.12980259
1	-0.26315845	-7.44975146	2.65465850
1	3.35955548	3.76608930	0.16683019
1	2.69527944	2.40910179	-0.77282092
1	1.82687244	3.00071584	0.64719210
1	-2.42961560	4.67618735	-2.33474381
1	-1.56650881	3.65242376	-3.49406413
1	-1.80582549	5.38935244	-3.82993513
1	3.33823374	7.78034272	-2.52053906
1	2.06136701	8.55983414	-1.57305850
1	1.84144965	8.32322671	-3.31564329
1	0.46021915	2.04236155	-1.01042772

Energy = -7584.953223 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 48

Atomic N.	X	Y	Z
8	0.60403900	0.66691455	-0.09859526
8	1.38198421	-0.64141992	-1.74326713
6	2.33050405	-1.58696919	-2.23813074
1	1.79026566	-2.20099759	-2.96953823
1	2.71765371	-2.23290026	-1.43642342
1	3.16769389	-1.08660571	-2.75352149
8	2.56951557	-0.38296566	0.31380353
6	1.78422880	0.31115266	-0.66468273
6	2.50524827	1.50289268	-1.32088713
1	3.27154655	1.14251396	-2.02668832
1	1.73430232	1.99753141	-1.92487630
6	3.13266826	2.50349248	-0.33732120
1	2.47807806	2.61040154	0.54216491
1	3.16463428	3.49281121	-0.81964926
6	4.55864386	2.13159732	0.09139426
1	5.18393741	2.05518407	-0.81571570

1	4.98817324	2.95101537	0.68968229
6	4.67031537	0.82375991	0.88231037
1	4.23493827	0.94270597	1.88618720
1	5.73610895	0.58049044	1.03227729
6	4.01027371	-0.38377709	0.21682617
1	4.34579703	-0.47654704	-0.82892249
1	4.31369535	-1.30386454	0.73815508
50	-0.89096591	-0.88720452	-0.49182429
7	-2.55064848	0.87813412	0.29054354
6	-3.68334007	0.18582000	0.93967948
1	-4.46394859	0.90091316	1.25792675
1	-3.33013317	-0.37790648	1.80825957
1	-4.12174924	-0.52201514	0.22611934
7	-0.63312947	0.26695121	2.59121853
6	-1.94160470	1.88871852	1.20163047
1	-2.65204929	2.72788591	1.33162962
1	-1.04538288	2.27681528	0.69723880
6	-1.57584046	1.39321664	2.60143398
1	-1.17558435	2.27566769	3.14261936
1	-2.48070605	1.09331674	3.15038251
6	-0.21438750	-0.16416423	3.89326472
6	-1.00168045	-1.08520078	4.61779494
6	-0.57901337	-1.49505300	5.88959450
6	0.61093119	-1.03546702	6.46224183
6	1.39127049	-0.14290853	5.71757205
6	0.99723819	0.30521710	4.45208378
7	-1.68841000	0.02130143	-2.28599821
6	-3.01787455	1.54366610	-0.96946187
1	-3.27327028	2.59767208	-0.75729716
1	-3.93065556	1.02886552	-1.29617444
6	-1.99072338	1.43269462	-2.09669544
1	-2.44860026	1.86578396	-3.00086369
1	-1.10467833	2.05263569	-1.85442407
6	-1.63080267	-0.51874144	-3.58493241
6	-0.93039208	0.11024549	-4.65511283
6	-0.94202446	-0.46604702	-5.93188651
6	-1.59704286	-1.66945375	-6.20904730
6	-2.25042758	-2.30047723	-5.14524946
6	-2.28554590	-1.75556304	-3.85693220
6	-2.26141615	-1.66703295	4.02889603
1	-1.19192702	-2.21570014	6.43695454
6	1.03408427	-1.47453955	7.84343000
1	2.33340527	0.22226050	6.13462156
6	1.86795901	1.27246296	3.68847486
6	-0.09092506	1.34526958	-4.43209374
1	-0.38956723	0.03538216	-6.73196404
6	-1.61744715	-2.25202570	-7.60188422
1	-2.77160981	-3.24499533	-5.32480862
6	-3.05075787	-2.48754568	-2.78246841
1	-2.55766916	-2.57598640	4.56827366
1	-2.11138477	-1.91572836	2.96882881
1	-3.10921378	-0.96472041	4.08779802
1	2.19829057	0.84525849	2.72988818
1	2.76161050	1.53037825	4.27121974
1	1.33674806	2.20811184	3.45498357
1	0.72742012	-0.73975717	8.60484190
1	2.12553339	-1.57921315	7.91515084
1	0.57825461	-2.43633654	8.11436512

1	0.63404299	1.46306348	-5.24858049
1	0.46076861	1.26210649	-3.48671769
1	-0.68360397	2.27211945	-4.38541068
1	-3.64934988	-1.78919869	-2.17881313
1	-2.38717073	-3.01751738	-2.07938253
1	-3.71941234	-3.23720879	-3.22666628
1	-1.67604023	-3.34914788	-7.57788617
1	-0.71774282	-1.97036440	-8.16689829
1	-2.48702399	-1.89225480	-8.17565424
1	0.17107075	0.51112444	2.00158612

Energy = -7584.958784 Hartree
Number of imaginary frequencies = 0.

Compound I3b isomer 49

Atomic N.	X	Y	Z
8	0.47048292	-0.03245373	-0.18679827
8	1.54214584	-1.50804226	-1.50489075
6	2.53398694	-2.51365398	-1.69886684
1	2.25520589	-3.03898822	-2.62079450
1	2.54485792	-3.23565385	-0.86756532
1	3.54672702	-2.09256036	-1.83160637
8	1.88273979	-1.47033732	0.83438507
6	1.67982379	-0.62893067	-0.35042239
6	2.80369533	0.39079967	-0.59090097
1	3.72015018	-0.12567511	-0.91928175
1	2.45672658	0.98091668	-1.44911247
6	3.11634108	1.31657259	0.59359055
1	2.17313890	1.58463584	1.09207957
1	3.53782192	2.25402209	0.19786704
6	4.11049222	0.72987401	1.60439514
1	5.04930577	0.48598859	1.07493564
1	4.37034184	1.50177846	2.34641546
6	3.61421605	-0.51721129	2.34297862
1	2.77091552	-0.26490941	3.00325012
1	4.42151605	-0.89755589	2.99223568
6	3.18231839	-1.66233851	1.43122006
1	3.93919450	-1.85598652	0.65228432
1	3.07165020	-2.58719794	2.01682409
50	-0.81792037	-1.43765193	0.84457598
7	-2.94874667	-0.17963537	0.42870645
6	-3.96235807	-1.12061467	0.96208063
1	-4.95962986	-0.64713454	0.99222871
1	-3.69090019	-1.44013459	1.97487873
1	-4.00304647	-2.00729352	0.31802280
7	-1.04163783	-0.13548974	2.56179075
6	-2.82908726	1.00650845	1.31847113
1	-3.81944381	1.49065872	1.42407232
1	-2.14406244	1.71308911	0.83072472
6	-2.26965270	0.63647321	2.68748070
1	-2.10263685	1.58160049	3.23020200
1	-3.04644671	0.10229024	3.27747457
6	-0.13519190	-0.04787326	3.64553084
6	0.18689216	-1.19051827	4.42787431
6	1.09723007	-1.07930862	5.48679591
6	1.70875836	0.13287250	5.82267443
6	1.38766735	1.25244598	5.04829381
6	0.49355999	1.18815731	3.97237198

7	-1.51948001	-0.00219895	-2.64571578
6	-3.38128752	0.22029833	-0.94327351
1	-4.26854811	0.87428307	-0.82911178
1	-3.70536593	-0.69350707	-1.45514843
6	-2.34018749	0.91513189	-1.83422919
1	-2.88610509	1.59073007	-2.50842929
1	-1.68283527	1.55561944	-1.22339461
6	-1.48771492	0.21964634	-4.05060730
6	-0.30303029	0.66226845	-4.69085783
6	-0.29368929	0.83948488	-6.07864899
6	-1.42694825	0.61259762	-6.86810597
6	-2.58418486	0.16781725	-6.22261554
6	-2.63413590	-0.04487197	-4.83867868
6	-0.45168883	-2.53194442	4.15878806
1	1.32027745	-1.97017729	6.08035309
6	2.70875144	0.21959350	6.95057140
1	1.86662421	2.20999333	5.27182271
6	0.26808609	2.42825940	3.14210455
6	0.94382679	0.95076717	-3.89384957
1	0.62949396	1.18172492	-6.55379474
6	-1.40442016	0.85826345	-8.35767334
1	-3.47665506	-0.04956727	-6.81533966
6	-3.88788752	-0.62087467	-4.23017493
1	-0.36978068	-3.18218731	5.04031715
1	0.02839529	-3.06249572	3.31993727
1	-1.51301619	-2.42538407	3.89486849
1	0.08361087	2.16039785	2.09213084
1	1.14571404	3.08687735	3.19030205
1	-0.59398568	3.02016211	3.49107795
1	2.49384806	-0.52024148	7.73405863
1	2.70896936	1.21671457	7.41177806
1	3.73278148	0.02570878	6.59232177
1	1.72282968	1.37566434	-4.53989432
1	1.34992378	0.04260100	-3.42217623
1	0.74632325	1.66785919	-3.08182142
1	-4.45968890	0.11828648	-3.64741401
1	-3.63776508	-1.44756452	-3.54823960
1	-4.55503133	-1.00299599	-5.01369486
1	-0.43404929	0.58602288	-8.79587641
1	-1.57833675	1.92137253	-8.58934138
1	-2.18555429	0.28012299	-8.86985462
1	-0.58522451	-0.08579284	-2.23894252

Energy = -7584.953271 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 50

Atomic N.	X	Y	Z
8	0.68661660	0.26910078	0.30871769
8	1.41292298	1.83392063	-1.13047232
6	2.30862624	2.23349302	-2.17248039
1	3.19981952	2.73206473	-1.75555765
1	1.76130919	2.95144856	-2.79498441
1	2.60612288	1.37721006	-2.79222770
8	2.51728567	-0.26121835	-0.89962766
6	1.85677682	0.76044669	-0.16660169
6	2.70489289	1.44889463	0.91668263
1	3.52960560	2.01766416	0.45655843

1	2.02834432	2.18965046	1.36383685
6	3.25761388	0.50541686	1.99731948
1	2.49733773	-0.25198715	2.24557290
1	3.42393817	1.08854886	2.91645985
6	4.57713825	-0.17344580	1.60954662
1	5.33568624	0.60805306	1.42517360
1	4.94738849	-0.76442195	2.46230502
6	4.48896274	-1.07450058	0.37366205
1	3.84829554	-1.94771548	0.57665066
1	5.49340564	-1.46581987	0.13882057
6	3.95192574	-0.38055000	-0.87899210
1	4.44215336	0.59735465	-1.02658917
1	4.17385305	-0.99174994	-1.76623541
50	-0.97988421	1.18687245	-0.72990981
7	-2.40790564	-0.84540228	-0.19082074
6	-3.77711406	-0.33166656	-0.42264345
1	-4.51534221	-1.15322376	-0.40390776
1	-3.83564665	0.17436634	-1.39377061
1	-4.02697307	0.39381544	0.36124670
7	-0.98320966	0.01940120	-2.54094251
6	-2.02557284	-1.80286743	-1.26424360
1	-2.77749667	-2.61467545	-1.31863114
1	-1.05838317	-2.23905881	-0.98274914
6	-1.87735311	-1.12662212	-2.62204316
1	-1.48838651	-1.89106845	-3.31675424
1	-2.88010514	-0.85882352	-3.02300855
6	-0.35633197	0.40380474	-3.75441940
6	-0.69233021	1.61719686	-4.41033621
6	-0.02356131	1.98468983	-5.58684418
6	0.96756157	1.18403096	-6.16104018
6	1.28749021	-0.01440448	-5.51202092
6	0.65397952	-0.41795762	-4.33127355
7	-0.46698504	-1.01076380	2.72480187
6	-2.39229875	-1.52645952	1.13905254
1	-3.02774006	-2.43011453	1.05124057
1	-2.88813598	-0.85958188	1.85866409
6	-1.00263043	-1.90865979	1.69780873
1	-1.06184502	-2.93301161	2.08531628
1	-0.25615119	-1.91398871	0.89331074
6	-1.20173436	-0.69118404	3.88433113
6	-1.69239396	-1.69945806	4.75428453
6	-2.40812335	-1.32865912	5.90061113
6	-2.63038436	0.00515957	6.25291083
6	-2.08145493	0.98729886	5.42003460
6	-1.38069898	0.67033289	4.25277524
6	-1.77363873	2.52919390	-3.87978608
1	-0.30122382	2.92242100	-6.07615859
6	1.64890881	1.57994265	-7.44915094
1	2.07301411	-0.65220771	-5.92738320
6	1.09682746	-1.69423903	-3.66042303
6	-1.39026564	-3.16228520	4.53575588
1	-2.77551227	-2.12140111	6.55792915
6	-3.42838800	0.37389207	7.48028749
1	-2.20747263	2.04163219	5.68014257
6	-0.80844299	1.77970083	3.40635759
1	-2.16059523	3.17341375	-4.68103048
1	-1.40764416	3.19372501	-3.07977286
1	-2.60901946	1.95704037	-3.45368696

1	1.10571877	-1.57370234	-2.56882345
1	2.10550103	-1.97320898	-3.99414005
1	0.43492473	-2.54238600	-3.90103153
1	1.18561748	1.08127568	-8.31545057
1	2.71113395	1.29682314	-7.44474606
1	1.58369020	2.66283077	-7.62093800
1	-1.51165227	-3.71642304	5.47575588
1	-0.35809675	-3.30265214	4.18265993
1	-2.05624214	-3.63451289	3.79489089
1	-1.18834732	1.75793387	2.37115474
1	0.29018630	1.72371243	3.33700992
1	-1.06106873	2.75876454	3.83265443
1	-3.00746792	1.25526408	7.98453322
1	-3.45387867	-0.45305317	8.20299989
1	-4.47197791	0.61654893	7.22270763
1	-0.02746821	-0.20921929	2.26911492

Energy = -7584.957151 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 51

Atomic N.	X	Y	Z
8	1.25707346	2.57381613	-0.16342651
8	3.00433902	2.13256297	1.17740511
6	3.70530248	2.32034982	2.40655455
1	4.23957717	1.38268951	2.60305615
1	3.01229091	2.52091401	3.23596323
1	4.44246761	3.13804714	2.32822362
8	1.30176139	3.65604959	1.81912621
6	2.07800029	3.20836714	0.70426700
6	2.93272072	4.29239331	0.02191911
1	3.71487397	4.66167425	0.70550476
1	3.44818897	3.75829832	-0.78741923
6	2.13156296	5.47271329	-0.54891020
1	1.19847682	5.08853990	-0.99049780
1	2.70613465	5.91783125	-1.37613913
6	1.82925291	6.57225514	0.47663123
1	2.78659684	6.97418453	0.85351185
1	1.32230880	7.41189766	-0.02555232
6	0.98458737	6.11635111	1.67084411
1	-0.03256521	5.84442847	1.34523238
1	0.87639207	6.95631045	2.37800780
6	1.56270265	4.92656511	2.43994755
1	2.64052890	5.07170819	2.63141963
1	1.06803871	4.84456240	3.41922215
50	1.66402974	0.45974857	-0.27647876
7	-0.67150789	0.53519259	-1.07914626
6	-0.93994927	1.61417137	-2.05540494
1	-2.01245029	1.64411268	-2.31908725
1	-0.35171724	1.45831440	-2.96693120
1	-0.63502645	2.56679360	-1.60927696
7	-0.69937104	-2.62621234	-3.25632160
6	-1.10707196	-0.78964670	-1.59308011
1	-2.20199456	-0.77775020	-1.75266752
1	-0.89400597	-1.52484586	-0.80502618
6	-0.40003122	-1.23712637	-2.88422754
1	-0.66649069	-0.57947698	-3.71864713
1	0.69070305	-1.15781919	-2.75080839

6	-2.03425599	-3.01467915	-3.54746420
6	-2.65214546	-4.04018917	-2.78694496
6	-3.94619385	-4.45667543	-3.11380358
6	-4.66710264	-3.88593434	-4.16947207
6	-4.02749794	-2.90196001	-4.92913088
6	-2.72411673	-2.46695431	-4.65555842
7	0.48523947	-0.27010109	1.36001015
6	-1.36614697	0.84845111	0.20599845
1	-2.46140603	0.81881147	0.05474400
1	-1.06373811	1.87120541	0.46863530
6	-0.96112831	-0.09872792	1.33257132
1	-1.36184798	0.34264547	2.26391236
1	-1.48162218	-1.07484970	1.22359534
6	1.03865887	-0.92595963	2.49015759
6	1.67719128	-2.18826971	2.35000583
6	2.24839881	-2.81186729	3.46671582
6	2.20754125	-2.23883467	4.74154776
6	1.56614877	-1.00302747	4.87362734
6	0.98989811	-0.33695305	3.78466353
6	-1.92610182	-4.69904463	-1.63719781
1	-4.40663903	-5.24808511	-2.51695724
6	-6.08208464	-4.31586399	-4.47276802
1	-4.54613269	-2.47249642	-5.79030707
6	-2.06797582	-1.48348045	-5.59384604
6	1.73593774	-2.89608999	1.01677447
1	2.72777970	-3.78589137	3.33541561
6	2.85718113	-2.91489505	5.92526614
1	1.52387975	-0.52688828	5.85750226
6	0.35962646	1.01524609	4.00984130
1	-2.56267059	-5.45930941	-1.16816667
1	-1.64272856	-3.97864861	-0.85316643
1	-1.00213127	-5.20725055	-1.96037218
1	-2.13944671	-0.44306437	-5.23661500
1	-2.55263062	-1.51708320	-6.57834095
1	-1.00061874	-1.71400814	-5.72202571
1	-6.22531472	-5.38903815	-4.28510035
1	-6.34523431	-4.11360328	-5.51986894
1	-6.80704429	-3.77621690	-3.84266643
1	1.94953221	-3.96432435	1.15774740
1	2.52162623	-2.48640998	0.36196802
1	0.78780446	-2.79255480	0.47038626
1	-0.72026411	0.93514782	4.21781694
1	0.48067118	1.66527684	3.13260843
1	0.81348384	1.50801100	4.88102827
1	3.89795009	-2.57731597	6.05589258
1	2.88301691	-4.00601713	5.79861835
1	2.32333586	-2.69042155	6.85901332
1	-0.28641171	-3.25977589	-2.57407854

Energy = -7584.958954 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 52

Atomic N.	X	Y	Z
8	0.43047762	0.66193483	0.55261284
8	1.15702848	2.15279010	-0.98488812
6	2.16046080	2.59688186	-1.89135431
1	1.65325456	3.24981810	-2.61344418

1	2.61830792	1.75375909	-2.43077107
1	2.95048651	3.18450722	-1.38892038
8	2.33911214	0.16617376	-0.54063657
6	1.57181901	1.22164275	0.06768939
6	2.31733295	2.01361602	1.16410464
1	3.17693466	2.55835541	0.73964268
1	1.59181662	2.77654620	1.47945323
6	2.76350018	1.18135733	2.37565323
1	1.97757244	0.44899156	2.61309685
1	2.84050542	1.84792313	3.24906636
6	4.11319276	0.48017276	2.18330610
1	4.89126043	1.24503740	2.00805900
1	4.39381926	-0.03379944	3.11703927
6	4.14576259	-0.52372956	1.02670621
1	3.47343136	-1.37198468	1.23396188
1	5.16460103	-0.93818355	0.93514668
6	3.75357603	0.06499047	-0.33157684
1	4.25995075	1.03380379	-0.49357570
1	4.08746368	-0.60926374	-1.13545790
50	-1.49151744	1.41829491	0.07868229
7	-3.85790737	0.22899707	-0.59067274
6	-4.68341356	1.03061900	-1.49754309
1	-5.71008717	0.62292659	-1.58859985
1	-4.23388084	1.07182766	-2.49640721
1	-4.74420762	2.05905077	-1.11714049
7	-1.28761757	-0.58381516	-1.86453758
6	-3.60133131	-1.12093915	-1.10753946
1	-4.53980973	-1.61031809	-1.44314033
1	-3.20017107	-1.72598120	-0.28265680
6	-2.60239008	-1.13856277	-2.26368433
1	-2.50604242	-2.18006616	-2.62235876
1	-2.97469687	-0.55172327	-3.11259433
6	-0.32691522	-0.55100428	-2.94222812
6	-0.41101960	0.43774703	-3.94328957
6	0.53104862	0.42766645	-4.98091110
6	1.55610314	-0.52029544	-5.04969682
6	1.63166559	-1.47523377	-4.02929575
6	0.70901337	-1.51092756	-2.97894199
7	-2.13974010	0.14509721	1.70093275
6	-4.43205410	0.23161891	0.76595184
1	-5.40754675	-0.29823527	0.79263847
1	-4.62013356	1.28666195	1.02037794
6	-3.49572246	-0.37213385	1.81049121
1	-3.93844011	-0.13614941	2.79841690
1	-3.53186366	-1.48176632	1.74236621
6	-1.31998396	-0.18460921	2.81972339
6	-0.79765631	-1.48931617	2.99592758
6	-0.01293443	-1.78075432	4.11985577
6	0.27854296	-0.81967099	5.09165355
6	-0.24308398	0.46643894	4.90924365
6	-1.02715463	0.79943234	3.79882075
6	-1.46322272	1.51855503	-3.91767561
1	0.46735398	1.20278920	-5.74878156
6	2.54196394	-0.52242460	-6.19308584
1	2.43443265	-2.21632273	-4.04664413
6	0.85034115	-2.54622125	-1.88908149
6	-1.03999844	-2.56855794	1.97192290
1	0.39366481	-2.79008813	4.22870400

6	1.15830760	-1.14229248	6.27575610
1	-0.03349969	1.23803186	5.65522923
6	-1.54318053	2.21078239	3.65900624
1	-1.11300626	2.40575658	-4.46118733
1	-1.70499782	1.82127855	-2.88869964
1	-2.39900871	1.19490110	-4.40318205
1	1.10124885	-2.06807092	-0.92883511
1	1.65876695	-3.24762030	-2.13048335
1	-0.06758819	-3.13959605	-1.75063052
1	2.20517335	-1.18400106	-7.00693260
1	3.52913122	-0.88071783	-5.87070649
1	2.66320802	0.48283015	-6.61878177
1	-0.24998527	-3.33008671	2.01087247
1	-1.05964102	-2.13262255	0.96388901
1	-2.00174653	-3.08376544	2.12835019
1	-2.59689319	2.23200897	3.34922664
1	-0.98138484	2.77270613	2.89464971
1	-1.44021496	2.75678460	4.60638532
1	2.19290473	-0.80326713	6.10592372
1	1.19372647	-2.22347840	6.46583731
1	0.80186746	-0.64529510	7.18923059
1	-0.89844195	-1.16821316	-1.11903322

Energy = -7584.953729 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 53

Atomic N.	X	Y	Z
8	0.01278365	1.20349236	0.79627088
8	0.98079942	2.82447079	-0.42741210
6	2.11005352	3.33914885	-1.13409957
1	2.71123705	4.00920537	-0.49559941
1	1.71479283	3.91516688	-1.97941968
1	2.73582794	2.52449130	-1.52403084
8	2.22103538	0.96498478	0.42548828
6	1.18484858	1.88126883	0.73873224
6	1.44623718	2.76798643	1.97218189
1	2.24794416	3.49547478	1.76291879
1	0.52229809	3.34995115	2.09344097
6	1.76707769	1.99682330	3.26148645
1	1.14948097	1.08549339	3.30196196
1	1.46511467	2.61208005	4.12319503
6	3.25433565	1.65059117	3.41263617
1	3.83227662	2.59175048	3.40873991
1	3.42630165	1.19052839	4.39884014
6	3.81031581	0.72465528	2.32524424
1	3.38514603	-0.28585534	2.42520584
1	4.90027550	0.62084338	2.46191760
6	3.56613131	1.19959470	0.89270250
1	3.85409062	2.25804737	0.77828193
1	4.18964772	0.61697738	0.19882988
50	-1.42915439	2.24855595	-0.47659472
7	-3.11785186	0.36756349	-0.38426796
6	-4.33784034	1.01678925	-0.91695844
1	-5.15119721	0.28120993	-1.04875084
1	-4.12409299	1.48305268	-1.88605258
1	-4.66773211	1.80012229	-0.22296148
7	-1.11376847	1.11960793	-2.26901060

6	-2.59609548	-0.62388325	-1.36751815
1	-3.40175960	-1.33292864	-1.64062815
1	-1.80341931	-1.18991689	-0.86682413
6	-2.04216317	0.05357510	-2.61759160
1	-1.53971760	-0.73265634	-3.20916486
1	-2.87645841	0.40814648	-3.26366821
6	-0.15242603	1.45191897	-3.26039801
6	-0.26570159	2.63665330	-4.03038504
6	0.71690100	2.94561550	-4.98248911
6	1.81616076	2.11291630	-5.21151828
6	1.91970674	0.94592048	-4.44420144
6	0.96612785	0.60175023	-3.47960458
7	-1.41462474	-1.72138711	1.39530761
6	-3.46727751	-0.26926628	0.91926487
1	-4.10577536	-1.14768929	0.71480598
1	-4.08312381	0.46209818	1.46576633
6	-2.31365398	-0.64651277	1.85548412
1	-1.71048298	0.25396510	2.05206761
1	-2.76826129	-0.93717609	2.81287834
6	-1.15707379	-2.83767345	2.22620282
6	-2.20024284	-3.67095367	2.70211396
6	-1.88099994	-4.76892753	3.51274561
6	-0.56586265	-5.10341582	3.84659338
6	0.45381687	-4.30913511	3.30958048
6	0.18706644	-3.19265093	2.51241099
6	-1.43188084	3.58041759	-3.85016447
1	0.60968591	3.86122994	-5.57066644
6	2.84409500	2.44355655	-6.26734753
1	2.78084702	0.28722634	-4.58822421
6	1.16130876	-0.64124745	-2.64902395
6	-3.63788765	-3.47974479	2.28102341
1	-2.69815049	-5.40110462	3.87031230
6	-0.25634262	-6.27141152	4.75155105
1	1.49650100	-4.55945483	3.52212541
6	1.32747958	-2.38465680	1.94614121
1	-1.55527247	4.21566549	-4.73776169
1	-1.29300195	4.25124346	-2.98650584
1	-2.36831809	3.03430618	-3.67414709
1	0.91919510	-0.44297551	-1.59625642
1	2.19936260	-0.99268473	-2.71568252
1	0.51496884	-1.46874290	-2.98416768
1	2.65571593	1.88232063	-7.19643713
1	3.85921614	2.18370751	-5.93474119
1	2.82927854	3.51217416	-6.52065882
1	-4.21589758	-4.38898067	2.49114587
1	-3.70134086	-3.27661034	1.20143967
1	-4.14213074	-2.64891559	2.79754925
1	1.24253442	-1.31527553	2.19158678
1	1.37724024	-2.44745023	0.84657794
1	2.28631740	-2.74703094	2.33814782
1	0.67605322	-6.77281051	4.45638303
1	-1.06454714	-7.01544824	4.73497785
1	-0.13288556	-5.94624610	5.79717595
1	-0.54321790	-1.29351560	1.08150049

Energy = -7584.954872 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 54

Atomic N.	X	Y	Z
8	0.49979286	0.38937695	0.34661808
8	1.01048766	2.27179225	-0.78034106
6	1.90770541	2.96426857	-1.64724842
1	2.64573905	3.55296830	-1.07458302
1	1.29530870	3.65587047	-2.23976284
1	2.42516555	2.26940945	-2.32311566
8	2.53370529	0.45555975	-0.62347832
6	1.56507214	1.19134467	0.11025752
6	2.08468021	1.88367631	1.38472490
1	2.82701966	2.66001069	1.13389107
1	1.20585827	2.40774085	1.78472345
6	2.65244683	0.92544623	2.44311741
1	2.02573673	0.02106620	2.47598202
1	2.56133502	1.40166717	3.43176559
6	4.12361194	0.55616126	2.21697498
1	4.73019402	1.47894758	2.25295265
1	4.47486470	-0.07318845	3.05069787
6	4.40296547	-0.16165768	0.89245395
1	3.92079027	-1.15247643	0.88011414
1	5.48857628	-0.33473806	0.79649419
6	3.93689077	0.59853106	-0.35142049
1	4.23449953	1.66077389	-0.29422170
1	4.41706276	0.17499041	-1.24587259
50	-1.31445422	1.23768304	-0.40175175
7	-3.86533008	-0.08463908	-0.64275953
6	-4.83206143	0.95946604	-0.99824773
1	-5.82266576	0.53810265	-1.26403284
1	-4.46334077	1.53849964	-1.85397686
1	-4.95291921	1.65195507	-0.15438305
7	-1.34579248	0.06415860	-2.20924748
6	-3.55880091	-0.95154466	-1.79367149
1	-4.49522984	-1.27891359	-2.29449404
1	-3.04095314	-1.84535244	-1.41949902
6	-2.63830896	-0.26813033	-2.80535514
1	-2.48780636	-0.98003740	-3.63590727
1	-3.16859485	0.59857828	-3.25495574
6	-0.26094604	0.06846255	-3.14016645
6	-0.13795879	1.07569298	-4.13133902
6	0.92773835	1.02917645	-5.04148000
6	1.88489831	0.01127789	-5.00965211
6	1.75296152	-0.97516601	-4.02538695
6	0.70550369	-0.96777117	-3.09720215
7	-2.27092468	-0.51278274	1.83088053
6	-4.33187970	-0.84925642	0.52597092
1	-5.08061484	-1.61410163	0.23241885
1	-4.85195903	-0.14623889	1.19712183
6	-3.20992371	-1.52726614	1.30837915
1	-3.66799002	-2.11295565	2.12637056
1	-2.67054349	-2.23640672	0.66791924
6	-1.45748943	-0.83715477	2.95712347
6	-0.56522624	-1.93163315	2.94043769
6	0.21793529	-2.17988808	4.07590735
6	0.17385286	-1.37167818	5.21518247
6	-0.68360417	-0.26570652	5.19005910
6	-1.49824487	0.01397333	4.08918661
6	-1.12442090	2.21450419	-4.22500677

1	1.01329464	1.82007131	-5.79209205
6	3.00960293	-0.03786548	-6.01659774
1	2.48906075	-1.78217418	-3.97622667
6	0.61882850	-2.05816518	-2.06247602
6	-0.37297570	-2.78920410	1.71518235
1	0.91145330	-3.02411867	4.04817474
6	1.01701902	-1.67846407	6.42919382
1	-0.72477072	0.40195711	6.05432148
6	-2.39577915	1.23000100	4.11651236
1	-0.67821200	3.07446433	-4.74236498
1	-1.45888357	2.54104272	-3.22887510
1	-2.02769997	1.92910016	-4.78790741
1	0.82772830	-1.64488457	-1.06561998
1	1.34689664	-2.85247612	-2.27539058
1	-0.38723900	-2.50034624	-2.02923358
1	2.77423936	-0.72402268	-6.84588907
1	3.94322742	-0.39395858	-5.55855762
1	3.19823126	0.95195797	-6.45430338
1	0.57835936	-3.33252344	1.78070414
1	-0.34505367	-2.16748065	0.81023647
1	-1.16938570	-3.54009873	1.59428380
1	-3.46167419	0.96650609	4.00993988
1	-2.15157552	1.94519580	3.31350367
1	-2.28903137	1.76269582	5.06946145
1	1.40013188	-0.75949867	6.89473496
1	1.87479043	-2.31297458	6.16881236
1	0.43408752	-2.21207167	7.19670790
1	-2.80908595	0.32488669	2.05459875

Energy = -7584.949835 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 55

Atomic N.	X	Y	Z
8	0.31461575	1.53720433	0.84911358
8	1.79577628	1.26086271	-0.95088382
6	1.79256494	2.60855856	-1.41776335
1	0.89007485	3.14983115	-1.08670940
1	1.79721187	2.55741662	-2.51406581
1	2.68631218	3.16604025	-1.08675780
8	1.58304382	-0.32738631	0.64306135
6	1.54361470	1.09944965	0.48269859
6	2.62749740	1.84707794	1.29845998
1	3.58633811	1.80767751	0.75649013
1	2.31310848	2.89914375	1.31283145
6	2.82160765	1.34190357	2.73606607
1	1.84895307	1.05266782	3.16200289
1	3.19825191	2.17343060	3.35289804
6	3.82233526	0.18142230	2.83358438
1	4.77877487	0.50840330	2.38777917
1	4.03570893	-0.03191791	3.89372437
6	3.36758971	-1.11426113	2.15247961
1	2.54808773	-1.56945779	2.73005511
1	4.20004413	-1.83945366	2.15117577
6	2.87923196	-0.94942110	0.71254373
1	3.60688415	-0.40452136	0.08782393
1	2.74915929	-1.94684019	0.26227206
50	-1.65091251	1.25817208	0.11257124

7	-3.58598976	-0.42331735	-0.83029187
6	-4.57211653	0.17577179	-1.73417291
1	-5.43582559	-0.49839996	-1.90216845
1	-4.12137064	0.41493878	-2.70269572
1	-4.93943953	1.11356550	-1.29616504
7	-0.87731738	-0.38716793	-2.18457822
6	-2.93266738	-1.60618600	-1.40656147
1	-3.68058669	-2.34812729	-1.75916128
1	-2.34999635	-2.08895484	-0.60935693
6	-2.00014621	-1.27563367	-2.57202392
1	-1.63116129	-2.22967430	-2.99285309
1	-2.55146800	-0.78035865	-3.38108193
6	-0.10683889	0.05690386	-3.32571040
6	-0.56481048	1.12103180	-4.12710520
6	0.20479433	1.51637028	-5.23224622
6	1.41203332	0.89734605	-5.56204249
6	1.84950578	-0.15336744	-4.74510484
6	1.11255506	-0.58747905	-3.64043817
7	-2.03767537	-0.24488796	1.60212800
6	-4.21018466	-0.68132991	0.47861709
1	-5.01095135	-1.44666116	0.39723651
1	-4.68603032	0.26340503	0.78650688
6	-3.21319232	-1.10969599	1.54846239
1	-3.75782701	-1.08911287	2.51147527
1	-2.94467787	-2.17450608	1.39318394
6	-1.26387617	-0.44802231	2.78369820
6	-0.56583799	-1.66124276	3.00702751
6	0.10702552	-1.86282441	4.21990479
6	0.13763453	-0.89242996	5.22459692
6	-0.53371339	0.31122194	4.98213620
6	-1.22653243	0.55186751	3.78992079
6	-1.84673083	1.85994479	-3.83398877
1	-0.15161876	2.35092237	-5.84111865
6	2.22465865	1.34167334	-6.75415215
1	2.79573152	-0.65087797	-4.97137152
6	1.63431950	-1.71623147	-2.78690695
6	-0.48454769	-2.72848472	1.94491027
1	0.64105352	-2.80518108	4.37149922
6	0.90467016	-1.11317812	6.50635425
1	-0.52218912	1.09168896	5.74767692
6	-1.91506337	1.88052133	3.60271628
1	-1.78830575	2.89137236	-4.20566586
1	-2.05957433	1.89403096	-2.75667743
1	-2.70985836	1.38962809	-4.33410701
1	1.84280656	-1.36665748	-1.76482387
1	2.56863545	-2.11251771	-3.20320340
1	0.92085924	-2.55286504	-2.71898112
1	2.26325387	0.55714092	-7.52539286
1	3.26353041	1.56311650	-6.46892542
1	1.79859096	2.24277564	-7.21392987
1	0.41845608	-3.33878811	2.08109927
1	-0.44406023	-2.26632956	0.94898397
1	-1.34628957	-3.41519911	1.96927182
1	-2.91571875	1.76501344	3.16340307
1	-1.33635082	2.53126245	2.92683922
1	-2.00881902	2.40698177	4.56190918
1	1.91278245	-0.67218958	6.44672739
1	1.02722636	-2.18333473	6.72151030

1 0.39833070 -0.64665332 7.36309246
 1 -0.24496830 -0.89663027 -1.55933635
 Energy = -7584.950155 Hartree
 Number of imaginary frequencies = 0.

Compound I3b isomer 56

Atomic N.	X	Y	Z
8	1.99850946	1.41592871	1.31965376
8	2.81128765	0.83552626	-0.68588344
6	3.78348585	0.15940566	-1.48616574
1	3.29298461	-0.05964368	-2.44270801
1	4.11006508	-0.78042122	-1.01666288
1	4.65877001	0.80150150	-1.68078800
8	3.84137493	0.08578942	1.31229662
6	3.18969538	1.21999556	0.71658619
6	4.03137203	2.50400262	0.66087738
1	4.89853369	2.36950481	-0.00584942
1	3.37677983	3.24158305	0.17876919
6	4.49428375	3.02195423	2.03199347
1	3.68201664	2.87450650	2.76106044
1	4.65323521	4.10915828	1.95872113
6	5.79166311	2.37713414	2.53551835
1	6.59542538	2.59042482	1.80843057
1	6.09703054	2.85926207	3.47816809
6	5.71184325	0.86187683	2.74837240
1	5.01965675	0.62211547	3.57168163
1	6.70516539	0.48696465	3.04875843
6	5.26309636	0.07114068	1.51724756
1	5.80905810	0.40845636	0.61826958
1	5.49786779	-0.99454542	1.65780812
50	0.61631976	-0.01245286	0.45837041
7	-1.04232026	1.01024743	2.07791645
6	-0.32684142	1.98694665	2.93486026
1	-1.04590324	2.53091452	3.57359563
1	0.23828387	2.69069531	2.31879040
1	0.39465164	1.45504810	3.56606668
7	-0.50173222	1.39057838	-0.72136406
6	-1.99211851	1.70862555	1.16911860
1	-2.59761211	2.43715890	1.74290691
1	-2.65400454	0.95111717	0.73369800
6	-1.25074160	2.39515619	0.02089535
1	-2.01142982	2.86257680	-0.62927940
1	-0.63942471	3.22769743	0.42345363
6	-0.27727928	1.58274511	-2.10273568
6	0.25938304	2.78951988	-2.63046534
6	0.42601009	2.93199226	-4.01415217
6	0.11097314	1.91079567	-4.91534741
6	-0.37603912	0.71148049	-4.38363172
6	-0.57853951	0.52838794	-3.01096648
7	-2.21617298	-1.76718438	1.33605996
6	-1.71142336	0.03798407	2.99423632
1	-2.22647940	0.60500258	3.79349385
1	-0.90548650	-0.53492638	3.48036022
6	-2.74631529	-0.92275074	2.41116390
1	-3.10932794	-1.52447978	3.26863282
1	-3.61707362	-0.35904182	2.04867333
6	-2.94823747	-2.92890447	0.96830957

6	-4.23108299	-2.82500216	0.38321869
6	-4.90898748	-3.99569267	0.01783084
6	-4.35265786	-5.26723317	0.18409145
6	-3.06300553	-5.34501704	0.72384503
6	-2.35514269	-4.20701717	1.12196559
6	0.73701733	3.89695850	-1.72337171
1	0.84581276	3.86775174	-4.39455685
6	0.27024325	2.10039586	-6.40496181
1	-0.62782452	-0.10923440	-5.06119616
6	-1.13027689	-0.78833207	-2.52218050
6	-4.85685101	-1.48617055	0.07892854
1	-5.89722055	-3.90125809	-0.43961428
6	-5.11603168	-6.51289594	-0.19626239
1	-2.59187441	-6.32352468	0.84670131
6	-0.96588609	-4.35120037	1.69830099
1	1.44410966	4.54748507	-2.25530367
1	1.23987966	3.47915047	-0.83985392
1	-0.08408808	4.53555811	-1.36018044
1	-0.33690037	-1.45387806	-2.14159949
1	-1.63555199	-1.32404258	-3.33705157
1	-1.83394713	-0.64351198	-1.69124312
1	-0.67822843	2.40949047	-6.87344400
1	0.58607856	1.17038585	-6.89847347
1	1.01350743	2.87732326	-6.63156374
1	-5.62010020	-1.59033456	-0.70294247
1	-4.09860274	-0.77156843	-0.27317670
1	-5.35141390	-1.04020158	0.95674692
1	-0.88879362	-3.91580755	2.70775024
1	-0.20205343	-3.85707202	1.07555388
1	-0.68992551	-5.41029768	1.77357908
1	-4.44855665	-7.28514869	-0.60321271
1	-5.88639652	-6.29527344	-0.94831405
1	-5.62492800	-6.95111682	0.67715559
1	-1.24463983	-2.01021890	1.53401947

Energy = -7584.955874 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 57

Atomic N.	X	Y	Z
8	1.10581680	-1.89819343	0.69071220
8	1.52964618	0.21077556	1.39594784
6	2.39469793	1.34816808	1.32966669
1	1.76448809	2.23771300	1.45736462
1	2.91266471	1.40617258	0.36209273
1	3.13432751	1.32317797	2.14694299
8	3.09103516	-1.00893221	0.06002198
6	2.15541846	-1.18825284	1.11597648
6	2.72283084	-1.68991430	2.44894706
1	3.43642772	-0.96180053	2.86875293
1	1.85691263	-1.71720698	3.12248352
6	3.36803515	-3.08275760	2.36504139
1	2.75630478	-3.71628900	1.70439900
1	3.32702430	-3.54496718	3.36324254
6	4.82820861	-3.06362217	1.89704466
1	5.42306283	-2.47490654	2.61822149
1	5.23476709	-4.08713876	1.92948441
6	5.04282726	-2.48261986	0.49538581

1	4.57030167	-3.12246475	-0.26699393
1	6.12324356	-2.46780096	0.27253716
6	4.50829933	-1.06158755	0.30817576
1	4.79476063	-0.41952645	1.15996087
1	4.94539616	-0.61681355	-0.59756592
50	-0.32984175	-0.50867206	-0.08968697
7	-1.91022901	1.77065378	0.63932859
6	-1.26359447	3.01238434	1.07984558
1	-1.99583554	3.79561608	1.36195354
1	-0.61504646	3.39604709	0.28244884
1	-0.64417986	2.79314904	1.95864857
7	-1.00299446	2.52990346	-2.17785896
6	-2.80593101	1.97601427	-0.52069932
1	-3.77668269	2.38945285	-0.17556399
1	-3.02061932	0.98654842	-0.95798920
6	-2.30599171	2.91628184	-1.61897476
1	-3.09473726	2.92693889	-2.39622121
1	-2.25451429	3.94113721	-1.22293264
6	-0.65611899	3.02263354	-3.46328880
6	-0.46884686	4.40815174	-3.68018618
6	-0.11146937	4.85844818	-4.95809937
6	0.09379231	3.98474976	-6.02956988
6	-0.05608232	2.61434754	-5.78482751
6	-0.43052416	2.11850910	-4.53210671
7	-1.73063567	-1.13973757	1.36680866
6	-2.64625856	1.14586510	1.75656853
1	-3.59629282	1.68989992	1.94492789
1	-2.01675884	1.24200674	2.65110284
6	-2.94395342	-0.34210390	1.54512991
1	-3.49685180	-0.69115809	2.43209742
1	-3.64848485	-0.46532769	0.69711411
6	-1.65219387	-2.34900292	2.11406113
6	-1.73113375	-3.60627047	1.46324717
6	-1.67482660	-4.78332538	2.21843057
6	-1.52824088	-4.76922023	3.60983390
6	-1.43129674	-3.52460965	4.23886444
6	-1.48306179	-2.32189082	3.52195308
6	-0.57335563	5.40564037	-2.55264026
1	0.03648847	5.93119766	-5.10781738
6	0.45380481	4.49800822	-7.40303989
1	0.11442895	1.90363412	-6.59754813
6	-0.58307309	0.62950818	-4.33312835
6	-1.86346238	-3.70497655	-0.03664844
1	-1.75023403	-5.74299685	1.70007467
6	-1.43985294	-6.05499456	4.39683586
1	-1.29513502	-3.48326056	5.32308285
6	-1.30669075	-1.01828168	4.25966436
1	-0.02533706	6.32353270	-2.80245025
1	-0.15240032	4.99116463	-1.62476612
1	-1.61421641	5.69655395	-2.33910888
1	0.13907648	0.22886924	-3.60344321
1	-0.42394534	0.09718694	-5.27925383
1	-1.58608288	0.36261078	-3.96339147
1	-0.43732990	4.57748395	-8.04609690
1	1.16023203	3.82669321	-7.91101252
1	0.90867154	5.49644632	-7.34985653
1	-2.22745345	-4.69887880	-0.32970165
1	-0.88846269	-3.56013526	-0.53041191

1	-2.55078534	-2.94722255	-0.43765453
1	-2.25742316	-0.47748944	4.39388377
1	-0.63041649	-0.35132277	3.70501882
1	-0.88948204	-1.19372852	5.26006466
1	-0.42344139	-6.47800796	4.35524156
1	-2.12319601	-6.81781859	3.99752951
1	-1.68618924	-5.89461041	5.45509298
1	-0.88179730	1.51656160	-2.12072035

Energy = -7584.949418 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 58

Atomic N.	X	Y	Z
8	0.45110712	-1.90322757	1.21661450
8	1.76106704	-0.05856877	1.10791684
6	2.95109221	0.53708793	0.58362992
1	2.73460120	1.60173927	0.42695926
1	3.24355900	0.08176464	-0.37294773
1	3.77993369	0.45122478	1.30558129
8	2.45580396	-2.15838766	0.19692692
6	1.75137318	-1.60734574	1.30132367
6	2.34455602	-1.87749556	2.68886272
1	3.34412251	-1.42169090	2.78222882
1	1.68080609	-1.34305988	3.38019731
6	2.40063677	-3.36842572	3.05970082
1	1.48246491	-3.85720805	2.69898950
1	2.38694725	-3.45411062	4.15703634
6	3.64392011	-4.09336716	2.53024482
1	4.54189833	-3.61727687	2.96324277
1	3.64311569	-5.13275385	2.89577895
6	3.78012413	-4.09872495	1.00380902
1	2.96868683	-4.68493350	0.54352444
1	4.72634386	-4.59428045	0.72765589
6	3.77554100	-2.71076820	0.36083133
1	4.43811258	-2.02104872	0.91296802
1	4.15740501	-2.77667479	-0.66832123
50	-0.49386051	-0.32077726	0.11811357
7	-0.92086705	2.52095570	0.08353394
6	0.21437871	3.44477093	-0.02282773
1	-0.09829382	4.50798413	0.01156231
1	0.75752686	3.25918012	-0.95782701
1	0.89542620	3.26346089	0.81827867
7	-0.47050547	1.93129155	-2.88016865
6	-1.92018373	2.72246311	-0.98891803
1	-2.56663548	3.59019538	-0.74051420
1	-2.57483661	1.83510880	-1.00809850
6	-1.37841304	2.98052008	-2.39618089
1	-2.26482380	3.08537681	-3.05164466
1	-0.86836405	3.95485019	-2.41517757
6	-0.27178668	1.81526316	-4.28106662
6	0.35261028	2.85398889	-5.01114998
6	0.54752238	2.69962975	-6.39015766
6	0.16998477	1.54093294	-7.07460337
6	-0.40889364	0.50788519	-6.32762507
6	-0.64188533	0.62303932	-4.95359134
7	-1.65606170	0.17497030	1.81698993
6	-1.55754941	2.63339358	1.41089859

1	-2.17317041	3.55650217	1.46677932
1	-0.74978892	2.71862468	2.14986345
6	-2.41849033	1.42348236	1.78807133
1	-2.84500522	1.62691599	2.78348777
1	-3.29142122	1.35913580	1.10660342
6	-1.86153199	-0.66586669	2.94718300
6	-2.53720665	-1.90502644	2.81277866
6	-2.74768179	-2.70660608	3.94089506
6	-2.30040616	-2.33456622	5.21315535
6	-1.61882391	-1.11955334	5.33093244
6	-1.38618101	-0.28651068	4.22881918
6	0.87890147	4.09313693	-4.32939546
1	1.03756849	3.50829164	-6.93881163
6	0.36849434	1.41014904	-8.56556814
1	-0.69931457	-0.41827887	-6.83019879
6	-1.27704285	-0.52411006	-4.20488349
6	-3.02835258	-2.38850633	1.47047037
1	-3.28186970	-3.65274500	3.81944340
6	-2.51284257	-3.23332987	6.40790856
1	-1.23965874	-0.81239996	6.30955004
6	-0.58615978	0.97775999	4.42010627
1	1.65156383	4.56985262	-4.94665353
1	1.31913207	3.84410108	-3.35262934
1	0.09385737	4.84560667	-4.15299224
1	-0.60412437	-0.95021047	-3.44326574
1	-1.54478271	-1.33280173	-4.89638892
1	-2.19463764	-0.21624434	-3.67839892
1	-0.55289046	1.66184686	-9.11480624
1	0.64213229	0.38354182	-8.84647680
1	1.15759462	2.08487888	-8.92428929
1	-3.78554790	-3.17427852	1.59470206
1	-2.20474165	-2.82436482	0.88143167
1	-3.46292663	-1.57294721	0.87590525
1	0.15077023	1.09344639	3.61172106
1	-0.05613579	0.95684132	5.38152836
1	-1.21644064	1.88163364	4.41599561
1	-1.72510282	-4.00086805	6.47344480
1	-3.47453400	-3.76176450	6.34617961
1	-2.49417702	-2.66357661	7.34684373
1	-0.71673211	1.03185669	-2.46162117

Energy = -7584.949422 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 59

Atomic N.	X	Y	Z
8	2.99243518	-0.59542793	-0.64113663
8	2.45648337	-0.40020312	-2.83490929
6	2.62327981	-0.78745897	-4.20064937
1	1.78799479	-0.33517095	-4.75037356
1	2.58104151	-1.88133964	-4.31536497
1	3.56687743	-0.40730175	-4.62669345
8	2.97950778	-2.46156113	-1.98530816
6	3.32471002	-1.05304413	-1.87892947
6	4.80592756	-0.73178299	-2.19653090
1	5.12058370	-1.23982228	-3.12210204
1	4.81379791	0.34820120	-2.40497583
6	5.79512904	-1.02594029	-1.06126484

1	5.37160626	-0.62387730	-0.12926885
1	6.72451842	-0.46783551	-1.25682398
6	6.14187748	-2.50748774	-0.88284746
1	6.70679984	-2.85697921	-1.76550951
1	6.82029357	-2.61823861	-0.02164122
6	4.92706429	-3.42397927	-0.69804362
1	4.34195810	-3.12685990	0.18649982
1	5.28295320	-4.45198704	-0.51680454
6	3.99589196	-3.47034657	-1.91509036
1	4.60066964	-3.47374499	-2.84292109
1	3.41873619	-4.40690764	-1.90470426
50	1.69390340	0.61921592	0.48729901
7	-0.14313866	-0.94332878	0.05337107
6	0.26065603	-2.36763793	0.11406252
1	-0.58430764	-3.01948209	-0.16994919
1	0.58499240	-2.62600192	1.12865267
1	1.10338859	-2.52762275	-0.57004261
7	-2.21239422	-0.49483706	3.26124317
6	-1.31655511	-0.66692764	0.92441546
1	-2.16800932	-1.28810724	0.58829654
1	-1.58806219	0.38597118	0.76948235
6	-1.07322175	-0.89641997	2.42572303
1	-0.84311730	-1.94868513	2.62376573
1	-0.19750994	-0.31240235	2.75202951
6	-3.45352109	-1.17586740	3.13740012
6	-3.56483572	-2.54347560	3.48585583
6	-4.81195615	-3.17292999	3.38219664
6	-5.96597645	-2.49371860	2.97969557
6	-5.84609891	-1.12815813	2.69677854
6	-4.61906265	-0.46052334	2.76298210
7	0.36269197	1.66727112	-0.79720898
6	-0.45373829	-0.57794829	-1.36253581
1	-1.35909506	-1.11870685	-1.69474229
1	0.40342933	-0.91369133	-1.96141566
6	-0.63645508	0.92867622	-1.55894046
1	-0.57051767	1.10675993	-2.64969245
1	-1.66114903	1.24161161	-1.26636798
6	0.38424934	3.08271684	-0.96491883
6	-0.05065807	3.93247435	0.08647401
6	-0.00971036	5.32236691	-0.07775389
6	0.44435785	5.91774326	-1.25960570
6	0.86243065	5.07253666	-2.29127270
6	0.84635893	3.67678811	-2.16850596
6	-2.39456515	-3.32157694	4.03681818
1	-4.88345677	-4.22826677	3.65820979
6	-7.29057287	-3.20627405	2.85117078
1	-6.73446417	-0.56136187	2.40691286
6	-4.55707095	1.01613793	2.44905776
6	-0.57971753	3.36942790	1.38472188
1	-0.35292104	5.95880208	0.74233049
6	0.51249204	7.41938081	-1.40055377
1	1.23043801	5.51000911	-3.22353206
6	1.35092127	2.83328602	-3.31183502
1	-2.75127399	-4.15587918	4.65489912
1	-1.75062026	-2.67940844	4.65438414
1	-1.76375610	-3.75761006	3.24492749
1	-4.21768235	1.61453070	3.31112174
1	-5.54992577	1.39019150	2.17055362

1	-3.87535104	1.23722582	1.61221354
1	-7.44284730	-3.58368203	1.82730767
1	-8.13100234	-2.53626133	3.07866809
1	-7.34785113	-4.06956743	3.52814737
1	-1.02683278	4.16643842	1.99353903
1	0.21270982	2.89676167	1.98585497
1	-1.34511067	2.60074376	1.20441198
1	0.53285793	2.54032738	-3.99081504
1	1.81969710	1.90935777	-2.94785296
1	2.07900520	3.39543374	-3.91235003
1	1.47303094	7.80981037	-1.02794608
1	-0.28329382	7.91278093	-0.82546438
1	0.42002599	7.72841883	-2.45057868
1	-2.35036714	0.51225940	3.19429971

Energy = -7584.949989 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 60

Atomic N.	X	Y	Z
8	1.96421594	-0.59078923	-0.97478765
8	2.37858397	1.61461088	-0.85139746
6	2.82328219	2.82640709	-1.46127380
1	2.24931037	3.63568384	-0.99345537
1	2.62781531	2.82488353	-2.54283957
1	3.89711477	2.99988699	-1.27465401
8	2.88372409	0.36013929	-2.80446955
6	2.89236827	0.30724545	-1.37717453
6	4.27035442	0.06147620	-0.73627220
1	4.94772968	0.90974553	-0.92893716
1	4.06857348	0.05847271	0.34316491
6	4.94215667	-1.25613640	-1.15280810
1	4.17250197	-2.04096341	-1.22242993
1	5.62979791	-1.56646333	-0.35076300
6	5.73644036	-1.16174083	-2.46143631
1	6.53450379	-0.40868785	-2.33450682
1	6.24779647	-2.11955434	-2.64925983
6	4.90070443	-0.78842036	-3.69016820
1	4.18785930	-1.59293640	-3.93336017
1	5.56813024	-0.68269355	-4.56234363
6	4.10666999	0.51148023	-3.54627575
1	4.74031990	1.31212009	-3.12600813
1	3.77017711	0.85105777	-4.53714575
50	0.32897614	0.35455735	0.05663100
7	-0.74899996	-1.76035682	-0.65739529
6	0.08170075	-2.96608335	-0.45440905
1	-0.40374171	-3.86031042	-0.88510738
1	0.25118379	-3.11887681	0.61759805
1	1.04847338	-2.79869273	-0.94122658
7	-1.39623653	-1.84326953	2.33948603
6	-2.10851937	-1.90010404	-0.06189201
1	-2.73134985	-2.51825020	-0.73630973
1	-2.55605938	-0.89463723	-0.03954315
6	-2.19602697	-2.53999656	1.32378169
1	-3.27259772	-2.55216150	1.58528539
1	-1.88333230	-3.59188072	1.26340105
6	-1.69870269	-2.07750898	3.70815490
6	-1.50813588	-3.35401210	4.28597127

6	-1.80095533	-3.53819676	5.64380077
6	-2.25115667	-2.49746488	6.46126625
6	-2.39071768	-1.23133275	5.88015106
6	-2.13041002	-1.00292136	4.52553261
7	-0.93803856	0.91015441	-1.58765081
6	-0.86396758	-1.47773467	-2.12015735
1	-1.42138582	-2.29748140	-2.61191937
1	0.16395394	-1.45652378	-2.50661683
6	-1.53403736	-0.13752408	-2.40474180
1	-1.41634556	0.04247551	-3.48910464
1	-2.63033304	-0.21097832	-2.23519335
6	-1.23076704	2.25349861	-1.93733079
6	-1.97092209	3.08519128	-1.05429815
6	-2.22379237	4.42055854	-1.39614711
6	-1.78044621	4.97843641	-2.59848174
6	-1.06213200	4.15033120	-3.46796808
6	-0.77529935	2.81408282	-3.16478385
6	-0.92910852	-4.50178951	3.49590456
1	-1.64271706	-4.52848677	6.07875656
6	-2.58348722	-2.73034272	7.91540890
1	-2.72104423	-0.39217247	6.49758586
6	-2.30088376	0.38470024	3.95310273
6	-2.52033182	2.55679054	0.24970333
1	-2.80137234	5.03843200	-0.70308095
6	-2.04478466	6.42607869	-2.93730744
1	-0.69428822	4.56052025	-4.41300680
6	0.04910010	2.00900365	-4.13892425
1	-0.49796123	-5.25155005	4.17187282
1	-0.13666011	-4.14919188	2.81953761
1	-1.68398229	-5.01617870	2.88003939
1	-1.35089655	0.80039312	3.57865052
1	-2.67768020	1.07249665	4.72024475
1	-3.01356537	0.40133336	3.11299394
1	-3.65979599	-2.92154491	8.05290418
1	-2.32824986	-1.85671724	8.53107479
1	-2.04375369	-3.59985604	8.31445313
1	-3.32568413	3.20607854	0.61903782
1	-1.74989319	2.50881435	1.03582249
1	-2.91375736	1.53737161	0.13198057
1	-0.58245333	1.44969018	-4.84890743
1	0.68720518	1.28222334	-3.61804538
1	0.68726340	2.67280424	-4.73881679
1	-1.15874392	7.05139342	-2.74270174
1	-2.87046169	6.83155433	-2.33700628
1	-2.30036061	6.55106809	-3.99914194
1	-1.38166089	-0.84072732	2.14568408

Energy = -7584.958010 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 61

Atomic N.	X	Y	Z
8	2.03820392	-1.45958848	-0.24339811
8	2.80281838	-0.20786042	-1.95610358
6	3.81804506	0.17132004	-2.88565334
1	4.62264213	0.75446499	-2.40715511
1	3.32955875	0.80508587	-3.63720566
1	4.24731096	-0.71165924	-3.38408203

8	3.46237448	-2.40336928	-1.76382891
6	3.16759286	-1.23581793	-0.97401726
6	4.33702362	-0.72987068	-0.09714487
1	5.26947125	-0.67237053	-0.68150691
1	4.06020046	0.30288722	0.16467810
6	4.56369115	-1.52885477	1.19391706
1	3.58581101	-1.69594752	1.66915030
1	5.15159221	-0.90810888	1.88832651
6	5.28849275	-2.86407155	0.99675010
1	6.32338148	-2.66804782	0.66330931
1	5.37215862	-3.37582557	1.96888023
6	4.62654222	-3.80149713	-0.01924714
1	3.60189434	-4.06019485	0.29095700
1	5.19592806	-4.74544435	-0.05364236
6	4.58212007	-3.24052026	-1.44453811
1	5.53401585	-2.72103299	-1.67002102
1	4.48667090	-4.06626153	-2.16443100
50	0.56780981	0.07037658	-0.06985394
7	-0.74426531	-1.02158219	-1.89369250
6	0.08373230	-2.11074827	-2.47266177
1	-0.52594495	-2.71662823	-3.16593071
1	0.49597966	-2.73872789	-1.67907965
1	0.93464699	-1.67327199	-3.00633342
7	-0.77682760	-1.24152488	0.96109874
6	-1.90531357	-1.59094062	-1.15409449
1	-2.43655066	-2.31795645	-1.79781688
1	-2.58303525	-0.76450340	-0.90881290
6	-1.46154423	-2.24217378	0.15566769
1	-2.37271554	-2.59442141	0.67310359
1	-0.86686737	-3.15039830	-0.06715090
6	-0.70020445	-1.42628409	2.36513109
6	-0.16512309	-2.60213637	2.95780232
6	-0.13880686	-2.72344950	4.35381787
6	-0.59935989	-1.71264902	5.20259545
6	-1.09181592	-0.54504536	4.60886900
6	-1.15716361	-0.38560759	3.22015392
7	-1.68078142	1.93006496	-1.74156707
6	-1.15528743	-0.14090724	-3.02733913
1	-1.59150217	-0.77470616	-3.82293027
1	-0.22569181	0.28610087	-3.43583738
6	-2.15775058	0.97717264	-2.75025058
1	-2.34402253	1.46560736	-3.72812997
1	-3.12107925	0.55612105	-2.43435685
6	-2.39244162	3.15317502	-1.58448603
6	-3.71501776	3.16764837	-1.08813805
6	-4.36956112	4.39757557	-0.93353116
6	-3.75257024	5.61716887	-1.22387389
6	-2.42894910	5.58226022	-1.68073396
6	-1.74156502	4.38014010	-1.86857946
6	0.45051764	-3.69580717	2.11903601
1	0.28407511	-3.63337324	4.78924673
6	-0.58308777	-1.88068665	6.70313763
1	-1.45521603	0.26594697	5.24596581
6	-1.73096645	0.88750487	2.64925374
6	-4.41747125	1.90141745	-0.66505005
1	-5.39188342	4.39548626	-0.54700594
6	-4.46862245	6.92999792	-1.01565062
1	-1.91496576	6.52016896	-1.90602870

6	-0.31376774	4.40243791	-2.36370572
1	1.11545384	-4.31716202	2.73398028
1	1.03381770	-3.26884093	1.28981368
1	-0.30573358	-4.36650520	1.68034587
1	-0.95268363	1.54130529	2.22213419
1	-2.25037102	1.46133689	3.42806620
1	-2.43091856	0.67188609	1.83046004
1	-1.55087133	-2.25458225	7.07468059
1	-0.38734250	-0.92687753	7.21284111
1	0.18587677	-2.60032091	7.01628259
1	-5.21389837	2.12821380	0.05533621
1	-3.71144548	1.20491254	-0.19025637
1	-4.88795000	1.37547252	-1.51151689
1	-0.18808181	3.82821380	-3.29591249
1	0.38890612	3.98267700	-1.62492925
1	0.00580734	5.43217202	-2.56585273
1	-4.11587632	7.43660043	-0.10359785
1	-5.55175078	6.78206429	-0.91390706
1	-4.29519891	7.61921002	-1.85455707
1	-0.69430227	2.12996759	-1.90966185

Energy = -7584.955657 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 62

Atomic N.	X	Y	Z
8	2.25834271	-1.12371741	0.01063588
8	3.11612305	0.45192906	-1.35502100
6	4.21197279	1.09866311	-2.00258215
1	4.80064159	1.71701318	-1.30435153
1	3.77687009	1.75614266	-2.76647606
1	4.87065282	0.36514832	-2.49292194
8	4.07212612	-1.63836042	-1.28524728
6	3.45285130	-0.64753226	-0.44340874
6	4.34392051	-0.12087702	0.70609523
1	5.34762768	0.14227013	0.33517754
1	3.86368623	0.81824775	1.02116125
6	4.44934380	-1.05816011	1.91727902
1	3.43849971	-1.41696581	2.16105464
1	4.79440346	-0.47059621	2.78265662
6	5.39691029	-2.24612005	1.72248803
1	6.43259338	-1.87191305	1.63347910
1	5.37593373	-2.87578654	2.62637209
6	5.09076708	-3.10727970	0.49207251
1	4.07870473	-3.53753922	0.55238462
1	5.79571664	-3.95515045	0.46882762
6	5.22834445	-2.35957603	-0.83838967
1	6.11264544	-1.69362176	-0.80142720
1	5.40026523	-3.07953213	-1.65159478
50	0.55721012	0.15588422	0.05391508
7	-0.20833267	-0.83458717	-2.10874912
6	0.87604087	-1.70707253	-2.62828834
1	0.50825908	-2.28687311	-3.49317407
1	1.23365183	-2.37829722	-1.84362889
1	1.72751463	-1.08650996	-2.92857096
7	-0.72583460	-1.45799396	0.63808968
6	-1.37699814	-1.65665553	-1.68697330
1	-1.65678361	-2.35141938	-2.50195363

8	0.21378918	0.09193752	0.76260063
8	2.30678698	0.26150884	0.00470535
6	3.65693897	0.74139328	-0.00299419
1	3.98871376	0.68477589	-1.04681108
1	4.30866118	0.10434989	0.61633702
1	3.70922565	1.78281713	0.34006837
8	1.55244254	1.88682848	1.41964897
6	1.46128498	0.47478409	1.16901759
6	1.93550257	-0.37269164	2.37908961
1	1.03273181	-0.62667818	2.95416364
1	2.30452214	-1.31904845	1.95675057
6	2.96878926	0.23820988	3.34113806
1	3.77426187	0.74393548	2.78838356
1	3.44638094	-0.58891282	3.89081899
6	2.35920497	1.20715446	4.36648920
1	1.52961329	0.69225256	4.88252623
1	3.10872792	1.43461531	5.14137235
6	1.84417184	2.52388621	3.77467694
1	2.69155707	3.13628686	3.42530357
1	1.33588157	3.10819951	4.56070414
6	0.88078869	2.35308807	2.60164783
1	0.04528653	1.67851553	2.85606902
1	0.44471220	3.32766303	2.33206867
50	0.16277562	-0.35796398	-1.37047139
7	-2.25584740	0.39275819	-1.24557991
6	-3.05884298	-0.42973527	-2.17417569
1	-4.11140311	-0.09351246	-2.20247325
1	-3.01989737	-1.48083552	-1.87392236
1	-2.63357016	-0.34439238	-3.18135877
7	-1.93709218	-1.92217114	0.76992137
6	-2.81187936	0.34767558	0.13781305
1	-3.76428457	0.91162885	0.15644614
1	-2.09436548	0.86881896	0.78721238
6	-3.11097340	-1.04114187	0.70567984
1	-3.56240011	-0.86684209	1.70505211
1	-3.89235374	-1.53780533	0.11171720
6	-2.19723868	-3.20108609	1.36533119
6	-2.70012989	-4.25227861	0.56482976
6	-2.95592140	-5.49900965	1.14906932
6	-2.71882630	-5.74813466	2.50496077
6	-2.20109769	-4.70335432	3.27745862
6	-1.94352343	-3.43725240	2.73687274
7	0.17031522	1.67898804	-2.09373948
6	-2.21705509	1.81048479	-1.73121690
1	-3.04880698	2.37852134	-1.27553443
1	-2.37073503	1.78944830	-2.81807525
6	-0.86985108	2.48289555	-1.46601484
1	-0.91833387	3.48748489	-1.91473638
1	-0.72354573	2.62163959	-0.37705109
6	1.16008773	2.29929143	-2.88134685
6	1.83286757	3.49244045	-2.48317175
6	2.78563738	4.07016372	-3.33360966
6	3.14012935	3.51282020	-4.56471761
6	2.48868565	2.33361157	-4.94031259
6	1.51595392	1.72637172	-4.13918296
6	-2.92152146	-4.06838380	-0.91485865
1	-3.33314241	-6.30567113	0.51539649
6	-3.02918755	-7.09268957	3.11737479

1	-1.99669129	-4.87229920	4.33785538
6	-1.37592532	-2.35788407	3.62711594
6	1.60575637	4.13462919	-1.13477614
1	3.28755739	4.98294051	-2.99971005
6	4.20253073	4.13583557	-5.43828528
1	2.72782275	1.87582838	-5.90441291
6	0.83398455	0.48536971	-4.65914452
1	-2.98736714	-5.04076600	-1.41980738
1	-2.09876751	-3.49097868	-1.35905907
1	-3.85881832	-3.52889348	-1.12885728
1	-0.29960379	-2.21434256	3.44502953
1	-1.49479573	-2.62856302	4.68404034
1	-1.86132473	-1.38433016	3.46844566
1	-4.05932135	-7.12261398	3.50672873
1	-2.35697935	-7.31659371	3.95677168
1	-2.93693497	-7.89997246	2.37813539
1	2.45547194	4.78384554	-0.88292216
1	1.50164157	3.37819215	-0.34582140
1	0.70273089	4.76539695	-1.10810517
1	-0.24745702	0.51209372	-4.45689868
1	1.21726096	-0.43616864	-4.19029874
1	0.98931842	0.38526726	-5.74192575
1	5.18510839	3.66297301	-5.27804162
1	4.31739906	5.20757992	-5.22586138
1	3.96161747	4.02355257	-6.50519296
1	-1.16881587	-1.42775233	1.23763681

Energy = -7584.958192 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 64

Atomic N.	X	Y	Z
8	0.55361881	-0.79058208	0.65858290
8	2.09437945	-2.53535315	0.43600667
6	1.46530256	-3.47308432	1.31341169
1	1.42096593	-4.42228280	0.76376386
1	0.44383495	-3.16488563	1.58361082
1	2.05593559	-3.62800209	2.23236436
8	2.69023370	-0.55102973	-0.25981930
6	1.88469076	-1.13956730	0.77263968
6	2.35898059	-0.81102223	2.20135738
1	1.99065371	0.19500034	2.45170587
1	1.81732986	-1.49249073	2.87173224
6	3.87378112	-0.90015004	2.43417752
1	4.28843256	-1.74153974	1.85637441
1	4.05698427	-1.12911943	3.49611713
6	4.61115587	0.40129247	2.08549878
1	4.16430971	1.22062963	2.67594372
1	5.66218757	0.32703108	2.40878323
6	4.57279567	0.77853399	0.60000449
1	5.19619752	0.08050964	0.01781060
1	5.01105811	1.78282040	0.46662200
6	3.17929295	0.77903989	-0.03171037
1	2.45903865	1.37109328	0.55753856
1	3.23513731	1.23870750	-1.02888072
50	-0.29300771	-1.21254302	-1.22888718
7	-2.49220993	-0.21208449	-2.86222400
6	-2.59019968	-1.15505791	-3.98077676

1	-3.50872314	-0.99784406	-4.58177045
1	-2.59607168	-2.18655894	-3.60677968
1	-1.71386078	-1.04333396	-4.63319443
7	-2.16216576	-1.60683149	-0.24693143
6	-3.57819411	-0.40866327	-1.88936374
1	-4.56189539	-0.45095804	-2.40519171
1	-3.58775996	0.45460502	-1.20977615
6	-3.38874329	-1.66794904	-1.04307152
1	-4.26109676	-1.73647709	-0.37053042
1	-3.45089359	-2.56150629	-1.69753002
6	-2.24958885	-2.29391435	1.00414867
6	-2.32868747	-3.70919733	1.06032361
6	-2.42578470	-4.34997299	2.30395355
6	-2.44993109	-3.63758661	3.50571520
6	-2.36853856	-2.24181406	3.43528871
6	-2.27219760	-1.55981845	2.21680154
7	-0.38946033	1.79616491	-2.11229986
6	-2.43515197	1.17307101	-3.35596822
1	-3.44610358	1.54218424	-3.62932401
1	-1.84381399	1.17004482	-4.28611738
6	-1.79793161	2.16030924	-2.38181169
1	-1.86982718	3.16820529	-2.82981686
1	-2.35953715	2.18977760	-1.43826998
6	0.49605557	2.84390206	-1.71758666
6	0.31704856	3.52287456	-0.49351831
6	1.22636788	4.52908792	-0.13884388
6	2.31784841	4.87150873	-0.94149873
6	2.48828073	4.16798681	-2.14070416
6	1.60079668	3.16644291	-2.54399878
6	-2.27760344	-4.55404394	-0.18939850
1	-2.47131475	-5.44215673	2.32912945
6	-2.58244265	-4.34475493	4.83334882
1	-2.38370041	-1.65926925	4.36031393
6	-2.18866768	-0.05618262	2.21386745
6	-0.79091334	3.15404019	0.45989844
1	1.08241238	5.04420400	0.81412095
6	3.30110900	5.93659843	-0.51947044
1	3.33697878	4.40694217	-2.78642669
6	1.83887234	2.43587449	-3.84564725
1	-1.93466994	-5.57067670	0.04362545
1	-1.59864251	-4.12121510	-0.93925610
1	-3.26707478	-4.64440602	-0.66540896
1	-1.17416103	0.26113526	1.93260215
1	-2.42223121	0.34693368	3.20831358
1	-2.88138494	0.38310951	1.48231047
1	-3.62403150	-4.32729606	5.19180390
1	-1.96655339	-3.86546318	5.60727952
1	-2.27933888	-5.39772637	4.75722033
1	-0.54585882	3.48473735	1.47730694
1	-0.94413812	2.06646354	0.48065897
1	-1.75023314	3.62198088	0.18759016
1	0.98794643	2.53200299	-4.53961023
1	2.01877355	1.35898774	-3.69043671
1	2.72260511	2.83945854	-4.35482854
1	4.25326907	5.49192541	-0.19028540
1	2.90851300	6.53398969	0.31364638
1	3.53421034	6.61932584	-1.34924783
1	-0.01304863	1.34587853	-2.94710103

Energy = -7584.950729 Hartree
Number of imaginary frequencies = 0.

Compound I3b isomer 65

Atomic N.	X	Y	Z
8	0.24520564	-0.44273977	0.63741643
8	2.21568470	-0.59237253	-0.40122147
6	3.64192927	-0.70011941	-0.48230750
1	3.91882611	-0.27859113	-1.45617116
1	3.96469444	-1.75302308	-0.44209530
1	4.12929618	-0.12494915	0.31583310
8	2.21137422	0.09177339	1.77599207
6	1.54332640	-0.80244185	0.86962360
6	1.63399123	-2.28274391	1.32738905
1	0.70545091	-2.49529969	1.87769328
1	1.58890897	-2.88568870	0.40834449
6	2.82511473	-2.70706352	2.20346445
1	3.76718707	-2.28581211	1.82242019
1	2.92527233	-3.80183985	2.12691556
6	2.66004008	-2.34257603	3.68733472
1	1.68975996	-2.73690774	4.03766972
1	3.43303662	-2.86111384	4.27688179
6	2.73256205	-0.84159852	3.98882344
1	3.75839907	-0.47407810	3.82211914
1	2.50455264	-0.66709335	5.05429995
6	1.79009571	0.01703446	3.14770836
1	0.74821735	-0.34190400	3.20787874
1	1.80022261	1.05368335	3.51944180
50	-0.02829709	0.45136768	-1.33131683
7	-1.90324863	1.76175056	-0.23818540
6	-2.98084489	1.96713486	-1.22824553
1	-3.79575652	2.58788861	-0.81322757
1	-3.38524651	1.00262398	-1.54922932
1	-2.56319280	2.47319672	-2.10685185
7	-2.53279728	-1.23658795	0.11902919
6	-2.42152094	1.11267526	1.00013751
1	-3.06270523	1.83617750	1.53949207
1	-1.55017120	0.89182621	1.63280861
6	-3.25395851	-0.15583580	0.80421726
1	-3.59474640	-0.45272999	1.81841102
1	-4.17051862	0.07004124	0.23950936
6	-3.28324146	-2.45201163	-0.01289380
6	-4.15947332	-2.61323495	-1.11117592
6	-4.89177011	-3.79957146	-1.23727304
6	-4.77888295	-4.84539368	-0.31432229
6	-3.89299565	-4.67714741	0.75421106
6	-3.15041813	-3.50142903	0.92555578
7	0.82141270	2.38739615	-0.88159084
6	-1.27528320	3.07999662	0.10385881
1	-1.77885574	3.50848654	0.98967752
1	-1.44366259	3.75447361	-0.74578928
6	0.23459755	2.96904378	0.31831549
1	0.61168998	3.98943822	0.48938226
1	0.44429435	2.38752073	1.23691905
6	1.95885167	2.97818455	-1.46646459
6	3.08195546	3.41824757	-0.70522591
6	4.16529200	4.02763066	-1.35297351

6	4.21817182	4.20516688	-2.73774908
6	3.12186047	3.75333643	-3.47935166
6	2.00674976	3.15670409	-2.88158193
6	-4.28420117	-1.54858941	-2.17112752
1	-5.55583918	-3.91510952	-2.09770342
6	-5.59961972	-6.10414105	-0.46002859
1	-3.77819398	-5.48132847	1.48549361
6	-2.20524173	-3.39199184	2.09805793
6	3.18560830	3.19053140	0.78561572
1	5.01385934	4.35136211	-0.74325504
6	5.42001566	4.82491276	-3.40971788
1	3.12050872	3.88693650	-4.56488306
6	0.85417580	2.74827837	-3.76470424
1	-4.72767900	-1.96313864	-3.08561820
1	-3.29876051	-1.12608568	-2.41212447
1	-4.93122224	-0.71706619	-1.84652617
1	-1.16015028	-3.54025690	1.78479875
1	-2.43276779	-4.15967488	2.84864597
1	-2.25735773	-2.40986016	2.58916583
1	-6.61138850	-5.96817657	-0.04616778
1	-5.13805635	-6.94722403	0.07104200
1	-5.71697127	-6.38595268	-1.51568892
1	4.23902021	3.22918021	1.09520298
1	2.77769525	2.21150419	1.06913845
1	2.65151729	3.95447149	1.37311685
1	-0.11089175	3.01594646	-3.30830937
1	0.82405338	1.66077465	-3.94466863
1	0.92857324	3.23610255	-4.74606822
1	6.12688016	4.05581021	-3.76134478
1	5.96894370	5.48221221	-2.72145742
1	5.12712447	5.41862494	-4.28750038
1	-1.63007061	-1.38895352	0.58308485

Energy = -7584.958227 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 66

Atomic N.	X	Y	Z
8	0.10914687	-2.23837428	0.30131166
8	1.04921151	-0.32422815	1.00171840
6	1.74319410	0.48464090	1.95829372
1	1.58529135	1.52871566	1.65786225
1	2.82488507	0.27526659	1.94318456
1	1.34676381	0.32819839	2.97039287
8	0.38023890	-1.82780681	2.58123047
6	0.94036886	-1.77992073	1.26606446
6	2.33122954	-2.46817224	1.16741472
1	2.15435014	-3.43858251	0.68018575
1	2.91879739	-1.87565612	0.44971269
6	3.12957984	-2.69587284	2.46076667
1	3.16105544	-1.78100308	3.07267834
1	4.17231959	-2.90937316	2.17380259
6	2.61624477	-3.86671194	3.31451875
1	2.52238265	-4.75668848	2.66768412
1	3.37364650	-4.11769381	4.07476470
6	1.27857119	-3.60796323	4.01654188
1	1.40856629	-2.83599109	4.79344437
1	0.95107362	-4.52476010	4.53631559

6	0.15271018	-3.15745219	3.08951307
1	0.00456449	-3.85798256	2.25151466
1	-0.79666546	-3.10678883	3.64175090
50	-0.83081582	-0.68180204	-0.81110880
7	-1.64718692	1.98775263	-0.78963486
6	-2.34571431	2.11577485	-2.08140048
1	-3.03449185	2.98228739	-2.07536986
1	-2.92813607	1.20880701	-2.29330631
1	-1.61464259	2.25895300	-2.88376710
7	-2.53327661	-0.55639723	0.45219879
6	-2.61183537	1.92976967	0.32493113
1	-3.31967444	2.78364579	0.27884720
1	-2.04140459	2.00095179	1.26156982
6	-3.40058659	0.61863529	0.34235208
1	-4.09019562	0.66195291	1.19948432
1	-4.05506366	0.56570702	-0.55107013
6	-3.01989003	-1.59154471	1.29925001
6	-3.39509842	-2.85174492	0.76949810
6	-3.91078394	-3.83659139	1.62203738
6	-4.07203485	-3.62485496	2.99468487
6	-3.66556666	-2.38985583	3.51105366
6	-3.13579374	-1.37975489	2.69904849
7	0.77356533	2.52661399	-2.65365266
6	-0.64596689	3.06522973	-0.62048877
1	-0.51272875	3.23017154	0.45947039
1	-1.02854753	4.01027267	-1.05220978
6	0.74047244	2.75343072	-1.19546204
1	1.39232487	3.60479723	-0.96045688
1	1.15551540	1.87951539	-0.66061012
6	1.95282649	2.91098939	-3.35150230
6	2.76875123	1.93271977	-3.96986813
6	3.89558769	2.33752483	-4.69347303
6	4.25337963	3.68498305	-4.81944182
6	3.41972874	4.63647477	-4.22279130
6	2.27110341	4.28102259	-3.50459478
6	-3.24191245	-3.16931862	-0.69778280
1	-4.20198248	-4.79906573	1.19327210
6	-4.67396299	-4.68526937	3.88512907
1	-3.73851766	-2.21114351	4.58751926
6	-2.62852249	-0.11249464	3.34008176
6	2.42903975	0.46416345	-3.86705994
1	4.51686791	1.57245357	-5.16584283
6	5.50045608	4.09548248	-5.56383723
1	3.65197975	5.69807155	-4.34073845
6	1.36272231	5.36263476	-2.97221204
1	-3.85477256	-4.03833774	-0.97232182
1	-2.19758693	-3.42242147	-0.94533991
1	-3.53584527	-2.32171086	-1.33319510
1	-1.66566389	0.17433675	2.89503650
1	-2.48580147	-0.25939923	4.41867513
1	-3.32012159	0.73643772	3.21635206
1	-5.76877664	-4.57857396	3.94848154
1	-4.28159334	-4.61813705	4.90940076
1	-4.46711973	-5.69463765	3.50374979
1	3.21124914	-0.14549794	-4.33612721
1	1.48061815	0.21835010	-4.37308569
1	2.32759163	0.13115647	-2.82234025
1	1.53358609	5.57709257	-1.90511892

1	0.30781730	5.07027140	-3.07728827
1	1.52383420	6.30103387	-3.51862310
1	5.71320509	3.41366980	-6.39872840
1	6.38154174	4.08472767	-4.90234344
1	5.40879167	5.11307822	-5.96749737
1	0.57153209	1.54181097	-2.83309953

Energy = -7584.948538 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 67

Atomic N.	X	Y	Z
8	0.08480836	-0.70498390	0.17856058
8	2.11311654	-0.38138634	-0.73968328
6	3.47962075	-0.72834379	-0.96622895
1	3.90531346	0.09329933	-1.55586284
1	3.57514545	-1.66358180	-1.54409579
1	4.03466066	-0.82266358	-0.02069089
8	1.98793666	-1.04677489	1.42981430
6	1.35289729	-1.22270968	0.14770662
6	1.33363054	-2.71272958	-0.31102028
1	0.32706645	-3.09118822	-0.07744087
1	1.40521122	-2.69549948	-1.41055749
6	2.37171204	-3.68307293	0.27697710
1	3.37979380	-3.24174264	0.26349063
1	2.41341598	-4.56615698	-0.38177184
6	2.03852270	-4.16173871	1.69912860
1	1.00194830	-4.54118509	1.70660030
1	2.68480249	-5.01775433	1.95276335
6	2.18989516	-3.08968589	2.78393745
1	3.25352292	-2.82381902	2.90346412
1	1.85530839	-3.49698418	3.75364773
6	1.41060030	-1.80549631	2.50948802
1	0.34812827	-2.01037693	2.30052785
1	1.45316176	-1.14874576	3.39260175
50	-0.88370587	0.06972623	-1.55276209
7	-2.41801229	2.28860843	-1.35135964
6	-2.95518870	2.54067013	-2.69870251
1	-3.65086117	3.40103809	-2.70548868
1	-3.49501129	1.65540390	-3.05760563
1	-2.13022472	2.74139643	-3.39388550
7	-2.68718008	-0.44888262	-0.50574097
6	-3.49119310	1.87039969	-0.42385568
1	-4.38015571	2.52047125	-0.55137905
1	-3.11900940	1.99731355	0.60135207
6	-3.86307294	0.39904778	-0.61198503
1	-4.60189867	0.14280424	0.16704971
1	-4.40451353	0.27211551	-1.57626381
6	-2.87156042	-1.69569961	0.15265757
6	-2.94862387	-2.90691723	-0.57815175
6	-3.11727642	-4.12128452	0.10312841
6	-3.21890641	-4.18438756	1.49573967
6	-3.13210867	-2.98243063	2.20922369
6	-2.95889932	-1.75073487	1.56895829
7	0.42679925	2.23342524	-0.29844905
6	-1.68372354	3.46685029	-0.84629732
1	-2.38991719	4.21538212	-0.43504451
1	-1.17341207	3.93909059	-1.69513523

6	-0.64827478	3.10849708	0.22238741
1	-0.23842619	4.04594546	0.63503936
1	-1.14225662	2.58137589	1.05257374
6	1.68152471	2.89233121	-0.59252769
6	2.63312238	3.03434828	0.44948988
6	3.84636925	3.67464280	0.18578554
6	4.15475585	4.18299072	-1.08349234
6	3.21241465	4.01322348	-2.09800356
6	1.98215784	3.36897455	-1.88259084
6	-2.84715372	-2.92164904	-2.08539149
1	-3.17884063	-5.04544848	-0.47807232
6	-3.43672242	-5.49847820	2.20729329
1	-3.18129173	-3.00535473	3.30154106
6	-2.80275641	-0.49737218	2.39142337
6	2.36367337	2.48084655	1.82779562
1	4.57354945	3.77554300	0.99539005
6	5.47138314	4.87557798	-1.34036711
1	3.43995454	4.37555257	-3.10371729
6	1.05624510	3.19036914	-3.06153235
1	-3.28091499	-3.84462846	-2.49360272
1	-1.79937171	-2.87836694	-2.42582629
1	-3.35960676	-2.06081791	-2.53493260
1	-1.92074622	0.06333279	2.04977835
1	-2.68171872	-0.74181063	3.45502960
1	-3.67283675	0.17280076	2.30377939
1	-4.50130864	-5.65178273	2.44595715
1	-2.88457409	-5.53672588	3.15710488
1	-3.11367524	-6.34686710	1.58902618
1	3.18613664	2.73517374	2.50819505
1	2.27003280	1.38214636	1.80903319
1	1.43487634	2.88247197	2.26097196
1	0.44091779	4.08772763	-3.23679367
1	0.38514463	2.33317314	-2.92106149
1	1.63777187	3.02110992	-3.97794630
1	6.32107444	4.21668564	-1.10724710
1	5.57893347	5.77258748	-0.71203399
1	5.56096861	5.18556433	-2.38953912
1	0.60690537	1.47622412	0.36972405

Energy = -7584.953308 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 68

Atomic N.	X	Y	Z
8	0.65943228	0.26378936	-0.45634501
8	1.72956095	1.45467555	1.08917575
6	2.86812923	1.88046948	1.85219082
1	2.46575983	2.29389159	2.78502572
1	3.41419194	2.67473927	1.32089394
1	3.53916928	1.03957722	2.07115383
8	2.76175237	-0.42399813	0.30861941
6	1.92170987	0.65732865	-0.13264141
6	2.54534842	1.49851413	-1.27473503
1	2.10847647	1.11858434	-2.21103492
1	2.14959203	2.51633518	-1.14850296
6	4.07662071	1.53349961	-1.41201850
1	4.55667482	1.69442870	-0.43481102
1	4.33424729	2.41116494	-2.02677919

6	4.67513199	0.28631715	-2.07928676
1	4.14945812	0.11258884	-3.03455121
1	5.72777602	0.48400099	-2.33806479
6	4.60491910	-0.98532757	-1.22805566
1	5.26817072	-0.89067607	-0.35248538
1	4.97658467	-1.84290752	-1.81432807
6	3.20506180	-1.32591096	-0.72236169
1	2.47365249	-1.35360397	-1.54821775
1	3.21379401	-2.32357752	-0.25680969
50	-0.45943195	0.18559707	1.41223036
7	-2.53871270	-0.15374617	0.01245415
6	-3.57425269	-0.45584356	1.02760797
1	-4.58492273	-0.42459060	0.58307630
1	-3.52214627	0.26972670	1.84770322
1	-3.39498180	-1.45784325	1.43628667
7	-1.39037573	2.11474089	1.29564566
6	-2.74154545	1.21337103	-0.54508999
1	-3.73995993	1.27262289	-1.02080940
1	-1.97467136	1.36229797	-1.31657012
6	-2.59977955	2.30317868	0.51276155
1	-2.59755141	3.26780271	-0.02680931
1	-3.51252808	2.33048339	1.14810513
6	-0.88822918	3.24791693	1.98514486
6	-0.90055298	3.30237538	3.40383847
6	-0.35879137	4.41354525	4.06416022
6	0.19150042	5.49618747	3.37074560
6	0.19992370	5.43374857	1.97281156
6	-0.32046748	4.33963394	1.27190545
7	-0.45834253	-2.22796064	-1.82756505
6	-2.65232846	-1.17333177	-1.07551085
1	-3.60856279	-0.98230656	-1.60158016
1	-2.74460261	-2.15993312	-0.59924615
6	-1.49590772	-1.22902765	-2.09684656
1	-1.93459431	-1.41735279	-3.08439261
1	-0.98338816	-0.26021954	-2.15336712
6	-0.78619566	-3.60262107	-1.77509909
6	-1.30439415	-4.26503254	-2.91769491
6	-1.60136685	-5.63189463	-2.84316834
6	-1.37361901	-6.38898684	-1.69029892
6	-0.80576190	-5.73308409	-0.59222400
6	-0.51282644	-4.36518139	-0.60873353
6	-1.50010788	2.18654268	4.22750072
1	-0.38220785	4.43685420	5.15715057
6	0.73110492	6.70229235	4.10171357
1	0.64519349	6.25600752	1.40526293
6	-0.22456066	4.31677865	-0.23277413
6	-1.46501125	-3.55844996	-4.24173603
1	-1.99524928	-6.12532281	-3.73577800
6	-1.72826178	-7.85519194	-1.63013249
1	-0.58812390	-6.30069126	0.31629319
6	0.09643416	-3.72375967	0.61242118
1	-1.75309651	2.54434372	5.23473220
1	-0.80739115	1.33771420	4.34694016
1	-2.40753766	1.78500138	3.75639160
1	-0.11235664	3.28568121	-0.59486697
1	0.63178824	4.91339567	-0.57549720
1	-1.12236802	4.74113899	-0.71187452
1	-0.04520798	7.47466419	4.22354586

1	1.56357389	7.16428982	3.55282638
1	1.08742248	6.43713866	5.10648113
1	-1.43245834	-4.28457167	-5.06471446
1	-0.66278799	-2.82183269	-4.39283218
1	-2.42402619	-3.02120125	-4.32598817
1	-0.51818190	-2.89579581	1.00328934
1	1.09318180	-3.29756192	0.41586745
1	0.21009802	-4.45908446	1.41892530
1	-1.00896447	-8.41843735	-1.01936882
1	-1.74957148	-8.30264679	-2.63322818
1	-2.72354834	-8.00809159	-1.18261425
1	0.13637499	-1.90737996	-1.06343767

Energy = -7584.957394 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 69

Atomic N.	X	Y	Z
8	0.63428256	-0.16086821	-0.04930063
8	1.66150559	1.10788542	1.49668761
6	2.81231357	1.58617514	2.19206365
1	2.43169936	2.16682271	3.04239169
1	3.42216513	2.25331040	1.55872307
1	3.43556664	0.76010462	2.56563348
8	2.51134783	-0.95802305	1.08320330
6	1.87157465	0.16497510	0.42447144
6	2.72786653	0.76481668	-0.72872223
1	2.31515668	0.35872249	-1.66459428
1	2.51136928	1.84371116	-0.73838596
6	4.24832863	0.53422040	-0.71806945
1	4.67029727	0.73575323	0.27806792
1	4.69946316	1.27630948	-1.39767424
6	4.67739730	-0.86606590	-1.18169344
1	4.19227962	-1.08052919	-2.15017224
1	5.76304374	-0.86633838	-1.37259792
6	4.34709788	-1.98967044	-0.19408900
1	4.95518671	-1.87752026	0.71905003
1	4.62011617	-2.96267198	-0.63784220
6	2.87842316	-2.04991369	0.21916809
1	2.20909926	-2.08132986	-0.65574273
1	2.69769578	-2.96500563	0.80403541
50	-0.77424902	-0.71007791	1.47580102
7	-3.50183032	-0.49893538	1.52276889
6	-4.06095857	-0.12963320	2.82590162
1	-5.16203305	-0.25402990	2.85105106
1	-3.82128311	0.91120816	3.07076474
1	-3.61622195	-0.76573344	3.60288260
7	-1.77239607	1.65536749	0.43425394
6	-3.92472571	0.40831517	0.44880464
1	-5.02499926	0.55676584	0.45279347
1	-3.66410411	-0.06348555	-0.50892165
6	-3.24567386	1.77577359	0.52412657
1	-3.64791001	2.40920040	-0.28779841
1	-3.49014994	2.28438046	1.46462525
6	-1.06575560	2.90460518	0.58657901
6	-0.92584856	3.49600418	1.85907614
6	-0.23325006	4.70903188	1.96743624
6	0.33865570	5.34523197	0.86193917

6	0.20754561	4.72547728	-0.38554367
6	-0.48695515	3.52153767	-0.54488906
7	-1.63471107	-2.02505837	-0.00733748
6	-3.78279218	-1.91516795	1.23095525
1	-4.87144075	-2.09200823	1.10129145
1	-3.45765500	-2.48212816	2.11765384
6	-3.03131582	-2.43523619	0.00744875
1	-3.13656622	-3.53825539	0.02428321
1	-3.56188295	-2.12017511	-0.91995195
6	-0.85573829	-2.78682558	-0.93177516
6	-0.68952900	-2.35916205	-2.26980103
6	0.05666296	-3.13922217	-3.16215629
6	0.65390358	-4.34345626	-2.77331157
6	0.47911983	-4.75948674	-1.44904637
6	-0.25951354	-4.00665828	-0.52637582
6	-1.46527715	2.84896366	3.11032812
1	-0.12011537	5.15586150	2.95840058
6	1.05910887	6.66391251	1.00581391
1	0.65884772	5.19029738	-1.26547924
6	-0.58188176	2.89161319	-1.91424762
6	-1.27972127	-1.05235540	-2.73332968
1	0.17693453	-2.79190067	-4.19200796
6	1.48549924	-5.15049617	-3.74172521
1	0.93272422	-5.69845817	-1.12006924
6	-0.38714453	-4.49666833	0.89601245
1	-0.89935033	3.18644255	3.98814750
1	-1.39285463	1.75291942	3.05933322
1	-2.52129538	3.11106596	3.28950874
1	-0.03315943	1.93740365	-1.95430860
1	-0.14588784	3.55463037	-2.67171952
1	-1.62270627	2.68972115	-2.21319313
1	0.37220636	7.51042792	0.84727318
1	1.86984702	6.76052607	0.27095943
1	1.48979195	6.77703141	2.00987338
1	-1.11544435	-0.90825215	-3.80945595
1	-0.80065211	-0.22326567	-2.19304733
1	-2.36168913	-0.99596775	-2.54318438
1	-1.43310338	-4.52574233	1.23314038
1	0.14727144	-3.83817110	1.59847674
1	0.03450198	-5.50560074	0.99607283
1	2.54160858	-4.83750500	-3.71435045
1	1.13539157	-5.02225066	-4.77521242
1	1.45713771	-6.22172923	-3.49943824
1	-1.53026321	1.26451298	-0.48071127

Energy = -7584.956867 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 70

Atomic N.	X	Y	Z
8	0.62736957	-0.03104541	-0.54282383
8	2.07684098	1.32026948	0.46939586
6	3.36105558	1.71367254	0.97512965
1	3.95933447	2.18831595	0.18267047
1	3.90254438	0.85762780	1.39861172
1	3.16087311	2.45667398	1.75670452
8	2.66490236	-0.87243411	0.24354522
6	1.96948312	0.17737711	-0.45157770

6	2.57098361	0.50270313	-1.84195429
1	1.95810806	-0.04035638	-2.57767390
1	2.37204152	1.57030858	-2.01241719
6	4.05500255	0.18850497	-2.09460401
1	4.67935537	0.53046881	-1.25526233
1	4.37346406	0.77630175	-2.97079019
6	4.34232428	-1.29313483	-2.37934701
1	3.67484870	-1.63032042	-3.19165772
1	5.37033361	-1.39568970	-2.76247222
6	4.16988356	-2.21782507	-1.17029171
1	4.94815461	-2.00570594	-0.41875539
1	4.31166689	-3.26601896	-1.48412275
6	2.81091689	-2.10681152	-0.48300582
1	1.98355916	-2.22815911	-1.20307993
1	2.71207877	-2.90448015	0.26939620
50	-0.23609670	0.68292199	1.32624718
7	-2.51360957	0.37695272	0.26513609
6	-3.43674862	0.59674573	1.40255792
1	-4.47931231	0.69768924	1.05194842
1	-3.15448110	1.50452988	1.94854220
1	-3.37168069	-0.25694070	2.08821380
7	-0.82275621	2.63769618	0.66406784
6	-2.56162150	1.53414977	-0.67253222
1	-3.59388793	1.65491327	-1.05537119
1	-1.90029924	1.29261478	-1.51504309
6	-2.08713023	2.83124817	-0.02521551
1	-2.00425018	3.57703843	-0.83655548
1	-2.87926690	3.22592667	0.64885757
6	-0.03694265	3.79465160	0.89945404
6	0.17418755	4.27766899	2.21766442
6	0.99016622	5.39775474	2.42769800
6	1.60591952	6.07868701	1.37280820
6	1.39289410	5.59507343	0.07704167
6	0.59409581	4.47461762	-0.17873096
7	-1.07885079	-2.52028921	-0.98653089
6	-2.94148901	-0.87100418	-0.43880616
1	-3.91328223	-0.65379388	-0.92462824
1	-3.13449706	-1.63604311	0.32681845
6	-1.95642798	-1.45344082	-1.47532895
1	-2.54648912	-1.82625232	-2.32156006
1	-1.29708133	-0.66757928	-1.86559367
6	-1.62855143	-3.72129170	-0.48136835
6	-1.33744482	-4.14770586	0.84138580
6	-1.85880690	-5.35932856	1.30793284
6	-2.67439440	-6.17602530	0.51670604
6	-2.91939578	-5.76053862	-0.79547313
6	-2.40208888	-4.56790936	-1.31684606
6	-0.47530116	3.61501829	3.40998283
1	1.13604851	5.75582272	3.45056271
6	2.44656358	7.30877016	1.61861514
1	1.88087698	6.09418273	-0.76512271
6	0.45655567	3.97702470	-1.59552109
6	-0.46741084	-3.31699505	1.75066152
1	-1.62356227	-5.66760804	2.32997811
6	-3.26838606	-7.45297606	1.06048247
1	-3.50853544	-6.40182728	-1.45656809
6	-2.61177772	-4.26368664	-2.78024088
1	-0.51017353	4.30581723	4.26329880

1	0.07364779	2.71772561	3.73899787
1	-1.49778176	3.28757629	3.17773377
1	0.34060758	2.88462736	-1.60966506
1	1.33789880	4.25288080	-2.19038230
1	-0.42068963	4.41016193	-2.10397302
1	1.84167848	8.22655390	1.54205287
1	3.25773787	7.39380523	0.88203300
1	2.89380569	7.29593967	2.62191621
1	-0.37500520	-3.79121063	2.73589255
1	-0.87118431	-2.30289889	1.90772647
1	0.55225698	-3.18178054	1.35599358
1	-1.72008214	-3.78761025	-3.21300943
1	-3.46385972	-3.58740265	-2.95895810
1	-2.81741816	-5.18942950	-3.33370455
1	-3.47850285	-8.17071862	0.25569649
1	-4.21919484	-7.26111945	1.58337641
1	-2.59372471	-7.93504372	1.78151170
1	-0.34059247	-2.11857911	-0.40848144

Energy = -7584.957389 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 71

Atomic N.	X	Y	Z
8	0.66201529	0.09387938	0.00381545
8	1.55497925	0.79778468	1.92221218
6	2.58524446	0.87348299	2.91350204
1	3.38715345	1.55672678	2.59105102
1	3.00383265	-0.11766816	3.13594798
1	2.11211892	1.28709742	3.81300090
8	2.32425751	-1.16490151	1.06078922
6	1.85554202	0.13772869	0.64599578
6	2.89830021	0.93153793	-0.18381643
1	2.56975307	0.86569466	-1.23203686
1	2.78110608	1.98702405	0.10243305
6	4.37354043	0.50998627	-0.09559827
1	4.68444002	0.38215006	0.95288995
1	4.97811310	1.34071010	-0.49533351
6	4.71521411	-0.76010189	-0.89144553
1	4.32488108	-0.64595937	-1.91807956
1	5.81027409	-0.84316836	-0.98553506
6	4.17319579	-2.06004159	-0.28678160
1	4.68817464	-2.27109029	0.66531645
1	4.39957394	-2.90371402	-0.96149388
6	2.67031541	-2.05166851	-0.01869922
1	2.09313903	-1.78954181	-0.92046224
1	2.34224090	-3.05298456	0.29973719
50	-0.86133046	-0.19488504	1.48790606
7	-3.71868867	-0.39195689	1.07012130
6	-4.30554963	-0.66601721	2.38609768
1	-5.41286090	-0.61151464	2.36917429
1	-3.93609461	0.06016433	3.12081895
1	-4.00174814	-1.66576260	2.72438762
7	-1.67335319	1.75678022	1.08337360
6	-3.97740553	0.99431363	0.64312214
1	-5.04691596	1.25410066	0.79589720
1	-3.75806242	1.06720036	-0.43107556
6	-3.08475620	2.00136197	1.37045334

1	-3.36694929	3.00521564	1.00793809
1	-3.33609964	1.99834128	2.45277779
6	-0.85578733	2.92904667	1.09840567
6	-0.54198656	3.59790079	2.30902104
6	0.25406760	4.75114898	2.28045807
6	0.75717453	5.27529746	1.08623903
6	0.44127611	4.60590490	-0.10138320
6	-0.35283531	3.45257099	-0.11862799
7	-1.90928079	-2.06565835	-0.59664786
6	-4.17699637	-1.37753072	0.07643460
1	-5.17771473	-1.11087371	-0.32200975
1	-4.29552998	-2.34338645	0.59411143
6	-3.21157956	-1.56889078	-1.09114015
1	-3.66936498	-2.28031897	-1.80217744
1	-3.06839726	-0.62200663	-1.62769731
6	-1.06635852	-2.80229082	-1.48097275
6	-0.60242290	-2.25168835	-2.69611039
6	0.24568610	-3.02069027	-3.50448595
6	0.67162994	-4.30286955	-3.14640999
6	0.23219802	-4.81053163	-1.91823770
6	-0.62611236	-4.08921490	-1.08341041
6	-1.03348759	3.08529427	3.64053147
1	0.49466832	5.24753726	3.22481097
6	1.58839792	6.53619121	1.07402613
1	0.82093182	4.99454279	-1.05034322
6	-0.66208744	2.78310964	-1.43231558
6	-0.93030516	-0.83943117	-3.10990197
1	0.60572084	-2.58082560	-4.43790828
6	1.56658665	-5.11405700	-4.05187882
1	0.56456218	-5.80070443	-1.59669385
6	-1.05424994	-4.68443126	0.23840648
1	-0.41466980	3.47467370	4.45987311
1	-1.01401794	1.98578136	3.68016945
1	-2.07224270	3.39375433	3.84045061
1	-0.16928553	1.80179728	-1.47924936
1	-0.31263177	3.39799831	-2.27267027
1	-1.74117051	2.60788472	-1.54990629
1	0.96284268	7.42494903	0.89264357
1	2.34910312	6.50807317	0.28140513
1	2.09955576	6.68791513	2.03464238
1	-0.22429527	-0.49644513	-3.87701341
1	-0.85550832	-0.15848714	-2.25132849
1	-1.94233968	-0.74680045	-3.53371888
1	-2.14972662	-4.78709678	0.31585962
1	-0.71777031	-4.07702586	1.09494453
1	-0.62621675	-5.68665346	0.36286140
1	2.29165602	-5.70567846	-3.47567685
1	2.12415343	-4.46873131	-4.74387824
1	0.98214620	-5.82149688	-4.66145806
1	-2.08557606	-2.63786054	0.22955624

Energy = -7584.953813 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 72

Atomic N.	X	Y	Z
8	0.62308509	-0.20338048	-0.08233277
8	1.84234921	1.28023734	1.08534177

6	3.07150380	1.82103847	1.56850920
1	3.63967999	2.32114992	0.76534171
1	3.69892431	1.04994919	2.03992486
1	2.79591941	2.57321199	2.31908649
8	2.56779973	-0.87176442	1.01983451
6	1.91212172	0.13676171	0.20859258
6	2.67522751	0.44698291	-1.11173786
1	2.16594623	-0.12388317	-1.90286530
1	2.48898001	1.50978400	-1.32786767
6	4.18287982	0.15116716	-1.18323388
1	4.70119526	0.52439551	-0.28723680
1	4.59192034	0.72172231	-2.03367794
6	4.52402054	-1.33214221	-1.39067388
1	3.94911986	-1.70850446	-2.25502918
1	5.58813745	-1.42341362	-1.66339690
6	4.24507705	-2.22269353	-0.17565752
1	4.93553280	-1.96562399	0.64490327
1	4.44425414	-3.27619070	-0.43759387
6	2.81795246	-2.12649105	0.35915251
1	2.07229371	-2.29160168	-0.43542168
1	2.65924807	-2.90153210	1.12491321
50	-0.64341618	-0.40000225	1.64009589
7	-3.34540193	-0.04683194	1.90346580
6	-3.76357854	0.57516855	3.16252694
1	-4.86004793	0.50782399	3.30994146
1	-3.47169547	1.63097998	3.19006028
1	-3.26353398	0.06885482	3.99906465
7	-1.66245048	1.79404911	0.29194415
6	-3.84191301	0.67400433	0.72496283
1	-4.93111214	0.87507487	0.80131821
1	-3.69153606	0.02672351	-0.15026426
6	-3.11631274	1.99832798	0.48674193
1	-3.57433034	2.49046477	-0.39095870
1	-3.25506173	2.68104652	1.33379395
6	-0.90434137	3.01516324	0.15992572
6	-0.62934939	3.81150577	1.29029270
6	0.11035429	4.98983822	1.12238187
6	0.60046897	5.39440864	-0.12223771
6	0.33571830	4.57348196	-1.22428752
6	-0.41024497	3.39614349	-1.10798947
7	-1.69354796	-1.90646121	0.50093904
6	-3.69744507	-1.47703845	1.90127667
1	-4.79848530	-1.62159117	1.91042930
1	-3.30045602	-1.89278572	2.84099364
6	-3.09222431	-2.24138491	0.72588388
1	-3.22747445	-3.31768847	0.95253189
1	-3.70657776	-2.07114849	-0.18750898
6	-1.04132059	-2.85109800	-0.34996351
6	-1.00334019	-2.66368040	-1.75154969
6	-0.38169032	-3.61944678	-2.56492156
6	0.21342064	-4.76965737	-2.03487993
6	0.16587102	-4.94747166	-0.64802927
6	-0.44607703	-4.01381664	0.19906957
6	-1.07217864	3.41955768	2.67797187
1	0.32804444	5.59661660	2.00490731
6	1.37694293	6.67960313	-0.27721430
1	0.72064481	4.85470337	-2.20755527
6	-0.65079982	2.54143555	-2.32967433

6	-1.59743145	-1.42647495	-2.37384385
1	-0.35973107	-3.45692118	-3.64605055
6	0.91035199	-5.76925869	-2.92689273
1	0.62042340	-5.83938409	-0.20815155
6	-0.43995740	-4.25091124	1.69012098
1	-0.41542062	3.87506764	3.43025184
1	-1.04280057	2.32909159	2.81612123
1	-2.09710999	3.76187972	2.89777675
1	-0.14290021	1.56791512	-2.24285749
1	-0.26122278	3.03782427	-3.22703292
1	-1.72103291	2.34460269	-2.50059375
1	0.72166121	7.50220164	-0.60478013
1	2.17237302	6.57986648	-1.02853072
1	1.83731525	6.98533212	0.67178962
1	-1.54330761	-1.47472396	-3.46954613
1	-1.03783281	-0.54258248	-2.03580214
1	-2.65095103	-1.28554156	-2.09059589
1	-1.44693705	-4.18168106	2.12594281
1	0.17704399	-3.50471718	2.21453182
1	-0.03343057	-5.24437784	1.92139893
1	1.97084727	-5.50503961	-3.06719368
1	0.45048889	-5.80644713	-3.92406511
1	0.88093570	-6.77985304	-2.49696413
1	-1.52006479	1.24008104	-0.55739313

Energy = -7584.956874 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 73

Atomic N.	X	Y	Z
8	0.62455240	-0.20311278	-0.05814721
8	1.71881326	0.91349778	1.55748857
6	2.89263761	1.28066393	2.28133613
1	3.54817094	1.93951614	1.68611731
1	3.45952558	0.39825114	2.61361314
1	2.54353616	1.83947815	3.15936312
8	2.43905411	-1.17728295	1.03752912
6	1.87657765	0.01754015	0.43722114
6	2.77731338	0.62205117	-0.67911785
1	2.34590642	0.29362670	-1.63678485
1	2.62989009	1.71155250	-0.63172917
6	4.27993801	0.29477701	-0.67573243
1	4.70716547	0.41616461	0.33113641
1	4.78179507	1.04148954	-1.31341765
6	4.62231751	-1.10353323	-1.21169174
1	4.13064917	-1.23538061	-2.19158038
1	5.70695247	-1.16283930	-1.39909604
6	4.21525382	-2.25430316	-0.28600750
1	4.82306578	-2.22901138	0.63383188
1	4.42938086	-3.21794039	-0.77968896
6	2.74295948	-2.24323187	0.11849596
1	2.07882373	-2.18712571	-0.75915362
1	2.50147296	-3.17440125	0.65406822
50	-0.82645160	-0.74651771	1.42834074
7	-3.53745769	-0.36478162	1.48060643
6	-4.08429101	-0.03782212	2.80014671
1	-5.19112573	-0.09519198	2.81215297
1	-3.78353730	0.97031287	3.10665805

1	-3.68644523	-0.74419825	3.54101715
7	-1.66524668	1.73528383	0.52822192
6	-3.89242243	0.62902001	0.45993754
1	-4.98104581	0.84704574	0.46699218
1	-3.65367641	0.19861589	-0.52264408
6	-3.12864912	1.94355288	0.61956412
1	-3.48364257	2.64853500	-0.15451148
1	-3.34756113	2.40977275	1.58788873
6	-0.88166188	2.92497160	0.75985122
6	-0.71603747	3.42844392	2.06663501
6	0.05190234	4.58545568	2.25220065
6	0.67423019	5.24847491	1.19057241
6	0.51544139	4.71459824	-0.09287426
6	-0.25374872	3.57010935	-0.32889427
7	-1.75996604	-1.91196770	-0.13350721
6	-3.90418108	-1.74091736	1.10494573
1	-5.00091317	-1.84155671	0.96227422
1	-3.62072979	-2.37822138	1.95756680
6	-3.17939756	-2.23449800	-0.14531040
1	-3.35319549	-3.32790791	-0.19359964
1	-3.68407644	-1.83318121	-1.05362028
6	-1.02621772	-2.66194135	-1.10350991
6	-0.82980581	-2.16377173	-2.41267612
6	-0.13029452	-2.93192958	-3.35204095
6	0.39037349	-4.19231334	-3.03863994
6	0.18589157	-4.67765054	-1.74237620
6	-0.50767184	-3.93897564	-0.77456549
6	-1.30770950	2.74375327	3.27349439
1	0.18401950	4.96365320	3.26905443
6	1.47658730	6.50667656	1.41820535
1	1.00420029	5.20118502	-0.94044148
6	-0.37634591	3.03146533	-1.73453629
6	-1.33696804	-0.79709013	-2.79471569
1	0.01440208	-2.52968400	-4.35847067
6	1.17408318	-4.98804116	-4.05513015
1	0.57946039	-5.66145313	-1.47235276
6	-0.66975937	-4.50685408	0.61497088
1	-0.72757138	2.98807536	4.17265763
1	-1.30821843	1.65051123	3.15552685
1	-2.34522716	3.06491066	3.46426597
1	0.10813475	2.04682694	-1.82945437
1	0.11024228	3.70829178	-2.44765805
1	-1.42528755	2.91821940	-2.05126849
1	0.84649673	7.40380381	1.30996884
1	2.29727716	6.59588816	0.69353932
1	1.90616241	6.52991317	2.42883092
1	-1.15957197	-0.59731853	-3.85980491
1	-0.81025107	-0.03375683	-2.20421604
1	-2.41427159	-0.68615124	-2.60211358
1	-1.71569814	-4.48669151	0.95263318
1	-0.09325700	-3.93059201	1.35543649
1	-0.31649066	-5.54591947	0.65106945
1	2.24962820	-4.75583188	-3.99705943
1	0.84770535	-4.76250951	-5.07964824
1	1.06543636	-6.06876665	-3.88963291
1	-1.44134891	1.38619153	-0.40800658

Energy = -7584.956873 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 74

Atomic N.	X	Y	Z
8	1.52307404	0.03877374	1.01709385
8	2.29359019	0.96186845	-0.86378333
6	3.30776829	1.27021636	-1.82336747
1	2.80782564	1.81530304	-2.63356212
1	3.76401103	0.35892846	-2.24222612
1	4.08649465	1.90730564	-1.37891483
8	3.45224417	1.34985906	1.05860042
6	2.68566160	0.31151694	0.39328069
6	3.52621146	-0.97494851	0.14064813
1	3.24759601	-1.67669958	0.94134571
1	3.13394552	-1.41848389	-0.78815873
6	5.05980199	-0.87510146	0.08905543
1	5.38181904	-0.02974072	-0.53715484
1	5.43813955	-1.78524749	-0.40475128
6	5.72265775	-0.76849825	1.47142173
1	5.34550913	-1.59007312	2.10588647
1	6.80705055	-0.93445047	1.36645856
6	5.49488449	0.56722241	2.18715893
1	6.01856749	1.37460374	1.64904202
1	5.93585131	0.52407768	3.19810703
6	4.02713260	0.97080259	2.31857126
1	3.42779671	0.16964344	2.78561855
1	3.94603391	1.85826857	2.96658761
50	-0.22962123	0.08412499	-0.44863558
7	-0.74598730	1.86469051	1.34902772
6	0.31932906	2.89301929	1.32609529
1	0.08296192	3.71168331	2.03100881
1	0.41363553	3.30803677	0.31769324
1	1.27360756	2.42509004	1.59040483
7	-1.38250125	1.74179096	-1.33064895
6	-2.02965395	2.44391304	0.89609233
1	-2.30194611	3.31522971	1.52239638
1	-2.80743484	1.67586826	1.01260583
6	-1.94881459	2.84333979	-0.57731935
1	-2.97759588	3.07304890	-0.91718267
1	-1.38647097	3.79626735	-0.67343614
6	-1.49491066	1.81949878	-2.74644569
6	-0.70907497	2.72347469	-3.50853078
6	-0.82765502	2.74426848	-4.90464354
6	-1.70422539	1.89697149	-5.58868502
6	-2.47373899	1.00790381	-4.82929761
6	-2.38969627	0.95564970	-3.43292151
7	-1.03318776	-1.02441101	2.01372157
6	-0.82812279	1.31765222	2.72290458
1	-1.25150853	2.07753593	3.40834631
1	0.20698948	1.12266384	3.03761067
6	-1.62987829	0.02710832	2.85563936
1	-1.63163948	-0.25788992	3.92457994
1	-2.67858587	0.17465990	2.56798746
6	-1.55326060	-2.35085219	2.13836662
6	-2.85776925	-2.66263838	1.69702771
6	-3.31578037	-3.98171957	1.81720300
6	-2.52158866	-5.00503093	2.34173267
6	-1.22001688	-4.67859278	2.74147091

6	-0.72280392	-3.37476604	2.65439292
6	0.27755511	3.64681015	-2.83893420
1	-0.20408688	3.43937652	-5.47403040
6	-1.83522378	1.95274311	-7.09204547
1	-3.16944017	0.33539747	-5.33860669
6	-3.26814882	-0.01289098	-2.67702886
6	-3.75321602	-1.63150733	1.05598633
1	-4.32345692	-4.21524167	1.46447319
6	-3.04934192	-6.41227162	2.48181194
1	-0.56875395	-5.46170708	3.13743459
6	0.69081463	-3.07926758	3.09873356
1	1.05145106	3.97205102	-3.54721803
1	0.76090456	3.14876564	-1.98630900
1	-0.20868387	4.55575362	-2.44976066
1	-2.69065759	-0.86296488	-2.28222752
1	-4.05011883	-0.41642356	-3.33425523
1	-3.74559394	0.47125383	-1.81392268
1	-2.72242971	2.53201756	-7.39396456
1	-1.94361461	0.94781492	-7.52407420
1	-0.95937359	2.43041427	-7.55153566
1	-4.48800885	-2.11764481	0.40147231
1	-3.17425172	-0.92083001	0.44892118
1	-4.31969561	-1.04951337	1.80093419
1	0.72293012	-2.32103012	3.89724708
1	1.31309333	-2.70041612	2.27253310
1	1.16781597	-3.98810227	3.48577629
1	-2.26691494	-7.15671796	2.27953439
1	-3.88451031	-6.59632959	1.79291243
1	-3.41829936	-6.59796126	3.50303156
1	-0.01746423	-1.02431379	2.15759204

Energy = -7584.949539 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 75

Atomic N.	X	Y	Z
8	2.50074130	0.25897978	1.30509632
8	3.54946678	1.09136487	-0.50473630
6	4.61175045	1.79231044	-1.15388567
1	4.34102244	1.83441029	-2.21642243
1	5.57222388	1.25918295	-1.05814281
1	4.71582489	2.81526806	-0.76260788
8	3.42271260	2.38230061	1.35987763
6	3.58281081	1.01026720	0.93645150
6	4.89996059	0.36891983	1.46430486
1	4.61611721	-0.23435880	2.33942185
1	5.21798250	-0.35189961	0.69490440
6	6.06883360	1.28786106	1.85617827
1	6.24457353	2.05604299	1.08806835
1	6.98148122	0.67042594	1.88784829
6	5.89903873	1.96305124	3.22622824
1	5.66500542	1.18534240	3.97426276
1	6.86074325	2.40531273	3.53261770
6	4.81950276	3.04982301	3.27269330
1	5.12876352	3.91211537	2.65898702
1	4.71349114	3.42061795	4.30670088
6	3.44635742	2.59494018	2.78332643
1	3.10671860	1.68560637	3.30688868

1	2.70303970	3.38366075	2.97941108
50	1.48330018	-0.95126790	-0.11182780
7	-0.18336414	0.85544217	-0.13847060
6	0.38869974	2.19434997	-0.41253605
1	-0.39422870	2.96908441	-0.33031978
1	0.82269091	2.22429017	-1.41747284
1	1.19296638	2.39662616	0.30459535
7	-2.07175022	0.08500926	-3.39374609
6	-1.32155372	0.55355266	-1.04644409
1	-2.11425244	1.31077719	-0.89785511
1	-1.72880427	-0.42034878	-0.74275021
6	-0.94821717	0.48585413	-2.53713818
1	-0.56710720	1.45182522	-2.88424317
1	-0.13745762	-0.24652000	-2.68142648
6	-3.20727377	0.93161173	-3.50890294
6	-3.09527298	2.21321727	-4.09934440
6	-4.24273049	3.00726917	-4.22508203
6	-5.50772606	2.57000033	-3.82139448
6	-5.60644864	1.27664743	-3.29462417
6	-4.48736394	0.45525078	-3.12729931
7	-0.01343030	-1.57122844	1.27739051
6	-0.62290499	0.79621383	1.28920979
1	-1.46155656	1.49869634	1.44876075
1	0.24175769	1.12684709	1.87997786
6	-1.01898124	-0.61485752	1.72031005
1	-1.10688083	-0.59608689	2.82471082
1	-2.03629598	-0.85515433	1.34687650
6	-0.14605004	-2.90853257	1.74103276
6	-1.17988914	-3.76239170	1.27205843
6	-1.27464808	-5.07330547	1.75612133
6	-0.37040778	-5.58804437	2.69045059
6	0.65129435	-4.74381511	3.13771629
6	0.78106146	-3.42495804	2.68464579
6	-1.78996486	2.71666374	-4.66630799
1	-4.14172807	3.99326325	-4.68618902
6	-6.72199348	3.45819595	-3.94590650
1	-6.58538608	0.89345934	-2.99557708
6	-4.66035592	-0.93252643	-2.55537007
6	-2.15597037	-3.30173699	0.21891583
1	-2.07411889	-5.71585966	1.37685371
6	-0.47045196	-7.01570947	3.17175969
1	1.36836732	-5.11801102	3.87350724
6	1.90394155	-2.56938380	3.21928747
1	-1.97975116	3.45731875	-5.45421656
1	-1.20365637	1.89189997	-5.09576496
1	-1.15931441	3.21042603	-3.90897059
1	-4.35159963	-1.71966870	-3.26351164
1	-5.71369793	-1.11686263	-2.31081356
1	-4.07695095	-1.07906061	-1.63239443
1	-6.93151840	3.98276375	-2.99998709
1	-7.62008922	2.87843093	-4.20041480
1	-6.57868902	4.22453507	-4.71962653
1	-2.61895454	-4.16051397	-0.28462961
1	-1.64209950	-2.68700375	-0.53509870
1	-2.97046328	-2.69074022	0.64027353
1	1.58514731	-1.53186660	3.37806686
1	2.75019827	-2.51958101	2.51536825
1	2.28762792	-2.98356914	4.16147543

1	0.14796009	-7.68732546	2.55491177
1	-1.50375258	-7.38508533	3.12137482
1	-0.12051723	-7.11413776	4.20874170
1	-2.35755537	-0.86591402	-3.16620874

Energy = -7584.958712 Hartree
Number of imaginary frequencies = 0.

Compound I3b isomer 76

Atomic N.	X	Y	Z
8	1.99927636	-0.13768090	1.36013532
8	2.87117999	0.84632770	-0.46887956
6	3.96174608	1.29195863	-1.27590977
1	3.51304844	1.79684560	-2.14111464
1	4.57236596	0.44960928	-1.64158806
1	4.60152039	2.00223197	-0.73100947
8	3.76037582	1.35283330	1.55977713
6	3.18581124	0.25435348	0.81260662
6	4.15995595	-0.95465058	0.68238947
1	3.83857204	-1.68572525	1.43914397
1	3.94163596	-1.41884409	-0.29223900
6	5.67086023	-0.71528718	0.83744250
1	5.99686590	0.15692655	0.25095494
1	6.19194536	-1.58674324	0.40803639
6	6.13028556	-0.55259560	2.29495436
1	5.74302720	-1.40353196	2.88248907
1	7.22922016	-0.62385942	2.33741993
6	5.69517954	0.75831432	2.95875446
1	6.21354544	1.60841295	2.48486585
1	6.00067046	0.75405120	4.01930818
6	4.19360424	1.02962866	2.89268773
1	3.60837417	0.18088353	3.28515537
1	3.94921679	1.90945796	3.50880957
50	0.27789410	-0.44359595	0.12231529
7	-0.44025621	1.71166364	1.16578495
6	0.57221736	2.78362541	1.03709043
1	0.27387986	3.66731026	1.63042178
1	0.68642495	3.07666560	-0.01173727
1	1.53970934	2.40780423	1.38925370
7	-1.81372171	1.40367931	-1.59870353
6	-1.78258332	2.19272520	0.74889463
1	-2.05089810	3.07316651	1.36433004
1	-2.50495494	1.39954045	0.98932041
6	-1.93845286	2.57627608	-0.72142028
1	-2.92690856	3.06757779	-0.82259328
1	-1.19220849	3.32553350	-1.01245116
6	-1.98194639	1.60427399	-2.99988584
6	-1.00095923	2.29096063	-3.74994468
6	-1.18908813	2.44867433	-5.12919901
6	-2.30108732	1.92796970	-5.79809667
6	-3.23811650	1.21268215	-5.04270660
6	-3.10301171	1.04587821	-3.66098589
7	-0.99852598	-0.98244744	1.76692001
6	-0.48573617	1.26117062	2.58974821
1	-0.86251079	2.08210768	3.22888592
1	0.55375625	1.04096417	2.86491957
6	-1.33617390	0.00595498	2.78082129
1	-1.12349091	-0.36735287	3.80235290

1	-2.41354347	0.27350478	2.78481381
6	-1.57529223	-2.27221776	1.90546119
6	-2.97177474	-2.49008702	1.74704370
6	-3.49955162	-3.77906961	1.89052823
6	-2.69403221	-4.88554427	2.17755772
6	-1.32049795	-4.66532066	2.32007397
6	-0.74937924	-3.39273915	2.19202976
6	0.26906318	2.79580500	-3.11163697
1	-0.42096021	2.97532486	-5.70126014
6	-2.48973386	2.13337675	-7.28168656
1	-4.10583295	0.77370234	-5.54145620
6	-4.13977084	0.25604523	-2.89545032
6	-3.90201819	-1.36451518	1.37070509
1	-4.57546327	-3.92250207	1.75609403
6	-3.28048299	-6.27228185	2.29132593
1	-0.66713797	-5.51063994	2.55308083
6	0.74087866	-3.23702632	2.37821144
1	1.06038553	2.89773422	-3.86570586
1	0.61699678	2.10243655	-2.33240724
1	0.14124015	3.78637038	-2.64521594
1	-3.72148871	-0.66809251	-2.46278350
1	-4.96061952	-0.04345212	-3.55867208
1	-4.57891560	0.83593927	-2.06814751
1	-3.15878319	2.98492676	-7.48384337
1	-2.93827823	1.24948357	-7.75600481
1	-1.53392783	2.34216293	-7.78068168
1	-4.80588461	-1.75292182	0.88298246
1	-3.39902518	-0.67051641	0.68080415
1	-4.22781942	-0.77547777	2.24298694
1	0.99275722	-2.29209861	2.87527897
1	1.27376433	-3.22646512	1.41319473
1	1.14504332	-4.07695512	2.95962939
1	-3.31502843	-6.77174433	1.30973119
1	-4.30836952	-6.24392371	2.67844921
1	-2.68019889	-6.90685210	2.95777577
1	-2.46785217	0.68790577	-1.28033164

Energy = -7584.958389 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 77

Atomic N.	X	Y	Z
8	1.56313152	0.69827504	0.25753462
8	1.64379753	1.06619852	-1.94291438
6	2.22410696	1.51093222	-3.17444850
1	1.40499892	1.53353675	-3.90316631
1	3.00230099	0.81440944	-3.52623244
1	2.64262645	2.52036202	-3.06397935
8	2.74096013	2.52086941	-0.58017136
6	2.42339737	1.12833646	-0.71012323
6	3.68551918	0.22274659	-0.77710324
1	3.81974662	-0.19001475	0.23429003
1	3.41269508	-0.63196661	-1.41507478
6	5.01286697	0.84256043	-1.24374524
1	4.86738092	1.45403688	-2.14723750
1	5.68268846	0.01744688	-1.53588532
6	5.72228809	1.67777258	-0.16612670
1	5.80933725	1.06685049	0.74969195

1	6.75294518	1.88982033	-0.49316101
6	5.03071908	3.00221903	0.17508190
1	5.09518870	3.69132365	-0.68307006
1	5.55969899	3.49020007	1.01167996
6	3.55758824	2.86463775	0.55298306
1	3.41129613	2.13043734	1.36326395
1	3.17284110	3.83137136	0.91289575
50	-0.24591695	-0.06921828	-0.59202103
7	-1.13095888	0.26240314	1.76266562
6	-0.06527848	0.76284254	2.66415143
1	-0.48290583	0.97992363	3.66354651
1	0.38835191	1.66478583	2.24367415
1	0.72249497	0.00672224	2.75144095
7	-1.43824629	1.70865484	-0.72584182
6	-2.15654547	1.32948224	1.55459353
1	-2.39408766	1.79358631	2.53105466
1	-3.06571966	0.85164109	1.16586153
6	-1.69649804	2.37605692	0.54230785
1	-2.51301247	3.11091881	0.43037313
1	-0.83300768	2.93399751	0.95538532
6	-1.63338324	2.41291688	-1.93720363
6	-1.09879597	3.71016324	-2.17231470
6	-1.34916638	4.35116532	-3.39342812
6	-2.08963358	3.75590090	-4.41869890
6	-2.58819278	2.46936094	-4.18749689
6	-2.38457971	1.79620801	-2.97766944
7	-1.89524679	-3.00292497	0.91054351
6	-1.76582073	-0.93092747	2.40089262
1	-2.39940172	-0.56892612	3.23286469
1	-0.96810244	-1.53747935	2.85190565
6	-2.59074152	-1.83055484	1.45343222
1	-3.48614216	-2.16610311	1.99001523
1	-2.95149949	-1.24187594	0.59584056
6	-1.43489958	-4.01227705	1.79380085
6	-2.35359579	-4.76986219	2.56336331
6	-1.87111859	-5.77729584	3.40782372
6	-0.51223432	-6.09403449	3.49970709
6	0.37284761	-5.37721498	2.68704036
6	-0.05719736	-4.34736644	1.84304353
6	-0.19963280	4.39397640	-1.17056782
1	-0.92187801	5.34511668	-3.55383703
6	-2.36265406	4.48106452	-5.71473140
1	-3.17504686	1.97554776	-4.96690918
6	-2.99651371	0.42873680	-2.79441186
6	-3.84539554	-4.57847577	2.43534853
1	-2.59404387	-6.35519638	3.98971486
6	-0.01909851	-7.16691774	4.44023540
1	1.43808703	-5.62081739	2.71113142
6	0.95110652	-3.62332146	0.98443999
1	0.34134443	5.21924911	-1.65257777
1	0.54147770	3.69311652	-0.76074668
1	-0.75891632	4.82279305	-0.32405737
1	-2.25186616	-0.38052565	-2.87568064
1	-3.76165341	0.24259896	-3.55988913
1	-3.45457923	0.33112571	-1.79963839
1	-3.34492536	4.98021570	-5.69580961
1	-2.36789488	3.79011793	-6.56954989
1	-1.60719381	5.25560356	-5.90586984

1	-4.37082944	-5.50069692	2.71611909
1	-4.12076446	-4.31983374	1.40292646
1	-4.23072763	-3.77909328	3.08956788
1	0.96696303	-2.53821437	1.17664326
1	0.74955340	-3.74398098	-0.09250820
1	1.96169197	-4.00728559	1.17214365
1	0.87892198	-7.66333232	4.04765259
1	-0.78731944	-7.93360813	4.61088051
1	0.24498007	-6.74557673	5.42351070
1	-1.17307737	-2.70541748	0.25083520

Energy = -7584.956363 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 78

Atomic N.	X	Y	Z
8	2.30646796	1.16072870	1.06280687
8	2.41909714	1.21937551	-1.16629470
6	2.89341589	1.67175750	-2.43931366
1	2.15957575	1.32391414	-3.17636496
1	3.87831242	1.23786323	-2.67723575
1	2.94697247	2.76824118	-2.46850105
8	2.89258822	3.13384312	-0.02598182
6	3.04628425	1.70746388	0.05942942
6	4.53422705	1.26676585	0.15969724
1	4.72420198	1.07197473	1.22616748
1	4.59336765	0.28680666	-0.33820711
6	5.62094559	2.21207355	-0.37821197
1	5.34635881	2.60597423	-1.36856924
1	6.53766736	1.61836286	-0.52694676
6	5.95311265	3.37909855	0.56504120
1	6.17198517	2.96840534	1.56655405
1	6.88011491	3.86775055	0.22407727
6	4.85194969	4.43845029	0.68361696
1	4.74928972	4.98116066	-0.27052921
1	5.13920879	5.18643154	1.44259708
6	3.47847186	3.88154843	1.05269589
1	3.52179492	3.26279670	1.96525874
1	2.78219165	4.71111873	1.25210266
50	0.83086623	-0.20632392	0.29701642
7	-0.32044543	0.17389767	2.51745521
6	0.50618902	1.09779293	3.33191409
1	-0.03549770	1.38095753	4.25224290
1	0.76123109	1.98815188	2.75190339
1	1.44743375	0.60305183	3.59875084
7	-0.76540936	1.15985118	-0.15390383
6	-1.59023509	0.83453821	2.10782941
1	-2.06400480	1.31603500	2.98547511
1	-2.25841668	0.05869829	1.71646666
6	-1.34847914	1.84905768	0.98903162
1	-2.32947157	2.27693139	0.71752821
1	-0.74320030	2.69158011	1.37816584
6	-1.05618716	1.61883410	-1.45755653
6	-0.95318386	2.98981661	-1.83017597
6	-1.28726738	3.38220441	-3.13276275
6	-1.69655780	2.47169159	-4.11203872
6	-1.75889531	1.12332112	-3.74688203
6	-1.45696877	0.68236992	-2.45280442

7	-1.30745933	-2.59928503	1.52844060
6	-0.53763219	-1.05431379	3.34047627
1	-0.84091603	-0.74553698	4.35938411
1	0.44590819	-1.54179587	3.43601904
6	-1.57376896	-2.07430265	2.87162800
1	-1.56890881	-2.87595550	3.63741801
1	-2.57835519	-1.63060425	2.90623334
6	-1.97223751	-3.79192915	1.13037468
6	-3.37549742	-3.81802802	0.95853404
6	-3.98794283	-5.00863416	0.54633720
6	-3.25975712	-6.17000108	0.27060510
6	-1.86758326	-6.10922523	0.40360024
6	-1.21268760	-4.94984467	0.83095387
6	-0.40660526	4.03086000	-0.88263792
1	-1.19314505	4.43993421	-3.39524953
6	-2.07982308	2.93005598	-5.49883228
1	-2.07500779	0.38371872	-4.48784859
6	-1.58536158	-0.78835180	-2.13987155
6	-4.21858849	-2.58014039	1.14121635
1	-5.07251764	-5.01389453	0.41055547
6	-3.95031718	-7.44630301	-0.14560620
1	-1.26856317	-6.99414643	0.17442342
6	0.29314707	-4.94205605	0.95601533
1	-0.11309104	4.92967505	-1.44141656
1	0.47968189	3.65133681	-0.35418316
1	-1.14113066	4.34518841	-0.12440992
1	-0.61339192	-1.30921893	-2.17908664
1	-2.24203955	-1.28315927	-2.86812309
1	-1.98187706	-0.95056849	-1.12807796
1	-3.14712924	3.19983558	-5.55121708
1	-1.90667819	2.14216406	-6.24492534
1	-1.50686807	3.81843967	-5.80003721
1	-5.16538409	-2.67863835	0.59486678
1	-3.69380051	-1.69064415	0.76320881
1	-4.47223751	-2.39267773	2.19698265
1	0.62309662	-4.68245334	1.97497580
1	0.76518171	-4.21944795	0.27005359
1	0.70292224	-5.93162236	0.71872827
1	-3.31608984	-8.04771535	-0.81110190
1	-4.89455871	-7.23867591	-0.66727141
1	-4.19127930	-8.07174773	0.72884444
1	-0.30080819	-2.69465380	1.38847689

Energy = -7584.954986 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 79

Atomic N.	X	Y	Z
8	2.13949661	-0.16980360	1.12505994
8	2.57385908	1.57210630	-0.23522974
6	3.44955561	2.51130893	-0.85971231
1	2.80890355	3.17448892	-1.45520072
1	4.16537860	2.01698680	-1.53748122
1	3.99802322	3.10715261	-0.11478600
8	3.58375170	1.51101782	1.79900461
6	3.15083151	0.65050072	0.71853089
6	4.32082518	-0.17731619	0.10747775
1	4.24358779	-1.18239786	0.54825580

1	4.08151632	-0.30087188	-0.96047318
6	5.76265025	0.32823935	0.28006297
1	5.83728101	1.40156184	0.04885101
1	6.38885676	-0.19082652	-0.46410424
6	6.35459625	0.06297329	1.67329666
1	6.21640541	-1.00518387	1.91655526
1	7.44294421	0.23338890	1.64179406
6	5.75390935	0.91760298	2.79453032
1	6.03206834	1.97481523	2.65019382
1	6.18168270	0.60828221	3.76379408
6	4.23177136	0.84326456	2.89578000
1	3.87849314	-0.19939831	2.96584640
1	3.89530684	1.36558353	3.80539552
50	0.37093408	-0.38729515	-0.06482212
7	-0.61668762	1.03246002	1.74119758
6	0.14744337	2.27681597	1.98307118
1	-0.24056795	2.79844442	2.87712230
1	0.07435816	2.94376558	1.11776757
1	1.20476232	2.02660837	2.12730081
7	-2.22955553	1.43537556	-0.87744580
6	-2.06680705	1.31769520	1.59138179
1	-2.42262588	1.83584005	2.50294982
1	-2.58871556	0.35112374	1.54619770
6	-2.47082288	2.15651242	0.38035516
1	-3.54031690	2.41660961	0.51152895
1	-1.92409650	3.10713749	0.36160520
6	-2.59869817	2.08208398	-2.09294079
6	-1.86357197	3.19124921	-2.56822107
6	-2.24118024	3.78687897	-3.77864192
6	-3.30437634	3.30747020	-4.55000754
6	-3.99000872	2.17978585	-4.08272858
6	-3.66229562	1.56352532	-2.87102913
7	-0.56785795	-1.75014557	1.30804225
6	-0.40107640	0.10382582	2.89186491
1	-0.84838667	0.53451852	3.80772216
1	0.68696346	0.03839271	3.02082295
6	-0.96433088	-1.29278550	2.63177053
1	-0.56182290	-1.94937655	3.42869365
1	-2.06458869	-1.29291469	2.77981258
6	-0.86806401	-3.09675772	0.97351614
6	-2.20595573	-3.54514739	0.79716167
6	-2.45803938	-4.88192301	0.46507862
6	-1.42861524	-5.81101774	0.28512537
6	-0.11501837	-5.35977316	0.44869986
6	0.18406203	-4.03388125	0.78687833
6	-0.64696211	3.70243617	-1.83758663
1	-1.66178304	4.64005068	-4.14064383
6	-3.70440127	3.98439112	-5.83863637
1	-4.81033510	1.76755155	-4.67560216
6	-4.42979068	0.34254976	-2.41839430
6	-3.37123509	-2.59436003	0.90687189
1	-3.49506568	-5.20085533	0.32694876
6	-1.72197913	-7.23869356	-0.10929719
1	0.71019177	-6.06603298	0.32231925
6	1.62850564	-3.63044657	0.96182382
1	0.01594555	4.23808908	-2.52960349
1	-0.08377443	2.87215341	-1.38771320
1	-0.90533446	4.40791097	-1.03094906

1	-3.79358331	-0.55747666	-2.38107348
1	-5.25076029	0.12615396	-3.11303534
1	-4.87058967	0.47428994	-1.41745190
1	-4.53456096	4.69012462	-5.67611786
1	-4.04114075	3.25499947	-6.58826112
1	-2.86892750	4.55472968	-6.26633481
1	-4.23473339	-2.96987438	0.34201352
1	-3.09325766	-1.60593274	0.51157796
1	-3.69998684	-2.44660737	1.94806731
1	1.75173884	-2.89771537	1.76887845
1	2.03222734	-3.15475189	0.05297817
1	2.25117987	-4.51178778	1.16765429
1	-1.74787290	-7.35161178	-1.20508897
1	-2.69611327	-7.57022722	0.27567046
1	-0.95173310	-7.92470028	0.26944571
1	-2.69200345	0.52706650	-0.82573171

Energy = -7584.958391 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 80

Atomic N.	X	Y	Z
8	2.17910942	-1.11323944	-0.35153176
8	3.91798944	-0.61926072	-1.81877420
6	4.30392557	-1.98727108	-1.94456642
1	4.67522854	-2.10554417	-2.97002198
1	3.44859667	-2.66132861	-1.78440008
1	5.11237218	-2.26141624	-1.24281192
8	2.69122949	1.02503954	-0.86523057
6	3.24924412	-0.29850968	-0.57615977
6	4.24041138	-0.32721101	0.60962396
1	3.74662199	0.14576869	1.47401987
1	4.32971417	-1.39136036	0.87243274
6	5.64072228	0.25514400	0.37316943
1	6.03842713	-0.15243033	-0.56857863
1	6.30437203	-0.10448312	1.17590050
6	5.71188566	1.78469657	0.32948916
1	5.46917477	2.18848656	1.32836617
1	6.74968387	2.08958609	0.11967895
6	4.77387723	2.43335538	-0.69450280
1	4.97491656	2.05978824	-1.71038759
1	4.96309380	3.51939224	-0.71140171
6	3.29171377	2.24317832	-0.37693011
1	3.12160397	2.33508881	0.71170402
1	2.69409168	3.02178546	-0.87143029
50	0.39410671	0.06321955	-0.10649175
7	-0.60053236	-2.17666255	-0.46431394
6	0.05353500	-3.25631129	0.30432873
1	-0.35349273	-4.24555931	0.02765664
1	-0.09388778	-3.08471676	1.37659831
1	1.12762008	-3.22410382	0.09200533
7	-2.07906796	-1.33785462	2.09153654
6	-2.07901433	-2.16017440	-0.27312094
1	-2.52488294	-2.97162863	-0.87945012
1	-2.44491725	-1.20785268	-0.68618944
6	-2.59646716	-2.34290695	1.15354595
1	-3.70186413	-2.31061009	1.08215522
1	-2.34212069	-3.34915050	1.51429407

6	-2.75336407	-1.17792225	3.33374601
6	-2.74524358	-2.20832508	4.30147746
6	-3.40552622	-2.00357730	5.52051692
6	-4.05321332	-0.80417645	5.82953868
6	-4.01248292	0.21926151	4.87464711
6	-3.38353162	0.05504178	3.63696566
7	-0.36983275	0.10040128	-2.10196120
6	-0.28505662	-2.33689139	-1.91643505
1	-0.74185855	-3.27167207	-2.29306580
1	0.80791992	-2.41830609	-1.98022369
6	-0.74857376	-1.14525652	-2.75043672
1	-0.28977437	-1.26749072	-3.74954267
1	-1.84614622	-1.19865278	-2.92031253
6	-0.44306898	1.28897574	-2.87727583
6	-1.40363977	2.28700597	-2.56600772
6	-1.45077079	3.46965183	-3.31533659
6	-0.57829137	3.70716910	-4.38219661
6	0.36009087	2.71515234	-4.68563757
6	0.45086786	1.52171565	-3.95802317
6	-1.98425126	-3.49256283	4.08286855
1	-3.38608665	-2.80613610	6.26235834
6	-4.77676288	-0.61841600	7.14142155
1	-4.49248587	1.17628997	5.09429021
6	-3.37200023	1.19469779	2.64511856
6	-2.39770370	2.09209629	-1.44537707
1	-2.20304190	4.22222552	-3.06346945
6	-0.62637005	5.00143314	-5.15879622
1	1.06187698	2.87863094	-5.50839390
6	1.52130644	0.52278190	-4.31930297
1	-1.76415581	-3.97486361	5.04403852
1	-1.03246718	-3.29781373	3.56728511
1	-2.54604249	-4.22068803	3.47620183
1	-2.35080790	1.55489955	2.43766733
1	-3.94439556	2.04649952	3.03278470
1	-3.81679908	0.90806885	1.67881173
1	-5.86052429	-0.77887660	7.02561666
1	-4.64097711	0.39854870	7.53532193
1	-4.41927091	-1.32910207	7.89861213
1	-3.21015323	2.82749597	-1.51903385
1	-1.93108749	2.21251470	-0.45471914
1	-2.83385818	1.08338852	-1.46852634
1	1.14156964	-0.25480973	-5.00291463
1	1.91603231	0.02076210	-3.42635206
1	2.35417446	1.02136698	-4.83271315
1	0.08219932	5.73909209	-4.74895186
1	-1.62665331	5.45428331	-5.12044921
1	-0.35963099	4.84729206	-6.21355944
1	-1.99715698	-0.43614684	1.61951387

Energy = -7584.956340 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 81

Atomic N.	X	Y	Z
8	1.90638299	-0.49193627	-1.31080550
8	2.34491259	1.69128985	-1.19081058
6	3.17015168	2.82600990	-0.89633663
1	3.67653667	2.71547424	0.07196033

1	2.49389886	3.68899604	-0.86768595
1	3.91484251	2.98517621	-1.69287378
8	3.54883039	0.30136638	0.15037092
6	2.95401608	0.35982421	-1.16405533
6	3.98210758	0.17135493	-2.31284484
1	3.83365659	-0.84936557	-2.69646377
1	3.66736463	0.84730258	-3.12186219
6	5.47212628	0.37667355	-1.99786205
1	5.63134379	1.31997695	-1.45291371
1	6.00008136	0.48443818	-2.95948756
6	6.11954246	-0.78131024	-1.22107465
1	5.87641659	-1.72863305	-1.73399122
1	7.21563565	-0.67850981	-1.26988415
6	5.70124610	-0.87865578	0.25006792
1	6.08997195	-0.00957171	0.80611536
1	6.15771715	-1.77407904	0.70597987
6	4.19259416	-0.94254436	0.47315605
1	3.72978048	-1.76477345	-0.09905206
1	3.97720382	-1.12220501	1.53765398
50	0.23523132	0.34917885	-0.22243950
7	-0.80029413	-1.73129351	-1.07196880
6	0.01543504	-2.94378382	-0.85102767
1	-0.43967623	-3.82492615	-1.33782985
1	0.11479347	-3.12806556	0.22482152
1	1.01199416	-2.76512350	-1.26952365
7	-1.64096358	-1.88821565	1.87205081
6	-2.19633427	-1.88443772	-0.56972925
1	-2.77321385	-2.48402974	-1.29935031
1	-2.64189997	-0.87811355	-0.55123338
6	-2.37310711	-2.55956942	0.79037183
1	-3.46444581	-2.57804986	0.98094502
1	-2.05586076	-3.60977788	0.72500950
6	-2.02204008	-2.16724897	3.21301585
6	-1.84883901	-3.45750584	3.76420175
6	-2.22007960	-3.68505412	5.09629731
6	-2.73218130	-2.67423712	5.91450414
6	-2.85428851	-1.39315433	5.36237232
6	-2.51645313	-1.12206385	4.03323492
7	-0.95814846	0.95246791	-1.89387819
6	-0.82338453	-1.40610432	-2.53087608
1	-1.35308057	-2.20802976	-3.07937308
1	0.22615047	-1.38223852	-2.85263003
6	-1.46800149	-0.05187284	-2.81484879
1	-1.24843184	0.18261632	-3.87333530
1	-2.57530105	-0.13381153	-2.75477937
6	-1.16125867	2.31517004	-2.23685869
6	-2.02216343	3.12869635	-1.45277768
6	-2.19584150	4.47872301	-1.77953701
6	-1.54779155	5.06807775	-2.87121469
6	-0.70460956	4.25917703	-3.63885491
6	-0.49362940	2.90573205	-3.34320286
6	-1.20868127	-4.57482717	2.97774264
1	-2.07501165	-4.68570591	5.51162001
6	-3.14542426	-2.95178342	7.33973262
1	-3.23249558	-0.57643962	5.98242931
6	-2.66991827	0.27995791	3.49166191
6	-2.77123342	2.55559194	-0.27314798
1	-2.86915665	5.08536948	-1.16764673

6	-1.73042925	6.53347765	-3.18722649
1	-0.17609083	4.69705407	-4.49043897
6	0.46970005	2.11034770	-4.18867337
1	-0.80864835	-5.33916282	3.65648976
1	-0.38191970	-4.19326386	2.36077881
1	-1.91850413	-5.07971650	2.30321696
1	-1.70375970	0.71799917	3.19130624
1	-3.10394402	0.93989608	4.25296584
1	-3.32843848	0.31349605	2.60892080
1	-4.23421397	-3.10065627	7.41786357
1	-2.88513753	-2.11589256	8.00406709
1	-2.66203029	-3.85912854	7.72613908
1	-3.56438014	3.24269142	0.05094780
1	-2.10843117	2.38292186	0.58966665
1	-3.22463166	1.58543955	-0.52077604
1	0.97014721	1.34156909	-3.58524599
1	1.23108989	2.76851563	-4.62881430
1	-0.03832983	1.60256355	-5.02524814
1	-1.07887827	7.16165733	-2.55886361
1	-2.76470943	6.85766258	-3.00411593
1	-1.48394546	6.75069902	-4.23525733
1	-1.63123929	-0.87976390	1.71104945

Energy = -7584.959651 Hartree

Number of imaginary frequencies = 0.

Compound I3b isomer 82

Atomic N.	X	Y	Z
8	0.57942464	0.10156620	0.32712494
8	2.02817148	-1.59394594	0.33925560
6	3.33820481	-2.17007763	0.29532603
1	3.19635926	-3.22734082	0.03777492
1	3.82564672	-2.11082166	1.28161987
1	3.96671475	-1.68423536	-0.46346507
8	2.71950416	0.37703516	-0.57130729
6	1.90213396	-0.13926442	0.50227077
6	2.36520070	0.32536721	1.90752980
1	1.66464567	1.11612115	2.21581936
1	2.18227710	-0.52032214	2.58647617
6	3.80356242	0.84284677	2.06621389
1	4.52321871	0.15708539	1.59276630
1	4.03888989	0.83802950	3.14322644
6	4.02325638	2.26753246	1.53224635
1	3.24491667	2.92517150	1.95775411
1	4.98721918	2.64868245	1.90695864
6	4.00647185	2.38886331	0.00437417
1	4.88583134	1.87605129	-0.41985865
1	4.09220920	3.45121662	-0.28253625
6	2.75858877	1.81304591	-0.66040435
1	1.83369125	2.24135871	-0.24062247
1	2.76736130	2.04602759	-1.73612532
50	-0.13759505	-1.28828449	-1.14347042
7	-2.83314824	-1.54911145	-2.17017152
6	-2.78014811	-2.59083278	-3.20132662
1	-3.79038740	-2.87898939	-3.55610199
1	-2.28562945	-3.48661415	-2.80560194
1	-2.18925532	-2.23428696	-4.05575919
7	-1.38628800	-2.24313494	0.32581509

6	-3.49049137	-2.03698068	-0.94513864
1	-4.43564547	-2.56483014	-1.19579084
1	-3.74007649	-1.16710904	-0.32194615
6	-2.58116467	-2.95310904	-0.12407051
1	-3.16418265	-3.28730761	0.75180447
1	-2.36983614	-3.87589467	-0.70582446
6	-0.86245833	-2.69900135	1.57502187
6	-0.21408982	-3.95470201	1.69224238
6	0.27820604	-4.37001805	2.93724453
6	0.15042265	-3.58273887	4.08500439
6	-0.49187171	-2.34590037	3.95661985
6	-1.00000860	-1.89323997	2.73290008
7	-1.57655251	1.14820018	-2.11279029
6	-3.46357182	-0.32557552	-2.69383701
1	-4.57038795	-0.40091688	-2.66762877
1	-3.18320478	-0.23386203	-3.75589778
6	-3.03463185	0.94748329	-1.96773953
1	-3.60129479	1.79424585	-2.39568580
1	-3.29722754	0.88730447	-0.90360006
6	-1.04304040	2.46662773	-2.00330660
6	-1.22068715	3.24578090	-0.83866490
6	-0.64672139	4.52327940	-0.78797867
6	0.11578283	5.05020740	-1.83422235
6	0.31328305	4.24282266	-2.96039981
6	-0.25024168	2.96790255	-3.06548919
6	-0.02371068	-4.85564796	0.49672997
1	0.78518537	-5.33658575	3.00629389
6	0.66168976	-4.06066071	5.42331846
1	-0.60689063	-1.71003915	4.83876396
6	-1.68673202	-0.55419174	2.66348496
6	-1.94186677	2.71581380	0.37471808
1	-0.78312066	5.11332459	0.12175768
6	0.69943093	6.44025056	-1.75710902
1	0.92380453	4.61451050	-3.78708773
6	0.01212632	2.13684147	-4.30051917
1	0.79071311	-5.57059824	0.67403845
1	0.21027806	-4.27712610	-0.40958958
1	-0.93063518	-5.44144233	0.27650223
1	-1.08192012	0.14788963	2.07244822
1	-1.83119060	-0.13990669	3.67039774
1	-2.66659367	-0.62997354	2.17055788
1	-0.14519883	-4.51635889	6.01938106
1	1.07243856	-3.23128297	6.01617830
1	1.44777829	-4.81863238	5.30353414
1	-1.68229100	3.31158111	1.25914929
1	-1.65392876	1.67414954	0.57089450
1	-3.03695217	2.75380478	0.26615433
1	-0.91788884	1.86263760	-4.82633688
1	0.54659501	1.20162725	-4.06488499
1	0.63280116	2.69517878	-5.01200568
1	1.68776564	6.48856669	-2.23518242
1	0.80652891	6.77066092	-0.71519598
1	0.05514980	7.17268865	-2.26905628
1	-1.29472162	0.76151332	-3.01396300

Energy = -7584.953831 Hartree

Number of imaginary frequencies = 0.

Intermediate 4a (I4a)**Compound I4a isomer 1**

Atomic N.	X	Y	Z
8	2.95674345	-1.84488636	-0.28598917
6	4.18927602	-1.74415556	0.30053872
8	5.25248513	-1.51919063	-0.61932204
6	5.00131762	-0.50845986	-1.60261182
1	4.78126818	0.46651390	-1.13754985
1	4.17075490	-0.79121025	-2.26571558
1	5.92493419	-0.42572426	-2.18715718
8	4.03613288	-0.56297146	1.17215338
6	4.60325969	-3.00752897	1.07765305
1	5.70222975	-3.04309662	1.12364007
1	4.29004170	-3.84818926	0.44228729
6	4.01312453	-3.14103897	2.48812675
1	2.96430159	-2.80397041	2.49507617
1	3.99624876	-4.21003696	2.75279182
6	4.81804060	-2.39687562	3.56758152
1	5.87258159	-2.71788132	3.49615768
1	4.46527165	-2.71627324	4.56074910
6	4.74703837	-0.86548089	3.50292611
1	3.74252534	-0.51841391	3.78885574
1	5.45128155	-0.43673289	4.23634359
6	5.07008772	-0.26685395	2.13856636
1	6.03473725	-0.61731333	1.73644648
1	5.10995838	0.83063120	2.20131775
50	1.72461577	-0.18553207	0.22354494
7	0.08403225	-1.80270884	-0.93630406
6	0.57636394	-2.30913481	-2.23541467
1	-0.11220241	-3.06330008	-2.65936306
1	0.69254825	-1.48436467	-2.94741077
1	1.55977247	-2.76269648	-2.06993677
7	-0.52628198	0.82906716	-2.26476753
6	-1.26926013	-1.20341253	-1.03179705
1	-2.02874080	-2.00652801	-1.11329282
1	-1.46513266	-0.67082400	-0.08838980
6	-1.50801910	-0.26022333	-2.21388120
1	-2.54648583	0.10853581	-2.12974698
1	-1.42865876	-0.80515802	-3.16298774
16	-0.38401348	1.71171271	-3.71418127
7	0.57078699	-1.28775757	1.76088685
6	0.07234214	-2.92149574	0.04873212
1	-0.65084049	-3.69757031	-0.26772457
1	1.08335293	-3.34797323	0.03538370
6	-0.25804071	-2.45478193	1.46567874
1	-0.04746003	-3.28761943	2.15730835
1	-1.33691612	-2.22431181	1.55792957
16	0.43060511	-0.57746280	3.23290957
8	1.42740735	0.52919814	3.20306857
8	0.44788081	-1.57781028	4.32598361
6	-1.21348093	0.19417688	3.28245101
6	-2.27371500	-0.46623429	3.90530986
6	-3.53945649	0.12785055	3.90918503
6	-3.75917348	1.37597470	3.30909937
6	-2.67185369	2.02049519	2.69265522
6	-1.40501656	1.43884668	2.67446047
1	-2.09659163	-1.42181071	4.39791539

1	-0.55736771	1.95009344	2.21636236
1	-2.81984954	2.99952473	2.23188715
6	-5.11659238	2.03234420	3.35673854
1	-4.36968892	-0.38545811	4.39828434
8	0.61335883	2.75376114	-3.42021289
8	-0.20082905	0.70197930	-4.77386203
6	-1.97161334	2.52454303	-4.00358752
6	-2.91891478	1.91924665	-4.83038056
6	-4.14619758	2.55536937	-5.03384084
6	-4.43731548	3.78471854	-4.42499737
6	-3.45997711	4.37243613	-3.60129617
6	-2.23065859	3.75347018	-3.38697591
1	-2.68328221	0.97733212	-5.32448922
1	-4.88752681	2.09047088	-5.68598228
6	-5.75674881	4.47633427	-4.65706027
1	-3.66270693	5.33627916	-3.13058624
1	-1.46505067	4.22290235	-2.76912428
1	-5.91356001	1.29536318	3.51983420
1	-5.16845596	2.76195998	4.17991883
1	-5.33245065	2.57769165	2.42781981
1	-5.61093346	5.43798415	-5.17117972
1	-6.42913517	3.86358946	-5.27007011
1	-6.26308032	4.69485266	-3.70568393
1	-0.55343194	1.47520433	-1.47168592

Energy = -8524.641586 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 2

Atomic N.	X	Y	Z
8	2.53458869	-2.31784767	0.85221644
6	3.45141806	-2.35675310	1.86781785
8	4.80499799	-2.35506481	1.42763252
6	5.11376739	-1.39023145	0.41499610
1	4.90287731	-0.36265987	0.75398531
1	4.55664199	-1.58931118	-0.51200525
1	6.18868043	-1.49119369	0.22556984
8	3.17213552	-1.10594773	2.60133813
6	3.32915521	-3.60821914	2.75677439
1	4.30702431	-3.79988602	3.22381507
1	3.14949185	-4.43736705	2.05766013
6	2.23442223	-3.55484008	3.83120906
1	1.33063160	-3.06981476	3.42910421
1	1.94683760	-4.58872636	4.07901282
6	2.67733257	-2.86013612	5.13050942
1	3.61333979	-3.33463674	5.47538752
1	1.92724641	-3.05364410	5.91330594
6	2.88354235	-1.34321435	5.02838898
1	1.91588269	-0.83488271	4.89994420
1	3.31459716	-0.96969754	5.97302933
6	3.79334269	-0.89563304	3.89003430
1	4.76830545	-1.40994174	3.89533334
1	3.98271235	0.18595385	3.95438380
50	1.48955600	-0.46471388	0.83642759
7	0.16246110	-1.89406617	-0.84601292
6	1.01234482	-2.55772327	-1.85773792
1	0.41773464	-3.22844279	-2.50493832
1	1.51835441	-1.81013598	-2.47867867

1	1.77464339	-3.14016006	-1.32861987
7	0.54283738	0.68733776	-2.34907769
6	-0.93787242	-1.10375834	-1.45047027
1	-1.73887853	-1.78544708	-1.79961298
1	-1.37315974	-0.47784078	-0.65620729
6	-0.56469024	-0.22762634	-2.64867927
1	-1.48484580	0.30268600	-2.95551457
1	-0.24497513	-0.84752351	-3.49580031
16	1.28636317	1.48943368	-3.65541534
7	-0.31606539	-1.27256161	1.83225020
6	-0.40196440	-2.92653424	0.06904249
1	-1.07212424	-3.60509839	-0.49290453
1	0.45456025	-3.50041606	0.44494919
6	-1.15685222	-2.31669345	1.24927497
1	-1.36551080	-3.12105142	1.97427421
1	-2.13574083	-1.91791401	0.92038782
16	-0.89515836	-0.42404133	3.11185187
8	0.21021087	0.51077366	3.46303883
8	-1.48233071	-1.31749458	4.13759899
6	-2.26449504	0.59223096	2.48469231
6	-3.58292641	0.16694228	2.65306585
6	-4.62375897	0.94522966	2.13759181
6	-4.36690996	2.14841151	1.46504713
6	-3.02932169	2.55637729	1.31483079
6	-1.98030784	1.78818041	1.81757968
1	-3.78394414	-0.75303522	3.20124259
1	-0.94497062	2.11756342	1.72038017
1	-2.80975097	3.49778783	0.80663532
6	-5.49513591	3.00648406	0.94876744
1	-5.65570454	0.61470999	2.27082181
8	2.30575794	2.35191010	-3.03596415
8	1.61464646	0.43304377	-4.63107059
6	0.03357088	2.55619769	-4.40252821
6	-0.72023172	2.08916856	-5.48022807
6	-1.69407487	2.92175966	-6.03755784
6	-1.92243554	4.21088730	-5.53468005
6	-1.14029202	4.65643695	-4.45371507
6	-0.16532630	3.84042724	-3.88427404
1	-0.52408072	1.09890638	-5.88987590
1	-2.27964248	2.56541428	-6.88674547
6	-2.97410557	5.10751092	-6.13748395
1	-1.28955207	5.66430410	-4.06179008
1	0.46022491	4.19817155	-3.06650322
1	-6.41726769	2.42447259	0.82342238
1	-5.71453190	3.82645010	1.65023872
1	-5.24097492	3.46638619	-0.01610003
1	-2.54858153	6.08025372	-6.42274053
1	-3.42368119	4.65535647	-7.03006534
1	-3.78047370	5.30881753	-5.41628363
1	0.36040927	1.35595034	-1.59557948

Energy = -8524.641515 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 3

Atomic N.	X	Y	Z
8	2.15873212	-2.11022958	0.26001267
6	3.27080636	-1.64656608	0.93755368

8	4.30991935	-1.19455608	0.10952235
6	3.90771608	-0.38430243	-1.01320773
1	3.29516406	0.47613698	-0.70028385
1	3.35391489	-0.98416133	-1.74826320
1	4.84121119	-0.02436628	-1.45924738
8	2.67405545	-0.50216231	1.68119614
6	3.89637858	-2.69124570	1.87547150
1	4.97296875	-2.47781759	1.94763893
1	3.80051666	-3.65079324	1.34799285
6	3.28823594	-2.78102433	3.28183803
1	2.18890694	-2.72713017	3.22746378
1	3.53052216	-3.77537898	3.68789568
6	3.82601044	-1.71995667	4.25972770
1	4.92892048	-1.72407423	4.20464548
1	3.57025518	-2.02225727	5.28736200
6	3.30192028	-0.29411815	4.04334626
1	2.23237301	-0.23854018	4.29296035
1	3.82119220	0.39475179	4.73085171
6	3.47405511	0.25146614	2.63339555
1	4.51757117	0.22191605	2.28224531
1	3.10967115	1.28445682	2.56336026
50	0.67991855	-0.67598105	0.51349475
7	-0.67839783	-2.41386481	-0.55364738
6	0.02030991	-3.25417038	-1.56173624
1	-0.62114025	-4.09820018	-1.86815948
1	0.28489131	-2.66970475	-2.44887986
1	0.94364925	-3.63339835	-1.11330541
7	-1.54595259	-0.09565089	-2.79592517
6	-2.00009572	-1.89744378	-1.05565086
1	-2.72991100	-2.72105847	-0.94366370
1	-2.31433504	-1.07519830	-0.39829541
6	-2.10620827	-1.42994834	-2.51128069
1	-3.18778749	-1.34739521	-2.69653415
1	-1.73891635	-2.20198216	-3.21000035
16	0.15051962	-0.16414872	-3.28122904
7	-0.54033241	-1.37325389	2.10669298
6	-0.92435457	-3.26881708	0.65303784
1	-1.62439900	-4.08098273	0.38946071
1	0.04327298	-3.71352346	0.92379205
6	-1.46350752	-2.47847285	1.84103501
1	-1.51468819	-3.15471628	2.70880070
1	-2.49058885	-2.12326868	1.63992559
16	-0.98201899	-0.27016155	3.28158478
8	0.13697869	0.70137625	3.30733608
8	-1.38310156	-1.00805541	4.49972401
6	-2.45488201	0.58898598	2.67106173
6	-3.67351771	0.40853026	3.32700478
6	-4.80249269	1.08430096	2.85704897
6	-4.72594697	1.93266893	1.74252296
6	-3.48495103	2.08455883	1.09891956
6	-2.34322978	1.42482890	1.55306289
1	-3.72363934	-0.24418006	4.19787757
1	-1.38550240	1.54458582	1.02973709
1	-3.40762578	2.73273448	0.22365617
6	-5.93907487	2.68780986	1.25960911
1	-5.75801522	0.95062253	3.36778832
8	0.39892527	1.01735593	-0.26775707
8	0.28123061	-1.00646436	-4.54725097

6	0.20834243	1.58241256	-3.81582275
6	0.27343526	1.83791827	-5.18339164
6	0.35149937	3.16469371	-5.61641848
6	0.38245887	4.22372168	-4.69710750
6	0.33280828	3.92448413	-3.32342074
6	0.25095708	2.60865645	-2.86763120
1	0.26749643	1.00091493	-5.88352928
1	0.39751992	3.37905885	-6.68606030
6	0.49304830	5.65426123	-5.16445299
1	0.36609086	4.73842245	-2.59579104
1	0.23319218	2.35131225	-1.80290081
1	-6.86988806	2.20685713	1.58733920
1	-5.94056214	3.71511319	1.65629357
1	-5.95294328	2.76537577	0.16397200
1	1.47764955	6.07609290	-4.91095361
1	0.36468133	5.73269533	-6.25163579
1	-0.26215399	6.29095799	-4.68171204
1	-2.03973275	0.30868702	-3.60011259

Energy = -8524.611207 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 4

Atomic N.	X	Y	Z
8	0.18703573	-0.71562300	0.51284582
6	0.99986972	-0.06125565	1.41505234
8	1.30780804	-0.81699505	2.58364152
6	1.98262875	-2.06871965	2.35919227
1	2.96871961	-1.91353472	1.89584943
1	1.37990434	-2.75551333	1.74873105
1	2.11929864	-2.51097408	3.35294736
8	2.21150089	0.16479478	0.63243580
6	0.36811210	1.24034155	1.94391077
1	0.79712344	1.46284318	2.93212571
1	-0.69415480	1.00957964	2.10469357
6	0.52456023	2.45274164	1.01706365
1	0.37786802	2.13351490	-0.02786482
1	-0.28416806	3.16525958	1.24294900
6	1.86757078	3.18833650	1.18168305
1	1.99792578	3.42756170	2.25163859
1	1.81398017	4.15867334	0.66130544
6	3.10906327	2.43871632	0.67704051
1	3.11516292	2.39148752	-0.42233701
1	4.01521733	2.99463708	0.97132708
6	3.24482398	1.00967735	1.18747467
1	3.20408606	0.94525781	2.28692800
1	4.19705900	0.57342018	0.85381023
50	1.31539435	-1.39677100	-1.18619903
7	-1.01523594	-1.86641036	-2.22068740
6	-0.59604066	-2.52661190	-3.48186388
1	-1.43043903	-2.56025669	-4.20509760
1	0.25093613	-2.00041523	-3.94061741
1	-0.28353392	-3.55341651	-3.25528294
7	0.76524050	0.35870057	-2.50437480
6	-1.52970230	-0.49857002	-2.48300078
1	-2.46727772	-0.54637939	-3.07171303
1	-1.75286355	-0.03862483	-1.51180176
6	-0.52047446	0.37262603	-3.22233148

1	-0.93545277	1.39569768	-3.26088114
1	-0.40624108	0.03117875	-4.26433984
16	2.08706381	0.68438009	-3.44493562
7	-2.08461556	-2.29945994	0.90935970
6	-2.07913435	-2.72965066	-1.61924476
1	-2.85411245	-2.88468598	-2.39724687
1	-1.63005810	-3.71085484	-1.41218810
6	-2.80649606	-2.23622381	-0.35998827
1	-3.70134968	-2.86579449	-0.26381528
1	-3.16373831	-1.20368723	-0.48267758
16	-1.93519640	-3.81480787	1.64371607
8	-0.50888046	-4.21270424	1.65478110
8	-2.95968520	-4.70088461	1.04431943
6	-2.41479429	-3.48436875	3.35304937
6	-3.59532860	-4.04057356	3.84232117
6	-3.95576793	-3.80414188	5.17145897
6	-3.15397143	-3.01914225	6.01184382
6	-1.97212779	-2.46785934	5.48574668
6	-1.59186838	-2.69802179	4.16516273
1	-4.21376046	-4.65210862	3.18646330
1	-0.67280376	-2.26218174	3.77139559
1	-1.33726386	-1.84889332	6.12263711
6	-3.53303302	-2.78775029	7.45326436
1	-4.87777822	-4.23993987	5.56072589
8	3.24430101	0.45130425	-2.53270646
8	2.06405167	-0.02771491	-4.75101278
6	2.00150711	2.45049954	-3.85003771
6	2.36646952	2.86057395	-5.13343423
6	2.34213077	4.22122534	-5.44483932
6	1.95110714	5.17793692	-4.49550989
6	1.57220315	4.73376291	-3.21762446
6	1.59830778	3.37880306	-2.88786627
1	2.65402839	2.11406487	-5.87266202
1	2.62669236	4.54507679	-6.44772175
6	1.95407775	6.64833905	-4.83063170
1	1.24934733	5.46127929	-2.47020640
1	1.29451619	3.03795353	-1.89867300
1	-4.59344554	-3.00893999	7.62972302
1	-2.94310299	-3.43437511	8.12136460
1	-3.34035929	-1.74936536	7.75635988
1	2.89621568	7.11888515	-4.50851139
1	1.85709475	6.81404897	-5.91139870
1	1.13655370	7.17775452	-4.32304353
1	-1.18230147	-1.77673248	0.91803038

Energy = -8524.642337 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 5

Atomic N.	X	Y	Z
8	1.82084671	-4.28481534	0.52044188
8	3.26620557	-4.94417482	2.18145245
6	2.53647815	-5.35546225	0.96729220
6	1.64911757	-6.60104909	1.12942319
1	2.21530495	-7.40591497	1.62415994
1	1.45140057	-6.93532054	0.10051611
6	0.31436719	-6.35652024	1.84668697
1	-0.14243474	-5.44914722	1.42590140

1	-0.36134856	-7.19357365	1.61009460
6	0.42088210	-6.22912713	3.36946525
1	0.75447670	-7.19419217	3.79192763
1	-0.58332560	-6.04442657	3.78261905
6	1.37343549	-5.13063330	3.85496295
1	1.06305788	-4.14236084	3.48400608
1	1.32189208	-5.08177840	4.95554633
6	2.84090209	-5.36741184	3.49294745
1	3.09850043	-6.43420504	3.63193700
1	3.48994777	-4.78498422	4.16228992
50	3.00832745	-2.57215554	0.74112494
7	-1.01834396	0.48118520	-1.11155158
6	-2.40086335	0.03097636	-0.95362477
1	-2.43627087	-0.88818055	-0.35490507
1	-2.97624345	0.79815972	-0.41851602
1	-2.90044500	-0.16767591	-1.92764300
7	0.50424340	3.74957561	-2.26121489
6	-0.95051610	1.77232324	-1.80500234
1	-0.98422849	1.65753270	-2.90953910
1	-1.83693248	2.35619492	-1.51813755
6	0.30548321	2.55641643	-1.40648624
1	1.19989800	1.93398074	-1.54929839
1	0.25450051	2.82483106	-0.34211937
16	-0.24974102	5.21333838	-1.79559322
7	1.13774641	-1.39978486	0.18082929
6	-0.19617252	-0.53373441	-1.77676999
1	-0.70869531	-0.92679379	-2.68623052
1	0.73857598	-0.06353009	-2.11488504
6	0.17131504	-1.71962039	-0.88117602
1	0.64060720	-2.49241981	-1.51076955
1	-0.72839814	-2.18895648	-0.45435468
16	0.59432378	-1.12543716	1.69187324
8	1.78441592	-1.67955189	2.50676035
8	-0.75291065	-1.65044878	2.00023375
6	0.59297349	0.63570279	2.09003389
6	-0.61060310	1.25739481	2.42266040
6	-0.60812574	2.61906958	2.72533792
6	0.57763540	3.37076404	2.69572936
6	1.77551908	2.71115564	2.37188953
6	1.79179070	1.35032795	2.06832440
1	-1.52849744	0.67207424	2.44634883
1	2.72885082	0.84819097	1.82674409
1	2.71026283	3.27427736	2.35662733
6	0.55649667	4.85155494	2.96968063
1	-1.54781393	3.11166248	2.98085778
8	-0.69188365	5.14744794	-0.38376998
8	0.67556308	6.26696851	-2.26403451
6	-1.73562155	5.26777798	-2.81692400
6	-1.60848876	5.41503052	-4.20121077
6	-2.75969333	5.49474687	-4.97992026
6	-4.03872041	5.43690480	-4.39645691
6	-4.13244135	5.29483385	-3.00499286
6	-2.98762342	5.21158971	-2.20783765
1	-0.62018698	5.47076127	-4.65614186
1	-2.66718183	5.60690245	-6.06171439
6	-5.27478373	5.54668979	-5.25290942
1	-5.11608890	5.25046209	-2.53433782
1	-3.05581786	5.10606313	-1.12583780

1	-0.14161696	5.09918695	3.78091370
1	1.55229998	5.22520632	3.24029576
1	0.22319340	5.39476538	2.07179078
1	-5.40038000	6.57407942	-5.62764704
1	-5.21111254	4.88932287	-6.13138003
1	-6.17849681	5.28340009	-4.68922429
1	1.48944980	3.99881359	-2.37469204
8	3.58402759	-5.56911617	-0.00172908
6	4.53604530	-6.59256755	0.30373352
1	4.97465093	-6.44725133	1.30271955
1	5.32512399	-6.50561691	-0.45296726
1	4.09191330	-7.59970346	0.23536584

Energy = -8524.622832 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 6

Atomic N.	X	Y	Z
7	-1.29550382	-0.09069793	2.83903219
6	-2.01667119	1.17274360	3.00043808
1	-1.84077811	1.82502147	2.13648961
1	-3.09437938	0.96737735	3.05248704
1	-1.72486542	1.72355547	3.92195953
7	-2.12125678	-3.16172475	2.69797026
6	-1.67107234	-1.01090010	3.91834182
1	-1.22746318	-0.68332133	4.88915198
1	-2.76425355	-0.97035376	4.03398666
6	-1.27563439	-2.47345648	3.70075185
1	-1.41751236	-3.00511235	4.65300690
1	-0.21334521	-2.56699385	3.43847122
16	-1.45502019	-3.52199613	1.16528777
7	0.38584674	0.88013608	0.44427776
6	0.16371058	0.10387751	2.82096672
1	0.52350306	0.40520957	3.83303980
1	0.63828870	-0.85837074	2.58411538
6	0.70178874	1.16145760	1.85906462
1	1.79242024	1.19511176	2.01230971
1	0.31462660	2.15400499	2.14179062
16	0.74480958	2.09226012	-0.58892642
8	1.04677779	1.33280922	-1.87614169
8	1.73920329	3.06995336	-0.09371455
6	-0.76399892	3.03130918	-0.93759335
6	-0.93419630	4.28547291	-0.35051713
6	-2.11209442	4.99701724	-0.59390115
6	-3.11497545	4.47894894	-1.42535176
6	-2.91100222	3.21595275	-2.00993769
6	-1.74691051	2.48890741	-1.77039929
1	-0.14359446	4.69933167	0.27433221
1	-1.58934747	1.51557917	-2.23506395
1	-3.67594030	2.80073566	-2.66977785
6	-4.36913911	5.26508606	-1.71475873
1	-2.24847655	5.97807882	-0.13517459
8	-0.15464573	-2.81180033	1.07735042
8	-1.53277830	-4.98652779	0.97722209
6	-2.61262091	-2.77119261	0.00648296
6	-3.30778350	-3.60077196	-0.87295022
6	-4.19276428	-3.02324265	-1.78585444
6	-4.38919943	-1.63505557	-1.82539075

6	-3.67380827	-0.83009304	-0.92171828
6	-2.77828334	-1.38351804	-0.00809450
1	-3.15092749	-4.67783337	-0.83768656
1	-4.73903075	-3.66514320	-2.47920570
6	-5.32348458	-1.01487650	-2.83380745
1	-3.81470975	0.25236360	-0.93574606
1	-2.22105214	-0.75734966	0.69432419
1	-4.50535135	6.08204271	-0.99485472
1	-4.32807683	5.71121616	-2.72051543
1	-5.26086771	4.62362461	-1.68289526
1	-4.76874745	-0.69137064	-3.72874089
1	-6.09049994	-1.72758467	-3.16337233
1	-5.82574995	-0.12879597	-2.42280383
1	-2.50414065	-4.04380084	3.04121954
8	2.86757405	-0.68553854	0.14799233
8	3.75803928	-1.28874753	-1.89259467
6	3.81028409	-1.47881406	-0.44246515
6	5.19768190	-1.26585001	0.19162477
1	5.96677130	-1.77457964	-0.41108514
1	5.14918059	-1.78860833	1.15801223
6	5.57854505	0.20119408	0.43235269
1	4.72814872	0.70060257	0.91841443
1	6.41712384	0.22761663	1.14642820
6	5.98159800	0.97401149	-0.82752963
1	6.92565644	0.55722566	-1.22279720
1	6.19856800	2.01795961	-0.55079541
6	4.93708910	0.95606789	-1.94986649
1	3.97930168	1.37440100	-1.60680809
1	5.28933417	1.60728607	-2.76716662
6	4.70079813	-0.42827415	-2.55926212
1	5.66678869	-0.95817027	-2.66697982
1	4.27169973	-0.32382162	-3.56598751
50	1.04644392	-0.89805794	-0.87402969
8	3.34667461	-2.83398023	-0.26378492
6	4.12133643	-3.86422986	-0.88382108
1	4.27246194	-3.66361009	-1.95519786
1	3.54142059	-4.78729920	-0.76506277
1	5.09845838	-3.99408429	-0.38856683

Energy = -8524.618904 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 7

Atomic N.	X	Y	Z
8	2.50591633	-1.60065402	0.81807827
6	3.79124279	-1.20703489	0.56183631
8	3.80120178	-0.83038450	-0.84138540
6	5.01176121	-0.25365037	-1.34268050
1	5.82418461	-0.99785129	-1.40050341
1	5.33233080	0.59832283	-0.72595732
1	4.78161582	0.09788266	-2.35562947
8	4.08475339	0.03003703	1.25333788
6	4.77856400	-2.35982573	0.83347698
1	5.81301736	-1.98437539	0.78318628
1	4.64782306	-3.05211927	-0.01122950
6	4.53835676	-3.11820883	2.14632017
1	3.46769400	-3.35996426	2.21144635
1	5.08183146	-4.07542501	2.09715288

6	4.97563536	-2.36828956	3.40866734
1	6.07641347	-2.27041598	3.40939203
1	4.72070793	-2.97723061	4.29052767
6	4.36495235	-0.97059734	3.56442252
1	3.26570685	-1.01208156	3.58247526
1	4.67917745	-0.55714376	4.53722700
6	4.81535778	0.02608228	2.49399526
1	5.89416890	-0.11011762	2.28510290
1	4.68008696	1.05316749	2.86102697
50	1.15028230	-0.01499102	0.53173477
7	0.03232086	-1.68600504	-1.08438824
6	0.94484208	-2.11174989	-2.16562946
1	0.48863853	-2.90410105	-2.78737141
1	1.21174584	-1.25742774	-2.79684453
1	1.86547005	-2.48914706	-1.70667393
7	-0.31342044	0.93513296	-2.53812895
6	-1.26182320	-1.16831840	-1.59231651
1	-1.90313430	-2.01467904	-1.90987744
1	-1.77399623	-0.67507892	-0.75180488
6	-1.19133553	-0.21377084	-2.78667331
1	-2.23070820	0.08528128	-3.01707051
1	-0.79550092	-0.73069112	-3.67000921
16	0.11305130	1.91013147	-3.86744473
7	-0.43649254	-1.18022682	1.59041003
6	-0.20631049	-2.83408191	-0.16447696
1	-0.73047214	-3.64763723	-0.70295456
1	0.78586078	-3.18892712	0.14368992
6	-0.99796529	-2.42900967	1.08098616
1	-0.90483094	-3.24271247	1.81842429
1	-2.07233392	-2.31676821	0.84592339
16	-0.26316853	-0.95434581	3.19997358
8	0.76485598	0.13955378	3.26201043
8	-0.05678479	-2.21212900	3.95612796
6	-1.81003723	-0.23810316	3.81622993
6	-2.67955872	-1.02306502	4.57331987
6	-3.88160916	-0.46950716	5.02261850
6	-4.22242509	0.85919215	4.73241796
6	-3.32432690	1.62791664	3.97079806
6	-2.12400953	1.08950554	3.51163071
1	-2.40309648	-2.04868891	4.81541426
1	-1.42298389	1.69355764	2.93529776
1	-3.56868919	2.66696325	3.74063731
6	-5.50312371	1.46387460	5.25175437
1	-4.56334792	-1.08141078	5.61650079
8	0.94225003	2.98458239	-3.29801494
8	0.60493495	0.97826203	-4.89959720
6	-1.41361721	2.65485464	-4.48582814
6	-2.11506179	2.03825123	-5.52284382
6	-3.30074715	2.61987710	-5.97928903
6	-3.79176959	3.80655467	-5.41601545
6	-3.05845290	4.40848187	-4.37742663
6	-1.87456575	3.84327085	-3.90903018
1	-1.72007095	1.13133624	-5.97938516
1	-3.84905036	2.14608034	-6.79533166
6	-5.06670904	4.43761581	-5.91576329
1	-3.41615708	5.34143172	-3.93769694
1	-1.29282369	4.32634865	-3.12401260
1	-6.23814906	0.68943558	5.50642084

1	-5.31558109	2.05390022	6.16250003
1	-5.95490626	2.14201842	4.51489031
1	-4.87794185	5.44665578	-6.31095818
1	-5.52434456	3.84031625	-6.71397395
1	-5.80100818	4.54333702	-5.10374752
1	-0.58431132	1.52873098	-1.74941837

Energy = -8524.635875 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 8

Atomic N.	X	Y	Z
8	1.00918684	-0.29731182	0.34774346
6	2.20285887	-0.07658889	0.99364029
8	2.70433666	-1.37993063	1.31402154
6	3.96027653	-1.44480018	1.99900088
1	3.86449377	-1.10847714	3.04317280
1	4.73096434	-0.85639900	1.47782011
1	4.24665407	-2.50255584	1.99596248
8	3.16329861	0.41349638	-0.00067328
6	2.04434257	0.80746783	2.24155848
1	3.03854253	1.12220036	2.59566589
1	1.62740415	0.14108584	3.01135925
6	1.12613112	2.02291734	2.06514905
1	0.18780941	1.68623720	1.60009125
1	0.86520129	2.40412261	3.06508693
6	1.72963327	3.16608715	1.24348259
1	2.58240034	3.59892446	1.79640745
1	0.98406645	3.97208832	1.15046162
6	2.21347773	2.76277999	-0.15494016
1	1.39916923	2.30936095	-0.74090326
1	2.52208421	3.67492594	-0.69237218
6	3.42213709	1.82403562	-0.15657546
1	4.14299341	2.14113460	0.62006029
1	3.93854255	1.87171888	-1.12555914
50	1.60054703	-1.32042481	-1.46382397
7	-0.86427043	-1.95558507	-1.56527836
6	-0.87759446	-2.76417451	-2.80940234
1	-1.91187790	-2.92374073	-3.16267807
1	-0.30042666	-2.27308458	-3.60317463
1	-0.42071442	-3.73981923	-2.60156168
7	0.53612698	0.23165271	-2.71550840
6	-1.54368016	-0.65120974	-1.76986090
1	-2.62129867	-0.80153108	-1.97932942
1	-1.44601342	-0.07937503	-0.83863099
6	-0.91912441	0.15158089	-2.90866182
1	-1.37798375	1.15682153	-2.88890837
1	-1.17098830	-0.30164312	-3.88213983
16	1.41768805	0.50553687	-4.08923324
7	-0.93398085	-1.73949449	1.77983532
6	-1.52996259	-2.78357427	-0.50795781
1	-2.45381657	-3.20137872	-0.95546337
1	-0.86542535	-3.62693203	-0.27495202
6	-1.96024998	-2.10055761	0.79746511
1	-2.66077343	-2.79785313	1.28166717
1	-2.55231503	-1.19752359	0.58674530
16	-0.44928303	-2.95836904	2.84287642
8	0.66915514	-2.39098839	3.62125464

8	-0.30353971	-4.27185380	2.16719270
6	-1.89713326	-3.09329252	3.92195157
6	-2.54344942	-4.32135365	4.05053706
6	-3.62312542	-4.43281389	4.93185706
6	-4.06067690	-3.33460576	5.68455005
6	-3.38786248	-2.10774870	5.53347647
6	-2.30966920	-1.98041045	4.66180884
1	-2.19542420	-5.17262972	3.46628430
1	-1.78684366	-1.03086689	4.55074643
1	-3.71437605	-1.24163998	6.11237913
6	-5.21522134	-3.45918355	6.64681587
1	-4.13253155	-5.39254524	5.03555572
8	2.83097951	0.31086047	-3.65750247
8	0.89260805	-0.25557565	-5.25349991
6	1.20074317	2.25612978	-4.50218511
6	0.18498362	2.63430804	-5.38223907
6	0.01518701	3.98681274	-5.68696129
6	0.85497123	4.96615693	-5.13628301
6	1.87697871	4.55490560	-4.26363006
6	2.05409351	3.21001640	-3.94276939
1	-0.44636112	1.87250282	-5.83834245
1	-0.77816551	4.28511940	-6.37493827
6	0.69186049	6.42170410	-5.49672290
1	2.54783035	5.30133821	-3.83340256
1	2.85750781	2.88946672	-3.28103072
1	-5.71510441	-4.43105696	6.54981475
1	-4.87087890	-3.35968629	7.68738246
1	-5.96169389	-2.66970544	6.47856047
1	1.43422420	6.72282382	-6.25218171
1	-0.30362314	6.62301041	-5.91277981
1	0.83957148	7.07017202	-4.62218598
1	-0.10560179	-1.24121178	1.37480223

Energy = -8524.634159 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 9

Atomic N.	X	Y	Z
8	3.42561732	0.36610149	1.99915894
6	4.25696395	-0.03446689	1.01711542
8	4.68826856	-1.35070468	1.06654407
6	3.71211747	-2.32311358	1.50759630
1	2.88949075	-2.40412668	0.78518957
1	3.30682569	-2.05297074	2.48922430
1	4.26163550	-3.26915990	1.56483396
8	3.28865664	0.12712305	-0.22452174
6	5.53045963	0.80955081	0.81922640
1	6.26429102	0.20349051	0.26744226
1	5.92801153	0.93370118	1.83685966
6	5.37256610	2.17539915	0.14170827
1	4.45168791	2.67740417	0.49164822
1	6.20041734	2.81787709	0.47980388
6	5.40627137	2.12788201	-1.39551030
1	6.31202444	1.57608985	-1.70215325
1	5.52754062	3.15231938	-1.78249370
6	4.18084878	1.50037861	-2.07222192
1	3.30101371	2.15297914	-1.95087047
1	4.36227544	1.43153242	-3.15808704

6	3.80316014	0.10966500	-1.57322705
1	4.65737046	-0.58689135	-1.59074022
1	3.00276918	-0.31712834	-2.19368843
50	1.85321474	1.44709921	1.00063963
7	-1.24828002	2.86433061	1.70882937
6	-0.72290274	4.08182825	2.31833603
1	-1.49530391	4.64315646	2.88756222
1	0.09706962	3.83707916	3.00748353
1	-0.31513934	4.74050589	1.53911566
7	0.04557717	0.25706224	1.81579228
6	-1.62282547	1.86017821	2.71466860
1	-2.00346492	2.33326715	3.64387220
1	-2.43514349	1.23269712	2.32347898
6	-0.43433681	0.94570512	3.04235865
1	-0.71882618	0.22295898	3.82215667
1	0.38213335	1.54371541	3.48950657
16	0.03459809	-1.40913225	1.89006774
7	-1.63692811	1.04746250	-0.52098458
6	-2.27189733	3.17156898	0.71077626
1	-3.18511752	3.62944415	1.15720126
1	-1.83863803	3.91734663	0.02778377
6	-2.71927877	1.95112594	-0.11493943
1	-3.24832701	2.30937635	-1.00779222
1	-3.43513872	1.33565539	0.45125348
16	-0.70926205	1.39924896	-1.86470904
8	0.71528245	1.18400767	-1.45716601
8	-1.13667336	2.67984491	-2.46588303
6	-1.08084912	0.08173922	-3.03676614
6	-1.77716027	0.38471885	-4.20531659
6	-2.05466701	-0.64347553	-5.11047708
6	-1.64471456	-1.96033708	-4.85942331
6	-0.94384830	-2.23039306	-3.66946773
6	-0.65369989	-1.22083101	-2.75468914
1	-2.08582676	1.41094463	-4.40076249
1	-0.11016920	-1.44025075	-1.83336813
1	-0.61805684	-3.25018639	-3.45595163
6	-1.92730623	-3.06450409	-5.84688299
1	-2.59775203	-0.41463392	-6.02911713
8	0.47650192	-1.85122073	0.54162254
8	0.71690628	-1.93514456	3.09744650
6	-1.71247685	-1.88442127	2.08140067
6	-2.17352886	-2.28792075	3.33645685
6	-3.50929260	-2.66788403	3.48584182
6	-4.39143817	-2.66334472	2.39504470
6	-3.89849686	-2.26342927	1.14122064
6	-2.56847188	-1.87682132	0.97637066
1	-1.47966578	-2.32040616	4.17588770
1	-3.86987329	-2.98184598	4.46735506
6	-5.82311597	-3.11086742	2.55372538
1	-4.56661799	-2.26004140	0.27754609
1	-2.19658332	-1.57200224	-0.00092629
1	-2.64810301	-2.74619247	-6.61052390
1	-1.00525438	-3.37268533	-6.36320431
1	-2.32652086	-3.95643099	-5.34391221
1	-5.92790402	-4.17865342	2.30535000
1	-6.17303941	-2.97871336	3.58586568
1	-6.49405178	-2.55471264	1.88525779
1	-1.01559816	0.76148245	0.27215126

Energy = -8524.622258 Hartree
 Number of imaginary frequencies = 0.

Compound I4a isomer 10

Atomic N.	X	Y	Z
8	4.22914746	1.49824691	-2.32372579
6	4.23260238	2.74212521	-1.80304840
8	3.08867494	3.41850231	-2.32366915
6	2.80932479	4.72503368	-1.82006261
1	3.59237519	5.45744288	-2.07762267
1	2.65871664	4.71727037	-0.72789744
1	1.87472333	5.03596488	-2.30211487
8	3.97495766	2.55829925	-0.31516385
6	5.53424517	3.50319306	-2.10659650
1	5.48434369	4.53924640	-1.73844342
1	5.54341699	3.55990587	-3.20457299
6	6.82254159	2.83254591	-1.61017342
1	6.73524866	1.74349710	-1.74989187
1	7.65200957	3.15773095	-2.25659022
6	7.18798419	3.16388243	-0.15820649
1	7.31239486	4.25728235	-0.06371866
1	8.16989246	2.72407913	0.07800997
6	6.17131769	2.69497369	0.88777280
1	6.12386880	1.59346070	0.91820429
1	6.51029800	3.01700496	1.88701284
6	4.75349456	3.23369500	0.69389295
1	4.77275362	4.31716005	0.48707297
1	4.17155150	3.08910886	1.61724175
50	3.77988341	0.05821235	-0.85590125
7	-0.18401046	0.83414565	1.56987957
6	0.18747127	1.00743149	2.97413396
1	-0.09856840	2.00456587	3.37808604
1	-0.28407303	0.23317044	3.59190058
1	1.27519396	0.89615025	3.07312150
7	-2.12168661	-1.32677443	2.09395887
6	-1.62326633	0.99756332	1.36493038
1	-1.94851978	2.04346383	1.58172480
1	-1.84049029	0.81781866	0.30073095
6	-2.51719456	0.08681240	2.20809653
1	-3.55587777	0.25856165	1.87060436
1	-2.47247720	0.35817598	3.27053541
16	-3.19549088	-2.47308967	2.72234673
7	1.53770905	0.27812238	-0.99707790
6	0.55963977	1.77279152	0.71950571
1	0.14056542	2.80273081	0.80170701
1	1.59046377	1.82722895	1.10018981
6	0.62603206	1.40828816	-0.76616398
1	0.98318804	2.29048263	-1.32118795
1	-0.37565696	1.17402845	-1.15946612
16	1.27858590	-0.70435009	-2.26264984
8	2.69571555	-1.26762173	-2.45970857
8	0.59258473	-0.12421005	-3.43377317
6	0.28502739	-2.12148689	-1.73390277
6	-0.56441679	-2.72918546	-2.65932354
6	-1.28082750	-3.86581551	-2.27616962
6	-1.16369417	-4.39872556	-0.98334891
6	-0.31830811	-3.74824054	-0.06530962

6	0.40884582	-2.61671503	-0.43259365
1	-0.65721981	-2.31220294	-3.66138940
1	1.04936956	-2.10718647	0.28746191
1	-0.24788508	-4.12463652	0.95581464
6	-1.90815433	-5.64553079	-0.57892008
1	-1.94075101	-4.34943243	-2.99899549
8	-2.60694601	-3.78579764	2.39139148
8	-3.47105574	-2.06409001	4.11166079
6	-4.74338045	-2.31039831	1.79751862
6	-5.83922349	-1.68531487	2.39300165
6	-7.02590293	-1.55643671	1.66613187
6	-7.13085059	-2.04140485	0.35483476
6	-6.00822854	-2.66405531	-0.22039344
6	-4.81832325	-2.80340470	0.49037156
1	-5.75851068	-1.32050456	3.41631016
1	-7.88654035	-1.07100110	2.12970908
6	-8.41999084	-1.92252566	-0.41807637
1	-6.07111506	-3.04901528	-1.23995405
1	-3.95707320	-3.29813766	0.04055265
1	-2.72136654	-5.87378928	-1.28018892
1	-1.22939358	-6.51241072	-0.56445508
1	-2.32483116	-5.54380763	0.43248370
1	-8.93451844	-2.89439568	-0.47035887
1	-9.10599839	-1.20750968	0.05314191
1	-8.23757074	-1.59817074	-1.45197021
1	-1.80677043	-1.61202223	1.16173262

Energy = -8524.620440 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 11

Atomic N.	X	Y	Z
8	3.07821339	0.35947432	1.19218395
6	4.39315944	0.17874349	0.82576832
8	5.08060638	-0.70903056	1.68491847
6	4.39145797	-1.94557121	1.95212631
1	4.11556092	-2.45853169	1.01973970
1	3.48711377	-1.77478839	2.55037964
1	5.10308665	-2.55898642	2.51713194
8	4.30953049	-0.38232205	-0.52439487
6	5.21695216	1.48491770	0.87603396
1	6.27752223	1.22452005	1.00980921
1	4.90267860	1.98958030	1.80014170
6	5.05819054	2.41208769	-0.33534776
1	4.00670054	2.41575968	-0.67564002
1	5.27943459	3.44355760	-0.01821754
6	5.98984633	2.06247556	-1.50832895
1	7.02463754	2.03360008	-1.12492664
1	5.96145806	2.87611811	-2.25089378
6	5.68034239	0.73821989	-2.21891968
1	4.74781281	0.83195612	-2.79934631
1	6.48105743	0.51752208	-2.94496477
6	5.52410513	-0.46541800	-1.29082302
1	6.38351947	-0.58233199	-0.61031457
1	5.44238970	-1.39004283	-1.88203417
50	1.65464944	0.27400995	-0.34212462
7	0.42273803	2.20492993	1.17401008
6	1.36203799	2.54441578	2.26291407

8	3.38116910	0.87175076	0.57681059
6	4.46446033	0.96275599	-0.25464622
8	5.53363087	0.08717214	0.08625262
6	5.14609931	-1.26027782	0.37933036
1	4.62476174	-1.72837581	-0.47182108
1	4.50397161	-1.30824897	1.27082248
1	6.07892771	-1.80347729	0.56990602
8	3.90086856	0.56381927	-1.56050019
6	5.09950091	2.36513435	-0.28478320
1	6.15531910	2.26243634	-0.57765661
1	5.09725280	2.70119357	0.76190717
6	4.40032025	3.39040886	-1.18772537
1	3.30681971	3.27780254	-1.11471362
1	4.63421236	4.39737540	-0.80775599
6	4.84455149	3.32289659	-2.65911973
1	5.94708272	3.38320976	-2.69099992
1	4.47186260	4.21491500	-3.18660675
6	4.38052423	2.08073140	-3.43127568
1	3.29351876	2.11996612	-3.59847144
1	4.85387123	2.07350152	-4.42803273
6	4.69467035	0.75122790	-2.75475501
1	5.75869889	0.64994019	-2.48534073
1	4.43334751	-0.08704759	-3.41718826
50	1.71360752	0.02578500	-0.43955295
7	0.67790112	0.87860964	1.75851372
6	1.41744514	0.45628298	2.96721149
1	0.99247785	0.91493076	3.87900552
1	1.39390249	-0.63463993	3.06562058
1	2.46071493	0.77021042	2.85145258
7	-0.41401895	-1.91975814	1.57508240
6	-0.76426438	0.53634513	1.81852917
1	-1.28946309	1.24672353	2.48763439
1	-1.18183369	0.67783094	0.80969920
6	-1.10773952	-0.86661983	2.32550698
1	-2.20801852	-0.96270427	2.27759168
1	-0.81364573	-0.97966434	3.37660953
16	-0.43004259	-3.49631109	2.22087815
7	0.72272142	1.97123555	-0.80850918
6	0.84101892	2.34922220	1.57772191
1	0.37563629	2.88868859	2.42490473
1	1.92210545	2.53784836	1.58427099
6	0.24991671	2.84918967	0.26031582
1	0.58407064	3.88927309	0.10886520
1	-0.85556247	2.87057536	0.31348998
16	0.21252720	2.25943942	-2.34151423
8	0.88804907	1.21134693	-3.15653832
8	0.34140653	3.69156364	-2.69887541
6	-1.56607123	1.89000274	-2.37434104
6	-2.49517057	2.92640862	-2.27510303
6	-3.86009062	2.62329193	-2.26928275
6	-4.31076335	1.29966611	-2.37197986
6	-3.35292543	0.27507322	-2.47760924
6	-1.98850582	0.56068273	-2.47812119
1	-2.14594803	3.95732516	-2.22433421
1	-1.24765849	-0.23306679	-2.58300190
1	-3.68451818	-0.76109471	-2.57333569
6	-5.78479153	0.98087287	-2.40737641
1	-4.58782198	3.43358518	-2.19371026

8	0.30060007	-4.31347827	1.23854202
8	0.00188157	-3.35019267	3.62369234
6	-2.15126665	-4.04641278	2.22981205
6	-2.93135747	-3.86348681	3.37254450
6	-4.26426973	-4.28228368	3.35754469
6	-4.82484703	-4.88173903	2.22035811
6	-4.01138043	-5.05847066	1.08641498
6	-2.68052186	-4.64692946	1.08230640
1	-2.48914187	-3.42368340	4.26582775
1	-4.87644045	-4.14929269	4.25116545
6	-6.25905060	-5.34674776	2.21122420
1	-4.42547139	-5.53799104	0.19742706
1	-2.04352865	-4.81125639	0.21328213
1	-6.38364162	1.80667227	-2.00227675
1	-6.12142735	0.80338012	-3.44061572
1	-6.01350789	0.07251438	-1.83306531
1	-6.31707602	-6.43837597	2.08728908
1	-6.77236987	-5.08443260	3.14448834
1	-6.81616489	-4.89914471	1.37542902
1	-0.63110713	-1.95560973	0.57525463

Energy = -8524.641523 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 13

Atomic N.	X	Y	Z
8	2.98650424	0.04339381	0.75699172
6	4.23580753	0.22258778	0.22992919
8	4.56115074	-0.81717970	-0.73578604
6	4.71958768	-2.12880430	-0.17368208
1	3.87356262	-2.39254780	0.47836707
1	5.66541118	-2.21962432	0.38585270
1	4.74445620	-2.82005650	-1.02464280
8	4.17153937	1.41168274	-0.57769181
6	5.30217145	0.30066004	1.34813064
1	6.26330417	-0.06446666	0.95302917
1	4.98437644	-0.40851668	2.12388224
6	5.51065516	1.69472916	1.95956387
1	4.53965395	2.19713606	2.09273910
1	5.93063776	1.56672894	2.96968011
6	6.47349536	2.58405950	1.15453505
1	7.41828470	2.02968078	1.01643798
1	6.72771598	3.47565440	1.75021825
6	5.95827113	3.04057905	-0.21686868
1	5.15119077	3.78085057	-0.08653949
1	6.76909571	3.55453298	-0.76088382
6	5.41807986	1.91680978	-1.09897866
1	6.14131785	1.09528788	-1.21813728
1	5.18958352	2.29971018	-2.10510605
50	1.51222817	-0.14298722	-0.73889102
7	0.46698827	2.07119836	0.21587881
6	1.44565631	2.61542715	1.18359201
1	1.02315849	3.49427609	1.70516146
1	1.72986388	1.84681262	1.90802891
1	2.35753970	2.90557258	0.64814322
7	-0.02767427	-0.63561511	0.78741698
6	-0.77574230	1.64616114	0.90756355
1	-1.14973498	2.45269431	1.56759512

1	-1.53272018	1.43917650	0.14255613
6	-0.56962535	0.36009316	1.71077671
1	-1.55728497	0.05700252	2.10211000
1	0.08937150	0.52005931	2.57987674
16	0.27202859	-2.15778118	1.31284742
7	-0.93141478	1.61709473	-2.44050549
6	0.23402052	3.11683865	-0.81757366
1	0.07460068	4.09468579	-0.32175237
1	1.17000147	3.20355632	-1.39115605
6	-0.94558442	2.92656410	-1.77171951
1	-0.92399098	3.76444554	-2.48881355
1	-1.89576357	3.00844801	-1.22420858
16	-2.23196998	1.33232782	-3.52572108
8	-1.78034102	0.19499682	-4.34899024
8	-2.68794111	2.59192328	-4.15509141
6	-3.52455622	0.79834362	-2.38758119
6	-4.75424598	1.45670870	-2.40524044
6	-5.77056870	1.01085277	-1.55711477
6	-5.57016206	-0.07750409	-0.69485170
6	-4.31637861	-0.71506726	-0.69542496
6	-3.29274653	-0.28847979	-1.53916364
1	-4.90115120	2.30384211	-3.07439529
1	-2.32192144	-0.78379642	-1.52752449
1	-4.13552193	-1.55765793	-0.02550360
6	-6.67904385	-0.57114381	0.19980615
1	-6.73501392	1.52167885	-1.56390628
8	1.23276575	-2.66451978	0.27224439
8	0.60953185	-2.24170681	2.75138375
6	-1.25726127	-3.10408489	1.08914517
6	-2.09315599	-3.32776857	2.18336965
6	-3.28100268	-4.04230857	1.99883150
6	-3.63794189	-4.54547713	0.73974639
6	-2.76875768	-4.31536084	-0.34252809
6	-1.58607326	-3.59779956	-0.17745927
1	-1.80002388	-2.96572824	3.16834666
1	-3.93506291	-4.22244963	2.85408324
6	-4.91504811	-5.32369558	0.54285723
1	-3.02214532	-4.70883476	-1.32889551
1	-0.90736874	-3.43509351	-1.01455913
1	-7.43579219	0.20558189	0.36868052
1	-7.18783567	-1.43541514	-0.25502150
1	-6.29112556	-0.89922753	1.17345033
1	-4.70794968	-6.33573664	0.16518885
1	-5.47490477	-5.42000778	1.48161479
1	-5.56786230	-4.83497962	-0.19585469
1	-0.07319829	1.43097692	-2.97188856

Energy = -8524.635820 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 14

Atomic N.	X	Y	Z
8	2.67705550	1.50491908	-0.20607174
6	3.88848644	0.89097785	-0.37438921
8	3.91831087	-0.16998651	0.61780568
6	5.03803606	-1.06070778	0.57064430
1	5.97006269	-0.56082929	0.88469861
1	5.16623932	-1.48660311	-0.43491782

1	4.81288474	-1.86641864	1.27969659
8	3.92127064	0.18468653	-1.63752131
6	5.04069610	1.89087796	-0.15169027
1	5.99737017	1.42883862	-0.44300668
1	5.07765136	2.04417357	0.93688681
6	4.85889361	3.24884122	-0.84427106
1	3.84209428	3.60895948	-0.63108054
1	5.55720641	3.96702243	-0.38536574
6	5.09417708	3.23275254	-2.35806175
1	6.16084826	3.02333758	-2.55721093
1	4.89871252	4.23988593	-2.75925044
6	4.24819624	2.20920439	-3.12434570
1	3.17240324	2.38227095	-2.97168816
1	4.43645316	2.33605621	-4.20348617
6	4.57808352	0.75384956	-2.78517070
1	5.67360747	0.63174197	-2.68082806
1	4.25225651	0.09725164	-3.60412595
50	1.08878454	0.17987118	-0.59864792
7	0.37464011	0.82628513	1.79490885
6	1.41150392	0.50045890	2.79580524
1	1.13485506	0.87779846	3.79760981
1	1.56969109	-0.58229092	2.84178989
1	2.35213496	0.96241129	2.47584006
7	-0.31147944	-2.10870055	1.69654961
6	-0.95392306	0.26068230	2.13526083
1	-1.42322682	0.86643467	2.93605302
1	-1.59289841	0.35651616	1.24385780
6	-0.96984874	-1.18780862	2.62983643
1	-2.02828682	-1.45028442	2.81315723
1	-0.44013077	-1.27322817	3.58705025
16	0.02986723	-3.68452827	2.24398307
7	-0.33781999	1.90026297	-0.65035072
6	0.27628355	2.30703510	1.65751708
1	-0.06795543	2.75330601	2.61090942
1	1.29288586	2.66126763	1.44211118
6	-0.64871857	2.72711756	0.51322034
1	-0.46702564	3.79465530	0.30832043
1	-1.70976631	2.62204681	0.80507388
16	-0.29569905	2.56592051	-2.14263615
8	0.52979002	1.57455785	-2.91299193
8	0.07534661	4.00069621	-2.14135788
6	-1.97269960	2.47447995	-2.82434392
6	-2.74064591	3.63457290	-2.92226796
6	-4.04176308	3.55029611	-3.42574931
6	-4.58216907	2.32461771	-3.83950417
6	-3.78297127	1.17229799	-3.73308215
6	-2.48571731	1.23874806	-3.22918852
1	-2.31110742	4.58921130	-2.62042036
1	-1.86344895	0.34603188	-3.16364680
1	-4.18352636	0.20964746	-4.05738930
6	-5.97350426	2.24367995	-4.41670377
1	-4.64441788	4.45713562	-3.50511786
8	0.63477431	-4.36403725	1.08699034
8	0.73081965	-3.51295862	3.53043163
6	-1.55714670	-4.47900683	2.58725869
6	-2.08641745	-4.44129158	3.87809051
6	-3.32118698	-5.04783733	4.12268051
6	-4.03012514	-5.69157225	3.09814834

6	-3.46744406	-5.71902882	1.80923186
6	-2.23795962	-5.11932165	1.54616528
1	-1.52351446	-3.96566635	4.68049989
1	-3.73598577	-5.02803152	5.13194739
6	-5.35604959	-6.35723255	3.36686387
1	-3.99734368	-6.22871673	1.00230705
1	-1.79016361	-5.16596303	0.55354596
1	-6.57279695	3.12181439	-4.14383205
1	-5.93827849	2.19504508	-5.51626156
1	-6.49999429	1.34349935	-4.07063495
1	-5.29402849	-7.44152819	3.19126611
1	-5.68167416	-6.20027313	4.40258674
1	-6.13809238	-5.96828787	2.69866766
1	-0.72542114	-2.15190934	0.76134127

Energy = -8524.635867 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 15

Atomic N.	X	Y	Z
8	3.19303637	-1.55011998	0.10549227
6	4.21318374	-1.50757178	1.01717640
8	5.43777203	-1.00502812	0.49418762
6	5.32002909	0.18920582	-0.28790984
1	4.87996857	1.01543682	0.29432487
1	4.71718765	0.01896200	-1.19172394
1	6.34293583	0.45890942	-0.57502031
8	3.69440501	-0.57369457	2.03674170
6	4.57187740	-2.88645603	1.60135476
1	5.61792947	-2.85839685	1.94203449
1	4.54100858	-3.57525467	0.74513088
6	3.66281401	-3.38360513	2.73362012
1	2.61311669	-3.12780338	2.51809322
1	3.71514479	-4.48349781	2.75719780
6	4.06310498	-2.85914162	4.12344113
1	5.13257753	-3.08435392	4.28368856
1	3.51108017	-3.42343399	4.89136396
6	3.81775398	-1.36287778	4.35891198
1	2.73812642	-1.15834034	4.42053823
1	4.25115619	-1.07126629	5.33090202
6	4.40030263	-0.44281408	3.29211363
1	5.47209666	-0.62490487	3.11011450
1	4.28266132	0.60996690	3.58823167
50	1.67300221	-0.14370290	0.59446889
7	0.57925163	-1.55520645	-1.26161135
6	1.42488349	-1.70770228	-2.46470115
1	0.96147320	-2.39356749	-3.19759845
1	1.59296765	-0.73333234	-2.93684293
1	2.39376269	-2.11000915	-2.14816138
7	-0.03308370	1.25906265	-2.14909678
6	-0.77872915	-1.04842559	-1.57572845
1	-1.39031942	-1.86469429	-2.00923345
1	-1.25464767	-0.76150956	-0.62545491
6	-0.85949337	0.11949674	-2.56195280
1	-1.93022857	0.37832822	-2.65635509
1	-0.50687935	-0.18546178	-3.55535378
16	0.25746689	2.48966444	-3.29004330
7	0.33473444	-1.64833355	1.51674459

6	0.47649416	-2.87021698	-0.56710901
1	-0.04393886	-3.60107224	-1.21543513
1	1.50733128	-3.20857634	-0.40239839
6	-0.24292265	-2.76965604	0.77740286
1	-0.10253817	-3.72347283	1.31278263
1	-1.33217118	-2.64280307	0.62652309
16	-0.29002143	-1.27633331	2.98803122
8	0.54164034	-0.13550133	3.46295493
8	-0.46361700	-2.48508289	3.82697051
6	-1.95942849	-0.62197980	2.69348447
6	-3.07141753	-1.45146812	2.84530521
6	-4.34648724	-0.94080018	2.58433932
6	-4.52805517	0.39057144	2.18359989
6	-3.39075932	1.20603416	2.04385149
6	-2.11228567	0.70976390	2.29438202
1	-2.93342751	-2.47749404	3.18526283
1	-1.23341801	1.35010328	2.20806896
1	-3.51272992	2.24987221	1.74673491
6	-5.90925031	0.94896113	1.94672390
1	-5.21716559	-1.58827429	2.70519797
8	1.07407614	3.48219541	-2.57250195
8	0.72265886	1.79715077	-4.50653040
6	-1.33700001	3.25152741	-3.66752369
6	-2.08093644	2.79787251	-4.75772409
6	-3.31679970	3.39063585	-5.02876615
6	-3.81555880	4.42911568	-4.22902413
6	-3.03953831	4.86893756	-3.14135104
6	-1.80530771	4.28989513	-2.85515346
1	-1.68171653	2.01055846	-5.39622091
1	-3.89901801	3.04541357	-5.88482229
6	-5.14202567	5.07846483	-4.53247840
1	-3.40375871	5.68728543	-2.51736880
1	-1.19181407	4.65184025	-2.03016989
1	-6.63378031	0.15187124	1.73559101
1	-6.26723396	1.49387861	2.83416120
1	-5.91825844	1.65766521	1.10731509
1	-5.00874313	6.13776273	-4.79811215
1	-5.65078843	4.58172848	-5.36777659
1	-5.80807830	5.04852042	-3.65804179
1	-0.28564028	1.67657938	-1.24926055

Energy = -8524.641514 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 16

Atomic N.	X	Y	Z
8	0.87082743	-0.77168779	0.61399732
6	1.99444925	-0.47723053	1.34667539
8	3.01471212	-1.44482523	1.25900277
6	3.28627806	-1.93487259	-0.06530394
1	3.38401611	-1.11198220	-0.78843397
1	2.49974001	-2.62867109	-0.39239889
1	4.23958567	-2.47077055	0.00846814
8	2.44367896	0.77413552	0.68444037
6	1.74750649	-0.29670660	2.85671709
1	2.69807445	-0.46496141	3.38450081
1	1.08440502	-1.12605178	3.14102157
6	1.14517726	1.04721834	3.28484698

1	0.36838159	1.36517212	2.56735126
1	0.62388030	0.89863077	4.24304959
6	2.18624280	2.16370897	3.47492187
1	2.96625451	1.79361909	4.16309792
1	1.70963807	3.01663045	3.98413456
6	2.85078904	2.67471384	2.19008999
1	2.12160090	3.23458097	1.58204622
1	3.64900130	3.38979366	2.45080629
6	3.46112105	1.59607797	1.30132886
1	4.15027939	0.93550177	1.85135801
1	4.00638505	2.05027851	0.46361013
50	0.34133035	0.99838697	-0.52556063
7	-0.96205495	-0.89095723	-1.75171674
6	-0.27655500	-2.20819923	-1.72274473
1	-0.73158478	-2.88414544	-2.46940410
1	0.78565313	-2.07604840	-1.94829301
1	-0.35457055	-2.66808744	-0.73655964
7	1.18402931	0.69744885	-2.54764257
6	-0.92040244	-0.35902177	-3.13906472
1	-1.40889843	-1.06279066	-3.83959482
1	-1.48416031	0.58646854	-3.14805513
6	0.51592211	-0.08275317	-3.58941691
1	0.46106095	0.47535186	-4.53999688
1	1.05271977	-1.02110623	-3.80534359
16	2.32965738	1.79219751	-2.98082417
7	-1.83405206	-1.71012792	1.14696060
6	-2.37088082	-1.03005208	-1.28474403
1	-2.96641688	-0.24190988	-1.77166964
1	-2.77624885	-2.00272319	-1.61192385
6	-2.58431789	-0.85277678	0.23047864
1	-3.65721901	-0.99084032	0.42365161
1	-2.33708700	0.18551232	0.50809936
16	-2.30566433	-3.31288185	1.37381643
8	-1.12378630	-4.17063524	1.13908075
8	-3.57244068	-3.50310791	0.63215388
6	-2.68528140	-3.41136395	3.13587900
6	-3.99279263	-3.19128662	3.56942928
6	-4.27547357	-3.26679019	4.93460707
6	-3.27162521	-3.56208823	5.86931240
6	-1.96602935	-3.78650105	5.40008259
6	-1.66555971	-3.71749429	4.04060376
1	-4.77682253	-2.98182143	2.84264926
1	-0.65705119	-3.91114882	3.67640266
1	-1.17304052	-4.02608771	6.11110873
6	-3.58609216	-3.66647995	7.34061538
1	-5.29748921	-3.09908096	5.27913248
8	2.58007278	2.55253531	-1.72024488
8	3.46135244	1.17549140	-3.70933705
6	1.54114801	2.93583277	-4.15110105
6	1.91736913	2.92446949	-5.49408964
6	1.30120213	3.81006248	-6.38319883
6	0.31843086	4.70977233	-5.94725771
6	-0.04088614	4.69972863	-4.58727423
6	0.56165373	3.82070486	-3.68982736
1	2.69307164	2.23472599	-5.82536814
1	1.59412851	3.80274136	-7.43477074
6	-0.31999872	5.68688537	-6.90247007
1	-0.80130682	5.39592594	-4.22782226

1	0.28926218	3.82938973	-2.63351621
1	-4.56772791	-3.23453744	7.57287141
1	-3.59893910	-4.71865394	7.66434328
1	-2.82910396	-3.15162243	7.94845058
1	0.12871312	6.68675496	-6.79575716
1	-0.18586708	5.37383209	-7.94578590
1	-1.39604534	5.79358491	-6.70777857
1	-0.80532952	-1.58698412	1.12309744

Energy = -8524.640127 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 17

Atomic N.	X	Y	Z
8	2.42586309	-1.57806207	1.04073963
6	3.66005738	-1.01622201	1.22305502
8	3.92542532	-0.27654508	0.00065189
6	5.11425866	0.52080956	-0.02266294
1	6.02300533	-0.10404512	-0.05215103
1	5.15701120	1.19753486	0.84287783
1	5.06231452	1.11327711	-0.94400303
8	3.59669572	0.01233377	2.24012243
6	4.72811815	-2.10348149	1.45483947
1	5.67747929	-1.63381713	1.75775357
1	4.89506861	-2.55406587	0.46539563
6	4.32620232	-3.20365151	2.44698158
1	3.31762798	-3.55314376	2.18279142
1	5.00872869	-4.05784490	2.31075892
6	4.35673413	-2.77816626	3.91820626
1	5.40075611	-2.56538048	4.21124403
1	4.02506244	-3.62321729	4.54205919
6	3.50748619	-1.54281914	4.24019624
1	2.45330015	-1.69605285	3.96509007
1	3.52677718	-1.37809339	5.33038429
6	4.01900503	-0.25509215	3.59036158
1	5.12472991	-0.22377925	3.64210716
1	3.64050856	0.61654570	4.14256694
50	0.95542753	-0.08869331	0.79932082
7	0.49585216	-1.34847068	-1.40451543
6	1.68586681	-1.40386839	-2.27856989
1	1.50061653	-2.03214199	-3.16935187
1	1.97452297	-0.39546462	-2.59344299
1	2.51560541	-1.82364894	-1.69908619
7	0.15771280	1.53033621	-2.23188596
6	-0.70129555	-0.80742484	-2.09355761
1	-1.13047717	-1.58198246	-2.76011666
1	-1.45771501	-0.59177419	-1.32321398
6	-0.48170597	0.43213993	-2.96465787
1	-1.46923751	0.71164248	-3.37623565
1	0.17208567	0.19438552	-3.81332547
16	0.76828808	2.83973158	-3.13205212
7	-0.64984171	-1.61517319	1.09650521
6	0.20898862	-2.71482427	-0.88297935
1	-0.05658876	-3.39076349	-1.71915859
1	1.14062388	-3.06595875	-0.42021505
6	-0.90030529	-2.71712738	0.17099003
1	-0.87233097	-3.69061494	0.68695258
1	-1.89456885	-2.62215276	-0.30285458

16	-0.88721106	-1.81835857	2.70059136
8	-0.06441597	-0.70784015	3.28986965
8	-0.68789715	-3.21396034	3.15757794
6	-2.61901076	-1.41134103	3.04864724
6	-3.51845940	-2.43143453	3.35765048
6	-4.85645849	-2.10959124	3.60213162
6	-5.30537592	-0.78248328	3.54959261
6	-4.37506389	0.22549350	3.23914614
6	-3.03884138	-0.07930354	2.98873607
1	-3.16294414	-3.45946592	3.41844226
1	-2.31741345	0.70678627	2.76480237
1	-4.70405383	1.26597134	3.20054048
6	-6.74207255	-0.43543135	3.85120105
1	-5.56220483	-2.90601043	3.84601806
8	1.30067684	3.77390812	-2.12695703
8	1.60237053	2.23773053	-4.18932676
6	-0.64298171	3.63378498	-3.93530460
6	-1.00076263	3.26358957	-5.23269313
6	-2.10288466	3.87715006	-5.83325785
6	-2.84758480	4.85517456	-5.15785783
6	-2.45947890	5.21044771	-3.85357141
6	-1.36368936	4.60918580	-3.23814302
1	-0.40659375	2.52380654	-5.76806621
1	-2.38297421	3.59623014	-6.84998723
6	-4.02087580	5.53394491	-5.81810100
1	-3.01932403	5.97863435	-3.31681450
1	-1.04755705	4.90554961	-2.23802887
1	-7.39646089	-1.31053766	3.74756167
1	-6.84627671	-0.06430534	4.88275237
1	-7.11286680	0.35549028	3.18473850
1	-3.77926706	6.57924997	-6.06398878
1	-4.30611726	5.02822215	-6.74894052
1	-4.89587620	5.55443256	-5.15327473
1	-0.36379236	1.88010770	-1.42360193

Energy = -8524.635884 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 18

Atomic N.	X	Y	Z
8	2.19028803	-2.01398068	0.92449058
6	3.42682419	-1.49172003	0.98270346
8	4.25073595	-2.23792898	0.06965300
6	5.50959749	-1.67898182	-0.30478832
1	6.17232092	-1.50299588	0.56021351
1	5.38378570	-0.73997203	-0.86620016
1	5.98635716	-2.42126701	-0.95672032
8	3.25564238	-0.09967350	0.42047203
6	4.03823484	-1.50212410	2.39430798
1	5.10202699	-1.21897620	2.36155621
1	4.00713598	-2.56335499	2.67917837
6	3.30651615	-0.65197553	3.44190127
1	2.21905965	-0.72229879	3.27408852
1	3.48572326	-1.09581697	4.43301546
6	3.75472789	0.81524053	3.48218443
1	4.84312707	0.84516815	3.66829594
1	3.28478542	1.31287182	4.34548530
6	3.44472308	1.62481913	2.21886448

1	2.35764514	1.76000338	2.09638100
1	3.86442781	2.63936459	2.32475613
6	3.99651573	1.04690156	0.91961148
1	5.05808821	0.77186084	1.02280875
1	3.90338616	1.78666753	0.11430477
50	0.81450954	-0.39302572	0.30778613
7	0.55599091	-2.23629613	-1.53139505
6	1.86659230	-2.42189279	-2.19986864
1	1.76425687	-3.09161292	-3.07390189
1	2.25745449	-1.45390695	-2.52984878
1	2.57622805	-2.84197909	-1.47966633
7	0.59606713	0.45412159	-1.80513692
6	-0.41767770	-1.63172923	-2.46796326
1	-0.59479592	-2.30047966	-3.33266316
1	-1.36989575	-1.50260694	-1.93269279
6	0.07570580	-0.26585221	-2.96085240
1	-0.78257659	0.25565368	-3.42225612
1	0.83636414	-0.38926353	-3.75048104
16	1.02199158	2.01827113	-1.97440090
7	-0.64558161	-2.86251744	1.19717258
6	0.11481584	-3.56169859	-1.03388457
1	-0.16483984	-4.20673263	-1.88951679
1	0.99088703	-4.01733217	-0.55114617
6	-1.03931457	-3.56424083	-0.03635801
1	-1.31295393	-4.61361238	0.15977284
1	-1.93093151	-3.06660434	-0.44684732
16	-1.72070977	-3.00927540	2.53094060
8	-0.90607743	-2.64773257	3.70538319
8	-2.44774011	-4.29509101	2.45676126
6	-2.90975301	-1.69688053	2.19913319
6	-4.16435062	-2.02257530	1.68156441
6	-5.08199422	-0.99847122	1.43923790
6	-4.76165313	0.34109317	1.70914474
6	-3.49521746	0.63401363	2.24364841
6	-2.56502639	-0.37432899	2.48955025
1	-4.41690674	-3.06579570	1.49499841
1	-1.58778526	-0.14586669	2.91250879
1	-3.23463438	1.66841853	2.47477810
6	-5.74699127	1.44442093	1.41745094
1	-6.06764648	-1.24643342	1.04166680
8	1.51544364	2.40340009	-0.61694435
8	1.87860734	2.27228175	-3.15893586
6	-0.51810829	2.94043536	-2.25981343
6	-0.70063318	3.63472955	-3.45418596
6	-1.88912790	4.34373922	-3.65835604
6	-2.89504213	4.36897961	-2.68348610
6	-2.68439407	3.65739862	-1.48764171
6	-1.50761927	2.94452080	-1.27151494
1	0.08925107	3.62017856	-4.20452546
1	-2.03325355	4.88951968	-4.59276952
6	-4.16937186	5.14792524	-2.89657459
1	-3.45516702	3.66902316	-0.71359412
1	-1.34844604	2.39913891	-0.33993725
1	-6.78186901	1.08135866	1.46279628
1	-5.63824993	2.27685225	2.12501211
1	-5.58619520	1.85045647	0.40607774
1	-4.23494469	5.99574926	-2.19785372
1	-4.22790911	5.54832285	-3.91648736

1 -5.05533256 4.51969323 -2.72380311
 1 0.29487658 -3.11769258 1.53335513
 Energy = -8524.626465 Hartree
 Number of imaginary frequencies = 0.

Compound I4a isomer 19

Atomic N.	X	Y	Z
8	2.34383723	-2.52917564	-0.44407717
6	3.56872625	-2.65119943	0.15434824
8	4.58929671	-3.04580810	-0.73857035
6	4.62007184	-2.33157150	-1.98201927
1	4.78646683	-1.25475089	-1.82194726
1	3.68994671	-2.47866844	-2.54812553
1	5.46516412	-2.74955616	-2.54097060
8	3.84799413	-1.24771745	0.61174068
6	3.56436744	-3.67076321	1.30616568
1	2.96182618	-3.24455527	2.12375196
1	3.00136229	-4.52921586	0.91124454
6	4.93042651	-4.15684598	1.80817205
1	5.52239021	-4.48846538	0.94322916
1	4.76613691	-5.04702055	2.43636082
6	5.72738290	-3.13002069	2.62055576
1	5.21297666	-2.94660916	3.57985259
1	6.70803493	-3.56342395	2.87478344
6	5.93738159	-1.77739876	1.92673933
1	6.41869460	-1.90510132	0.94515067
1	6.62518579	-1.17311301	2.54099059
6	4.66013938	-0.95263819	1.77867447
1	4.03528876	-1.04540431	2.68091286
1	4.89952120	0.11226333	1.65560740
50	1.60271969	-0.56471454	-0.11030456
7	-0.55798773	-1.92451546	-0.58508656
6	-0.48023148	-2.75301879	-1.80616405
1	-1.38010322	-3.38489179	-1.92380461
1	-0.36685652	-2.11555963	-2.69003855
1	0.40613163	-3.39220652	-1.72512688
7	-0.91684894	0.47284517	-2.36721699
6	-1.74521537	-1.03670208	-0.56562716
1	-2.65009564	-1.62585345	-0.31514812
1	-1.60294846	-0.30795310	0.24734275
6	-2.06249389	-0.29545843	-1.86644263
1	-2.94483258	0.33867669	-1.66113697
1	-2.34319249	-1.00192493	-2.65783978
16	-1.04745551	1.17511307	-3.91269920
7	0.63673971	-1.09044268	1.81850090
6	-0.57098681	-2.81381388	0.60856205
1	-1.48919790	-3.43271176	0.61197777
1	0.30104565	-3.47216228	0.50715740
6	-0.47093943	-2.04127588	1.92296618
1	-0.30383517	-2.76889279	2.73474194
1	-1.42771060	-1.53025555	2.14335986
16	0.86803903	-0.04233015	3.06125421
8	2.03554485	0.78054796	2.63924161
8	0.87127114	-0.74167141	4.36741186
6	-0.57194978	1.06553664	3.08682233
6	-1.62990852	0.81575335	3.96259887
6	-2.74634001	1.65681323	3.94454112

6	-2.81771738	2.75112828	3.07044592
6	-1.73571276	2.98332357	2.20283325
6	-0.61790244	2.14983363	2.20465917
1	-1.56179675	-0.01653261	4.66260575
1	0.23030827	2.34509355	1.54724596
1	-1.76629369	3.83876220	1.52461821
6	-4.00522134	3.68121739	3.08688706
1	-3.57314031	1.46323429	4.63073094
8	0.22222542	1.89329836	-4.11012679
8	-1.50220165	0.09068533	-4.80294661
6	-2.37100310	2.40301903	-3.82429641
6	-3.67410261	2.04388379	-4.17480791
6	-4.68789106	3.00019596	-4.08637259
6	-4.41726686	4.30878556	-3.65806301
6	-3.09495433	4.64107031	-3.31529632
6	-2.07003540	3.69980747	-3.39642478
1	-3.87998291	1.03570869	-4.53280239
1	-5.70720721	2.72604322	-4.36398033
6	-5.50936467	5.34669181	-3.60193244
1	-2.86346856	5.65720162	-2.99061011
1	-1.04081024	3.96681544	-3.15680569
1	-4.90041046	3.18275074	3.48090947
1	-3.80695514	4.55558246	3.72634343
1	-4.23259325	4.06056264	2.08141307
1	-5.51184368	5.95684606	-4.51858916
1	-6.50016407	4.88322311	-3.51256157
1	-5.36782400	6.03307942	-2.75639939
1	-0.53165063	1.15651762	-1.70908955

Energy = -8524.638858 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 20

Atomic N.	X	Y	Z
8	0.46576915	-0.54734300	0.44758603
6	1.62230976	0.17576240	0.58744181
8	2.39611343	-0.14021729	1.71672232
6	2.58710777	-1.54339777	1.98269012
1	3.00389798	-2.07083158	1.10952686
1	1.65431123	-2.02841541	2.29589563
1	3.31265495	-1.58697226	2.80314843
8	2.35337089	-0.16668661	-0.68063826
6	1.34671730	1.68519112	0.61451407
1	0.83921757	1.91222879	-0.33474030
1	0.61667747	1.85185860	1.42091225
6	2.55347295	2.60628266	0.81763086
1	2.97528781	2.43291403	1.81998691
1	2.18443100	3.64460761	0.81109030
6	3.67940927	2.47224069	-0.21915954
1	3.27993566	2.60806203	-1.23831105
1	4.39200673	3.29640222	-0.05789164
6	4.44777675	1.14549892	-0.12185152
1	4.62758903	0.92161626	0.93908436
1	5.43792245	1.25290253	-0.59480392
6	3.79555623	-0.05718444	-0.80702204
1	3.94408513	-0.01203462	-1.89525114
1	4.26396884	-0.98670857	-0.44400178
50	0.71401833	-1.93109385	-1.20448273

7	-1.92909285	-1.92684934	-1.19993701
6	-2.19126189	-2.94825471	-2.24051788
1	-3.23918574	-2.90095046	-2.58912009
1	-1.52533324	-2.80993091	-3.10118346
1	-2.00572319	-3.94238703	-1.81566380
7	-0.03149624	-0.52324348	-2.77365032
6	-2.22667725	-0.56451168	-1.70550300
1	-3.31217946	-0.45402370	-1.90178867
1	-1.94148861	0.14740273	-0.92017814
6	-1.45481948	-0.23020915	-2.97864664
1	-1.61371759	0.84319783	-3.18784174
1	-1.85995793	-0.78944043	-3.83784294
16	0.86949381	-0.71623891	-4.14023393
7	-1.61107140	-1.45067205	2.07605397
6	-2.80069537	-2.26399224	-0.03728013
1	-3.84933939	-2.28226554	-0.40048173
1	-2.55121274	-3.28202516	0.28850939
6	-2.76557986	-1.34085847	1.18982582
1	-3.66807776	-1.57570756	1.77261867
1	-2.86062114	-0.28418969	0.90138030
16	-1.55567759	-2.70111052	3.18912422
8	-0.12342611	-2.94576672	3.46030071
8	-2.45970021	-3.79528751	2.76344389
6	-2.28483876	-1.98472724	4.68003020
6	-3.55143202	-2.39347262	5.09401244
6	-4.09847684	-1.83896971	6.25524173
6	-3.39405858	-0.88920576	7.00701806
6	-2.11467653	-0.50206065	6.56698753
6	-1.55561532	-1.04226782	5.41228658
1	-4.08881575	-3.14571539	4.51787356
1	-0.55994828	-0.74744288	5.08153126
1	-1.54773468	0.23158564	7.14334622
6	-3.97714032	-0.30440440	8.26909836
1	-5.08932422	-2.15725022	6.58435993
8	2.15779573	-1.28403330	-3.63868321
8	0.14364906	-1.42793146	-5.22316356
6	1.19668402	0.95218194	-4.76505869
6	0.96141622	1.24475371	-6.10762387
6	1.24205534	2.52930060	-6.58160814
6	1.75152530	3.52181753	-5.73227592
6	1.96986124	3.19866983	-4.38078885
6	1.69754153	1.92236317	-3.89312547
1	0.56112128	0.47127782	-6.76196140
1	1.05880347	2.76377840	-7.63187127
6	2.07492942	4.90004559	-6.25273485
1	2.35762206	3.96170723	-3.70250587
1	1.85907427	1.67178965	-2.84425359
1	-5.02186727	-0.60985969	8.40727922
1	-3.40984630	-0.63318564	9.15301971
1	-3.93914929	0.79432201	8.25364377
1	3.16250119	5.03099803	-6.36349649
1	1.61740627	5.07553670	-7.23464846
1	1.72468042	5.68093016	-5.56333834
1	-0.69050911	-1.18789895	1.67194589

Energy = -8524.642192 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 21

Atomic N.	X	Y	Z
8	2.35481154	-2.67607721	-0.19242016
6	3.63150990	-2.66662758	0.28012624
8	4.61699012	-2.40749971	-0.73774662
6	4.56911756	-3.31274990	-1.84087136
1	3.55750114	-3.35983233	-2.27168183
1	4.89190939	-4.32898685	-1.55456619
1	5.26636135	-2.91806065	-2.58945352
8	3.69267131	-1.49116950	1.15801707
6	3.92332102	-3.93187023	1.10585512
1	3.17583663	-3.92702715	1.91322988
1	3.69650212	-4.80363190	0.47256331
6	5.33244218	-4.06457514	1.69216210
1	6.06233673	-4.19928555	0.87657167
1	5.35730190	-4.99333456	2.28471009
6	5.79969927	-2.89586485	2.57583631
1	5.04200322	-2.67426347	3.34520728
1	6.70654202	-3.21470446	3.11336242
6	6.13462652	-1.62852089	1.77396451
1	6.68906553	-1.92155896	0.87064715
1	6.80501440	-0.98095833	2.36213675
6	4.93229315	-0.76496331	1.38207591
1	4.65355552	-0.08494639	2.19852387
1	5.16799462	-0.16612329	0.48986986
50	1.66318335	-0.63259303	-0.00511876
7	-0.55908020	-1.99796995	-0.45419252
6	-0.38820802	-2.86977703	-1.63434998
1	-1.24142994	-3.56583326	-1.74408125
1	-0.30332881	-2.26443500	-2.54463662
1	0.54038296	-3.43887372	-1.51395811
7	-1.08975478	0.97052792	-1.35147067
6	-1.82918631	-1.24066914	-0.53169201
1	-2.66635108	-1.95610210	-0.66401218
1	-1.98603590	-0.74274614	0.43516637
6	-1.93888631	-0.19110617	-1.63865575
1	-3.00662339	0.08236627	-1.72313173
1	-1.62671484	-0.59562900	-2.60980944
16	-0.81611438	2.09026127	-2.60132686
7	0.57713473	-1.00023211	1.89095772
6	-0.56147548	-2.83131220	0.78107722
1	-1.46207152	-3.47540944	0.81050136
1	0.32980886	-3.46844557	0.72111070
6	-0.48674689	-1.98724413	2.05591526
1	-0.28142374	-2.66505051	2.90103285
1	-1.46301462	-1.50983285	2.26854371
16	0.78907655	0.12762722	3.06095778
8	2.02856396	0.85240212	2.66869014
8	0.63630575	-0.45346518	4.41465909
6	-0.57547025	1.31473654	2.86231532
6	-1.73779865	1.18288688	3.62392812
6	-2.80035377	2.06816629	3.41369504
6	-2.71419486	3.09436368	2.46227289
6	-1.52739987	3.21196729	1.71506012
6	-0.46262397	2.33089875	1.90619151
1	-1.79350575	0.40763842	4.38789420
1	0.45986511	2.43940863	1.33424974
1	-1.42423449	4.01756819	0.98467665

6	-3.84355539	4.07675401	2.27373972
1	-3.70839220	1.96561456	4.01128851
8	-0.03374854	3.16878381	-1.97254661
8	-0.32476345	1.30235720	-3.74619997
6	-2.42631387	2.77245070	-3.06644232
6	-3.15147937	2.18703667	-4.10650293
6	-4.39930194	2.71429206	-4.44509569
6	-4.93018391	3.82069703	-3.76430671
6	-4.17493223	4.39207284	-2.72569154
6	-2.92807912	3.87774207	-2.37315393
1	-2.72844568	1.34553942	-4.65414303
1	-4.96732049	2.26242475	-5.26024189
6	-6.26073035	4.40827587	-4.16093514
1	-4.56622588	5.26054629	-2.19246058
1	-2.33129056	4.33960055	-1.58700021
1	-4.79587613	3.66823224	2.63588473
1	-3.64934033	5.00638415	2.83111449
1	-3.96396356	4.35407343	1.21726862
1	-6.12157137	5.24088191	-4.86805203
1	-6.89857289	3.66285765	-4.65301598
1	-6.79894854	4.80758835	-3.29107279
1	-1.33866478	1.47433370	-0.49301450

Energy = -8524.634632 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 22

Atomic N.	X	Y	Z
8	0.47188539	-0.24116087	0.38416128
6	1.72895585	0.30642120	0.46185166
8	2.55673678	-0.28586940	1.46066460
6	2.15259013	-0.05108265	2.81319436
1	1.11033501	-0.35328901	2.98288284
1	2.29204827	1.00357805	3.10436116
1	2.79690054	-0.68460867	3.43255828
8	2.36497650	-0.07536321	-0.80791365
6	1.65358269	1.84077920	0.53905756
1	1.10297036	2.14991198	-0.36168122
1	1.01586324	2.10400186	1.39679232
6	2.99005189	2.58694510	0.63363865
1	3.46170299	2.38178156	1.60877701
1	2.76630043	3.66589179	0.62431860
6	4.01801868	2.28283704	-0.46988363
1	3.55989839	2.41368373	-1.46411373
1	4.82176267	3.03226506	-0.40018624
6	4.65169793	0.88731509	-0.35280452
1	4.89545425	0.70269021	0.70310135
1	5.60419961	0.86515432	-0.90656463
6	3.80613880	-0.26934708	-0.89524468
1	3.95421470	-0.39598941	-1.97621633
1	4.07618059	-1.20891073	-0.39289767
50	0.62076652	-1.82620846	-1.11052097
7	-2.01030496	-1.74457352	-1.08475704
6	-2.33140902	-2.77730840	-2.09793076
1	-3.38807119	-2.70696266	-2.41444739
1	-1.68925437	-2.67187160	-2.98063246
1	-2.15946360	-3.76780938	-1.65941812
7	-0.10985722	-0.49880180	-2.75076936

6	-2.26710757	-0.38188130	-1.61142468
1	-3.35190249	-0.23145731	-1.78261180
1	-1.93156902	0.33391123	-0.84955825
6	-1.51509435	-0.11159500	-2.91341932
1	-1.61006888	0.96735715	-3.13249260
1	-1.98380706	-0.65393186	-3.75087727
16	0.72961368	-0.80332778	-4.13288156
7	-1.47570175	-1.28099960	2.12912939
6	-2.85828461	-2.02973568	0.10547550
1	-3.92057215	-1.96488440	-0.20951590
1	-2.66719117	-3.06611542	0.41073173
6	-2.69461227	-1.12807571	1.33621732
1	-3.55766298	-1.33284011	1.98843924
1	-2.76964626	-0.06433154	1.06795296
16	-1.31603530	-2.62396553	3.12595093
8	0.11768614	-2.68415320	3.47374424
8	-2.01002479	-3.80777609	2.56424537
6	-2.25388800	-2.13858651	4.59503842
6	-3.37415511	-2.87820650	4.97045026
6	-4.06810507	-2.52007379	6.13007108
6	-3.65335348	-1.43834266	6.91864987
6	-2.51823233	-0.71133865	6.51470089
6	-1.81661857	-1.05437112	5.36228616
1	-3.68680528	-3.72429517	4.35972959
1	-0.93484548	-0.49117842	5.05753423
1	-2.18000043	0.13439115	7.11638940
6	-4.38778711	-1.06955573	8.18303141
1	-4.94657828	-3.09586576	6.42679723
8	1.98952419	-1.44570276	-3.64981725
8	-0.07997673	-1.49534378	-5.16850023
6	1.15836633	0.81454382	-4.82641400
6	0.91229234	1.07644131	-6.17311592
6	1.27347150	2.31994968	-6.70001303
6	1.87349163	3.30145922	-5.89891608
6	2.10165696	3.01014238	-4.54156964
6	1.74970378	1.77533427	-4.00124775
1	0.44188914	0.31177316	-6.79014184
1	1.08313163	2.53013517	-7.75418162
6	2.27685189	4.63663251	-6.47343171
1	2.56157217	3.76557894	-3.90073009
1	1.91981810	1.54824920	-2.94801020
1	-4.54472371	0.01596742	8.25235995
1	-5.36556021	-1.56448715	8.23807751
1	-3.81081507	-1.36938702	9.07141159
1	1.89039179	4.76780988	-7.49201441
1	1.90565372	5.46641339	-5.85502405
1	3.37269689	4.73143704	-6.51503292
1	-0.59195818	-1.00982071	1.65315061

Energy = -8524.638949 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 23

Atomic N.	X	Y	Z
8	3.50818786	0.03087524	-1.28857994
6	3.96974843	1.30307405	-1.38168383
8	4.28745551	1.69827410	-2.68643894
6	3.38006930	1.25725381	-3.71088604

1	2.40206894	1.75351064	-3.61102859
1	3.24669478	0.16897134	-3.68066598
1	3.84336600	1.55738577	-4.65733381
8	2.73593408	2.13120829	-0.92742039
6	5.20980193	1.56734294	-0.51356787
1	4.91829157	1.45863586	0.54332935
1	5.86703154	0.71505091	-0.73838709
6	5.97301413	2.87576985	-0.75629921
1	6.12072583	2.99701111	-1.83894824
1	6.97639133	2.77379844	-0.31362592
6	5.31319490	4.13028010	-0.17426906
1	5.33706714	4.07573754	0.92833397
1	5.91534620	5.01099409	-0.44892389
6	3.86019559	4.35789474	-0.60923690
1	3.77900679	4.41959859	-1.70577210
1	3.52344808	5.32968692	-0.21224067
6	2.88306195	3.30224378	-0.09029711
1	3.16157703	2.99936379	0.93481363
1	1.86649480	3.71585881	-0.03989656
50	1.72370310	0.03704868	-0.17962016
7	-0.87988603	2.07544746	-0.83228227
6	-0.97546787	3.51600257	-0.57571379
1	-1.90513704	3.95614564	-0.99458972
1	-0.94054047	3.71703201	0.50183856
1	-0.12376204	4.02232196	-1.04873236
7	-1.07569552	1.52103834	1.97527821
6	-2.04074176	1.34748409	-0.30322299
1	-2.97313172	1.60618802	-0.85383185
1	-1.85820948	0.27478117	-0.45813041
6	-2.31363647	1.59584820	1.18439382
1	-3.05814633	0.84648528	1.50555839
1	-2.76415453	2.58442218	1.34624164
16	-1.18226094	1.17842116	3.62367196
7	0.35363295	-0.33333647	-1.90981558
6	-0.70469322	1.85921304	-2.27844156
1	-1.53325236	2.32680534	-2.85590554
1	0.22594139	2.37261470	-2.56413265
6	-0.62415878	0.39526173	-2.71285677
1	-0.35258715	0.38820925	-3.78279008
1	-1.62221692	-0.07384559	-2.63281719
16	0.58073825	-1.92134001	-2.17762069
8	1.57481840	-2.23989734	-1.07056961
8	0.91409924	-2.29479843	-3.56749420
6	-0.95378429	-2.79154570	-1.76920424
6	-1.68650893	-3.40273792	-2.78687950
6	-2.88619312	-4.04507963	-2.46959080
6	-3.36045531	-4.08724119	-1.15067614
6	-2.60052069	-3.46238388	-0.14536082
6	-1.40346290	-2.81560338	-0.44555247
1	-1.30786738	-3.37948556	-3.80803056
1	-0.81651683	-2.34587249	0.34492226
1	-2.94972302	-3.48381135	0.88886256
6	-4.64034342	-4.80761527	-0.80854739
1	-3.46210726	-4.52388874	-3.26354291
8	0.20057224	1.25551470	4.12644460
8	-2.27276353	2.02245965	4.14736708
6	-1.71434611	-0.54600583	3.76807463
6	-3.05413579	-0.84219406	4.02090619

6	-3.44652372	-2.18043364	4.12287853
6	-2.51935513	-3.22250267	3.97946558
6	-1.17507098	-2.89270525	3.72566245
6	-0.76660580	-1.56510098	3.62030153
1	-3.76829040	-0.03114354	4.15970807
1	-4.49218344	-2.41664426	4.32856922
6	-2.93904213	-4.66463843	4.11750269
1	-0.43665431	-3.68943140	3.61707593
1	0.27993442	-1.31312368	3.44684280
1	-5.27483723	-4.94132074	-1.69389070
1	-4.42691811	-5.80764407	-0.39994176
1	-5.21518586	-4.26262636	-0.04746157
1	-2.52741951	-5.10606594	5.03789422
1	-4.03115458	-4.76269057	4.15909391
1	-2.56849488	-5.27085215	3.27823254
1	-0.30747041	0.99504062	1.53948410

Energy = -8524.627349 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 24

Atomic N.	X	Y	Z
8	2.15179867	2.34415740	0.00360705
6	3.44895719	2.10662915	0.35178131
8	3.34909219	0.88727450	1.16643248
6	4.53624652	0.17776496	1.56294127
1	5.11248556	0.78164374	2.27888936
1	5.15401830	-0.07753464	0.69253652
1	4.17573478	-0.72746691	2.06389543
8	4.26217919	1.69393282	-0.75452488
6	4.03165335	3.29169074	1.15794277
1	3.47830741	4.18684085	0.83529803
1	3.74217498	3.11796545	2.20458065
6	5.53936255	3.56721811	1.04895854
1	6.11850449	2.63961524	1.17601882
1	5.81746673	4.21942534	1.89245439
6	5.95716397	4.26317040	-0.25634703
1	5.31940070	5.15345797	-0.39837485
1	6.98784889	4.63814247	-0.15078133
6	5.88160505	3.38160666	-1.50805879
1	6.64260594	2.58596232	-1.45185656
1	6.12289276	3.98523950	-2.39969101
6	4.52617137	2.71729308	-1.73355325
1	3.70377033	3.45239921	-1.74032949
1	4.51533746	2.20345399	-2.70627152
50	1.24351840	0.40734774	-0.01972889
7	-0.92157685	1.93380208	-0.51688607
6	-0.45223137	3.27004760	-0.95162337
1	-1.31103234	3.94417758	-1.12689733
1	0.20989773	3.69742549	-0.19280672
1	0.12423430	3.17088703	-1.87884494
7	0.12624248	0.73263419	1.83046562
6	-1.59929637	2.04999727	0.80668528
1	-2.19320341	2.98332277	0.83743113
1	-2.29220399	1.20511620	0.91347161
6	-0.61160832	1.98784381	1.97081040
1	-1.18373433	2.01632440	2.91283252
1	0.06483588	2.85906384	1.97338910

16	0.69304344	-0.04391203	3.16341907
7	-1.29543482	-0.99294542	-2.15018584
6	-1.87996239	1.42536460	-1.53896390
1	-2.82171422	2.00243287	-1.45306817
1	-1.46910021	1.63869899	-2.53339505
6	-2.20732473	-0.07591539	-1.45501668
1	-3.21071872	-0.23079590	-1.87364622
1	-2.25226670	-0.40753255	-0.40623890
16	-1.40506909	-1.12527351	-3.84138856
8	-0.02495546	-1.36996615	-4.30430655
8	-2.22800582	-0.01439544	-4.37229715
6	-2.35565256	-2.64165110	-4.07375419
6	-3.70047496	-2.56343422	-4.43360533
6	-4.42205791	-3.74592243	-4.61742337
6	-3.81559436	-4.99926236	-4.45245557
6	-2.45551938	-5.04391853	-4.09628903
6	-1.72083492	-3.87602994	-3.90797834
1	-4.16438620	-1.58889216	-4.58065989
1	-0.66390243	-3.91363877	-3.64584652
1	-1.96480396	-6.01072855	-3.96969652
6	-4.58959108	-6.27362578	-4.67778088
1	-5.47476147	-3.69140936	-4.90049570
8	1.55607686	-1.12448778	2.60377248
8	1.22193368	0.87409527	4.19958047
6	-0.75957118	-0.84567215	3.89804697
6	-1.26670940	-0.38305372	5.11127210
6	-2.38807488	-1.00913536	5.66563848
6	-3.00399922	-2.09305785	5.02631381
6	-2.46473092	-2.54469683	3.80720782
6	-1.35227302	-1.92854722	3.23993205
1	-0.77181625	0.44596994	5.61617775
1	-2.78477517	-0.65136555	6.61767972
6	-4.21417223	-2.76698852	5.62370427
1	-2.92173957	-3.39763101	3.30118880
1	-0.92790040	-2.29192808	2.30377361
1	-5.67174553	-6.09175977	-4.67816460
1	-4.32671287	-6.72378033	-5.64754867
1	-4.36347061	-7.02035259	-3.90409703
1	-4.06013570	-3.85189019	5.71555144
1	-4.44308456	-2.36868887	6.62016907
1	-5.10179514	-2.62113319	4.98953947
1	-0.30483607	-0.91101545	-1.88251095

Energy = -8524.633301 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 25

Atomic N.	X	Y	Z
8	1.13604401	1.39043715	-0.16052042
6	2.46305761	1.39316979	-0.56676675
8	2.92363366	0.08077085	-0.87856609
6	3.10949476	-0.78344976	0.25258176
1	2.22174555	-0.81062562	0.89842705
1	3.97681390	-0.48249543	0.86017537
1	3.29890746	-1.78097806	-0.16229276
8	2.45997494	2.11219888	-1.82820663
6	3.34643429	2.14822024	0.44160751
1	2.91288167	3.15791911	0.50411417

1	3.21149485	1.68992142	1.43277929
6	4.83980357	2.24403917	0.10382704
1	5.31135650	1.25259842	0.20477097
1	5.30656009	2.87988384	0.87274421
6	5.18944466	2.80339738	-1.28595694
1	4.67039603	3.76216653	-1.45152677
1	6.26760601	3.02692745	-1.30121928
6	4.88218714	1.82509489	-2.43088586
1	5.19897029	0.81695359	-2.12662160
1	5.47759361	2.08838298	-3.32014801
6	3.41400504	1.79205688	-2.87047185
1	3.21909101	2.57703080	-3.61532558
1	3.15598763	0.82119545	-3.31555292
50	-0.09574049	2.41826156	-1.57100750
7	-2.14348200	2.90564231	0.34505262
6	-2.29820128	4.37083138	0.33942692
1	-3.28126055	4.67628840	0.74784829
1	-1.51086817	4.84266549	0.93896233
1	-2.20669344	4.74537604	-0.68863494
7	0.13505841	1.77452444	2.48753306
6	-2.22577799	2.38785741	1.73283827
1	-3.12629729	2.81989676	2.21865107
1	-2.37333894	1.30188215	1.68726655
6	-1.00355463	2.68163355	2.61762515
1	-1.31587263	2.65388437	3.67102085
1	-0.63553205	3.70413359	2.44121969
16	0.27479666	0.46265072	3.51435501
7	-1.59917956	0.74346439	-1.44147973
6	-3.21361931	2.30681414	-0.48985781
1	-4.19752403	2.39129386	0.01525111
1	-3.26649802	2.89442649	-1.41935375
6	-2.93832783	0.84845204	-0.86439542
1	-3.71138155	0.54129231	-1.58788959
1	-3.03055772	0.19119611	0.01718108
16	-1.37539366	-0.01724647	-2.86517227
8	-0.08020034	0.63210781	-3.32474797
8	-2.55150677	-0.00659408	-3.76542371
6	-0.97580769	-1.75172427	-2.55203091
6	-1.92053285	-2.73326925	-2.85134672
6	-1.62149242	-4.06968476	-2.57171845
6	-0.39215584	-4.43380160	-2.00396903
6	0.54341396	-3.42036641	-1.72632198
6	0.26325945	-2.08164807	-1.99338774
1	-2.86625818	-2.44929493	-3.31143936
1	0.99678487	-1.30163177	-1.78075672
1	1.51020983	-3.68770170	-1.29535538
6	-0.07408899	-5.87435621	-1.69130647
1	-2.35488014	-4.84289749	-2.80783531
8	1.59698093	-0.12304432	3.21363982
8	-0.08166415	0.92646108	4.87139777
6	-0.97125362	-0.77335787	3.05216498
6	-1.94044165	-1.14774454	3.98315151
6	-2.88470679	-2.11604790	3.63062506
6	-2.87230306	-2.71477810	2.36264387
6	-1.88885871	-2.31146776	1.44133334
6	-0.94011538	-1.34687018	1.77667417
1	-1.94227351	-0.68441777	4.96910189
1	-3.64381392	-2.41163137	4.35738783

6	-3.87468757	-3.78076953	1.99658152
1	-1.86849209	-2.75360932	0.44309369
1	-0.19626239	-1.03108737	1.04404987
1	-0.84016672	-6.55069602	-2.09078289
1	0.89769476	-6.16797065	-2.11305377
1	-0.01354914	-6.03634735	-0.60431060
1	-3.42882607	-4.78343269	2.08829959
1	-4.75328494	-3.74869555	2.65365587
1	-4.21267782	-3.67173977	0.95700161
1	0.52771874	1.59807269	1.53957774

Energy = -8524.638561 Hartree
Number of imaginary frequencies = 0.

Compound I4a isomer 26

Atomic N.	X	Y	Z
8	2.77282628	1.92740027	0.93173120
6	4.03782855	1.63157113	0.50989926
8	5.00174992	1.68554851	1.52574579
6	4.62969145	1.05229733	2.76161446
1	4.31495290	0.01176833	2.59980801
1	3.82360648	1.60997837	3.25877671
1	5.53133228	1.07374853	3.38420925
8	3.87720791	0.17622471	0.07546077
6	4.52777888	2.53570233	-0.63189550
1	3.91497987	2.31522737	-1.52098473
1	4.25473439	3.55197923	-0.31273878
6	6.02561323	2.49032523	-0.95765180
1	6.58908535	2.63551889	-0.02483779
1	6.26086928	3.35152767	-1.60308827
6	6.50530432	1.21433932	-1.65897468
1	6.06824518	1.16887404	-2.67228549
1	7.59592624	1.27989142	-1.80084174
6	6.17298004	-0.09711283	-0.93389895
1	6.54736430	-0.08518455	0.10085981
1	6.69337422	-0.92253041	-1.44710403
6	4.69122963	-0.46198676	-0.94202157
1	4.25973920	-0.24467061	-1.93574876
1	4.55160304	-1.53256295	-0.73815362
50	1.51902625	0.40143819	0.14760431
7	-0.31382239	1.61655574	1.80039231
6	0.31429141	2.83829056	2.35162961
1	-0.33964127	3.30641263	3.11161278
1	1.28470789	2.59825213	2.79585166
1	0.49439074	3.55195327	1.53971892
7	1.41075995	-0.69912577	2.02877784
6	-0.48983612	0.60493727	2.87431207
1	-0.92386181	1.08503517	3.77439097
1	-1.20292798	-0.15111771	2.51960465
6	0.81919198	-0.10722628	3.22578383
1	0.61801094	-0.87384028	3.99094758
1	1.53653961	0.59667216	3.67878414
16	1.57996299	-2.32671271	1.89922178
7	-1.84250279	0.88886711	-1.06418441
6	-1.63615832	2.00058374	1.23364328
1	-2.32457142	2.23329710	2.07149236
1	-1.50686552	2.92860396	0.66278033
6	-2.31406378	0.96352372	0.32492075

1	-3.38690041	1.19802312	0.29670869
1	-2.23207198	-0.04994509	0.74663563
16	-2.35878852	2.07810189	-2.16443741
8	-1.23122380	2.25583460	-3.10064920
8	-2.95520319	3.21633409	-1.42853248
6	-3.70543012	1.26423875	-3.04898460
6	-5.02563004	1.60662309	-2.75833440
6	-6.05810181	0.97982787	-3.46071574
6	-5.78674311	0.02468044	-4.45084862
6	-4.44447436	-0.29404869	-4.72452237
6	-3.40237821	0.31963461	-4.03363559
1	-5.23312332	2.36430187	-2.00371892
1	-2.36298510	0.08245922	-4.25878065
1	-4.21402230	-1.03077359	-5.49631331
6	-6.90289054	-0.62416394	-5.23014026
1	-7.09343045	1.24472271	-3.23878432
8	2.16108597	-2.50762747	0.53746707
8	2.24308996	-2.89984755	3.09215830
6	-0.08338275	-3.05703284	1.85964601
6	-0.59635468	-3.67793514	2.99919009
6	-1.88968326	-4.20744929	2.96630651
6	-2.67514375	-4.13502771	1.80690065
6	-2.13041532	-3.51137990	0.66997650
6	-0.84442880	-2.97417528	0.68896421
1	0.02498719	-3.75746199	3.89078584
1	-2.29122519	-4.69417333	3.85720835
6	-4.05535821	-4.74175684	1.76346209
1	-2.72198955	-3.45146584	-0.24583815
1	-0.42250913	-2.50760970	-0.20221437
1	-7.86265349	-0.53758202	-4.70504156
1	-7.01922769	-0.14563014	-6.21499346
1	-6.69984446	-1.68858411	-5.41043232
1	-4.03120423	-5.73235039	1.28314697
1	-4.46756251	-4.87409044	2.77202540
1	-4.74947063	-4.11862734	1.18311561
1	-0.82596550	0.75968182	-1.17194448

Energy = -8524.635493 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 27

Atomic N.	X	Y	Z
8	4.08254936	1.81580925	-2.89975195
6	4.57235339	2.85189885	-2.17993334
8	4.03169012	4.09222910	-2.52728662
6	2.61806553	4.11073566	-2.79526775
1	2.04409146	4.02588931	-1.85954089
1	2.33193056	3.30388049	-3.48018269
1	2.42086373	5.08654437	-3.25280691
8	4.08741697	2.48769422	-0.74144520
6	6.10389999	2.98495958	-2.24339649
1	6.54173198	2.11796785	-1.72149286
1	6.33850286	2.85225570	-3.30946668
6	6.71361408	4.30238011	-1.75033387
1	6.18034399	5.13359956	-2.23315691
1	7.75565893	4.35158475	-2.10410724
6	6.70823486	4.49571116	-0.23019272
1	7.40385730	3.77321935	0.23258388

1	7.10961639	5.49516209	0.00152158
6	5.33788218	4.33774672	0.44172570
1	4.59345511	5.00849122	-0.01339164
1	5.43055265	4.63722623	1.49874482
6	4.80279316	2.90507900	0.44335300
1	5.63281437	2.20156086	0.64157761
1	4.06728344	2.78507769	1.25386419
50	3.73781956	0.19976622	-1.58528103
7	0.31411552	0.05640504	1.71221628
6	0.91958675	-0.34163014	2.98370669
1	0.80818360	0.43071654	3.77759475
1	0.47475792	-1.27779552	3.34231735
1	1.99141904	-0.52093432	2.82803187
7	-1.76207957	-2.05927506	1.85100959
6	-1.11366739	0.34392692	1.85210334
1	-1.28419611	1.26358137	2.46248288
1	-1.52280700	0.55480072	0.85180933
6	-1.95271725	-0.75658153	2.50512052
1	-3.00534700	-0.41909357	2.47251378
1	-1.68236905	-0.88171990	3.56135331
16	-2.64341290	-3.36773331	2.46440598
7	1.53596705	0.52435931	-1.16742642
6	1.01238788	1.22031998	1.15575697
1	0.73998914	2.15041767	1.70814806
1	2.09051424	1.06689126	1.31533575
6	0.79211857	1.47861400	-0.33962570
1	1.13109074	2.50687430	-0.54965055
1	-0.28001480	1.45173187	-0.59041622
16	0.93292447	0.03526515	-2.59140009
8	2.20194048	-0.55119665	-3.22142071
8	0.17180424	1.03720351	-3.36853810
6	-0.17206059	-1.37498984	-2.34903381
6	-1.28998060	-1.50426497	-3.17485089
6	-2.09956351	-2.63495075	-3.04574582
6	-1.80761201	-3.63451391	-2.10478907
6	-0.68903330	-3.46218086	-1.26837471
6	0.13152916	-2.34084505	-1.38576301
1	-1.51130675	-0.72805850	-3.90626053
1	0.98692876	-2.20470472	-0.72435133
1	-0.47213237	-4.20979717	-0.50438273
6	-2.65238980	-4.87864184	-1.99959690
1	-2.97068319	-2.74479251	-3.69445227
8	-2.35547605	-4.49150074	1.55115279
8	-2.34072290	-3.42703974	3.90600390
6	-4.39836149	-2.95737745	2.30159498
6	-5.09804221	-2.47551277	3.40874871
6	-6.44907079	-2.14805846	3.26897985
6	-7.10915348	-2.29561252	2.04054003
6	-6.37799658	-2.78301737	0.94245540
6	-5.03047532	-3.11555649	1.06394960
1	-4.58886686	-2.37906805	4.36699869
1	-7.00069285	-1.77480916	4.13361501
6	-8.57416666	-1.96782337	1.90080031
1	-6.87612289	-2.90978912	-0.02058644
1	-4.47455606	-3.51026992	0.21355321
1	-2.18511086	-5.70820482	-2.55304212
1	-2.75225708	-5.20203221	-0.95469751
1	-3.65215450	-4.72320396	-2.42654539

1	-9.17881323	-2.88764143	1.87940240
1	-8.93031498	-1.35550316	2.73875645
1	-8.77579431	-1.42734910	0.96570533
1	-1.82275725	-2.04450699	0.82845123

Energy = -8524.626220 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 28

Atomic N.	X	Y	Z
8	2.72554796	0.59753070	1.25485582
6	3.95319481	1.05721457	0.86599912
8	4.73906961	0.04367247	0.21040473
6	4.97967033	-1.12331077	1.01088306
1	4.04260950	-1.52339200	1.42371916
1	5.68749252	-0.91275732	1.82996011
1	5.42597139	-1.86276236	0.33568473
8	3.71806748	2.06309168	-0.16248665
6	4.65760423	1.69923300	2.07745845
1	4.00232540	2.52541361	2.39246416
1	4.64535709	0.96671029	2.89816221
6	6.08326358	2.21381367	1.85681504
1	6.76345731	1.36189235	1.69118545
1	6.41154526	2.68983096	2.79489488
6	6.26636139	3.20813366	0.69917553
1	5.54140458	4.03470443	0.79057974
1	7.26676049	3.66019225	0.78869775
6	6.15336453	2.54627844	-0.68185951
1	6.69309182	1.58885266	-0.65610033
1	6.65225021	3.17082638	-1.44123028
6	4.71984140	2.31259874	-1.17533151
1	4.34319106	3.22352486	-1.66573721
1	4.70759854	1.49617656	-1.91426047
50	1.49641736	0.12466899	-0.38739825
7	0.05228048	2.19705292	0.27657254
6	0.79630260	2.92135875	1.33283301
1	0.17691781	3.73935740	1.74438971
1	1.09031836	2.23204497	2.12952365
1	1.71695974	3.33483188	0.90414857
7	-0.13787868	-0.52084926	0.97022612
6	-1.20694923	1.62718953	0.81961044
1	-1.78235052	2.40236261	1.36145002
1	-1.80699345	1.27062363	-0.02542944
6	-0.94293264	0.42982423	1.73512208
1	-1.92545234	0.00430047	2.00743599
1	-0.44783885	0.73134742	2.67272530
16	0.30604719	-1.94536781	1.64813856
7	-0.88238158	1.43855384	-2.51471836
6	-0.17399051	3.15355671	-0.84225905
1	-0.53268697	4.11812430	-0.43253886
1	0.81258756	3.34894789	-1.29047264
6	-1.17233902	2.75620543	-1.93008142
1	-1.16955897	3.56072481	-2.68469027
1	-2.19105650	2.71863214	-1.51774523
16	-1.97521146	0.91818138	-3.73429310
8	-1.25372980	-0.15963470	-4.43652127
8	-2.53212214	2.07054914	-4.47742816
6	-3.30653775	0.22384496	-2.73629548

6	-4.60621777	0.69402897	-2.92236179
6	-5.64317908	0.12268164	-2.18048268
6	-5.39434258	-0.90436600	-1.25840076
6	-4.07118468	-1.35217669	-1.08948296
6	-3.02542709	-0.79885283	-1.82477939
1	-4.79128318	1.49504295	-3.63722784
1	-2.00241171	-1.14684816	-1.68247750
1	-3.85344821	-2.14461145	-0.37103796
6	-6.51815950	-1.53162555	-0.47269903
1	-6.66287406	0.48569144	-2.31986555
8	1.46923868	-2.35546479	0.78911362
8	0.43989543	-1.89059392	3.12100740
6	-1.02277100	-3.12700985	1.29767285
6	-1.97520873	-3.40173348	2.27940901
6	-3.00941933	-4.29858512	1.99395071
6	-3.09765398	-4.93249616	0.74637044
6	-2.11459746	-4.64698724	-0.21884828
6	-1.08289976	-3.74893366	0.04647090
1	-1.88801939	-2.93560343	3.26039123
1	-3.75321466	-4.51927133	2.76195637
6	-4.21395342	-5.89919695	0.43855979
1	-2.15702296	-5.14034523	-1.19187143
1	-0.31379213	-3.54221635	-0.69755898
1	-7.42927856	-0.92180395	-0.51675687
1	-6.76323448	-2.52778524	-0.87241907
1	-6.23993793	-1.66713957	0.58153632
1	-3.81941942	-6.86519673	0.09212010
1	-4.84071086	-6.08262649	1.32028002
1	-4.86153908	-5.51315954	-0.36351591
1	0.05520573	1.36328425	-2.92529118

Energy = -8524.634369 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 29

Atomic N.	X	Y	Z
8	2.47219467	1.72223537	-1.22402741
6	3.47906073	1.95692007	-0.32597964
8	3.39908163	3.31131127	0.18709408
6	3.52769429	4.33545309	-0.80122130
1	2.89729514	4.12538977	-1.67898645
1	4.57327820	4.46642787	-1.12713983
1	3.19210462	5.26554190	-0.32471925
8	3.20883247	1.12132126	0.81950426
6	4.85458130	1.66037318	-0.95293319
1	4.76234524	0.67613451	-1.43649599
1	5.00357144	2.38089114	-1.77060172
6	6.06882590	1.65207133	-0.01232300
1	6.11012454	2.58209495	0.57806854
1	6.97277576	1.65287659	-0.64171330
6	6.11888273	0.41540947	0.90224487
1	5.84734111	-0.46043742	0.29206751
1	7.15528010	0.24226043	1.23090232
6	5.21011090	0.46086653	2.15109595
1	5.77634707	0.84766972	3.01577745
1	4.90428177	-0.56249035	2.41578083
6	3.97565850	1.35154029	2.02438329
1	3.28288069	1.14818832	2.85418941

1	4.24548880	2.41486532	2.06805793
50	1.21404281	0.08532167	-0.84785655
7	-0.44167622	1.79023221	0.15454978
6	0.11921340	2.52771711	1.30655801
1	-0.58489518	3.30210761	1.66413717
1	0.34781394	1.83788643	2.12625870
1	1.05612644	3.00434074	0.99231399
7	-0.78861198	-0.63274373	1.91072268
6	-1.74572100	1.15525050	0.46327930
1	-2.53883155	1.92892586	0.49585079
1	-1.99072205	0.47704652	-0.36837392
6	-1.82678619	0.39739514	1.79120705
1	-2.84828544	-0.01788588	1.86557298
1	-1.68966589	1.08665008	2.63388605
16	-0.44237116	-1.24618520	3.46094262
7	-0.19777344	0.80328785	-2.41520138
6	-0.58880922	2.72441829	-0.99748142
1	-1.31433186	3.52257689	-0.74719215
1	0.40074071	3.17439633	-1.15051803
6	-1.00930206	2.00958221	-2.28297115
1	-0.84087958	2.70207224	-3.12379183
1	-2.08864433	1.76901288	-2.26467499
16	0.31786426	0.31703831	-3.89139576
8	1.45892778	-0.59508574	-3.55582920
8	0.50254200	1.43789774	-4.84231905
6	-0.98609224	-0.73101194	-4.59221757
6	-1.81168615	-0.22585282	-5.59675030
6	-2.82863986	-1.03275020	-6.11434536
6	-3.02629797	-2.34030014	-5.64824872
6	-2.17596571	-2.82463577	-4.63852751
6	-1.16022457	-2.03095371	-4.10896715
1	-1.64141466	0.78182253	-5.97447159
1	-0.49037858	-2.41624130	-3.33995550
1	-2.30853455	-3.84348926	-4.26864245
6	-4.09921479	-3.22151738	-6.23826109
1	-3.47453935	-0.64006441	-6.90212510
8	0.58104570	-2.28000985	3.23564092
8	-0.21196442	-0.06277859	4.31136034
6	-1.93980574	-2.06448058	4.05569614
6	-2.85358962	-1.35526116	4.83769950
6	-4.01457439	-1.99754015	5.27329300
6	-4.27243956	-3.33651958	4.94238288
6	-3.33139356	-4.02527882	4.15713459
6	-2.16712831	-3.40108171	3.71299390
1	-2.64190317	-0.32372774	5.11708768
1	-4.72970403	-1.44939086	5.88917414
6	-5.51078637	-4.03466750	5.44435070
1	-3.50983529	-5.07055130	3.89824990
1	-1.42606362	-3.94469277	3.12710411
1	-3.67599046	-3.89709202	-6.99806240
1	-4.56837380	-3.85209889	-5.47060938
1	-4.88325494	-2.62767818	-6.72572581
1	-5.27866109	-4.64914246	6.32805172
1	-6.28708065	-3.31604319	5.73615012
1	-5.92776368	-4.70778183	4.68310753
1	-0.86574636	-1.40735910	1.24673372

Energy = -8524.632476 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 30

Atomic N.	X	Y	Z
8	2.97117897	0.17274656	2.23963409
6	4.10718369	-0.11529759	1.55695756
8	4.76448169	-1.26637257	2.00614444
6	3.91714104	-2.37599420	2.35000299
1	3.43488955	-2.79501130	1.45302741
1	3.15149397	-2.08000548	3.07749468
1	4.58532818	-3.12697239	2.78593081
8	3.56336518	-0.41131630	0.13054900
6	5.13410609	1.02758532	1.57087091
1	4.70032445	1.88530231	1.03242458
1	5.17696242	1.32130945	2.62953092
6	6.54987077	0.70740711	1.07438040
1	6.88006983	-0.22994586	1.54445622
1	7.22704670	1.49551529	1.43965656
6	6.69804776	0.61022904	-0.44765168
1	6.54044205	1.60829701	-0.89294324
1	7.73573452	0.32944729	-0.68858433
6	5.73891529	-0.37330604	-1.12953502
1	5.85458146	-1.38908409	-0.72013104
1	5.99905521	-0.43217995	-2.19923615
6	4.26784308	0.03692276	-1.05097702
1	4.17415566	1.13295761	-1.15201832
1	3.70196037	-0.41316760	-1.87827050
50	1.41482680	0.49014815	0.86406184
7	0.65001696	-1.63737114	-1.64646283
6	1.38874504	-1.85893884	-2.89365702
1	0.97160301	-2.70189181	-3.48433731
1	1.37956433	-0.95269951	-3.51125868
1	2.43235660	-2.10299564	-2.65516535
7	-0.23729053	0.92510896	-2.57667970
6	-0.77751668	-1.39729415	-1.89236751
1	-1.28411913	-2.30436260	-2.29178510
1	-1.24469673	-1.15953652	-0.92570749
6	-1.06302371	-0.25527281	-2.87429449
1	-2.14259924	-0.03404149	-2.80805645
1	-0.86223248	-0.56206000	-3.90975369
16	-0.76873340	2.44252520	-3.08664289
7	0.34571599	-1.43882425	1.24337043
6	0.87065843	-2.78553589	-0.75072250
1	0.57744592	-3.73919996	-1.24379050
1	1.95342084	-2.83333281	-0.55939717
6	0.12685112	-2.72301165	0.58400448
1	0.49484198	-3.56136969	1.20072008
1	-0.95245961	-2.89701334	0.41861800
16	-0.37417115	-1.14239900	2.67119384
8	0.05954118	0.29911139	2.89446067
8	-0.12229482	-2.13703808	3.73422049
6	-2.16576678	-1.11580471	2.41036076
6	-2.95893598	-2.10111715	2.99868666
6	-4.33699695	-2.09213356	2.76803909
6	-4.93156927	-1.11241911	1.95986525
6	-4.10677593	-0.13215477	1.37917500
6	-2.73079389	-0.12755291	1.59879399
1	-2.49442205	-2.85351259	3.63491224

1	-2.10358068	0.64553063	1.15280056
1	-4.54713813	0.63856530	0.74349615
6	-6.42293233	-1.09011708	1.73757776
1	-4.96047259	-2.86172419	3.22664026
8	0.30615357	3.37710461	-2.70969396
8	-1.22796108	2.26942895	-4.47765909
6	-2.21881548	2.85560540	-2.08452626
6	-3.50021668	2.67199136	-2.60486622
6	-4.60742191	2.99306107	-1.81325155
6	-4.45039409	3.49619576	-0.51397105
6	-3.14553935	3.67182022	-0.01695367
6	-2.03137594	3.35711382	-0.79136254
1	-3.62048069	2.30732750	-3.62450000
1	-5.61161536	2.85913858	-2.21961285
6	-5.64461692	3.86423046	0.33055651
1	-3.00191914	4.06890998	0.98976472
1	-1.02198803	3.51682616	-0.41132963
1	-6.87282001	-2.07188399	1.93278944
1	-6.90589648	-0.36522061	2.41132290
1	-6.67006548	-0.79187089	0.70970829
1	-5.68383482	4.95019950	0.50326635
1	-6.58440325	3.56624799	-0.15109977
1	-5.59629342	3.38591358	1.31965443
1	0.13826049	0.96852982	-1.62086819

Energy = -8524.627329 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 31

Atomic N.	X	Y	Z
8	3.14220951	-1.26478425	-0.59515124
6	4.04936526	-0.26582903	-0.38690703
8	4.72404905	0.13806220	-1.54851631
6	3.89452921	0.34922102	-2.70430331
1	3.08961871	1.06932599	-2.50079005
1	3.46518463	-0.60075864	-3.05401690
1	4.56439104	0.75174716	-3.47300945
8	3.14990219	0.86756607	0.07962724
6	5.12618325	-0.62580353	0.65280913
1	4.63245183	-0.69532908	1.63630857
1	5.43547684	-1.64711534	0.38718489
6	6.36367497	0.27813310	0.71228753
1	6.77276015	0.37186606	-0.30378752
1	7.13235802	-0.23246259	1.31438045
6	6.12900708	1.67193869	1.30579536
1	5.89542848	1.57583603	2.38116367
1	7.07036090	2.24174039	1.24880887
6	5.00896784	2.48549154	0.64279801
1	5.16865192	2.57067439	-0.44240063
1	5.03531422	3.51100632	1.04693868
6	3.60278947	1.95927774	0.91920445
1	3.52622332	1.65212023	1.97856881
1	2.85235774	2.74134255	0.73990760
50	1.40130499	-0.73737107	0.54445897
7	0.43479100	-2.92735896	-0.86609080
6	1.60172416	-3.58613625	-1.49572919
1	1.27650907	-4.42107381	-2.14556754
1	2.17258624	-2.85937843	-2.08001649

1	2.27061524	-3.97076913	-0.71670873
7	0.20709309	-0.09621658	-1.19081171
6	-0.41573379	-2.30929889	-1.91764917
1	-0.51211612	-3.00113371	-2.77776706
1	-1.41671777	-2.14435516	-1.49845847
6	0.12163750	-0.95306302	-2.37268630
1	-0.58001277	-0.53953878	-3.11622666
1	1.09769785	-1.05712744	-2.87570036
16	-0.02172047	1.51959853	-1.34876312
7	-0.89875752	-2.88457575	2.02468316
6	-0.32529627	-3.97224953	-0.13295266
1	-0.77342267	-4.67332093	-0.86569481
1	0.40473405	-4.55928246	0.44662492
6	-1.44083047	-3.51390559	0.80685509
1	-2.05315123	-4.39833122	1.04825158
1	-2.10397803	-2.78876039	0.31342871
16	-1.99298020	-2.70408795	3.34081776
8	-1.12278916	-2.71844489	4.53371860
8	-3.12695368	-3.64603972	3.20850241
6	-2.63530372	-1.04126964	3.08906520
6	-4.01270579	-0.85578059	2.97872327
6	-4.50969557	0.44425620	2.84783131
6	-3.64862977	1.55061061	2.81654285
6	-2.26307130	1.32831239	2.92658631
6	-1.75068709	0.04232673	3.06963792
1	-4.67645259	-1.71921553	3.00339576
1	-0.67653383	-0.12336108	3.15021832
1	-1.57481661	2.17330923	2.87915450
6	-4.18221765	2.95056439	2.65471601
1	-5.58723994	0.59853427	2.76765956
8	0.21434336	2.05306614	0.02490003
8	0.70876296	2.11896572	-2.49323140
6	-1.78588445	1.71608931	-1.73540428
6	-2.16495949	2.43256866	-2.87040749
6	-3.52424152	2.59390398	-3.15286479
6	-4.50916897	2.05062371	-2.31568650
6	-4.09783893	1.32835117	-1.18114588
6	-2.74618661	1.15853680	-0.88632846
1	-1.39498166	2.85085431	-3.51776567
1	-3.82328690	3.15151083	-4.04249228
6	-5.97512342	2.25223095	-2.60857991
1	-4.84797249	0.89235568	-0.51798443
1	-2.43519554	0.59967594	-0.00341260
1	-5.27929884	2.96579272	2.65185232
1	-3.83039525	3.60417855	3.46581532
1	-3.83022555	3.39472062	1.71164263
1	-6.56014464	1.35478831	-2.36529951
1	-6.38353364	3.07886205	-2.00629344
1	-6.14298003	2.50008368	-3.66455644
1	-0.10982319	-3.40649203	2.42029280

Energy = -8524.634102 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 32

Atomic N.	X	Y	Z
8	2.71732303	-1.15013549	0.54579939
6	3.83573916	-0.39483671	0.30635533

8	3.54521925	0.34013492	-0.90735801
6	4.50552713	1.30880234	-1.34549808
1	5.42243330	0.82291799	-1.71919386
1	4.75962729	2.01529452	-0.54330313
1	4.02915462	1.84989725	-2.17196321
8	3.99986668	0.63670794	1.29939951
6	5.07059935	-1.32398204	0.15692719
1	4.83563054	-2.24636210	0.70860755
1	5.11495505	-1.60563068	-0.90590486
6	6.43692235	-0.79558894	0.62333098
1	6.61485731	0.22246178	0.24449286
1	7.21076411	-1.43299386	0.16500417
6	6.63404666	-0.81921336	2.14716128
1	6.38499365	-1.82866375	2.51847466
1	7.70101813	-0.66172590	2.37386058
6	5.80763210	0.21877126	2.91422360
1	6.16573274	1.23394313	2.67532937
1	5.95654386	0.07898817	3.99849161
6	4.30978680	0.16647834	2.63133934
1	3.89443888	-0.84330800	2.77740963
1	3.76921199	0.84010424	3.31108039
50	0.99992147	0.08126004	0.56751948
7	0.21117789	-1.57169765	-1.24096714
6	1.12985904	-1.61075940	-2.39753714
1	0.83061609	-2.39080811	-3.12171178
1	1.15654094	-0.63640159	-2.89696854
1	2.13714278	-1.82626093	-2.02418471
7	-0.82620582	1.06581997	-2.26783984
6	-1.19675247	-1.31682577	-1.63278360
1	-1.63768728	-2.23921808	-2.06068416
1	-1.75951847	-1.08734084	-0.71490383
6	-1.42330314	-0.21285039	-2.66886385
1	-2.51527676	-0.14286753	-2.82766943
1	-0.96910578	-0.48810359	-3.62914984
16	-0.68964886	2.28508471	-3.44882357
7	-0.18514409	-1.57406458	1.49517176
6	0.30735310	-2.86036302	-0.49698991
1	-0.04498856	-3.69289628	-1.13669550
1	1.37270413	-3.00454331	-0.27467925
6	-0.47391465	-2.83576443	0.81854888
1	-0.14643874	-3.69941056	1.41980903
1	-1.55810177	-2.95165482	0.63612366
16	0.06890758	-1.54572165	3.11000098
8	0.82260686	-0.25903183	3.29459079
8	0.61503735	-2.81414417	3.64684523
6	-1.54193355	-1.30880741	3.90738240
6	-2.14786956	-2.37753818	4.56764147
6	-3.40088734	-2.19206183	5.15838701
6	-4.05216138	-0.95159369	5.10534832
6	-3.41534515	0.10888290	4.43640484
6	-2.16831887	-0.06107144	3.83858374
1	-1.63025261	-3.33440157	4.62658203
1	-1.67013023	0.76810771	3.33585421
1	-3.90318551	1.08472540	4.39087958
6	-5.38687765	-0.74513602	5.77724717
1	-3.87639243	-3.02657488	5.67740258
8	-0.10839501	3.43566078	-2.73829950
8	-0.03618598	1.64354679	-4.60527251

6	-2.36935987	2.73007681	-3.94632280
6	-2.95528047	2.10263813	-5.04746907
6	-4.26038748	2.44516670	-5.40768887
6	-4.98468205	3.40671819	-4.68692368
6	-4.36623206	4.02392903	-3.58547111
6	-3.06483458	3.69488827	-3.21070481
1	-2.38424086	1.37524430	-5.62346919
1	-4.72127525	1.96141956	-6.27069622
6	-6.38057368	3.79758155	-5.10137316
1	-4.91046702	4.78170648	-3.01884459
1	-2.57770828	4.19359108	-2.37285929
1	-5.89997882	-1.69952428	5.95241154
1	-5.26065469	-0.25311816	6.75435279
1	-6.04465642	-0.10306454	5.17537228
1	-6.36594942	4.73469024	-5.67931033
1	-6.84316815	3.02760535	-5.73174026
1	-7.02533541	3.96639819	-4.22829210
1	-1.19508505	1.46681733	-1.40133647

Energy = -8524.637066 Hartree

Number of imaginary frequencies = 0.

Compound I4a isomer 33

Atomic N.	X	Y	Z
8	2.65267266	-1.36734107	0.91776888
6	3.67822572	-0.63656084	0.45010452
8	4.54129554	-1.36260406	-0.45968102
6	5.21378718	-2.47451457	0.13220459
1	4.51549926	-3.10682820	0.70383548
1	6.03894487	-2.15782656	0.79205214
1	5.63381936	-3.05694234	-0.69745882
8	3.01665818	0.35847117	-0.44092728
6	4.48194814	0.07546720	1.55251096
1	3.74091966	0.49507382	2.25011263
1	5.01223833	-0.70691781	2.11656916
6	5.45873577	1.17952877	1.11891028
1	6.12427775	0.81478051	0.31955338
1	6.11123040	1.39663954	1.97916282
6	4.75881815	2.48667891	0.70290030
1	3.93755863	2.66699935	1.41474994
1	5.45447352	3.32999238	0.83136057
6	4.19526192	2.53823968	-0.73485304
1	4.94864246	2.96489093	-1.41878039
1	3.32701403	3.21144959	-0.76466472
6	3.80704714	1.19233905	-1.33509194
1	3.18363563	1.33867574	-2.22740203
1	4.68560710	0.59976380	-1.62036175
50	0.83085270	-0.12682582	0.36502925
7	0.56288536	-2.28270081	-1.03595154
6	1.66744970	-2.32596149	-2.02445492
1	1.53105244	-3.17385650	-2.72049238
1	1.69593143	-1.39179861	-2.59394755
1	2.61910108	-2.42401165	-1.49141024
7	-0.18525840	0.24098084	-1.66405381
6	-0.73715074	-2.09931255	-1.72370005
1	-0.94400701	-2.95299564	-2.39728497
1	-1.52428112	-2.06779289	-0.95658818
6	-0.75667613	-0.78937147	-2.52036257

1	-1.80742867	-0.57409081	-2.78801517
1	-0.20153845	-0.90054950	-3.46750377
16	-0.05629078	1.76408689	-2.22595540
7	0.16455824	-2.57479738	1.96778584
6	0.61247306	-3.54027364	-0.25047348
1	0.34214893	-4.39434601	-0.90114809
1	1.66070634	-3.67094742	0.05253715
6	-0.26226842	-3.59728267	0.99807911
1	-0.18831553	-4.61480593	1.41469593
1	-1.32191888	-3.42453754	0.75804897
16	-0.59070708	-2.63703672	3.51309463
8	0.33936251	-1.93093248	4.41215880
8	-1.04793247	-4.01579318	3.79120293
6	-2.05676445	-1.62243422	3.25499183
6	-3.29508398	-2.23939030	3.07067778
6	-4.42516966	-1.44212885	2.87852039
6	-4.33182121	-0.04168271	2.87095950
6	-3.07269027	0.54836663	3.07520797
6	-1.93276481	-0.23064824	3.26545965
1	-3.36662850	-3.32610158	3.10050328
1	-0.95968378	0.22931450	3.43217742
1	-2.98370404	1.63607966	3.08839136
6	-5.55128169	0.81208559	2.63177216
1	-5.39797004	-1.91732770	2.74097856
8	0.67232883	2.48415562	-1.13749080
8	0.46567523	1.83829018	-3.61511496
6	-1.74115135	2.43933915	-2.28038314
6	-2.27076344	2.89238730	-3.48730538
6	-3.56687700	3.41727636	-3.51018654
6	-4.33834304	3.49662301	-2.34304494
6	-3.77968758	3.02730736	-1.13987431
6	-2.49115977	2.49994329	-1.10161136
1	-1.66402054	2.83479260	-4.39042380
1	-3.98364890	3.77320450	-4.45435460
6	-5.72586714	4.08838270	-2.36460759
1	-4.36549186	3.08193897	-0.21953200
1	-2.06216638	2.14068144	-0.16509698
1	-6.46863127	0.30204433	2.95304196
1	-5.48087934	1.77021035	3.16325476
1	-5.66061251	1.03880006	1.55929621
1	-5.73209630	5.09020357	-1.90801060
1	-6.10295827	4.18820261	-3.39033965
1	-6.43451937	3.47037726	-1.79527021
1	1.18337290	-2.55479545	2.12354891

Energy = -8524.624513 Hartree

Number of imaginary frequencies = 0.

Intermediate 4b (I4b)

Compound I4b isomer 1

Atomic N.	X	Y	Z
8	1.91737850	-1.69559932	-1.93892962
6	2.14024068	-0.38350964	-2.09584940
8	2.34132946	0.03758940	-3.43989867
6	1.60010989	-0.68460475	-4.43046228
1	0.50896142	-0.59214431	-4.28810107
1	1.86926785	-1.74941004	-4.42609514

1	1.87382708	-0.23129142	-5.39075088
8	0.81932723	0.25276012	-1.57580698
6	3.33525491	0.16391412	-1.28491990
1	4.19458312	0.16239236	-1.97082894
1	3.54233451	-0.57943241	-0.50402794
6	3.19527507	1.54975486	-0.63500092
1	2.58001012	1.46432839	0.27506642
1	4.20043784	1.84208339	-0.29144005
6	2.61289160	2.67312169	-1.51319292
1	2.97894039	2.57575618	-2.54792538
1	2.98122948	3.64189622	-1.14013433
6	1.07754303	2.71631480	-1.49589772
1	0.73714229	2.81676151	-0.45282475
1	0.71948325	3.61524434	-2.02616135
6	0.39647383	1.51583282	-2.14241825
1	0.59401074	1.50936296	-3.22389660
1	-0.69210812	1.55288968	-1.98630294
50	-0.18051486	-2.00978428	-1.53717959
7	-2.63685323	-2.12999346	0.07257424
6	-3.09546613	-3.38827656	-0.52389209
1	-3.88302145	-3.87376525	0.08792163
1	-2.26185554	-4.09352113	-0.63899733
1	-3.50148931	-3.18748665	-1.52441109
7	0.28076884	-2.63636441	0.44602149
6	-2.03415837	-2.33689213	1.39331912
1	-2.74477401	-2.82764685	2.09525700
1	-1.78206609	-1.35207199	1.81051678
6	-0.75012628	-3.17039290	1.34385942
1	-0.36086791	-3.20417032	2.37495819
1	-1.00077045	-4.22294914	1.09934396
6	1.61167123	-2.85038043	0.92533403
6	2.42213150	-3.88786120	0.40448578
6	3.70986905	-4.08138151	0.91989424
6	4.23744214	-3.27274234	1.93206471
6	3.42854832	-2.24808524	2.43385161
6	2.13244456	-2.02488508	1.95274865
7	-2.48417982	0.98969802	0.15754245
6	-3.76751553	-1.18202908	0.06493463
1	-4.65341747	-1.64911708	0.55144041
1	-4.02790594	-1.01036362	-0.99106863
6	-3.56100421	0.17126058	0.74198119
1	-4.50491692	0.71903034	0.61926977
1	-3.43540316	0.04330638	1.83435532
6	-2.62230359	2.40118962	0.33564631
6	-1.85072842	3.10232755	1.29181098
6	-1.98868540	4.49089218	1.39892855
6	-2.88222350	5.21139360	0.59751129
6	-3.64058918	4.49850111	-0.33723110
6	-3.52178454	3.11162828	-0.49226942
6	1.94022675	-4.78185198	-0.71099695
1	4.32096277	-4.89089670	0.51217385
6	5.64548564	-3.47655311	2.43772580
1	3.81843309	-1.59383971	3.21833449
6	1.31790540	-0.88773122	2.51445026
6	-0.88621464	2.37274126	2.19667338
1	-1.38795558	5.02223278	2.14150713
6	-2.99557121	6.71245880	0.71484639
1	-4.33486968	5.03879276	-0.98575945

6	-4.32214377	2.40341291	-1.55690994
1	2.51883213	-5.71484682	-0.73820009
1	2.07080347	-4.28497396	-1.68532614
1	0.87623040	-5.03566793	-0.60677222
1	0.79346773	-0.35863909	1.70721200
1	1.95839824	-0.17645461	3.05233328
1	0.54801218	-1.23667275	3.22206879
1	5.76170831	-3.10304107	3.46416960
1	6.37346538	-2.93982658	1.80862719
1	5.92673954	-4.53872331	2.42428519
1	-0.48165399	3.05331517	2.95627197
1	-0.02760281	1.96056252	1.64255967
1	-1.36503459	1.53229023	2.72135661
1	-5.22817277	1.92565023	-1.15011622
1	-3.72469529	1.60874062	-2.02575663
1	-4.64981545	3.11065095	-2.32980995
1	-2.23359319	7.21723846	0.09997284
1	-2.84853022	7.04570722	1.75151893
1	-3.97789078	7.06793767	0.37610428
1	-1.58112556	0.67490933	0.51273305

Energy = -7584.947166 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 2

Atomic N.	X	Y	Z
8	0.51228930	0.07117905	-0.06432108
6	1.33785316	0.94907195	-0.71443523
8	2.46079360	0.32643924	-1.35950361
6	2.15006633	-0.74344901	-2.26088416
1	1.54399573	-0.39327802	-3.11185435
1	1.62004781	-1.56561892	-1.75600178
1	3.11459080	-1.11050861	-2.63128538
8	0.46765861	1.55821695	-1.72607751
6	1.98074178	1.99421186	0.22557804
1	2.98089529	2.23950745	-0.16189632
1	2.13066779	1.47634900	1.18311209
6	1.17535256	3.28277739	0.43893624
1	0.10826550	3.04441917	0.55090611
1	1.49940580	3.73208336	1.39105649
6	1.35556856	4.32971782	-0.67337722
1	2.43571835	4.47594807	-0.85134554
1	0.96716682	5.29820664	-0.32036825
6	0.66156398	3.98633145	-1.99718056
1	-0.43152368	4.03240629	-1.86816640
1	0.92377305	4.74002365	-2.75940206
6	1.01528172	2.61035814	-2.54981782
1	2.10392627	2.46458131	-2.64100603
1	0.57334112	2.47027784	-3.54846208
50	-1.28717050	-0.32470723	-1.19827843
7	-2.04330342	-1.86845151	0.60690684
6	-2.34205363	-3.19919606	0.03841360
1	-2.83822027	-3.85025086	0.77984782
1	-1.41540342	-3.66894901	-0.30589646
1	-3.00922077	-3.07229850	-0.82353132
7	0.91902505	-2.78442811	0.65835119
6	-1.15445221	-1.95650192	1.80835363
1	-1.78171234	-2.21106269	2.68380213

8	0.55512284	0.18543802	-0.22483193
6	1.49209365	0.68297446	-1.05514311
8	1.74630226	-0.43103937	-2.02530253
6	2.36940060	-0.09593971	-3.26373729
1	3.39404778	0.28548749	-3.11262730
1	1.78106603	0.64418010	-3.82684363
1	2.43068447	-1.02703473	-3.84223453
8	0.93395175	1.77718020	-1.81186235
6	2.80267765	0.98945341	-0.31407341
1	3.60679369	1.22769854	-1.02949811
1	3.07289769	0.03609162	0.15891219
6	2.69233550	2.09455633	0.74785900
1	1.73032338	1.98597524	1.27217901
1	3.47944156	1.93320656	1.50128223
6	2.83903095	3.51522805	0.18984638
1	3.83671093	3.61082529	-0.27539256
1	2.82020626	4.23752509	1.02223814
6	1.77582480	3.90822211	-0.84110616
1	0.77870282	3.95006897	-0.37475158
1	1.99659015	4.92270566	-1.21592413
6	1.69028232	2.97277091	-2.05020339
1	2.70086316	2.74498964	-2.43621250
1	1.14069336	3.47268378	-2.86227501
50	-0.79126834	-1.08416395	-1.30417776
7	-3.11527816	-2.27924831	-0.30917035
6	-3.59379457	-3.16040623	-1.38145729
1	-4.45236623	-3.78084790	-1.05585210
1	-2.78773087	-3.82829712	-1.70811143
1	-3.89808612	-2.55359819	-2.24474009
7	-0.24761655	-2.68107003	0.01781331
6	-2.55394089	-3.04840808	0.81491064
1	-3.26619297	-3.83224317	1.14979186
1	-2.38991935	-2.35341141	1.64979876
6	-1.20724628	-3.68173134	0.46359232
1	-0.83886269	-4.17791999	1.38032580
1	-1.36252730	-4.50821873	-0.26574151
6	1.11807123	-3.05809996	0.21643774
6	1.82895849	-3.78063097	-0.77187159
6	3.15812601	-4.15589802	-0.53599455
6	3.81936315	-3.83007110	0.65272399
6	3.10629074	-3.11464013	1.62087153
6	1.77562188	-2.72329812	1.42447674
7	-2.77939071	0.66964374	0.05313753
6	-4.18748214	-1.35878523	0.10642670
1	-4.94907780	-1.88542611	0.71874251
1	-4.70086663	-1.02415672	-0.80995880
6	-3.71156349	-0.12751865	0.87442258
1	-4.60679112	0.45758186	1.15698974
1	-3.21856891	-0.42093860	1.80870465
6	-2.48827676	2.00788377	0.46065801
6	-1.88520556	2.28838990	1.70583287
6	-1.61694943	3.62265389	2.04054034
6	-1.89553672	4.68644852	1.17830812
6	-2.45595407	4.37989560	-0.06720133
6	-2.75449206	3.06686160	-0.44150595
6	1.18512083	-4.13868664	-2.09002831
1	3.69151171	-4.71919091	-1.30662901
6	5.26426673	-4.21127937	0.87095569

1	3.60071559	-2.84567084	2.55838645
6	1.06601354	-1.92082866	2.48407607
6	-1.46293582	1.19638000	2.65601645
1	-1.14552201	3.82731590	3.00510490
6	-1.55057099	6.10858066	1.54931671
1	-2.66818923	5.18651091	-0.77336099
6	-3.33474702	2.79536521	-1.81009495
1	1.05569329	-3.24761414	-2.72444774
1	0.18804695	-4.58136823	-1.95882437
1	1.80892754	-4.85298806	-2.64381648
1	0.79665755	-0.93446591	2.08054090
1	1.70983184	-1.78242860	3.36297536
1	0.13449646	-2.40352649	2.81490957
1	5.48486019	-4.35523789	1.93762428
1	5.94208408	-3.42533252	0.50084983
1	5.51970754	-5.13811418	0.33892026
1	-0.68281553	1.56614611	3.33389779
1	-1.05322433	0.34002153	2.10396819
1	-2.29416765	0.83750797	3.28384209
1	-4.30983645	2.28229006	-1.76058117
1	-2.66155013	2.17329852	-2.42264821
1	-3.49180085	3.73596221	-2.35220945
1	-0.57106312	6.39921719	1.13671770
1	-1.49866232	6.23728863	2.63868732
1	-2.29140945	6.81820270	1.15518989
1	-3.14892831	0.69906631	-0.89835919

Energy = -7584.952332 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 4

Atomic N.	X	Y	Z
8	0.89834050	0.09105311	-0.35980195
6	1.34270322	1.13341139	-1.12166664
8	0.22443291	1.50528900	-1.97252543
6	0.40520938	2.64536871	-2.81110517
1	1.08830942	2.43713994	-3.65274779
1	0.77992314	3.50609405	-2.23601884
1	-0.58555512	2.88956460	-3.21476795
8	1.55797042	2.27119808	-0.25672492
6	2.56185420	0.74112325	-1.98932934
1	2.97279755	1.62409584	-2.50518401
1	2.14173464	0.08803250	-2.76990415
6	3.67249592	-0.01577369	-1.24744872
1	3.20598092	-0.78612307	-0.61660929
1	4.28871870	-0.54523846	-1.99147587
6	4.58814325	0.87117697	-0.39822376
1	5.16484069	1.54020513	-1.06237519
1	5.32755659	0.23625495	0.11579407
6	3.85321495	1.73343509	0.63349185
1	3.30166842	1.10293288	1.34804998
1	4.59753160	2.30123553	1.21712616
6	2.88263332	2.74703799	0.01816224
1	3.33222731	3.19274017	-0.89027002
1	2.70801308	3.56978885	0.72724726
50	-0.60378103	-1.23530767	-1.07346700
7	-2.92437600	-2.22499547	0.19337295
6	-3.70430467	-2.99077445	-0.78579355

1	-4.60085119	-3.45526674	-0.32997161
1	-3.08165356	-3.78836478	-1.21180608
1	-4.02023863	-2.33603943	-1.60811630
7	-0.06418509	-2.50578552	0.59300624
6	-2.34412666	-3.11594540	1.22058569
1	-3.03582073	-3.95539364	1.43353500
1	-2.21201325	-2.54547579	2.14934863
6	-0.97112388	-3.63498913	0.78666304
1	-0.59012101	-4.29944890	1.58003489
1	-1.09967914	-4.27826290	-0.11122801
6	1.28232591	-2.70665688	1.00823781
6	2.11788253	-3.67956376	0.39986624
6	3.43696620	-3.84372396	0.84626256
6	3.97323512	-3.06960086	1.87865091
6	3.13914604	-2.11550964	2.47420053
6	1.81530075	-1.92199572	2.06404741
7	-1.99235261	0.64793315	0.24009852
6	-3.69921772	-1.11748067	0.77306540
1	-4.35570138	-1.47211501	1.59382559
1	-4.35696395	-0.71033860	-0.00585265
6	-2.79604686	-0.00566664	1.30883236
1	-3.41920717	0.73235031	1.84086175
1	-2.08835339	-0.42886278	2.03614353
6	-2.56278921	1.88367459	-0.27305897
6	-2.25170543	3.09033704	0.40405270
6	-2.79966269	4.29117966	-0.05177537
6	-3.65054870	4.34109475	-1.16429285
6	-3.92406652	3.14447798	-1.82598963
6	-3.39100727	1.91204108	-1.40967612
6	1.62632002	-4.52431189	-0.75005261
1	4.06653085	-4.59236311	0.35728876
6	5.40947176	-3.23133331	2.31625603
1	3.52829208	-1.50518226	3.29396872
6	0.96910379	-0.88713667	2.75974591
6	-1.31318493	3.10115015	1.58700421
1	-2.54907604	5.21545251	0.47449335
6	-4.23781896	5.65096508	-1.63099239
1	-4.56251981	3.15914204	-2.71292093
6	-3.71896423	0.69070800	-2.23408031
1	1.01551056	-3.93136545	-1.44814127
1	0.99719238	-5.36276824	-0.41156319
1	2.47108060	-4.95137705	-1.30626683
1	0.74694792	-0.05604420	2.07438875
1	1.49223745	-0.48430807	3.63756023
1	0.01011921	-1.31256557	3.08951287
1	5.51709469	-3.08987937	3.40104228
1	6.06149858	-2.48964942	1.82711854
1	5.79694342	-4.22685074	2.06050888
1	-1.24163228	4.11249062	2.00623362
1	-0.29772657	2.78989676	1.29060442
1	-1.64719269	2.42968371	2.39250043
1	-4.72400964	0.30326948	-2.00180962
1	-2.99283822	-0.11737994	-2.08047608
1	-3.71524024	0.94481197	-3.30287571
1	-3.45135125	6.39712620	-1.81717731
1	-4.91196211	6.07751753	-0.87272415
1	-4.81193872	5.52340710	-2.55775278
1	-1.06859142	0.88132712	0.62125001

Energy = -7584.953267 Hartree
 Number of imaginary frequencies = 0.

Compound I4b isomer 5

Atomic N.	X	Y	Z
8	0.50946317	0.09716762	-0.21148428
6	1.17876237	0.97729127	-1.00966762
8	1.74088748	0.34790776	-2.19949211
6	2.71061821	-0.66646565	-1.94462783
1	2.28202846	-1.49864534	-1.36496858
1	3.59996493	-0.27285598	-1.42196786
1	3.02112672	-1.04359024	-2.92671996
8	0.14418593	1.82450733	-1.56587408
6	2.26384867	1.78222616	-0.25501932
1	3.09125158	1.99745530	-0.94958805
1	2.66376410	1.11696606	0.52215627
6	1.78973617	3.09698113	0.38426383
1	0.81262707	2.94776582	0.86726188
1	2.49830798	3.35700267	1.18688528
6	1.72638582	4.28172723	-0.59600985
1	2.69812636	4.35469840	-1.11613402
1	1.61751658	5.21496789	-0.02041334
6	0.59675145	4.22001768	-1.63248387
1	-0.37674240	4.35600056	-1.13648621
1	0.70875435	5.05413758	-2.34623108
6	0.54105666	2.92056907	-2.42621785
1	1.49665798	2.67592829	-2.91393304
1	-0.22947549	2.97996596	-3.20830102
50	-1.31637302	-0.33359199	-1.34516855
7	-2.15070576	-1.88851417	0.45123795
6	-2.40320471	-3.22858903	-0.11479259
1	-2.93195691	-3.87849456	0.60544025
1	-1.45499448	-3.69160827	-0.40495122
1	-3.02423126	-3.11856418	-1.01281989
7	0.81290299	-2.77344874	0.69088417
6	-1.32743552	-1.94318493	1.69802296
1	-1.99521391	-2.17355560	2.55027591
1	-0.91357738	-0.93850162	1.86430897
6	-0.19698254	-2.97034438	1.73658360
1	0.23318050	-2.89634083	2.75739558
1	-0.60429047	-3.99015900	1.65889136
6	1.98572978	-3.58185127	0.84787964
6	1.99313971	-4.90212985	0.34472593
6	3.14426718	-5.68658694	0.49493152
6	4.29865228	-5.20084983	1.11788962
6	4.27864728	-3.88498914	1.59453697
6	3.14427911	-3.07246542	1.48061859
7	-2.66227436	0.89519512	-0.15962255
6	-3.45356386	-1.22151625	0.73582025
1	-3.94397033	-1.71970455	1.59430126
1	-4.08614022	-1.35690673	-0.15398140
6	-3.28726546	0.26817971	0.99721079
1	-4.29695927	0.68584870	1.16594772
1	-2.74290552	0.40593894	1.95298465
6	-2.85211404	2.28249974	-0.33280124
6	-2.58679931	3.22527122	0.69959506
6	-2.84110104	4.58713435	0.48445172

6	-3.32622671	5.07797313	-0.73038066
6	-3.55573496	4.14792108	-1.75102842
6	-3.33529088	2.77724295	-1.57838609
6	0.80259179	-5.45932199	-0.39348751
1	3.14139603	-6.70271897	0.09243566
6	5.51921459	-6.07261525	1.29038189
1	5.16912485	-3.47813427	2.08067118
6	3.17423239	-1.66586779	2.02851878
6	-1.95176462	2.81212386	2.00545407
1	-2.62159554	5.29025944	1.29306991
6	-3.55112764	6.55458509	-0.95156784
1	-3.94297644	4.49692037	-2.71238460
6	-3.65246249	1.84155061	-2.71824554
1	1.07274130	-6.38062675	-0.92535364
1	0.42467335	-4.72751748	-1.12133950
1	-0.03114138	-5.70576780	0.28358469
1	3.12698629	-0.91417909	1.22631618
1	4.09948207	-1.49186393	2.59221094
1	2.32521390	-1.46565203	2.69864091
1	5.52968659	-6.54792535	2.28415680
1	6.44588275	-5.48922502	1.20019855
1	5.54535360	-6.87674460	0.54277524
1	-1.46700125	3.67517437	2.48129921
1	-1.19121890	2.03578929	1.83649659
1	-2.67921824	2.40840822	2.72753931
1	-4.17918418	0.94405824	-2.36304583
1	-2.74443879	1.48495939	-3.23394214
1	-4.27215928	2.34498786	-3.47250154
1	-2.69163438	7.01920716	-1.46156486
1	-3.69318539	7.08513124	-0.00032852
1	-4.43507887	6.73669326	-1.57933511
1	1.04051684	-1.77472224	0.61439757

Energy = -7584.958412 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 6

Atomic N.	X	Y	Z
8	-1.07574737	-0.94578312	-0.29270707
6	-2.16644500	-0.37948887	-0.89348439
8	-3.17629033	-0.03284346	0.06016468
6	-2.69524473	0.68461683	1.19900445
1	-2.22183020	1.63437483	0.90376173
1	-1.98037988	0.07580912	1.77270658
1	-3.57869946	0.89415915	1.81484801
8	-1.66790516	0.82360925	-1.54744337
6	-2.89891327	-1.33836166	-1.86481805
1	-3.96106949	-1.05303536	-1.90227778
1	-2.85865004	-2.32318092	-1.37970542
6	-2.33427285	-1.41035106	-3.28842737
1	-1.22911131	-1.39439302	-3.26596285
1	-2.61324780	-2.38302837	-3.72410308
6	-2.85392743	-0.30187724	-4.21907598
1	-3.95769309	-0.32439725	-4.19700286
1	-2.56324385	-0.53234402	-5.25704494
6	-2.37539647	1.11447292	-3.87557462
1	-1.30009096	1.21030414	-4.09978291
1	-2.89959327	1.84367963	-4.51721849

6	-2.57874308	1.51674535	-2.41457748
1	-3.61790888	1.35244380	-2.08345572
1	-2.36116274	2.58916468	-2.28616516
50	0.85086471	-0.78214974	-1.13723538
7	3.55010888	-0.38451779	-0.58412179
6	4.29505477	0.06175067	-1.76233621
1	5.39131759	-0.01556003	-1.61442789
1	4.04874620	1.10290689	-2.00363453
1	4.01073713	-0.55421843	-2.62624799
7	1.51630806	1.60008755	0.45040021
6	3.75020948	0.49770242	0.56998519
1	4.82635543	0.72836502	0.72041841
1	3.41240022	-0.03594459	1.47023953
6	2.98295566	1.81477835	0.46232061
1	3.28477914	2.46004994	1.30867228
1	3.25762888	2.35343169	-0.45348550
6	0.75183792	2.82139833	0.42133251
6	0.61862936	3.54908215	-0.77966566
6	-0.13760742	4.72843110	-0.77240183
6	-0.77260547	5.20408368	0.37910390
6	-0.63613082	4.45730500	1.55433040
6	0.11978998	3.28065592	1.59927213
7	1.46303118	-2.15238922	0.39950031
6	3.82738395	-1.80068474	-0.29655175
1	4.87122240	-1.94938523	0.05397609
1	3.72135970	-2.33861750	-1.25200006
6	2.86294545	-2.40954131	0.71915434
1	3.06890173	-3.49735782	0.72919878
1	3.13039170	-2.06165442	1.74016764
6	0.56144266	-2.96643935	1.15108805
6	0.31827384	-2.72557915	2.52455645
6	-0.55652525	-3.55924497	3.23467025
6	-1.20719680	-4.63725303	2.63023498
6	-0.95416108	-4.87030802	1.27315350
6	-0.09151437	-4.05998551	0.52777456
6	1.24508237	3.08398652	-2.07018020
1	-0.24828056	5.28009227	-1.70930234
6	-1.56489153	6.48879093	0.35939397
1	-1.13199315	4.79762708	2.46649181
6	0.23313356	2.51563731	2.89774812
6	0.96606277	-1.56911220	3.24387321
1	-0.74113734	-3.34831579	4.29173496
6	-2.17646836	-5.50118571	3.40083490
1	-1.44557348	-5.71107442	0.77609673
6	0.12186623	-4.36236373	-0.93452120
1	0.69082470	3.48213854	-2.92998517
1	1.25042774	1.98700872	-2.14249878
1	2.28624580	3.43313673	-2.16957569
1	-0.25302470	1.52849710	2.84001334
1	-0.25465412	3.06752462	3.71059297
1	1.28044635	2.35009397	3.19562226
1	-0.92877429	7.35105863	0.61479484
1	-2.38743319	6.46352554	1.08681060
1	-1.99094635	6.68062230	-0.63460433
1	0.31940032	-1.19735186	4.05017454
1	1.16326446	-0.74794343	2.54110396
1	1.92930010	-1.85003069	3.69986163
1	1.18254111	-4.30384611	-1.21509563

1	-0.41589944	-3.64182695	-1.57185193
1	-0.25525751	-5.36365681	-1.18188707
1	-3.21555266	-5.17465335	3.23593451
1	-1.98457993	-5.45358222	4.48131112
1	-2.11419813	-6.55276057	3.08689834
1	1.26870105	1.08847035	1.30111112

Energy = -7584.956819 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 7

Atomic N.	X	Y	Z
8	-0.22079061	-0.77424416	-1.37876934
6	-1.48170271	-0.42723054	-1.77432384
8	-2.45911983	-0.55266600	-0.75662946
6	-2.12544505	0.07772928	0.49254601
1	-2.01693691	1.16522691	0.37079548
1	-1.19703562	-0.33622127	0.90725704
1	-2.96411339	-0.13933883	1.16379393
8	-1.32292168	1.01173880	-2.13059254
6	-2.03827253	-1.26951264	-2.94359392
1	-3.13759221	-1.23361679	-2.90890435
1	-1.75167696	-2.30352719	-2.70656362
6	-1.55154320	-0.89021042	-4.34774587
1	-0.47729891	-0.63669087	-4.32550620
1	-1.63781492	-1.77931022	-4.99176997
6	-2.35651484	0.24748485	-4.99731539
1	-3.42623875	-0.02428198	-4.96672547
1	-2.08881571	0.31750919	-6.06383272
6	-2.17335080	1.62951108	-4.35761903
1	-1.15882377	2.00713156	-4.56707306
1	-2.87405242	2.34372985	-4.82227385
6	-2.38734929	1.67184971	-2.84651903
1	-3.34737215	1.21836840	-2.55101108
1	-2.38583032	2.71124946	-2.48554113
50	1.18539287	0.69351469	-2.12052778
7	2.98950628	-0.44917798	-0.81079656
6	4.18426580	-0.14729197	-1.62987908
1	5.10248229	-0.50398618	-1.13034967
1	4.26751635	0.93379028	-1.79875941
1	4.09164808	-0.63601612	-2.60863424
7	1.43154910	1.93324277	-0.37681850
6	3.03700065	0.27315411	0.48803960
1	4.02805403	0.15169133	0.96496741
1	2.26473786	-0.17097223	1.12788006
6	2.71133884	1.75690361	0.30508984
1	2.68946144	2.20999035	1.30876841
1	3.54559189	2.26892355	-0.22323846
6	0.63812816	3.03919095	0.01314549
6	0.34632057	4.09421489	-0.89347396
6	-0.47567347	5.15566674	-0.49268411
6	-1.02182599	5.23329667	0.79206281
6	-0.71508193	4.20130374	1.68460619
6	0.09174135	3.11454943	1.32658350
7	0.98875246	-2.19254864	0.97401257
6	2.85111041	-1.94421671	-0.71091712
1	3.84416548	-2.39132333	-0.88985452
1	2.19829245	-2.26689648	-1.53806470

6	2.36032403	-2.55191420	0.60341210
1	2.47164746	-3.64718389	0.46967596
1	3.05463969	-2.27621371	1.41319544
6	0.35363821	-3.02737630	1.93550757
6	0.77302362	-2.99980862	3.28669607
6	0.12875675	-3.81899823	4.22307455
6	-0.93509523	-4.65575627	3.87409826
6	-1.35319176	-4.65039926	2.53826927
6	-0.72871900	-3.86401298	1.56359162
6	0.93528390	4.12328666	-2.28335729
1	-0.67837104	5.95889640	-1.20661921
6	-1.93060903	6.37111787	1.19121949
1	-1.13482075	4.22753703	2.69418949
6	0.32449730	2.02091267	2.33978162
6	1.85905027	-2.06237164	3.75341625
1	0.45775677	-3.77848711	5.26479890
6	-1.60029497	-5.54648378	4.89588910
1	-2.18828431	-5.28820540	2.23697085
6	-1.22145656	-3.91514886	0.13764922
1	0.88454461	5.13766771	-2.70197032
1	0.39988442	3.46141384	-2.98448092
1	1.98452840	3.79579876	-2.28368872
1	0.40846093	1.04312928	1.84688595
1	-0.50134637	1.98206436	3.06269283
1	1.24930644	2.17610054	2.91950923
1	-1.72594511	7.27329394	0.59839325
1	-1.81329463	6.62581275	2.25367702
1	-2.98984364	6.11064885	1.03462076
1	1.77233318	-1.88014865	4.83252604
1	1.79301894	-1.09806311	3.22969184
1	2.86912744	-2.46479233	3.57318131
1	-0.39853130	-4.07659803	-0.57525756
1	-1.72273320	-2.98058192	-0.15864725
1	-1.94333639	-4.73242199	0.01290808
1	-2.68343151	-5.61613658	4.72358997
1	-1.43886588	-5.17378545	5.91644444
1	-1.19889026	-6.57166379	4.85319276
1	0.41337621	-2.02281022	0.14203170

Energy = -7584.959434 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 8

Atomic N.	X	Y	Z
8	-0.76805781	-1.22509371	0.08350680
6	-1.74925024	-0.58384887	0.74989498
8	-1.12376733	0.47267039	1.49762610
6	-1.96463075	1.49202526	2.03774907
1	-2.72126433	1.09503986	2.73756997
1	-2.46357181	2.06642263	1.24190633
1	-1.30099358	2.16430993	2.59522267
8	-2.59998327	0.03715307	-0.31707132
6	-2.54345427	-1.51405969	1.68642948
1	-3.22280884	-0.93542629	2.33200052
1	-1.77305665	-1.93512900	2.34751601
6	-3.31689655	-2.64490852	0.99314978
1	-2.72086313	-3.02297143	0.14646954
1	-3.41198160	-3.48413455	1.69948678

6	-4.72444112	-2.25052894	0.52568517
1	-5.29977953	-1.89437173	1.39869464
1	-5.24970048	-3.14702362	0.15939854
6	-4.76403300	-1.17391724	-0.56399701
1	-4.33606136	-1.56342896	-1.50298885
1	-5.81456674	-0.91737944	-0.78258092
6	-4.03721125	0.12253888	-0.21034204
1	-4.31711345	0.46907635	0.79756840
1	-4.31063837	0.91955428	-0.91765224
50	-1.07478817	-1.00047265	-2.04695251
7	1.40930166	-1.14522987	-2.40580476
6	1.51604406	-1.83402866	-3.70993143
1	2.56926104	-1.89730046	-4.03534578
1	0.93908645	-1.29552602	-4.47237553
1	1.10516146	-2.84820732	-3.62175007
7	-0.45536366	1.01614097	-2.44403660
6	1.87941258	0.26181194	-2.51498708
1	2.82582556	0.30352891	-3.08729900
1	2.06447252	0.63280887	-1.50135479
6	0.81201424	1.15339900	-3.15200830
1	1.17755147	2.19311197	-3.10401427
1	0.72810920	0.92699556	-4.23870068
6	-1.26011939	2.18097382	-2.35086532
6	-2.44340634	2.33019474	-3.11709825
6	-3.22686538	3.48454249	-2.97279976
6	-2.87515227	4.51711018	-2.09853594
6	-1.70494751	4.36016122	-1.34579439
6	-0.89925620	3.22074664	-1.45093081
7	2.48125907	-2.27251546	1.03036641
6	2.14723520	-1.94363851	-1.38426088
1	3.13058613	-2.24238758	-1.79381434
1	1.57247868	-2.86858198	-1.22750490
6	2.33707064	-1.25046744	-0.02665888
1	3.23726362	-0.62506454	-0.03204047
1	1.46991962	-0.60464829	0.18296516
6	3.30110324	-1.95941624	2.14739314
6	2.73364463	-1.80902904	3.43587281
6	3.56993959	-1.56127131	4.52977780
6	4.95777158	-1.43988293	4.39268912
6	5.50079553	-1.61095399	3.11469684
6	4.70588769	-1.88036983	1.99393065
6	-2.87956700	1.27024009	-4.10093149
1	-4.13370775	3.58261156	-3.57606746
6	-3.71116448	5.76983924	-1.98751325
1	-1.41731944	5.14229235	-0.63746772
6	0.31398292	3.08178373	-0.56672227
6	1.23985634	-1.91226450	3.63563209
1	3.11778033	-1.44670144	5.51841781
6	5.83559490	-1.12112524	5.57920062
1	6.58500102	-1.55936989	2.98398860
6	5.36120317	-2.14850285	0.66153945
1	-3.59039614	1.68599380	-4.82794254
1	-3.38280484	0.42250423	-3.60671829
1	-2.02457011	0.84879160	-4.64702461
1	0.34435929	2.08004773	-0.11462152
1	0.29932271	3.83411792	0.23303060
1	1.25505180	3.21880580	-1.12362789
1	-3.30607511	6.57753618	-2.61784867

1	-3.73324443	6.14735994	-0.95533541
1	-4.74606537	5.59126406	-2.30948531
1	0.97733725	-1.69601715	4.67896806
1	0.85920509	-2.92239762	3.40792578
1	0.69063338	-1.20375262	2.99587399
1	5.33385586	-1.27468165	-0.00936593
1	4.85132915	-2.97119465	0.13905512
1	6.41668080	-2.41736459	0.79931424
1	6.85094898	-1.51870794	5.44427351
1	5.42422568	-1.54046524	6.50775148
1	5.92816232	-0.03304659	5.72648212
1	1.54321258	-2.52669909	1.34114929

Energy = -7584.954747 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 9

Atomic N.	X	Y	Z
8	-0.72449397	-0.21997543	0.13565389
6	-1.85892009	0.31704007	-0.36024256
8	-2.35298004	1.23091684	0.63179295
6	-3.33699078	2.17614383	0.22412524
1	-4.26086378	1.69772573	-0.15134615
1	-2.94505607	2.86691006	-0.53858652
1	-3.58919875	2.75403931	1.12181483
8	-1.44250801	1.09759216	-1.56242979
6	-2.92596746	-0.75381330	-0.66786121
1	-3.89748214	-0.28795424	-0.89893561
1	-3.04965412	-1.27311845	0.29235133
6	-2.55362976	-1.76129584	-1.76412264
1	-1.47934741	-1.99521598	-1.68341550
1	-3.08664223	-2.70457187	-1.56842560
6	-2.89461154	-1.29917463	-3.18705647
1	-3.97824776	-1.09154443	-3.24075638
1	-2.70713345	-2.12404191	-3.89362453
6	-2.13081712	-0.05747594	-3.65960930
1	-1.05749649	-0.28512327	-3.77111428
1	-2.49626088	0.23452985	-4.65917902
6	-2.26268319	1.15977657	-2.74314421
1	-3.31719856	1.33108874	-2.46980232
1	-1.91529356	2.06272336	-3.26894194
50	0.99317313	0.11317011	-1.08944030
7	3.61215631	-0.23312256	-0.19815861
6	4.45744060	0.02886696	-1.37053299
1	5.53354463	0.05221958	-1.10793446
1	4.18943868	0.99236890	-1.82032969
1	4.28992355	-0.75247504	-2.12374313
7	1.60183621	1.88192810	-0.03633801
6	3.69793474	0.86106556	0.78568400
1	4.75820061	1.08312553	1.03066703
1	3.19479458	0.52706960	1.70363181
6	2.99792780	2.12876506	0.30148500
1	3.06198997	2.86244238	1.12579022
1	3.58105668	2.58408470	-0.53034872
6	0.78382721	3.04863473	0.09061474
6	0.56358361	3.91061008	-1.00896786
6	-0.21065810	5.06720611	-0.83920155
6	-0.77528814	5.40421460	0.39485157

6	-0.55523011	4.53799177	1.47232743
6	0.20538561	3.37029638	1.34257708
7	1.63775644	-2.37912353	0.47359755
6	3.95281561	-1.54065216	0.39245690
1	4.89025006	-1.47424918	0.98208686
1	4.15600639	-2.23383544	-0.44024402
6	2.85855870	-2.14363319	1.26914262
1	3.25189023	-3.08342146	1.70001494
1	2.62541148	-1.48087882	2.11173006
6	0.65439580	-3.27517422	0.99676479
6	-0.02296375	-3.00506665	2.20644735
6	-0.98911231	-3.91577925	2.65409168
6	-1.32981594	-5.06753262	1.93872674
6	-0.67456327	-5.29226681	0.72294908
6	0.31062846	-4.42370271	0.24302598
6	1.13734945	3.60044224	-2.37103235
1	-0.37132827	5.72510233	-1.69773403
6	-1.57629541	6.67292514	0.56823864
1	-1.00074285	4.76929671	2.44384501
6	0.36967498	2.44437535	2.51955872
6	0.21288998	-1.73933869	2.99059076
1	-1.51368271	-3.69274290	3.58645837
6	-2.36047964	-6.03874728	2.46176926
1	-0.93203851	-6.17241218	0.12846887
6	0.98008929	-4.71816678	-1.08038578
1	1.05134696	4.47101374	-3.03507350
1	0.60626223	2.76283632	-2.85033589
1	2.19586681	3.31069644	-2.31609074
1	-0.06050540	1.46202191	2.28001143
1	-0.14252388	2.84694762	3.40350577
1	1.42746156	2.28901752	2.78052291
1	-0.95955631	7.47978826	0.99537728
1	-2.42539088	6.52085188	1.24964886
1	-1.96838299	7.03345374	-0.39247670
1	-0.62841296	-1.55392227	3.67035378
1	0.29288500	-0.87924539	2.31201596
1	1.12402977	-1.79038003	3.60788616
1	2.07310603	-4.82669099	-0.98213617
1	0.79309905	-3.92840332	-1.82708423
1	0.59837930	-5.65661610	-1.50094293
1	-2.93490425	-6.49444389	1.64333318
1	-3.06677705	-5.54339846	3.14159328
1	-1.88648922	-6.85980997	3.02304121
1	1.92625161	-2.72277871	-0.44349548

Energy = -7584.948107 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 10

Atomic N.	X	Y	Z
8	-0.83271213	-1.96992020	-1.49176228
6	0.41457429	-2.45385634	-1.68035641
8	0.95786566	-2.25657907	-2.98456244
6	0.71064730	-0.97410796	-3.56859171
1	1.16075906	-0.16091644	-2.97419744
1	-0.36748343	-0.78884999	-3.68293193
1	1.18683196	-0.99898008	-4.55586642
8	1.22487761	-1.64614712	-0.69938731

6	0.55122122	-3.96847280	-1.43149775
1	1.36726311	-4.35501473	-2.06042901
1	-0.38122721	-4.40195488	-1.81808405
6	0.76926384	-4.38823526	0.02685077
1	0.12852981	-3.78240650	0.68481420
1	0.42650585	-5.42854614	0.13778664
6	2.23766026	-4.32037602	0.48243852
1	2.85665308	-4.86145819	-0.25445816
1	2.34758579	-4.86804106	1.43240182
6	2.80782520	-2.90822288	0.67373096
1	2.33715262	-2.43668379	1.55268622
1	3.88748851	-2.97292828	0.89240436
6	2.61480377	-1.97345899	-0.51753469
1	3.00171214	-2.40771772	-1.45374589
1	3.13971430	-1.01964918	-0.35225189
50	-0.77355897	-0.14228523	-0.37719897
7	0.31490942	1.04882939	1.97033971
6	1.75405845	0.95397932	2.24386720
1	2.03615427	1.43356939	3.20255389
1	2.31723148	1.42172756	1.42707550
1	2.03507353	-0.10515811	2.29479772
7	1.02213814	3.09890732	-0.19074744
6	-0.16243215	2.44943452	1.92390559
1	-0.29475444	2.83209407	2.95731714
1	-1.16148214	2.44787047	1.45662019
6	0.72991962	3.46138514	1.20290433
1	0.20475164	4.43425292	1.26940928
1	1.66886526	3.58300914	1.76254199
6	1.45025750	4.12859681	-1.07058180
6	2.69137053	4.77802159	-0.87307375
6	3.09147193	5.77612125	-1.77142463
6	2.31882002	6.14145050	-2.87753157
6	1.11235647	5.45989302	-3.07796175
6	0.66179186	4.47072165	-2.19808345
7	-1.81689247	-0.97091206	1.27548793
6	-0.46183468	0.27508922	2.96111576
1	-0.54966005	0.84341128	3.91078459
1	0.10043941	-0.64467771	3.16891401
6	-1.85826430	-0.12255852	2.47067068
1	-2.35860045	-0.65288154	3.29482145
1	-2.46654266	0.78921869	2.30274450
6	-2.66134804	-2.11522073	1.27821107
6	-3.72574469	-2.23387721	0.34559955
6	-4.55663469	-3.35977773	0.37858871
6	-4.37684136	-4.39547572	1.30097974
6	-3.31993224	-4.27509121	2.20726864
6	-2.46209511	-3.16777604	2.21247268
6	3.62584547	4.37277428	0.24019221
1	4.05646604	6.26357794	-1.60973274
6	2.76150413	7.23793390	-3.81617564
1	0.49317066	5.71076887	-3.94301587
6	-0.65402869	3.77842121	-2.46275690
6	-3.99296172	-1.17267569	-0.69286798
1	-5.37643363	-3.42481964	-0.34169552
6	-5.26778066	-5.61428979	1.29047714
1	-3.14145152	-5.07693603	2.92894744
6	-1.31112625	-3.15319110	3.18807212
1	4.65400786	4.67896365	0.00727475

1	3.61173406	3.28227371	0.38327019
1	3.36014940	4.83393831	1.20475844
1	-0.52951193	2.69944527	-2.64983301
1	-1.14477955	4.20979064	-3.34416131
1	-1.34882019	3.87278666	-1.61292102
1	2.29324657	8.20032461	-3.55458077
1	2.48305687	7.01457343	-4.85547313
1	3.84965647	7.38248434	-3.77689584
1	-5.01692913	-1.25954266	-1.08028212
1	-3.31295635	-1.28032616	-1.55360361
1	-3.86428375	-0.15888096	-0.28517859
1	-1.50626714	-2.52183063	4.06983518
1	-0.40060096	-2.76531066	2.70955741
1	-1.10706250	-4.16732368	3.55569660
1	-4.91080118	-6.36152125	0.56379042
1	-6.29794337	-5.35538383	1.00845341
1	-5.29359403	-6.10106290	2.27482940
1	0.23799130	2.57567036	-0.58582527

Energy = -7584.952604 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 11

Atomic N.	X	Y	Z
8	2.59333935	-1.13026794	0.83439263
6	3.42824142	-1.76676245	-0.03982238
8	3.74136868	-3.11999927	0.34561479
6	2.61028707	-3.93424056	0.64523046
1	1.89195103	-3.96244882	-0.19108700
1	2.08916704	-3.58665585	1.55277342
1	3.00042767	-4.94434639	0.82094984
8	2.70933961	-1.78517261	-1.30838378
6	4.80720811	-1.07860540	-0.14177380
1	5.56085383	-1.83756903	-0.40072721
1	5.03933717	-0.73921684	0.87701791
6	4.88177078	0.09188355	-1.13266975
1	3.95500041	0.68443083	-1.08641644
1	5.69520184	0.76303949	-0.81510578
6	5.15506444	-0.34094694	-2.58272746
1	6.04674551	-0.99221891	-2.59196095
1	5.41552292	0.54587892	-3.18238723
6	3.99187046	-1.06869133	-3.26816175
1	3.16718560	-0.36157245	-3.45477188
1	4.31833041	-1.44219603	-4.25383097
6	3.42387340	-2.24120364	-2.47207041
1	4.20650986	-2.95624342	-2.16937772
1	2.68827592	-2.79086704	-3.08006233
50	0.58129086	-0.77283250	0.21835799
7	0.05942464	-0.57106007	2.66666577
6	1.27145943	-0.91665783	3.45063731
1	1.11170320	-0.68235177	4.51792063
1	2.14159766	-0.37700460	3.06877244
1	1.47995024	-1.98757176	3.34318237
7	0.67139458	1.34420499	0.60875426
6	-0.25685426	0.87747886	2.80484489
1	-0.25764642	1.16204894	3.87478224
1	-1.25651694	1.03927547	2.38526148
6	0.73033169	1.73249564	2.01242122

1	0.41997222	2.78602644	2.12961917
1	1.73372328	1.65701446	2.47529040
6	0.96472329	2.31325337	-0.37787928
6	2.12187945	3.13969269	-0.32142657
6	2.33482431	4.10630114	-1.31396471
6	1.46243395	4.28185478	-2.39124202
6	0.33988268	3.44838229	-2.45054533
6	0.07243918	2.48139597	-1.47584789
7	-2.65104614	-1.11608710	1.27016847
6	-1.04237192	-1.45723325	3.15341069
1	-1.03444795	-1.45060177	4.25998229
1	-0.77922920	-2.48027313	2.84015853
6	-2.47416146	-1.13940675	2.72567054
1	-3.10822818	-1.90971689	3.20926809
1	-2.78877692	-0.17772849	3.15342869
6	-3.97782209	-1.14860185	0.75565516
6	-4.86223275	-0.06491916	0.95848836
6	-6.15241115	-0.12965843	0.41553024
6	-6.59200245	-1.21704263	-0.34498684
6	-5.68518653	-2.25981514	-0.57050780
6	-4.39438069	-2.24930640	-0.03352638
6	3.17878069	2.95805379	0.74290062
1	3.23404652	4.72558919	-1.25030246
6	1.73611321	5.30391835	-3.46861119
1	-0.36905578	3.56656342	-3.27481616
6	-1.18092407	1.65053460	-1.59788065
6	-4.43027738	1.18533480	1.68410600
1	-6.82465175	0.71754918	0.57345292
6	-7.99559885	-1.27062172	-0.89803743
1	-5.99175810	-3.11390094	-1.17956673
6	-3.45700430	-3.40147693	-0.31199273
1	4.12725799	3.40272039	0.41364646
1	3.34937634	1.89177160	0.94759508
1	2.90949438	3.43557769	1.69830387
1	-0.97623288	0.64714996	-2.00867716
1	-1.90057618	2.13270377	-2.27293235
1	-1.65343211	1.49231344	-0.61857911
1	0.80519841	5.76055551	-3.83401863
1	2.23475779	4.84687224	-4.33854955
1	2.38933143	6.10722144	-3.10167585
1	-5.06854694	2.03185015	1.40028789
1	-3.38969543	1.44083735	1.43640865
1	-4.49644076	1.08362902	2.77931526
1	-3.09951525	-3.87850458	0.61489167
1	-2.56556418	-3.08577381	-0.87881181
1	-3.96303561	-4.17272000	-0.90567727
1	-8.01953736	-1.74487961	-1.88895879
1	-8.42777020	-0.26506393	-0.98907415
1	-8.66011975	-1.85531321	-0.24209110
1	-2.09520802	-1.86005458	0.84635805

Energy = -7584.958325 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 12

Atomic N.	X	Y	Z
8	1.33032401	-1.77031534	0.82157974
6	1.51455011	-2.84662057	0.02552998

8	0.15749297	-3.07947540	-0.56773218
6	0.07439562	-3.85532540	-1.76476228
1	0.39778074	-4.89611086	-1.59306510
1	0.67023472	-3.41186776	-2.57612109
1	-0.98450029	-3.86249236	-2.05137527
8	2.40148320	-2.49380968	-1.04587784
6	1.91560320	-4.09464389	0.82779279
1	1.85964890	-4.99461388	0.19403471
1	1.12983060	-4.19627899	1.58775753
6	3.29514324	-4.00728523	1.49964836
1	3.43996631	-2.98579082	1.88522971
1	3.29907422	-4.67388920	2.37619622
6	4.46009245	-4.40521303	0.58479653
1	4.31106016	-5.45062275	0.26061784
1	5.39784563	-4.39589301	1.16337816
6	4.62688980	-3.52448440	-0.65778718
1	4.91805116	-2.50098168	-0.37156135
1	5.44676721	-3.92635519	-1.27719449
6	3.37864331	-3.42540208	-1.53740553
1	2.94087774	-4.42555026	-1.70548986
1	3.65331618	-3.02183364	-2.52325096
50	-0.12403759	-0.47295229	-0.11225767
7	0.42879338	0.84883584	1.90717919
6	1.88002117	0.99867089	2.14422971
1	2.07662912	1.49751080	3.11029125
1	2.32618386	1.58199662	1.33074285
1	2.33059447	0.00017864	2.14364352
7	0.63656314	3.04116430	-0.23106097
6	-0.28857486	2.15597065	1.92045067
1	-0.42220682	2.47742254	2.97102219
1	-1.29190482	1.97442864	1.50586867
6	0.37650541	3.32048034	1.18698232
1	-0.29977587	4.18835698	1.31891547
1	1.31669304	3.58580355	1.69020985
6	0.88610096	4.14201981	-1.09511545
6	2.04508839	4.93721918	-0.94215005
6	2.26250980	6.00208793	-1.82675646
6	1.38810153	6.29394438	-2.87747718
6	0.26992682	5.46671529	-3.03879648
6	-0.00006675	4.40553445	-2.16963187
7	-1.75116421	-0.79540531	1.24194798
6	-0.15644650	-0.05416996	2.94430377
1	-0.08220303	0.42728385	3.93792092
1	0.46017206	-0.96244759	2.93782684
6	-1.60644749	-0.42599608	2.64175487
1	-1.86894549	-1.24780194	3.33478766
1	-2.28240241	0.41444581	2.91219381
6	-2.93864341	-1.47895617	0.86880886
6	-3.89655937	-0.84560690	0.03326183
6	-5.05107372	-1.53667536	-0.35361028
6	-5.30638480	-2.84826423	0.06266870
6	-4.35983495	-3.46265160	0.88825364
6	-3.18648799	-2.81217660	1.29222184
6	3.08789195	4.62244657	0.10183057
1	3.16565665	6.60489450	-1.70091743
6	1.63414038	7.46231035	-3.80135248
1	-0.42182539	5.65583914	-3.86357480
6	-1.22276514	3.54620987	-2.39225523

6	-3.69892881	0.57612314	-0.43632531
1	-5.77938232	-1.02801772	-0.99124035
6	-6.54487950	-3.58313562	-0.39199045
1	-4.52825621	-4.49150218	1.21894569
6	-2.18868608	-3.55547338	2.14447130
1	4.05195666	5.06858113	-0.17473473
1	3.22498416	3.53552728	0.19941789
1	2.82350784	5.01316667	1.09740625
1	-0.95965662	2.49960553	-2.61806071
1	-1.80849869	3.92459300	-3.23918132
1	-1.88425790	3.53083639	-1.51130402
1	1.05366479	8.34576234	-3.49087535
1	1.33908852	7.22781180	-4.83363770
1	2.69364225	7.75187253	-3.80568779
1	-4.62780817	0.97232088	-0.86808788
1	-2.91590093	0.64889812	-1.20756682
1	-3.38859851	1.23087808	0.39031660
1	-1.16795910	-3.21638495	1.92430958
1	-2.25263959	-4.63662990	1.96179999
1	-2.36904137	-3.39874672	3.22086191
1	-6.39092373	-4.05353829	-1.37645140
1	-7.40201762	-2.90214612	-0.48985434
1	-6.81909079	-4.38040931	0.31208966
1	-0.10871101	2.45619585	-0.61191977

Energy = -7584.958521 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 13

Atomic N.	X	Y	Z
8	2.52966506	-0.55189108	0.25557524
6	3.05718459	-1.76129827	-0.06161279
8	2.24372771	-2.75390562	0.67698368
6	2.34458499	-4.11004307	0.24845784
1	3.36746586	-4.51101380	0.36306566
1	2.02275526	-4.22829504	-0.79739277
1	1.67512618	-4.68951376	0.89773364
8	2.85296216	-2.00199069	-1.46841148
6	4.51753612	-1.85557898	0.41520794
1	4.89466661	-2.88520925	0.30451965
1	4.46400313	-1.65556045	1.49406752
6	5.48082335	-0.86416390	-0.25598671
1	4.96524491	0.10048290	-0.38128671
1	6.32502718	-0.68112805	0.42722389
6	6.04144185	-1.34925456	-1.59824131
1	6.59635648	-2.28997063	-1.43134537
1	6.78030915	-0.62041732	-1.96832178
6	4.98519294	-1.58825405	-2.68197341
1	4.50279619	-0.64068222	-2.97024189
1	5.48039851	-1.98377570	-3.58518449
6	3.88425719	-2.57477323	-2.28617233
1	4.32125407	-3.47471403	-1.81653828
1	3.34716536	-2.90785463	-3.18685035
50	0.42948106	-0.36738583	-0.08572418
7	0.09156332	-0.29876277	2.39556726
6	1.38523172	-0.61689297	3.05055931
1	1.30493653	-0.45641409	4.14030265
1	2.18120060	0.00665131	2.63508589

1	1.64663960	-1.66080796	2.84212481
7	0.45879690	1.71998981	0.39864323
6	-0.27470698	1.12554753	2.63103913
1	-0.19892305	1.35820932	3.71073201
1	-1.31260235	1.26021529	2.30423308
6	0.60465925	2.06457638	1.80514396
1	0.24748793	3.09458345	1.98716278
1	1.64387157	2.03131737	2.19011465
6	0.71907456	2.71203360	-0.57985117
6	1.94429663	3.42946848	-0.63594243
6	2.12321939	4.42059630	-1.61065799
6	1.14543135	4.71778641	-2.56417692
6	-0.04591570	3.98467070	-2.51830784
6	-0.27878977	2.99962649	-1.55232761
7	-2.64967596	-1.04201284	1.15576777
6	-0.91582128	-1.25844924	2.93908689
1	-0.84100470	-1.25736296	4.04353174
1	-0.60124432	-2.25815443	2.60006379
6	-2.38802289	-1.03593398	2.59883386
1	-2.94259604	-1.83909006	3.12511929
1	-2.73866428	-0.09122186	3.03525499
6	-3.99986879	-1.14151605	0.71780354
6	-4.92460001	-0.10174536	0.96676069
6	-6.23829334	-0.23349768	0.49757039
6	-6.66555296	-1.34561511	-0.23375674
6	-5.72188074	-2.34296818	-0.50768586
6	-4.40500583	-2.26527367	-0.04460128
6	3.09176681	3.09743756	0.28683732
1	3.07473693	4.95933739	-1.63667356
6	1.37895188	5.76249980	-3.62935172
1	-0.83230702	4.19802821	-3.24765024
6	-1.59936326	2.27019010	-1.54645652
6	-4.51625640	1.17250031	1.66364938
1	-6.94183083	0.58034958	0.69091350
6	-8.09417030	-1.47198926	-0.70488126
1	-6.01896233	-3.21426636	-1.09675579
6	-3.42773583	-3.36966326	-0.37493257
1	4.03498008	3.47860224	-0.12703665
1	3.18007400	2.00876728	0.41858336
1	2.97241782	3.54299418	1.28746754
1	-1.51050075	1.24946726	-1.95420718
1	-2.33945150	2.80270535	-2.15848879
1	-1.98558982	2.15765787	-0.52442697
1	0.45456237	6.30886846	-3.86500053
1	1.73272885	5.30585610	-4.56776544
1	2.13688695	6.49267530	-3.31462260
1	-5.20315594	1.98783349	1.40282488
1	-3.49996422	1.47060276	1.36785041
1	-4.52968622	1.07735960	2.76142975
1	-2.99383412	-3.82448282	0.53032093
1	-2.58803142	-3.01121778	-0.99305853
1	-3.92721413	-4.16804537	-0.93748268
1	-8.15304878	-1.97608008	-1.67940565
1	-8.57242579	-0.48770583	-0.79899656
1	-8.69666771	-2.06251568	0.00372682
1	-2.08957558	-1.77112840	0.71284430

Energy = -7584.956644 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 14

Atomic N.	X	Y	Z
8	0.53778202	-1.23705111	2.24856968
6	1.82342393	-1.47145590	1.90630918
8	2.30179531	-2.75467839	2.24431178
6	1.38344959	-3.83092250	1.99654121
1	1.17557444	-3.92891455	0.91987313
1	0.44177105	-3.67950337	2.53819312
1	1.88782683	-4.73543297	2.35587669
8	1.77226007	-1.36265379	0.38375064
6	2.85563388	-0.50112683	2.51844431
1	3.84251324	-0.98830998	2.51437641
1	2.55259733	-0.41684860	3.57146983
6	2.95913327	0.88969564	1.88112390
1	1.95710602	1.26470484	1.60893006
1	3.34136876	1.58772692	2.64198061
6	3.89931171	0.95053410	0.66662821
1	4.88063509	0.54223601	0.96603589
1	4.07432936	2.00426919	0.39704128
6	3.40750572	0.20496685	-0.58000108
1	2.52999331	0.72492752	-0.99946628
1	4.19484566	0.22693706	-1.35330525
6	3.00799216	-1.25053009	-0.34465155
1	3.78782894	-1.81443303	0.19342222
1	2.83993722	-1.75932603	-1.30748394
50	-0.46209961	-0.24194476	0.62772143
7	-1.07416400	-0.60821739	-2.14843547
6	-0.56809980	-1.87642679	-2.68794077
1	-1.14480973	-2.21702887	-3.57236553
1	-0.61193635	-2.65105819	-1.91506190
1	0.48134492	-1.74978510	-2.98411208
7	-1.89932299	-1.82295070	0.42359025
6	-2.49135267	-0.71975335	-1.74702140
1	-3.13064062	-0.89018318	-2.63992727
1	-2.78854415	0.24703616	-1.31065787
6	-2.78031798	-1.83832208	-0.74296063
1	-3.83910116	-1.71346933	-0.44178286
1	-2.74111152	-2.80670820	-1.27676834
6	-2.26297878	-2.75189549	1.43991873
6	-2.20354203	-4.15507716	1.22234864
6	-2.60582786	-5.03645902	2.23487382
6	-3.06188125	-4.58930170	3.47702227
6	-3.09027853	-3.20758650	3.69228047
6	-2.70359358	-2.28923465	2.70959860
7	0.35826640	2.30789385	-2.10098918
6	-0.91450010	0.45779054	-3.16178336
1	-1.69935411	0.34333143	-3.93863618
1	0.04722150	0.28709962	-3.67216063
6	-0.94412314	1.90404635	-2.65866302
1	-1.22838354	2.54689680	-3.51444658
1	-1.72807648	2.02753983	-1.89969146
6	0.63163744	3.69355894	-1.94681175
6	-0.12923020	4.49890266	-1.06828938
6	0.19800714	5.85497460	-0.93427254
6	1.27000436	6.44200439	-1.61256981
6	2.02940881	5.62089744	-2.45458452

6	1.72916078	4.26794467	-2.63811268
6	-1.65059521	-4.74072384	-0.05318337
1	-2.53758410	-6.11167384	2.04726451
6	-3.51734291	-5.55693259	4.54249343
1	-3.42701590	-2.82592710	4.65973067
6	-2.75482877	-0.81852083	3.04305693
6	-1.24513607	3.92500461	-0.23067163
1	-0.39818022	6.46478239	-0.25052906
6	1.62395925	7.89644384	-1.41500074
1	2.87760110	6.04731069	-2.99641641
6	2.57899588	3.43636187	-3.57129606
1	-1.25734871	-5.75013605	0.12742756
1	-0.83532942	-4.11639930	-0.44385649
1	-2.41193293	-4.82756841	-0.84508255
1	-1.75449280	-0.43462970	3.30406013
1	-3.40008594	-0.64101391	3.91385308
1	-3.13534579	-0.22053188	2.20217143
1	-4.61307414	-5.67198429	4.53514473
1	-3.23504851	-5.21087017	5.54663644
1	-3.08247837	-6.55391278	4.38886557
1	-1.43010532	4.56094456	0.64489616
1	-0.99383463	2.91347192	0.12248462
1	-2.19442625	3.85594787	-0.78641501
1	1.98244947	2.96648594	-4.37035125
1	3.11396782	2.62850328	-3.04381406
1	3.33999330	4.06109941	-4.05499268
1	2.44532499	8.01306229	-0.69023845
1	0.76696844	8.46808347	-1.03464123
1	1.95437357	8.36056792	-2.35506191
1	1.09415606	1.88342883	-2.66381341

Energy = -7584.948889 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 15

Atomic N.	X	Y	Z
8	2.16244046	-1.08342665	-1.34034973
6	3.39383316	-1.19306226	-0.75154548
8	4.42904410	-1.40101729	-1.71757429
6	4.44542773	-0.46431860	-2.79851210
1	4.68468401	0.55168492	-2.44739299
1	3.48006549	-0.44534175	-3.32514596
1	5.23296499	-0.80812107	-3.48000769
8	3.59577089	0.07895396	-0.06648875
6	3.53081270	-2.41683482	0.18834882
1	4.59125917	-2.70799882	0.22946030
1	3.00559150	-3.23368982	-0.32594502
6	2.99094950	-2.23984690	1.61313264
1	2.04630265	-1.66815071	1.59985370
1	2.73711979	-3.23456072	2.01295687
6	3.99247391	-1.57963946	2.57450322
1	4.93030171	-2.16208832	2.54797938
1	3.61187222	-1.65691768	3.60570044
6	4.30851753	-0.10901448	2.27546742
1	3.43070872	0.51824253	2.50083755
1	5.12040913	0.23258348	2.94004325
6	4.71714720	0.17391514	0.83036518
1	5.52707675	-0.49315272	0.49103414

1	5.08312522	1.20868090	0.74096509
50	0.66896428	0.12433431	-0.39593973
7	-0.70517510	-1.37228148	-1.86457284
6	-0.29536955	-2.79224451	-1.82142741
1	-0.84768610	-3.38203463	-2.57565810
1	-0.48772656	-3.21018377	-0.82742074
1	0.78076514	-2.84428966	-2.01582104
7	-2.22927274	-1.20338994	0.81189397
6	-2.17310500	-1.23084749	-1.67640978
1	-2.68790208	-1.70152971	-2.53665692
1	-2.40313074	-0.15654333	-1.71112346
6	-2.76582075	-1.83307108	-0.40288635
1	-3.86502322	-1.71227368	-0.48343707
1	-2.58017333	-2.91408683	-0.36227164
6	-2.81642796	-1.58111726	2.05552918
6	-2.56876456	-2.85824356	2.60679990
6	-3.14564528	-3.19039224	3.83950850
6	-3.93863155	-2.29225130	4.56038160
6	-4.13411173	-1.01646349	4.01758030
6	-3.59459604	-0.64681555	2.78150892
7	0.06113757	1.33953204	-2.05686161
6	-0.31367322	-0.79399926	-3.18657677
1	-0.89113571	-1.28390956	-3.99349125
1	0.75020135	-1.03250954	-3.31526605
6	-0.50632842	0.72055741	-3.24481985
1	-0.00604866	1.06852870	-4.17090684
1	-1.58118848	0.96237254	-3.38312428
6	0.04784782	2.76177415	-2.00458836
6	-1.14958648	3.49424232	-1.79012549
6	-1.11172458	4.89421975	-1.74209862
6	0.07934144	5.61103783	-1.88865253
6	1.25569532	4.88055274	-2.08974400
6	1.26262130	3.48206064	-2.15105491
6	-1.64431989	-3.83940449	1.93095383
1	-2.94229270	-4.17874379	4.25946165
6	-4.56927209	-2.68475238	5.87454087
1	-4.73017010	-0.28518717	4.56920673
6	-3.83210578	0.74628731	2.24531572
6	-2.46706350	2.79593656	-1.56651665
1	-2.04452779	5.43847173	-1.57036457
6	0.10337911	7.11799542	-1.79828347
1	2.20116702	5.41535639	-2.21467140
6	2.56152245	2.75487768	-2.39100919
1	-1.26051170	-4.56829583	2.65622914
1	-0.79081007	-3.31430650	1.47812067
1	-2.14467941	-4.41184101	1.13298337
1	-2.89696697	1.32471967	2.16286582
1	-4.49847470	1.30606003	2.91313810
1	-4.29862418	0.73405497	1.24752076
1	-5.60894407	-3.01997631	5.73176248
1	-4.59470746	-1.83988554	6.57656209
1	-4.02176954	-3.50947954	6.35014965
1	-3.18934074	3.46951397	-1.08726471
1	-2.32834023	1.91548692	-0.92184239
1	-2.92123756	2.44214396	-2.50598782
1	2.44917780	1.98300098	-3.16387737
1	2.91763132	2.23138284	-1.48992681
1	3.34546094	3.45890635	-2.70117345

1	0.35905356	7.45136690	-0.77972910
1	-0.87465518	7.55062877	-2.04875297
1	0.85327655	7.54775651	-2.47707738
1	-2.28808001	-0.18968785	0.70771367

Energy = -7584.961696 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 16

Atomic N.	X	Y	Z
8	2.11576220	-1.26415590	-0.84738094
6	3.34965996	-0.71621086	-0.76349382
8	3.83492829	-0.61476204	-2.11926662
6	5.03225980	0.13023641	-2.32938113
1	5.90609437	-0.31166283	-1.81887707
1	4.91891096	1.18052288	-2.01600992
1	5.21740286	0.10521729	-3.41046548
8	3.15850512	0.65880955	-0.24609454
6	4.30612160	-1.57720549	0.08551750
1	5.33873705	-1.19949754	0.02410552
1	4.29861307	-2.55050093	-0.42492206
6	3.90284459	-1.75270851	1.55641182
1	2.80748770	-1.85573663	1.61847034
1	4.32188007	-2.70352204	1.92099277
6	4.38849893	-0.62748067	2.47890466
1	5.49032859	-0.57339444	2.42101114
1	4.14972155	-0.88465352	3.52330402
6	3.81008787	0.75547866	2.16242128
1	2.72449818	0.77333141	2.35417819
1	4.26054247	1.49946281	2.84136992
6	4.04664132	1.23657790	0.73020856
1	5.09800444	1.08052226	0.43407202
1	3.84370143	2.31572040	0.66166724
50	0.54069243	0.01672448	-0.15740074
7	-0.70286668	-1.53564690	-1.62223263
6	-0.33172801	-2.95788345	-1.46034992
1	-0.84466530	-3.58791006	-2.20905228
1	-0.59749426	-3.29537056	-0.45228910
1	0.75308846	-3.04273633	-1.58299873
7	-2.40418505	-1.70094005	0.92871371
6	-2.17571606	-1.32570849	-1.53517827
1	-2.63862304	-1.66129849	-2.48276522
1	-2.34162399	-0.24031137	-1.46000382
6	-2.91325924	-2.04500655	-0.40587169
1	-3.98278473	-1.77827831	-0.52144573
1	-2.85075963	-3.13167852	-0.55359957
6	-3.20777056	-2.04180126	2.05251863
6	-3.42929864	-3.39364341	2.40243677
6	-4.21113379	-3.68685344	3.52770440
6	-4.76138937	-2.68982759	4.33843460
6	-4.49318138	-1.35796425	4.00011099
6	-3.73598741	-1.01599077	2.87551747
7	0.07076588	1.15641929	-1.90615681
6	-0.20183091	-1.04328356	-2.94313552
1	-0.72313995	-1.58035916	-3.75774983
1	0.86752120	-1.29158347	-2.97195465
6	-0.37397778	0.46429042	-3.10784810
1	0.20359853	0.74529768	-4.00800700

1	-1.43176203	0.71008804	-3.34486328
6	0.23310726	2.56517093	-1.98929250
6	-0.61393937	3.43066170	-1.24704752
6	-0.42708629	4.81728420	-1.31251896
6	0.57238114	5.39645180	-2.10081656
6	1.39542722	4.53729950	-2.83586963
6	1.25246466	3.14468874	-2.79354287
6	-2.78752072	-4.52414956	1.63701002
1	-4.36961959	-4.73602487	3.79026130
6	-5.62104025	-3.03427953	5.53063831
1	-4.89191633	-0.55553032	4.62590446
6	-3.47899254	0.43902944	2.55980066
6	-1.73547926	2.88762069	-0.39350453
1	-1.09507667	5.46485876	-0.73791752
6	0.77604446	6.89239829	-2.13214423
1	2.19171334	4.96110548	-3.45453625
6	2.21049494	2.28706798	-3.58156388
1	-2.74368630	-5.42914781	2.25658714
1	-1.76293355	-4.25877025	1.33823764
1	-3.34190143	-4.78494200	0.72132678
1	-2.40755398	0.69310703	2.61533510
1	-4.00294064	1.08521895	3.27491930
1	-3.82540139	0.71233687	1.55038898
1	-6.69186864	-2.99567279	5.27443685
1	-5.46080027	-2.33008030	6.35883504
1	-5.40877917	-4.04777696	5.89691000
1	-2.44119928	3.68721824	-0.13097030
1	-1.36390328	2.45233960	0.54787439
1	-2.28440577	2.09095385	-0.91526107
1	1.82734134	2.06897987	-4.59227422
1	2.38983180	1.32647059	-3.08061645
1	3.17048001	2.80542483	-3.71141843
1	1.51987065	7.20905534	-1.38337960
1	-0.15719967	7.42824533	-1.91060370
1	1.13995281	7.22799327	-3.11311084
1	-2.16958637	-0.70773901	0.95864599

Energy = -7584.956704 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 17

Atomic N.	X	Y	Z
8	1.42513779	-1.90531236	1.11300402
6	1.99961818	-2.53437242	0.07696739
8	2.09468612	-3.91921292	0.20473510
6	0.95527095	-4.56594502	0.80091151
1	0.08290044	-4.50125766	0.13450602
1	0.71176423	-4.11818720	1.77119292
1	1.24874220	-5.61455601	0.92453771
8	0.94776251	-2.22408233	-1.07998003
6	3.39504516	-2.00744494	-0.30318538
1	3.27529510	-0.98024178	-0.68570858
1	3.91723211	-1.91718212	0.66084522
6	4.23591675	-2.86482268	-1.25555102
1	4.24935862	-3.89633731	-0.87546033
1	5.27587011	-2.50303390	-1.21544453
6	3.77847379	-2.85909998	-2.71793332
1	3.93935281	-1.85409089	-3.14741145

1	4.42472152	-3.54235136	-3.29209336
6	2.31204250	-3.24953903	-2.94617270
1	2.08449247	-4.21921148	-2.47841603
1	2.14940648	-3.37354411	-4.02984840
6	1.29912974	-2.20286396	-2.47940511
1	1.66535819	-1.19487589	-2.75411453
1	0.34240585	-2.36247165	-3.00230467
50	0.24034209	-0.31544306	0.25231100
7	-2.00209520	0.48055708	-1.35377173
6	-2.48019996	-0.69119799	-2.09541537
1	-3.54104852	-0.58505498	-2.40166888
1	-2.37208119	-1.59519162	-1.48591026
1	-1.87352457	-0.81340326	-3.00320060
7	-1.55119667	-1.04746764	1.13111500
6	-2.78665076	0.73650385	-0.13463497
1	-3.82921457	1.03186474	-0.38176294
1	-2.31002201	1.58096408	0.38680655
6	-2.85534133	-0.46185921	0.81334662
1	-3.35045729	-0.09662610	1.73336249
1	-3.54490570	-1.21597271	0.38787766
6	-1.60447734	-2.01702004	2.17693544
6	-2.24097023	-3.27076864	1.98678458
6	-2.31524601	-4.18077322	3.05010147
6	-1.77027686	-3.90368932	4.30643495
6	-1.11948864	-2.67658091	4.47349673
6	-1.02606414	-1.73504609	3.44197332
7	-0.45579488	3.10882488	-0.93894720
6	-1.98084853	1.63727263	-2.27644720
1	-2.95651922	1.70677606	-2.80440828
1	-1.21717419	1.42431106	-3.04260344
6	-1.72591950	3.01494828	-1.66820905
1	-1.74738276	3.72863646	-2.51190132
1	-2.57131821	3.28692691	-1.01637852
6	0.27621917	4.31837904	-0.96721935
6	-0.29688399	5.52185750	-0.49242238
6	0.46035302	6.70005250	-0.52974501
6	1.77911933	6.72923336	-0.99263161
6	2.34356092	5.51884193	-1.41365616
6	1.62158075	4.32165407	-1.41544733
6	-2.79098839	-3.68277620	0.64386539
1	-2.80065507	-5.14554931	2.88034536
6	-1.89102817	-4.88482624	5.44682876
1	-0.66896368	-2.43971073	5.44056589
6	-0.29060292	-0.44335710	3.70180249
6	-1.67191638	5.54530967	0.12983218
1	0.00610060	7.62054731	-0.15378715
6	2.56420979	8.01777681	-1.04544720
1	3.37921613	5.50415578	-1.76295679
6	2.28084336	3.04938693	-1.89165480
1	-2.82719392	-4.77734089	0.56221353
1	-2.16009506	-3.29337613	-0.16759600
1	-3.81502336	-3.31226895	0.47575495
1	0.72783453	-0.47753220	3.28096031
1	-0.18539430	-0.26837606	4.78071014
1	-0.80528242	0.41887650	3.25562190
1	-2.73200254	-4.62431766	6.10914216
1	-0.98305317	-4.89536801	6.06595561
1	-2.06743552	-5.90491765	5.07961469

1	-1.80111495	6.45148135	0.73565326
1	-1.81878325	4.66964713	0.77973890
1	-2.47986858	5.53384989	-0.61823987
1	1.73053100	2.58912212	-2.72875527
1	2.34371361	2.28964005	-1.09532096
1	3.30271269	3.25201859	-2.23600285
1	3.62281572	7.85464149	-0.79941687
1	2.16081114	8.76013313	-0.34348241
1	2.53024175	8.46573887	-2.05155155
1	0.13431470	2.29591885	-1.11222843

Energy = -7584.948371 Hartree
Number of imaginary frequencies = 0.

Compound I4b isomer 18

Atomic N.	X	Y	Z
8	0.65339408	-1.38326517	-2.08783446
6	1.99303739	-1.63187030	-2.21870584
8	2.35417258	-1.94200076	-3.55442530
6	1.90626791	-1.01186463	-4.54507835
1	2.41579470	-0.04203511	-4.43901288
1	0.81858664	-0.86169627	-4.48822804
1	2.16818588	-1.45763545	-5.51216297
8	2.61984745	-0.34035898	-1.81753455
6	2.46141024	-2.83236623	-1.36737486
1	2.42301553	-2.52736216	-0.30823759
1	1.67333912	-3.58699053	-1.50151028
6	3.81764307	-3.45683196	-1.71843683
1	3.82767175	-3.67886604	-2.79501712
1	3.89518402	-4.42469108	-1.19721519
6	5.04028856	-2.60829624	-1.35457515
1	5.13170222	-2.55189875	-0.25528660
1	5.94858203	-3.12062238	-1.71073258
6	5.01665053	-1.17690489	-1.90576617
1	4.89323611	-1.17661045	-2.99933661
1	5.99047283	-0.70408818	-1.69586330
6	3.95327376	-0.28249594	-1.26566567
1	3.90577106	-0.48939304	-0.17988536
1	4.23088165	0.77484435	-1.38659393
50	0.33140839	-0.02877527	-0.45468427
7	-2.00931501	-0.58973951	-1.06562571
6	-2.24388839	-2.03058984	-1.29881663
1	-3.26708184	-2.21063369	-1.67504262
1	-2.09378359	-2.58163481	-0.36380149
1	-1.50943542	-2.38296445	-2.03082035
7	-2.10361087	-1.09775088	1.95702266
6	-2.99423635	-0.00623302	-0.11188529
1	-3.95758270	0.13732991	-0.63794644
1	-2.62289990	0.99264641	0.16249417
6	-3.29804448	-0.81310705	1.15055239
1	-4.04815211	-0.22446550	1.71557764
1	-3.79051816	-1.75670964	0.87904076
6	-2.29860170	-1.54863328	3.29289160
6	-2.87043205	-2.81475500	3.55500663
6	-3.02755751	-3.22937402	4.88434705
6	-2.61439679	-2.44777990	5.96703337
6	-2.01053476	-1.21656306	5.68445327
6	-1.85067188	-0.75140351	4.37569511

7	-0.41443934	1.69856319	-1.47492035
6	-2.07836186	0.14094119	-2.36708051
1	-3.10592219	0.08000911	-2.77309056
1	-1.39508356	-0.38662753	-3.04584996
6	-1.64584443	1.60019945	-2.24485721
1	-1.54272708	1.98218330	-3.27870336
1	-2.45812279	2.20487120	-1.78671791
6	0.22831958	2.96691777	-1.45053729
6	0.26224380	3.73882997	-0.25913952
6	0.91952529	4.97569907	-0.24738071
6	1.54876282	5.49534951	-1.38333870
6	1.50274747	4.73290407	-2.55456780
6	0.86476149	3.48751042	-2.60942083
6	-3.24966913	-3.75817599	2.44057682
1	-3.46558240	-4.21295594	5.07265232
6	-2.81800294	-2.90834657	7.39018194
1	-1.65759997	-0.59128396	6.50844250
6	-1.19137306	0.58597228	4.13177559
6	-0.41499246	3.26319485	1.00416828
1	0.92829327	5.55662232	0.67892209
6	2.27809491	6.81665319	-1.33740365
1	1.99376109	5.10917659	-3.45648076
6	0.89406393	2.70260956	-3.89600591
1	-3.29771800	-4.78972423	2.81254159
1	-2.50987017	-3.71755428	1.62789491
1	-4.23397135	-3.52502085	2.00400883
1	-0.24645743	0.48735298	3.57227831
1	-0.95448470	1.07623000	5.08413485
1	-1.83823369	1.26938470	3.55894844
1	-3.72743426	-2.46511600	7.82631467
1	-1.97550973	-2.61549297	8.03207286
1	-2.92702111	-3.99981610	7.44508423
1	-0.49850530	4.08423916	1.72870694
1	0.14524709	2.44838204	1.48922131
1	-1.42289557	2.87628632	0.79710416
1	0.88593401	1.62521663	-3.68807703
1	1.79160692	2.94752802	-4.47979029
1	0.02303837	2.92568744	-4.53386233
1	3.34257882	6.67528014	-1.09049801
1	1.85257758	7.48243590	-0.57400035
1	2.23520118	7.33311938	-2.30618657
1	-1.48600910	-0.28479901	1.95186673

Energy = -7584.958481 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 19

Atomic N.	X	Y	Z
8	0.32913883	-2.44646930	-0.76128219
6	1.32333998	-2.81286157	-1.61916869
8	1.21894572	-1.92062283	-2.76321264
6	2.20360359	-2.06562056	-3.79055321
1	2.07990362	-3.01498535	-4.33896102
1	3.22323042	-2.00455624	-3.38468718
1	2.04005795	-1.23492478	-4.48935474
8	2.63927410	-2.52652972	-1.09488419
6	1.13726102	-4.30383677	-2.02614177
1	0.54390427	-4.77105096	-1.22616602

1	0.49380855	-4.30319508	-2.91916453
6	2.39101131	-5.15700235	-2.27847552
1	3.09998499	-4.63109126	-2.93613039
1	2.07147355	-6.05752513	-2.82840337
6	3.11564561	-5.60686154	-0.99988439
1	2.37607304	-6.06018405	-0.31675507
1	3.83045248	-6.40629405	-1.25389584
6	3.86606819	-4.49091646	-0.26539922
1	4.71544383	-4.14582340	-0.87802096
1	4.29359212	-4.88779097	0.67128613
6	3.00785017	-3.27630512	0.07781698
1	2.10355074	-3.56081761	0.64172323
1	3.58064841	-2.57851956	0.70778467
50	0.28993161	-0.36080147	-0.28198244
7	-1.82841872	-0.16375942	-1.59096504
6	-2.04851608	-1.43956379	-2.31831237
1	-3.04505772	-1.43401830	-2.79409227
1	-1.96174055	-2.28523552	-1.63119234
1	-1.26922434	-1.55778469	-3.08004901
7	-1.25948521	-0.67063775	1.16804754
6	-2.85353236	0.00930137	-0.52342379
1	-3.86392028	-0.15103354	-0.94600987
1	-2.77607506	1.03800077	-0.15232217
6	-2.59344369	-0.93512803	0.65019496
1	-3.35540951	-0.71894631	1.42141637
1	-2.77389541	-1.98098074	0.32996932
6	-0.95673387	-1.03045979	2.50544090
6	-1.15181409	-2.34409536	3.01248344
6	-0.84865553	-2.62127709	4.35237216
6	-0.33054176	-1.65454238	5.21915215
6	-0.10826520	-0.37425798	4.69971169
6	-0.41336371	-0.04397093	3.37457834
7	-0.69229892	2.70515543	-1.30417337
6	-1.85914165	0.92742178	-2.61124961
1	-2.76390639	0.79814812	-3.23539201
1	-0.99227782	0.75670820	-3.26903544
6	-1.86200933	2.37529838	-2.12529410
1	-1.91759684	2.99946474	-3.04017100
1	-2.78065691	2.58414799	-1.56133671
6	-0.43586874	4.07714360	-1.02421584
6	-1.31678876	4.83217328	-0.21687444
6	-1.01295280	6.17379564	0.04985191
6	0.14618057	6.79005423	-0.43045664
6	1.02740633	6.01128933	-1.19028835
6	0.75810107	4.67460597	-1.49907849
6	-1.60287355	-3.47458468	2.11916619
1	-0.99964429	-3.64032685	4.72001802
6	-0.03838601	-1.97364610	6.66584788
1	0.30149678	0.40270033	5.35092542
6	-0.17294198	1.36469396	2.89096115
6	-2.53687257	4.21334238	0.41909605
1	-1.69865431	6.74504706	0.68083989
6	0.43558229	8.24432344	-0.14726226
1	1.95358167	6.45768738	-1.56085131
6	1.74830817	3.88057236	-2.31944493
1	-1.35455097	-4.44147363	2.57713863
1	-1.11211626	-3.41403529	1.13634962
1	-2.69121260	-3.46790878	1.94685023

1	0.71754608	1.43595745	2.24445956
1	-0.01681560	2.04471208	3.73890900
1	-1.01689046	1.72449078	2.28700819
1	-0.88329418	-1.69452487	7.31597737
1	0.84326236	-1.42683988	7.02864908
1	0.14193696	-3.04792138	6.80951875
1	-2.84321878	4.79122063	1.30049040
1	-2.32900689	3.18191245	0.73868597
1	-3.40126694	4.18358923	-0.26380937
1	1.29436004	3.47152932	-3.23660549
1	2.16822241	3.03028003	-1.75707052
1	2.58981476	4.51499606	-2.62389876
1	1.51113247	8.42042873	-0.00753044
1	-0.08774657	8.58740397	0.75535548
1	0.10689953	8.88556537	-0.98066528
1	0.13905762	2.27837736	-1.71448204

Energy = -7584.958215 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 20

Atomic N.	X	Y	Z
8	0.89289322	-1.51153247	-1.69807060
6	2.21939535	-1.41295811	-1.98869458
8	2.46118762	-0.96767858	-3.33791823
6	1.89051699	-1.80607306	-4.34101838
1	0.81889819	-1.97793236	-4.15495037
1	2.40598657	-2.77983741	-4.40979699
1	2.01371615	-1.27455880	-5.29263127
8	2.73997410	-0.34408980	-1.13824385
6	2.96063808	-2.72235489	-1.64866580
1	2.79213929	-2.87656418	-0.57204638
1	2.44003042	-3.54539492	-2.16218767
6	4.45942387	-2.77522487	-1.96280499
1	4.61101394	-2.76198060	-3.05514122
1	4.83729170	-3.74944493	-1.61257068
6	5.31407526	-1.65721636	-1.34255885
1	5.11734249	-1.58710134	-0.25965839
1	6.37414469	-1.93641048	-1.44937796
6	5.10350555	-0.29123104	-2.01336876
1	5.06023361	-0.43806491	-3.10231193
1	5.96955102	0.36149521	-1.81565687
6	3.85881668	0.47588625	-1.55110817
1	4.08212052	1.04971070	-0.63985609
1	3.53198682	1.18015699	-2.32944664
50	0.33296024	-0.11885371	-0.15808596
7	-1.90671288	-0.75918071	-0.99476931
6	-2.08137426	-2.21256537	-1.20058038
1	-3.05329570	-2.43368857	-1.67707049
1	-2.01701584	-2.72969520	-0.23648843
1	-1.26527624	-2.56674171	-1.83970587
7	-2.31446934	-1.25253099	2.00621544
6	-2.98527876	-0.16927332	-0.15037826
1	-3.88958863	-0.03157316	-0.77320275
1	-2.64550738	0.83306618	0.15235942
6	-3.41775176	-0.96620580	1.08033173
1	-4.21635339	-0.36885940	1.56315263
1	-3.88857390	-1.90721275	0.76293285

6	-2.63975396	-1.62216632	3.33993810
6	-3.31287820	-2.83512605	3.61315833
6	-3.59906732	-3.17109708	4.94310799
6	-3.21971174	-2.36254896	6.01837879
6	-2.51513295	-1.18770509	5.72884605
6	-2.22396521	-0.80040558	4.41735841
7	-0.29832570	1.54486261	-1.35997479
6	-1.87092166	-0.06867629	-2.31903034
1	-2.85657612	-0.16401641	-2.81289281
1	-1.11621261	-0.59798292	-2.91547132
6	-1.47704748	1.40029503	-2.20215920
1	-1.31438289	1.76058313	-3.23496168
1	-2.33109854	1.99689311	-1.81379683
6	0.36872994	2.79767910	-1.39524433
6	0.38684386	3.64004401	-0.25141912
6	1.07108565	4.86166853	-0.29367978
6	1.74265933	5.29935298	-1.43956493
6	1.71294555	4.46785122	-2.56384852
6	1.05066926	3.23393213	-2.56511100
6	-3.66549119	-3.80859503	2.51557539
1	-4.11446024	-4.11463013	5.14046035
6	-3.56437373	-2.73571058	7.44002606
1	-2.18653071	-0.54437805	6.54900497
6	-1.46190585	0.47953604	4.16543518
6	-0.33894081	3.25700489	1.01656065
1	1.06521555	5.49732153	0.59605876
6	2.49871707	6.60640801	-1.45223183
1	2.23853501	4.77893557	-3.47118584
6	1.11352391	2.37210802	-3.80204694
1	-3.80577817	-4.81581554	2.92880720
1	-2.86587215	-3.85222251	1.76163135
1	-4.59762240	-3.53951776	1.99355494
1	-0.48840482	0.29615702	3.68155147
1	-1.26298400	0.99991010	5.11049336
1	-2.01985269	1.17278668	3.51574967
1	-4.48243658	-2.22637713	7.77398632
1	-2.76376966	-2.45005214	8.13637710
1	-3.73525207	-3.81615171	7.53936349
1	-0.47543468	4.13480086	1.66247269
1	0.21449035	2.50262747	1.59833193
1	-1.32489678	2.82369272	0.79678272
1	1.14381062	1.30569169	-3.53899988
1	2.00822366	2.61268910	-4.39220965
1	0.24357702	2.52975286	-4.46090226
1	3.55264381	6.46048804	-1.16567921
1	2.06577862	7.32602674	-0.74375783
1	2.49421697	7.06346193	-2.45136095
1	-1.64922954	-0.47767138	2.00589184

Energy = -7584.957278 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 21

Atomic N.	X	Y	Z
8	2.30246617	-1.76758119	-0.07649463
6	2.88709923	-0.55032504	-0.17386705
8	3.55310412	-0.32965137	-1.38996484
6	2.84266984	-0.74134640	-2.56909490

1	1.94576362	-0.12298650	-2.72197983
1	2.55507161	-1.79780487	-2.51049871
1	3.54139112	-0.58325681	-3.39913360
8	1.66788938	0.38947884	-0.09904917
6	3.90642316	-0.25889427	0.94722942
1	3.34638752	-0.14745632	1.89096201
1	4.48123077	-1.19201728	1.03703000
6	4.87338508	0.91118663	0.73152017
1	5.34687865	0.79135502	-0.25334629
1	5.67959268	0.83375333	1.47889786
6	4.24482211	2.30465381	0.83673839
1	3.94240728	2.49084065	1.88273150
1	5.01300738	3.05920798	0.60213676
6	3.02178200	2.53459643	-0.06082410
1	3.25722800	2.31564574	-1.11309604
1	2.74762236	3.60139298	-0.01094491
6	1.77642151	1.75610290	0.36568354
1	1.69466195	1.77269283	1.46780732
1	0.87795230	2.24533462	-0.03712132
50	0.53147026	-1.52288047	1.11638953
7	-2.30100411	-1.85892477	2.06524699
6	-2.32280744	-2.01885606	3.51823752
1	-3.24368788	-2.52930963	3.87261858
1	-2.25581611	-1.04345590	4.01520103
1	-1.45149222	-2.60965400	3.83288330
7	-2.04136616	1.07818589	1.19695770
6	-3.37922745	-0.98297383	1.59691174
1	-4.36009085	-1.30230104	2.01592698
1	-3.45768007	-1.09296800	0.50477713
6	-3.18826598	0.49976265	1.91953090
1	-4.13492536	1.01915406	1.66853376
1	-3.03633774	0.64473700	2.99659325
6	-1.80356661	2.46887063	1.40148987
6	-1.26248679	2.92185747	2.62725698
6	-1.00176099	4.28772599	2.79238521
6	-1.23985511	5.22359949	1.78003612
6	-1.74705430	4.75052317	0.56448981
6	-2.03975453	3.39745520	0.35899186
7	-0.59863313	-2.58783156	-0.32784974
6	-2.32298994	-3.17179941	1.40581452
1	-3.32001917	-3.65807063	1.49647330
1	-1.60222068	-3.81128922	1.94102791
6	-1.92925042	-3.14246159	-0.06853195
1	-1.96952291	-4.19236815	-0.41679433
1	-2.70940469	-2.62043410	-0.66090404
6	-0.18026137	-2.85101946	-1.67166562
6	-0.56046643	-1.98853348	-2.72475911
6	-0.19975967	-2.30443668	-4.04165048
6	0.54253214	-3.44886365	-4.34979994
6	0.92809287	-4.28229677	-3.29282011
6	0.58554550	-4.00454800	-1.96392887
6	-0.90871810	1.95900497	3.73349354
1	-0.57410334	4.62451410	3.74028824
6	-0.97486253	6.69396174	1.99697021
1	-1.92977394	5.45593907	-0.25002758
6	-2.58451806	2.94524448	-0.97627634
6	-1.30182069	-0.70473064	-2.44358468
1	-0.50236561	-1.63055497	-4.84762786

6	0.94857933	-3.75869312	-5.77085517
1	1.52068124	-5.17575215	-3.50627557
6	1.06910454	-4.91126178	-0.86076681
1	-0.11338310	2.37564942	4.36545398
1	-0.56601315	0.99789957	3.32348284
1	-1.76699695	1.75130135	4.39339610
1	-1.86149813	2.32524295	-1.53187652
1	-2.81659590	3.81115015	-1.60870347
1	-3.50739047	2.35385767	-0.87165301
1	-1.86664593	7.20390816	2.39488638
1	-0.70417050	7.19622956	1.05829784
1	-0.16123599	6.85197499	2.71799356
1	-1.50688707	-0.16312957	-3.37639648
1	-0.70137516	-0.05185758	-1.79089396
1	-2.26282300	-0.87935489	-1.93664454
1	0.26399932	-5.18320754	-0.16399644
1	1.85030893	-4.40757783	-0.27126315
1	1.49595496	-5.83344225	-1.27629239
1	1.99321991	-3.46352770	-5.95809506
1	0.31954983	-3.22117117	-6.49295734
1	0.87440624	-4.83426897	-5.98477019
1	-2.15781716	0.89113509	0.20030248

Energy = -7584.951080 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 22

Atomic N.	X	Y	Z
8	1.91457612	-2.07611604	-0.72921001
6	2.72601513	-1.01654536	-0.50544584
8	3.42254373	-0.57543571	-1.64128147
6	2.64770722	-0.48406013	-2.84786609
1	1.89372463	0.31313882	-2.76988229
1	2.15381387	-1.43618575	-3.07529183
1	3.36657538	-0.23111659	-3.63616538
8	1.71162027	0.07124122	-0.09258930
6	3.78125891	-1.26100104	0.59333489
1	3.25252999	-1.32861332	1.55901607
1	4.16372726	-2.26949387	0.37903746
6	4.95740781	-0.28045021	0.66933530
1	5.39969331	-0.19245545	-0.33324380
1	5.73237677	-0.72201900	1.31661494
6	4.61157033	1.11258365	1.20578142
1	4.34977783	1.03712870	2.27628530
1	5.51212059	1.74581403	1.15567428
6	3.45781656	1.81926856	0.48198877
1	3.64691514	1.87708281	-0.60039020
1	3.39760813	2.85660220	0.85078969
6	2.08390269	1.19785260	0.73683501
1	2.00536551	0.90789746	1.80047074
1	1.29891382	1.94250749	0.54114094
50	0.22808716	-1.86180397	0.58780597
7	-2.61248716	-1.92818395	1.57271177
6	-2.65779236	-2.51381201	2.91138621
1	-3.65968991	-2.92551381	3.15812239
1	-2.39583191	-1.76543765	3.66919240
1	-1.91924629	-3.32444489	2.97965927
7	-1.78130628	1.03106079	1.59223756

6	-3.49856655	-0.76604797	1.45592039
1	-4.52020938	-1.00758116	1.82677854
1	-3.60525184	-0.52469385	0.38756001
6	-3.01490653	0.48688425	2.18741322
1	-3.84146426	1.22523455	2.16433500
1	-2.82934256	0.26854401	3.24671292
6	-1.27502524	2.22929017	2.17559992
6	-0.64967854	2.19035360	3.44335266
6	-0.12597947	3.37315687	3.98023155
6	-0.18181591	4.59388603	3.29949114
6	-0.77841627	4.60482515	2.03331135
6	-1.33110835	3.45233802	1.46381853
7	-1.09577273	-2.20881227	-1.03170250
6	-2.89780827	-2.95044914	0.55640136
1	-3.97146419	-3.24359812	0.56172254
1	-2.31727898	-3.84627722	0.83095306
6	-2.51025770	-2.55013144	-0.86452430
1	-2.76279966	-3.41580485	-1.50629004
1	-3.17023603	-1.73302490	-1.22376306
6	-0.74343214	-2.12929882	-2.41761180
6	-0.93593608	-0.93002675	-3.14007430
6	-0.65557503	-0.89833301	-4.51288953
6	-0.17172842	-2.01955616	-5.19442166
6	0.03469981	-3.19300168	-4.45905009
6	-0.23719128	-3.26817319	-3.08760785
6	-0.48544810	0.89500392	4.19912403
1	0.36376703	3.32884769	4.95643580
6	0.36689914	5.85866719	3.91472060
1	-0.82423402	5.54098377	1.47118993
6	-1.96125007	3.52509780	0.09204405
6	-1.39020796	0.32849745	-2.44300497
1	-0.81220137	0.03428480	-5.06154907
6	0.15414464	-1.95896494	-6.66769175
1	0.42544519	-4.07911394	-4.96610223
6	0.05003292	-4.54288552	-2.33557889
1	0.37865147	0.95120930	4.87420199
1	-0.33835168	0.05245819	3.50787666
1	-1.36474669	0.66345466	4.82237647
1	-1.37529403	2.97689659	-0.66420958
1	-2.02522573	4.56700539	-0.24555002
1	-2.98046386	3.10870977	0.07843554
1	-0.42046284	6.41566840	4.44711866
1	0.78020988	6.53111083	3.15049088
1	1.15940575	5.63812704	4.64257404
1	-1.48481721	1.15567171	-3.15882147
1	-0.66168018	0.62237740	-1.67118348
1	-2.36247597	0.20118327	-1.94349116
1	-0.79371592	-4.85090663	-1.70241493
1	0.91761382	-4.40458349	-1.67251606
1	0.27891433	-5.36034154	-3.03174834
1	1.23483216	-1.81928642	-6.82934492
1	-0.36305887	-1.12342322	-7.15806523
1	-0.13114479	-2.88815780	-7.18070796
1	-1.93788567	1.17321661	0.59367020

Energy = -7584.951089 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 23

Atomic N.	X	Y	Z
8	0.13200889	-0.31452975	0.35593649
6	1.21168405	-0.82152940	1.02209828
8	1.77486509	-1.94721153	0.39150643
6	1.99987004	-1.80808159	-1.02022742
1	2.66584693	-0.95944666	-1.23282850
1	1.05171686	-1.67466051	-1.55760769
1	2.47792254	-2.74374904	-1.33334916
8	2.19088050	0.33086492	0.94654355
6	0.89953784	-1.23687061	2.47426754
1	0.71245956	-0.31627107	3.05164516
1	-0.06469541	-1.76212273	2.41637841
6	1.91905786	-2.14012386	3.17844236
1	2.11995976	-3.00723206	2.53312285
1	1.45125464	-2.53336639	4.09510708
6	3.23921101	-1.46165520	3.55795910
1	3.05167706	-0.71506414	4.35011484
1	3.91013586	-2.21475628	4.00152567
6	3.96386812	-0.76167719	2.40104205
1	4.13368218	-1.45388105	1.56293138
1	4.95861537	-0.44168245	2.75326658
6	3.26873122	0.50281524	1.89736497
1	2.89519015	1.08367235	2.76160594
1	3.99003779	1.13211827	1.35530369
50	0.18725859	1.82506982	0.68496832
7	-2.00570337	2.34419472	-0.55550442
6	-2.21803180	3.74003050	-0.10899280
1	-3.02869688	4.21990010	-0.68677200
1	-1.30064103	4.32758667	-0.23307375
1	-2.48516020	3.74159969	0.95497481
7	0.77632655	2.35409870	-1.31803819
6	-1.59621867	2.31859260	-1.98264338
1	-2.35530381	2.83818539	-2.60083400
1	-1.55354858	1.26691914	-2.29396483
6	-0.22126260	2.94554232	-2.19954839
1	0.03900553	2.78330368	-3.25894533
1	-0.28905171	4.04991387	-2.08832845
6	2.11470744	2.37176064	-1.78787909
6	3.10732813	3.16763512	-1.15633078
6	4.42800822	3.13746846	-1.62271610
6	4.81646587	2.35138572	-2.71231571
6	3.82912129	1.58566653	-3.34040509
6	2.49860162	1.57749898	-2.90427763
7	-2.76816923	-0.70459401	0.50792183
6	-3.29167418	1.61710918	-0.33810546
1	-4.05280762	2.09309765	-0.99001987
1	-3.58665847	1.79586592	0.70518574
6	-3.32866163	0.10501835	-0.58024712
1	-4.39155340	-0.15403820	-0.68416600
1	-2.87227905	-0.14619439	-1.55640273
6	-3.45589911	-1.91270149	0.81534935
6	-2.92473365	-3.17725094	0.46402990
6	-3.61834590	-4.33764571	0.83231041
6	-4.83466160	-4.29321714	1.52159522
6	-5.34386818	-3.03471472	1.86178437
6	-4.67717997	-1.84947026	1.53131209
6	2.76647550	4.08231909	-0.00359508

1	5.17362481	3.76463200	-1.12612413
6	6.25333448	2.30922528	-3.17439676
1	4.10398319	0.95529392	-4.19079380
6	1.50544750	0.68842138	-3.61109477
6	-1.63054275	-3.29941099	-0.30428364
1	-3.19726457	-5.30753969	0.55473181
6	-5.58504424	-5.55703504	1.86802812
1	-6.27843750	-2.97012914	2.42539181
6	-5.23294562	-0.52622254	1.99568231
1	3.53346354	4.86049042	0.11012381
1	2.70854140	3.54622896	0.95823725
1	1.79171900	4.56778058	-0.14996025
1	0.75094475	0.31675591	-2.90466989
1	2.01339459	-0.16885619	-4.07317506
1	0.97219335	1.21704288	-4.41825494
1	6.76922501	3.25670337	-2.96574378
1	6.32309535	2.11115576	-4.25276184
1	6.81416834	1.51258178	-2.65954408
1	-1.52145999	-4.31451308	-0.70774289
1	-0.74850554	-3.09823499	0.32238663
1	-1.58398392	-2.59060943	-1.14353897
1	-5.72173256	0.03669610	1.18401812
1	-4.42623916	0.11160761	2.38575150
1	-5.98318400	-0.67611711	2.78298532
1	-6.11404330	-5.45891542	2.82640785
1	-4.90791526	-6.41908589	1.93717613
1	-6.34149531	-5.79491606	1.10301114
1	-1.75704763	-0.83852565	0.38967759

Energy = -7584.957708 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 24

Atomic N.	X	Y	Z
8	0.63987745	0.47715555	-0.00114480
6	2.00796853	0.39343406	-0.00211373
8	2.60917438	1.59465672	-0.44671783
6	2.09961811	2.79056854	0.16477059
1	2.27689967	2.78882171	1.25032704
1	1.02569033	2.90461134	-0.02937793
1	2.65700386	3.61436548	-0.29733442
8	2.34852609	0.17504844	1.43275559
6	2.53733551	-0.71950550	-0.93208574
1	2.29484703	-1.68918274	-0.46502517
1	1.91552770	-0.64510506	-1.83443408
6	4.01533324	-0.65587248	-1.33628248
1	4.22595806	0.35433721	-1.71532143
1	4.16986050	-1.34732669	-2.18049109
6	5.00878912	-1.00954125	-0.22547919
1	4.90451052	-2.07997713	0.02772817
1	6.03548273	-0.87981698	-0.60440557
6	4.83391580	-0.20096069	1.06615605
1	4.88358787	0.87996411	0.86569117
1	5.66844094	-0.43958055	1.74665283
6	3.54319352	-0.52401089	1.82460227
1	3.36120023	-1.61573426	1.78253998
1	3.66161894	-0.25543082	2.88560830
50	-0.27337964	-0.77473649	1.43734465

7	-2.94689150	-1.79616751	1.50463844
6	-3.03523948	-2.58066615	2.74169234
1	-4.07106706	-2.91663959	2.94882396
1	-2.69073917	-1.98082715	3.59322783
1	-2.38238386	-3.46063401	2.66680107
7	-1.62114510	0.81150085	1.93680342
6	-3.68784196	-0.52833064	1.61646031
1	-4.70240118	-0.70515170	2.03339854
1	-3.80307814	-0.11222615	0.60634232
6	-2.94766894	0.50445098	2.46722939
1	-3.56798335	1.41619018	2.48185601
1	-2.91533254	0.16290722	3.52408711
6	-1.23775656	2.17838306	2.08011697
6	-0.33093783	2.58365685	3.09091008
6	0.00557968	3.93796025	3.21677475
6	-0.52138854	4.91825955	2.36975371
6	-1.41883919	4.50667062	1.37876582
6	-1.78557181	3.16480608	1.22028479
7	-1.37280115	-2.21147256	-1.02136162
6	-3.38795661	-2.59831881	0.35055964
1	-4.49556386	-2.64282390	0.29669919
1	-3.04342667	-3.63250822	0.51516091
6	-2.84731679	-2.11679040	-0.99384691
1	-3.30683291	-2.73788182	-1.78501146
1	-3.15185889	-1.07944710	-1.18468145
6	-0.72799325	-2.24492984	-2.29621027
6	-0.77135388	-1.13489100	-3.16885850
6	-0.09683616	-1.21547508	-4.39448268
6	0.63948774	-2.34055781	-4.77746943
6	0.70141983	-3.41134953	-3.87850140
6	0.02975677	-3.38701674	-2.65222662
6	0.28988583	1.58554976	4.03802774
1	0.70111011	4.23418701	4.00676057
6	-0.11084317	6.36546002	2.50119210
1	-1.84085313	5.25052198	0.69749663
6	-2.73872194	2.78321404	0.11674713
6	-1.44813949	0.15512763	-2.78198168
1	-0.12630284	-0.34705530	-5.05697824
6	1.33895211	-2.40133722	-6.11372577
1	1.28684215	-4.29686046	-4.13801652
6	0.13847088	-4.57263320	-1.72038507
1	0.68684823	2.09322292	4.92750128
1	1.12967743	1.05493772	3.56045177
1	-0.43293673	0.82457355	4.36307910
1	-2.40980541	1.85516250	-0.36953569
1	-2.80230668	3.57946459	-0.63642163
1	-3.75960896	2.60636602	0.49345415
1	0.10369284	6.62811611	3.54645576
1	-0.89468107	7.04026568	2.13108155
1	0.80164031	6.57361962	1.91976935
1	-1.10876335	0.97086629	-3.43271213
1	-1.19229655	0.42132118	-1.74622552
1	-2.54462416	0.10175166	-2.87059268
1	-0.84572928	-5.00795932	-1.48139015
1	0.62302143	-4.30997646	-0.76502834
1	0.74177235	-5.36546006	-2.17939639
1	2.28751191	-2.95178116	-6.04588811
1	1.55362064	-1.39498150	-6.49741788

1 0.71836348 -2.91406345 -6.86577642
 1 -1.10481506 -3.04848173 -0.50224431
 Energy = -7584.953397 Hartree
 Number of imaginary frequencies = 0.

Compound I4b isomer 25

Atomic N.	X	Y	Z
8	1.08477825	-0.82279380	0.36848200
6	1.55010915	0.15591099	-0.44840967
8	0.43090381	0.69266847	-1.19843916
6	0.76669403	1.60844317	-2.24217740
1	1.25816129	1.09782084	-3.08670323
1	1.41569393	2.42177485	-1.88149432
1	-0.17939484	2.03671377	-2.59831292
8	1.99582723	1.31254861	0.30314739
6	2.66714956	-0.42432473	-1.36877098
1	3.02796370	-1.33136645	-0.86285223
1	2.17537489	-0.77698006	-2.28700793
6	3.87743867	0.45848958	-1.71183634
1	3.56010361	1.45547464	-2.05424035
1	4.39103543	-0.00960195	-2.56819820
6	4.89452086	0.60934023	-0.56841708
1	5.14246402	-0.39610622	-0.18487599
1	5.83247885	1.02374853	-0.97308760
6	4.42779213	1.49358046	0.59326427
1	4.33670550	2.53848036	0.25186038
1	5.19033127	1.48850945	1.39150638
6	3.09025353	1.07949213	1.20329059
1	3.09411468	0.02372302	1.52157288
1	2.88175083	1.68975711	2.09606648
50	-0.72030271	-1.67560635	1.03813893
7	-3.36198916	-1.34711453	1.00237007
6	-4.04414031	-1.61654837	2.27363828
1	-5.14338608	-1.65469982	2.14277831
1	-3.80510821	-0.84966559	3.01670429
1	-3.70276807	-2.58298990	2.66772070
7	-1.54508847	1.02213982	1.40681343
6	-3.64504858	0.00084819	0.48393803
1	-4.73809751	0.18198411	0.41545470
1	-3.24029411	0.05746630	-0.53619235
6	-3.02207079	1.11427658	1.32877673
1	-3.34738038	2.08286816	0.90528137
1	-3.41130708	1.08690929	2.35465899
6	-0.98235734	1.94335377	2.37740312
6	-0.93594570	1.60188125	3.74561058
6	-0.38779575	2.51671521	4.65628207
6	0.11311053	3.75836103	4.25894719
6	0.03737040	4.08379058	2.90061949
6	-0.50353370	3.20577126	1.95515693
7	-1.42433543	-2.19033884	-0.95535613
6	-3.67376336	-2.42571221	0.04342789
1	-4.75341691	-2.42592831	-0.21386062
1	-3.45352457	-3.37219448	0.56184994
6	-2.84759210	-2.34624156	-1.23358336
1	-3.03750504	-3.28260758	-1.79156923
1	-3.26227595	-1.54164793	-1.87255642
6	-0.56807969	-2.45749229	-2.05584856

6	-0.67465964	-1.75207309	-3.28616604
6	0.16743906	-2.08219181	-4.35733251
6	1.13542213	-3.08521651	-4.26853861
6	1.23877724	-3.76983490	-3.05294894
6	0.41645375	-3.48107540	-1.95841677
6	-1.46551917	0.29437987	4.27868460
1	-0.34582369	2.23577329	5.71148966
6	0.73914649	4.70555726	5.25338436
1	0.40912572	5.05329661	2.56007689
6	-0.54342199	3.62363490	0.50639938
6	-1.63934276	-0.60655726	-3.47072828
1	0.06978532	-1.51672605	-5.28854774
6	2.05765597	-3.39607987	-5.42284558
1	1.97954439	-4.56779310	-2.95233711
6	0.59527904	-4.28786099	-0.69657589
1	-0.94914667	0.02267196	5.20855317
1	-1.33311932	-0.52810788	3.56244838
1	-2.53970305	0.36375239	4.51857927
1	0.22153331	3.08037724	-0.06520118
1	-0.33901021	4.69770912	0.41418245
1	-1.51856438	3.42816175	0.03540484
1	0.52963448	5.75316610	4.99660925
1	1.83417040	4.58858133	5.27280187
1	0.37119842	4.51984546	6.27122936
1	-1.28180041	0.06875956	-4.25981454
1	-1.73555493	-0.03327163	-2.53870026
1	-2.64466518	-0.94590129	-3.76765233
1	-0.37095639	-4.55316208	-0.24430982
1	1.16744414	-3.72972775	0.06355381
1	1.15353319	-5.21088528	-0.90393167
1	3.03448087	-2.90164964	-5.29830106
1	1.63517653	-3.05288674	-6.37687931
1	2.25115819	-4.47530661	-5.50297732
1	-1.13129519	1.22776025	0.48783636

Energy = -7584.949097 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 26

Atomic N.	X	Y	Z
8	0.08114573	-0.37705445	0.31150059
6	1.07318047	-1.03354139	0.98333139
8	1.64245079	-2.08680138	0.24276135
6	2.00285328	-1.75940569	-1.10844006
1	2.72668213	-0.93215820	-1.13514955
1	1.11592283	-1.49054444	-1.69723687
1	2.46088952	-2.66792496	-1.51687080
8	2.10358436	0.06155260	1.16122105
6	0.61312536	-1.63479617	2.32709931
1	0.41471096	-0.79745454	3.01654673
1	-0.36376109	-2.09146741	2.11234056
6	1.52492886	-2.68509141	2.97264269
1	1.74642253	-3.46033159	2.22523595
1	0.95947089	-3.17928263	3.77873146
6	2.83294937	-2.14244675	3.55728183
1	2.60632852	-1.50782973	4.43248104
1	3.42798650	-2.98744791	3.93930897
6	3.68892266	-1.32517969	2.58110307

1	3.90445809	-1.89830363	1.66705161
1	4.66039652	-1.11493044	3.05861254
6	3.09722896	0.03519200	2.21366700
1	2.67196014	0.50582016	3.12000991
1	3.89085249	0.69477783	1.83253731
50	0.19819250	1.68610138	0.95998395
7	-1.84123691	2.50198195	-0.37480027
6	-2.03299718	3.82951689	0.25267842
1	-2.76205590	4.43352788	-0.31728020
1	-1.08258810	4.37436346	0.29850998
1	-2.40065088	3.69429701	1.27732748
7	0.99699172	2.46691653	-0.88163453
6	-1.30098145	2.65728205	-1.74925328
1	-1.97606336	3.30072437	-2.34801928
1	-1.27327750	1.65987071	-2.20659393
6	0.11337120	3.23179563	-1.75122805
1	0.46537281	3.20714916	-2.79623408
1	0.08228767	4.31126204	-1.48583892
6	2.37489090	2.48664445	-1.21846947
6	3.32836588	3.13240856	-0.38672846
6	4.68647716	3.10577061	-0.72942280
6	5.15201909	2.46893820	-1.88429182
6	4.20467014	1.85242270	-2.70765657
6	2.83839460	1.84573617	-2.40117391
7	-2.83468722	-0.62020875	0.15380935
6	-3.17256822	1.82577129	-0.37868085
1	-3.84806481	2.43380223	-1.01498456
1	-3.55505923	1.86854464	0.65053628
6	-3.25368166	0.36924594	-0.84586374
1	-4.31248908	0.18975145	-1.07894248
1	-2.71902034	0.23567980	-1.80530396
6	-3.60161224	-1.81788363	0.21764928
6	-3.09574313	-3.04769930	-0.26875509
6	-3.87158067	-4.20700444	-0.13777301
6	-5.14478720	-4.19187156	0.44120136
6	-5.62813766	-2.96776050	0.91730055
6	-4.88139528	-1.78770281	0.82537788
6	2.90924080	3.88518955	0.85397951
1	5.40133814	3.61682676	-0.07851168
6	6.62480435	2.42478485	-2.21420613
1	4.53909405	1.34038080	-3.61433550
6	1.88896476	1.12100628	-3.32315025
6	-1.74112093	-3.13279628	-0.93046460
1	-3.46895632	-5.14990170	-0.51713914
6	-5.97926396	-5.44727078	0.53019750
1	-6.60841403	-2.93080454	1.39992356
6	-5.41997292	-0.51495521	1.42996011
1	3.68829050	4.60009487	1.15187774
1	2.73958431	3.21840575	1.71563720
1	1.97089019	4.43393645	0.69391831
1	1.05153463	0.69320415	-2.75562806
1	2.40816158	0.31231950	-3.85509331
1	1.46382638	1.78780815	-4.09121773
1	6.79251645	2.38096937	-3.29905581
1	7.10526885	1.53630785	-1.77373480
1	7.14993051	3.30646831	-1.82141527
1	-1.63949580	-4.08381761	-1.46929446
1	-0.91435162	-3.07530762	-0.20633903

1	-1.58361498	-2.31448675	-1.64774775
1	-5.80488043	0.18537988	0.67103760
1	-4.62648288	0.01328259	1.97869670
1	-6.24693315	-0.73284693	2.11830933
1	-6.60008149	-5.45235801	1.43706894
1	-5.34955785	-6.34716681	0.54125232
1	-6.66143503	-5.53529048	-0.33058476
1	-1.82392969	-0.79408664	0.10484714

Energy = -7584.957718 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 27

Atomic N.	X	Y	Z
8	0.65297425	0.47712518	0.04027752
6	2.01770285	0.35831337	0.09665648
8	2.66607560	1.54576009	-0.31923033
6	2.17914485	2.75067895	0.29118317
1	2.33910703	2.73721843	1.37950068
1	1.11220223	2.89947048	0.08232235
1	2.76718276	3.56170086	-0.15544421
8	2.29441548	0.12733687	1.54191093
6	2.55888617	-0.76368966	-0.81555029
1	2.27798024	-1.72951582	-0.36254416
1	1.97523701	-0.67394283	-1.74161756
6	4.05287766	-0.72717680	-1.16114741
1	4.29583367	0.28034090	-1.52753890
1	4.22743719	-1.41835473	-2.00162298
6	4.99805361	-1.10230119	-0.01527435
1	4.88187109	-2.17630547	0.21668983
1	6.03955821	-0.97371571	-0.35220435
6	4.78071736	-0.30927893	1.27933669
1	4.86171771	0.77305154	1.09746763
1	5.57884914	-0.57474032	1.99272371
6	3.44968774	-0.61280108	1.97347576
1	3.24073625	-1.69802143	1.90190620
1	3.52638489	-0.36701139	3.04371260
50	-0.35932772	-0.73826166	1.44192881
7	-3.06186229	-1.69964556	1.39350235
6	-3.22829682	-2.46677701	2.63317567
1	-4.28083018	-2.77495276	2.79454118
1	-2.90973876	-1.86530034	3.49365700
1	-2.59475908	-3.36325341	2.59930926
7	-1.69361647	0.88413182	1.85079498
6	-3.77541959	-0.41297659	1.45562910
1	-4.81169849	-0.55947159	1.82871362
1	-3.83549536	-0.00829543	0.43614815
6	-3.04904964	0.61378982	2.32559293
1	-3.64776117	1.53963316	2.30260013
1	-3.07061087	0.28493183	3.38668980
6	-1.28986921	2.24625949	1.98263322
6	-0.42162795	2.65620248	3.02438317
6	-0.06510533	4.00690926	3.13729694
6	-0.53434459	4.97799573	2.24729157
6	-1.39355354	4.56151412	1.22442497
6	-1.77820815	3.22372638	1.07732468
7	-1.37322968	-2.19259620	-1.04248574
6	-3.46677728	-2.50378944	0.22773472

1	-4.57102163	-2.51756084	0.11740874
1	-3.16119893	-3.54523168	0.42097475
6	-2.84411107	-2.05434012	-1.09203002
1	-3.28024948	-2.67120129	-1.89944332
1	-3.10754983	-1.01082711	-1.30884477
6	-0.66743029	-2.27472556	-2.28226038
6	-0.63469121	-1.18388140	-3.18003282
6	0.09511040	-1.31232580	-4.36883859
6	0.81397644	-2.46792342	-4.69116443
6	0.80030526	-3.51843130	-3.76729716
6	0.07149316	-3.44598769	-2.57550999
6	0.13882495	1.66703577	4.01736772
1	0.60005650	4.30755567	3.95135629
6	-0.10271341	6.42018448	2.36569222
1	-1.76909458	5.29781802	0.50861370
6	-2.68522692	2.83477418	-0.06191801
6	-1.28946055	0.13400693	-2.85351688
1	0.12445512	-0.45878663	-5.05047044
6	1.57196955	-2.57943776	-5.99180038
1	1.37039995	-4.42639385	-3.97876527
6	0.10002417	-4.61198510	-1.61349600
1	0.50677787	2.18583784	4.91287344
1	0.98843863	1.11156585	3.58747681
1	-0.61149486	0.92606119	4.32589858
1	-2.34593812	1.89501169	-0.51773476
1	-2.70467171	3.61889546	-0.83007807
1	-3.72418074	2.67577798	0.27067434
1	-0.88780156	7.10477860	2.01617258
1	0.79523919	6.61673897	1.75820738
1	0.14346434	6.68068355	3.40424416
1	-0.89776472	0.92377217	-3.50689564
1	-1.07230870	0.41793679	-1.81349690
1	-2.38201970	0.10974037	-2.98995584
1	-0.90689387	-5.01384086	-1.41374446
1	0.54492643	-4.34034505	-0.64151364
1	0.70163720	-5.43198015	-2.02449209
1	2.44012653	-3.24537068	-5.89455107
1	1.92903386	-1.59765909	-6.33137812
1	0.93343604	-2.98874079	-6.79080612
1	-1.15732454	-3.02511470	-0.49280109

Energy = -7584.953395 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 28

Atomic N.	X	Y	Z
8	0.22507933	-1.69174108	-1.95693859
6	0.95319166	-2.69231159	-1.44569241
8	2.26931351	-2.81275884	-1.94633613
6	2.88894796	-1.58753292	-2.35930881
1	3.00704563	-0.88038429	-1.52028328
1	2.31132522	-1.09973248	-3.15559760
1	3.88069161	-1.87138547	-2.73039826
8	1.02580752	-2.31699894	0.07486471
6	0.27478426	-4.06160224	-1.53119221
1	-0.69787828	-3.94856104	-1.03320910
1	0.06661716	-4.23048319	-2.59852001
6	1.03807549	-5.26100760	-0.96011844

1	1.94208608	-5.44276369	-1.56299078
1	0.39723819	-6.14819175	-1.08782994
6	1.44797678	-5.15616732	0.51838286
1	0.57361712	-4.89618769	1.13851164
1	1.78123382	-6.15107965	0.85329318
6	2.59220224	-4.15922207	0.76212276
1	3.32686677	-4.26528142	-0.04834531
1	3.11550197	-4.40742311	1.70018416
6	2.16408033	-2.69088252	0.87838922
1	1.83624013	-2.48124953	1.90943449
1	3.02069418	-2.03152738	0.65774323
50	0.01929801	-0.16284152	-0.44470733
7	-0.61830158	0.79112909	2.33229875
6	0.35979379	0.36536369	3.33925925
1	0.00289077	0.54752722	4.37426606
1	1.30942025	0.89800817	3.20506647
1	0.55406193	-0.70861776	3.22372073
7	0.58490707	3.31783510	0.85394617
6	-0.95377856	2.22391726	2.48661237
1	-1.35701402	2.39061764	3.50977030
1	-1.75602998	2.46154916	1.77337683
6	0.18242046	3.21997296	2.26326285
1	-0.19581635	4.19979620	2.58463122
1	1.03782647	2.99624047	2.93118049
6	1.50243949	4.35513697	0.52441766
6	2.83355434	4.05522445	0.14491612
6	3.69783489	5.09523038	-0.21406527
6	3.29375730	6.43549110	-0.19955254
6	1.97018408	6.71038946	0.15860819
6	1.06478760	5.70086150	0.50910836
7	-1.95689942	-0.73385168	0.03450111
6	-1.84941215	-0.01883633	2.43303748
1	-2.49216895	0.35326522	3.25963213
1	-1.55157632	-1.04730017	2.67927895
6	-2.65872729	-0.06096387	1.13449586
1	-3.59735710	-0.59526659	1.35062610
1	-2.96682977	0.96535442	0.85219067
6	-2.74531411	-1.65081436	-0.72115786
6	-3.12326664	-1.35351751	-2.05455908
6	-3.91688306	-2.26128053	-2.76610588
6	-4.34848011	-3.47039495	-2.21064676
6	-3.95865922	-3.75794396	-0.89902753
6	-3.16708654	-2.87883298	-0.14886034
6	3.32644453	2.62789016	0.10735295
1	4.72132794	4.84782568	-0.50726019
6	4.25691837	7.54476166	-0.54798999
1	1.61594592	7.74443769	0.14059819
6	-0.37171473	6.06036897	0.79875321
6	-2.68415694	-0.07938185	-2.73277100
1	-4.20866148	-2.01111895	-3.78944110
6	-5.17403327	-4.44642945	-3.01415148
1	-4.26679571	-4.70356311	-0.44483614
6	-2.73409936	-3.28218445	1.23873724
1	4.40411361	2.59808458	-0.09778323
1	2.82276241	2.03766464	-0.67520897
1	3.14982457	2.10417098	1.06003373
1	-1.04766122	5.26663022	0.45043704
1	-0.64032593	7.00024081	0.29872825

1	-0.56071549	6.20415700	1.87513569
1	4.84472752	7.85331398	0.33133277
1	3.72653915	8.43426908	-0.91426433
1	4.97110177	7.22906505	-1.32102495
1	-3.32834415	0.14290925	-3.59386303
1	-1.65454577	-0.17381273	-3.11382777
1	-2.70804549	0.77926879	-2.04758485
1	-1.66957612	-3.05174065	1.39238988
1	-2.88858494	-4.35804190	1.39405138
1	-3.29568671	-2.75515351	2.02659248
1	-4.53185425	-5.09498998	-3.63120369
1	-5.85890788	-3.92496994	-3.69725338
1	-5.76999920	-5.09969850	-2.36259229
1	0.91368891	2.40805405	0.52122668

Energy = -7584.951638 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 29

Atomic N.	X	Y	Z
8	1.56494788	-2.10266440	1.64348877
6	2.78435085	-2.22385914	1.06981578
8	3.07814187	-3.51062934	0.53405860
6	1.97185047	-4.21062791	-0.04176097
1	1.51763470	-3.65662666	-0.88150948
1	1.19390160	-4.41379885	0.70830666
1	2.38239787	-5.15600429	-0.41709876
8	2.75449242	-1.19845201	-0.04076477
6	3.92159712	-1.86395180	2.03611853
1	3.71962336	-0.83311559	2.35940649
1	3.79480133	-2.51222060	2.91632128
6	5.35652233	-1.97804215	1.51291407
1	5.59105552	-3.03623633	1.31566512
1	6.02966756	-1.65667097	2.32419717
6	5.67104935	-1.15906923	0.25086116
1	5.36782502	-0.10823632	0.39154673
1	6.76325521	-1.15216412	0.10852679
6	5.02220284	-1.73692104	-1.01598895
1	5.11767593	-2.83189377	-0.98972447
1	5.56769600	-1.39149357	-1.90960102
6	3.55497389	-1.35079363	-1.23365719
1	3.49444120	-0.35604298	-1.70048206
1	3.07649891	-2.07429794	-1.91569762
50	0.27007959	-0.99393350	0.30255257
7	-1.29812824	-0.89288481	2.29198640
6	-0.66020611	-1.57399945	3.44414660
1	-1.25663101	-1.41394086	4.36044211
1	0.35923090	-1.20715583	3.58734628
1	-0.59088869	-2.64815137	3.23668892
7	0.54373206	0.98270203	1.10769073
6	-1.39626921	0.57134863	2.53017988
1	-1.85233232	0.76587524	3.52086783
1	-2.03842414	0.99111969	1.74669472
6	-0.02645370	1.24177428	2.42451373
1	-0.18447701	2.32554744	2.56418647
1	0.60701461	0.91475863	3.27269473
6	1.36029548	1.97063428	0.51464372
6	2.44829927	2.57535805	1.20530119

6	3.21150064	3.56728321	0.57588595
6	2.96570731	3.98528930	-0.73475229
6	1.90333340	3.37724935	-1.41153003
6	1.10031765	2.39472112	-0.82082472
7	-3.13552060	-0.61154694	-0.19037389
6	-2.62632387	-1.54276494	2.07809630
1	-3.12209306	-1.66175976	3.06063218
1	-2.42009086	-2.55737769	1.70105078
6	-3.63777732	-0.84858206	1.16723158
1	-4.53479746	-1.49969304	1.16771221
1	-3.95427862	0.10178671	1.61957266
6	-4.07972721	-0.33106691	-1.21597407
6	-4.84026425	0.86037694	-1.19521648
6	-5.74637349	1.10745055	-2.23518633
6	-5.90849408	0.23100295	-3.31202031
6	-5.11341690	-0.92137392	-3.33557867
6	-4.21042765	-1.22104570	-2.31110012
6	2.85488606	2.12989562	2.58908065
1	4.04543207	4.00921076	1.12866471
6	3.82998523	5.02633358	-1.40505655
1	1.67128651	3.69376236	-2.43235790
6	-0.05452563	1.83464314	-1.61490266
6	-4.64902107	1.90228517	-0.12089561
1	-6.32365906	2.03526710	-2.21073007
6	-6.90958893	0.51075309	-4.40682050
1	-5.20187802	-1.61603986	-4.17471272
6	-3.37886843	-2.48022010	-2.38893746
1	3.89264598	2.42430846	2.79447419
1	2.77842313	1.03821554	2.68514687
1	2.22759904	2.56842736	3.38110105
1	0.18769900	0.86353534	-2.07970568
1	-0.32817500	2.51733822	-2.43071368
1	-0.93565363	1.66390237	-0.98050259
1	3.24849287	5.63519353	-2.11175656
1	4.64932832	4.56095289	-1.97658954
1	4.28827401	5.70136625	-0.66934601
1	-5.01233926	2.87858378	-0.46657831
1	-3.58538007	2.00345558	0.14027980
1	-5.19647547	1.66251258	0.80469237
1	-3.53175508	-3.13199671	-1.51359268
1	-2.29925254	-2.26406389	-2.44483605
1	-3.64270949	-3.05923684	-3.28260946
1	-6.53259432	0.19058549	-5.38809547
1	-7.14936137	1.58100338	-4.46480191
1	-7.85417739	-0.02809802	-4.23030470
1	-2.52135584	-1.37706515	-0.47209603

Energy = -7584.956532 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 30

Atomic N.	X	Y	Z
8	0.05323932	-1.90091894	-1.67083647
6	1.07187485	-2.59664307	-1.14035075
8	2.37973266	-2.13134741	-1.57521206
6	2.54450619	-2.10210732	-2.99362449
1	1.69459473	-1.60105016	-3.48075513
1	2.66195727	-3.11523884	-3.41576822

1	3.46343485	-1.53382242	-3.18353907
8	1.06332186	-2.24856348	0.30962891
6	0.91354473	-4.11060692	-1.34200624
1	-0.13185552	-4.34993968	-1.09781584
1	1.02825861	-4.30341001	-2.41942078
6	1.85516824	-5.02097345	-0.53856416
1	2.90546154	-4.72961074	-0.70221119
1	1.75627094	-6.03784467	-0.94931845
6	1.52598463	-5.07504066	0.96481698
1	0.42970655	-5.09686614	1.06715759
1	1.88626375	-6.02561505	1.38743135
6	2.08933838	-3.92164351	1.82356437
1	3.09514024	-4.18387672	2.19387300
1	1.45553313	-3.79591441	2.71539434
6	2.23573930	-2.58866657	1.09026204
1	2.37134261	-1.76716985	1.81045171
1	3.10847864	-2.59014244	0.42637859
50	-0.13343048	-0.10735844	-0.49695025
7	-0.73778750	0.86049834	2.21176031
6	0.24666536	0.43009397	3.21195181
1	-0.08360166	0.65373306	4.24708941
1	1.21046972	0.92613950	3.04376537
1	0.40072315	-0.65255617	3.12154829
7	0.57935229	3.33565074	0.72612976
6	-1.03367207	2.30673714	2.33377514
1	-1.45195080	2.50045296	3.34539232
1	-1.81532269	2.55306648	1.60057686
6	0.13322573	3.27004960	2.12378140
1	-0.23322451	4.26321665	2.41744790
1	0.96243278	3.03869574	2.82156148
6	1.55950310	4.32132818	0.41730154
6	2.88319901	3.94692120	0.07948599
6	3.81165772	4.93679045	-0.26026095
6	3.47949359	6.29688226	-0.26636422
6	2.16288786	6.64508544	0.05071673
6	1.19484327	5.68783529	0.38054108
7	-2.11625311	-0.64576153	-0.02436764
6	-1.98896859	0.08683766	2.35464141
1	-2.60624849	0.49825274	3.18121657
1	-1.71221844	-0.94205729	2.62162351
6	-2.81865430	0.03018797	1.06913441
1	-3.74871169	-0.51291961	1.30270076
1	-3.14023244	1.05188722	0.78345050
6	-2.88823046	-1.58764470	-0.76759634
6	-3.30899022	-1.29137978	-2.08735512
6	-4.08715520	-2.21911340	-2.78967153
6	-4.45696359	-3.44984024	-2.23640449
6	-4.01928394	-3.73776742	-0.94010430
6	-3.24141117	-2.83730454	-0.20091566
6	3.30069811	2.49529981	0.06800256
1	4.82881181	4.63326575	-0.52116090
6	4.51069030	7.34984999	-0.59429552
1	1.86532641	7.69642927	0.01602463
6	-0.22831894	6.12541211	0.62513517
6	-2.92458581	0.00318932	-2.76203513
1	-4.41439647	-1.96978696	-3.80254386
6	-5.26945703	-4.44620572	-3.02836838
1	-4.27770906	-4.70036950	-0.49050464

6	-2.75422281	-3.23352244	1.17006389
1	4.37861078	2.40629374	-0.11704612
1	2.78248183	1.91811195	-0.71436931
1	3.08219505	1.99501437	1.02462845
1	-0.93524574	5.36765575	0.25846998
1	-0.43069565	7.07600745	0.11426521
1	-0.44184479	6.28432545	1.69483719
1	5.11019120	7.61115768	0.29240623
1	4.03781278	8.27412657	-0.95296018
1	5.21028009	7.00089795	-1.36653505
1	-3.58279675	0.20405686	-3.61786971
1	-1.89478566	-0.04261798	-3.15327541
1	-2.97326013	0.85740588	-2.07341033
1	-3.30521743	-2.72180179	1.97557424
1	-1.69160551	-2.97632207	1.28995945
1	-2.87745692	-4.31326190	1.32676708
1	-4.63065750	-5.02025648	-3.71828436
1	-6.03499163	-3.94575195	-3.63798897
1	-5.77251637	-5.16679706	-2.36966036
1	0.87348609	2.40856696	0.40903607

Energy = -7584.948970 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 31

Atomic N.	X	Y	Z
8	2.00780848	-0.95442207	1.31649828
6	2.48156076	-2.21393182	1.09839639
8	1.33018989	-3.09877029	1.18414461
6	1.55645611	-4.48652909	0.92192068
1	2.15767137	-4.95660835	1.71873588
1	2.04748425	-4.63955107	-0.04942998
1	0.56585551	-4.95944923	0.90713816
8	2.94500867	-2.40262468	-0.25743560
6	3.55984685	-2.55849635	2.16682274
1	3.95308996	-1.59763596	2.53079728
1	3.02205450	-3.00680795	3.01611654
6	4.73901422	-3.45487528	1.75489565
1	4.38624120	-4.34610547	1.21368378
1	5.21154655	-3.82380780	2.68012880
6	5.81274320	-2.73993797	0.91931921
1	6.09821529	-1.80735883	1.43697022
1	6.72003401	-3.36476268	0.88850820
6	5.39123721	-2.41289226	-0.51714845
1	5.26808719	-3.34521905	-1.09313984
1	6.19145379	-1.83888872	-1.01501400
6	4.09372677	-1.61656274	-0.62627860
1	4.12773165	-0.69448499	-0.02196192
1	3.92467365	-1.31699464	-1.67198018
50	0.34510243	-0.40658216	0.08362317
7	-1.09658090	-0.45256997	2.12630111
6	-0.31147376	-1.04679359	3.23788965
1	-0.87204561	-0.95559068	4.18498133
1	0.65831394	-0.54961653	3.32242629
1	-0.11768020	-2.10268765	3.01637640
7	0.40145892	1.60772568	0.81835952
6	-1.34393905	0.99473968	2.38078642
1	-1.74665303	1.13046379	3.40287024

8	0.98293921	-2.32718950	-0.70144741
6	1.12451303	-3.01262059	0.44179269
8	2.26602804	-3.80913937	0.51739963
6	3.46045517	-3.23470219	-0.04412840
1	3.79550085	-2.37748160	0.55770956
1	3.29425587	-2.91540605	-1.07933531
1	4.21211743	-4.03115404	-0.00339721
8	1.29604642	-1.81734269	1.48550584
6	-0.08045776	-3.89233636	0.82039910
1	-0.92825262	-3.22441388	1.04652530
1	-0.33778386	-4.40843165	-0.11645060
6	0.12563992	-4.92992515	1.92939769
1	1.03154901	-5.50922499	1.70041826
1	-0.71642659	-5.63973876	1.89612479
6	0.22177153	-4.36058355	3.34871144
1	-0.75604905	-3.93659458	3.63940714
1	0.41414276	-5.18943114	4.04881108
6	1.29230868	-3.27945457	3.54897454
1	2.27784773	-3.63248095	3.20999440
1	1.38227186	-3.07439554	4.62882925
6	0.96974907	-1.93946333	2.88560908
1	-0.10218028	-1.70793388	3.03780449
1	1.55420933	-1.14202635	3.37224302
50	0.16054913	-0.40706662	-0.13851326
7	0.49657065	2.08526376	1.21265628
6	1.66492547	1.98677980	2.09402476
1	2.08467976	2.98354772	2.33997900
1	2.44355464	1.37576096	1.62410431
1	1.36638927	1.50114217	3.03325535
7	1.79162407	0.64656069	-1.00508239
6	0.80430525	2.75390592	-0.06211471
1	1.07445637	3.82012836	0.09655494
1	-0.11086330	2.72246703	-0.67312180
6	1.94533085	2.09337596	-0.83739874
1	1.97841982	2.59644201	-1.82266216
1	2.90503065	2.34472660	-0.34640744
6	2.73737978	0.07612269	-1.90842486
6	4.11659918	0.00484927	-1.58307914
6	5.02367226	-0.52244038	-2.51227973
6	4.61800050	-0.99861139	-3.76160212
6	3.25198419	-0.94895162	-4.05993858
6	2.31098789	-0.42549889	-3.16586380
7	-2.48481139	2.07048408	0.45769608
6	-0.59716870	2.74360985	1.96159972
1	-0.20869746	3.66164768	2.45276253
1	-0.89663437	2.05309538	2.76748695
6	-1.83087896	3.17420357	1.17056858
1	-2.51840311	3.63333590	1.90487796
1	-1.55171529	3.97695212	0.47019650
6	-3.88879129	2.09176974	0.28321350
6	-4.51418188	3.14563552	-0.42401383
6	-5.90589992	3.12883778	-0.58446215
6	-6.70407620	2.09025309	-0.09603222
6	-6.06076834	1.03368287	0.56009802
6	-4.67763066	1.01584224	0.76342048
6	4.63253496	0.42475656	-0.22909948
1	6.08055252	-0.57868793	-2.23715275
6	5.61573359	-1.53677439	-4.75876577

1	2.90254340	-1.32935925	-5.02327702
6	0.85463730	-0.42683728	-3.56057099
6	-3.70768273	4.24065613	-1.07868203
1	-6.37399975	3.94674707	-1.13853694
6	-8.20474011	2.10969494	-0.26060318
1	-6.65459843	0.19681511	0.93664738
6	-4.04133635	-0.14689677	1.48704423
1	5.57261304	-0.09371843	0.00223991
1	3.89997354	0.18459011	0.55439651
1	4.83762197	1.50592509	-0.17244631
1	0.31645240	-1.26138304	-3.08164262
1	0.74799154	-0.55796139	-4.64556456
1	0.34958400	0.50444182	-3.26890856
1	5.88102811	-0.77448849	-5.50856710
1	5.21170702	-2.40054985	-5.30515304
1	6.54604354	-1.84816268	-4.26472793
1	-4.30365972	4.74336631	-1.85130363
1	-2.80408081	3.82774132	-1.55170500
1	-3.37847373	5.01282283	-0.36584092
1	-3.48052019	0.17991315	2.37808733
1	-3.33200872	-0.69755057	0.84753742
1	-4.80769204	-0.85873658	1.81834960
1	-8.60494093	1.09915810	-0.42279286
1	-8.50523477	2.73691347	-1.11085406
1	-8.69987378	2.51497232	0.63642389
1	-2.15430951	1.16620913	0.79307208

Energy = -7584.948396 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 33

Atomic N.	X	Y	Z
8	0.50889572	-0.88450881	2.38546223
6	0.17539092	-2.18491227	2.65905620
8	0.14364446	-2.43586999	4.05712002
6	-0.65257122	-1.52739840	4.82492770
1	-1.72490698	-1.66187818	4.61559160
1	-0.37189979	-0.48378836	4.62417506
1	-0.45285224	-1.77095248	5.87536027
8	-1.18850447	-2.32877945	2.09695249
6	1.19355261	-3.19033203	2.07650636
1	1.07309716	-3.19193480	0.98024897
1	2.17378760	-2.73657710	2.28044985
6	1.17752544	-4.61636727	2.64187431
1	1.22468280	-4.55320795	3.73831551
1	2.09908277	-5.12543799	2.31619372
6	-0.02429245	-5.46986047	2.22462197
1	0.04239228	-5.69181848	1.14468648
1	0.03161244	-6.44203109	2.74048447
6	-1.39045354	-4.82804399	2.49657613
1	-1.49799325	-4.56349637	3.55952476
1	-2.17702350	-5.56731759	2.27134009
6	-1.68067137	-3.60086098	1.62924818
1	-1.30947299	-3.78071995	0.60254227
1	-2.76692463	-3.44110878	1.56007163
50	-0.30162612	-0.20110320	0.52941018
7	1.36033244	1.58143159	1.03496621
6	2.67035335	1.07854688	1.49981213

1	3.32596068	1.91143785	1.81212084
1	3.15361737	0.51399948	0.69470833
1	2.49735680	0.40125532	2.34258401
7	2.09331497	0.90253269	-1.85900243
6	1.50328156	2.55784482	-0.08063124
1	1.86891377	3.51828642	0.33118355
1	0.49554716	2.73910363	-0.48151688
6	2.45153305	2.17442496	-1.21709779
1	2.42907705	3.02043206	-1.93277658
1	3.48211036	2.11798188	-0.84152422
6	2.69747661	0.59671932	-3.11111914
6	4.08303259	0.33180191	-3.20257923
6	4.63480205	0.01416673	-4.45091189
6	3.86031831	-0.07828867	-5.61088855
6	2.48324819	0.14460347	-5.49051937
6	1.89042510	0.48422867	-4.27067701
7	-1.45960647	1.46296834	1.19453637
6	0.64471116	2.22611593	2.17786157
1	1.19836335	3.12750359	2.50217755
1	0.65268123	1.49015911	2.99262750
6	-0.79904606	2.58935014	1.83613633
1	-1.28876016	2.87349487	2.78991951
1	-0.82371257	3.50658835	1.20907047
6	-2.84422972	1.63330790	0.89815325
6	-3.27478427	2.31550873	-0.26785101
6	-4.64516017	2.46159955	-0.52261486
6	-5.61846850	1.95048588	0.34143384
6	-5.18293858	1.27797648	1.48875297
6	-3.82367142	1.10943868	1.77971776
6	4.96704072	0.31280097	-1.98038356
1	5.70634383	-0.19417545	-4.50672326
6	4.48478530	-0.39891637	-6.94737486
1	1.84740300	0.05920683	-6.37531175
6	0.39858273	0.71466686	-4.20134230
6	-2.28278546	2.87089292	-1.25978406
1	-4.95865886	2.98712838	-1.42872372
6	-7.08968277	2.08985643	0.03175632
1	-5.92325844	0.87270868	2.18391156
6	-3.41122498	0.36810521	3.02594061
1	5.87663931	-0.26983112	-2.17507092
1	4.44087371	-0.14102787	-1.12790191
1	5.28767108	1.32097977	-1.67282101
1	-0.10649419	-0.01381742	-3.54566746
1	-0.05083520	0.61973081	-5.19754824
1	0.15240311	1.71933808	-3.82187896
1	4.67902963	0.51778051	-7.52673591
1	3.82658235	-1.03358979	-7.55687939
1	5.44466032	-0.91858213	-6.82544172
1	-2.79259224	3.21210406	-2.17002942
1	-1.54259066	2.10840025	-1.54401250
1	-1.72497554	3.72855196	-0.85178257
1	-2.68795121	0.94378202	3.62022262
1	-2.91588184	-0.58308943	2.78091576
1	-4.28570276	0.15169586	3.65415421
1	-7.47585222	1.18988017	-0.47287270
1	-7.28087172	2.94464440	-0.63092410
1	-7.68108140	2.22578606	0.94796371
1	1.07787359	0.83828877	-1.94244688

Energy = -7584.958305 Hartree
Number of imaginary frequencies = 0.

Compound I4b isomer 34

Atomic N.	X	Y	Z
8	1.75718161	-1.56239582	1.07546027
6	1.41921221	-2.54929946	1.95330287
8	0.60064025	-1.91767164	2.97605245
6	0.06162943	-2.76794492	3.99208438
1	0.85178348	-3.15363448	4.65866102
1	-0.49898118	-3.60887223	3.56010634
1	-0.61943872	-2.14235649	4.58360606
8	0.52689241	-3.52543384	1.37065061
6	2.71113724	-3.17994353	2.55050296
1	3.51670744	-2.97572851	1.82960351
1	2.95439769	-2.59438640	3.45021071
6	2.70869241	-4.68116757	2.88151679
1	1.80845229	-4.95766439	3.45149131
1	3.56568265	-4.87296809	3.54804757
6	2.83944231	-5.59769629	1.65467054
1	3.69815069	-5.25675259	1.05010594
1	3.08617072	-6.61742627	1.99203778
6	1.58998809	-5.66121595	0.76981517
1	0.77026006	-6.15660595	1.31616822
1	1.79754367	-6.28247713	-0.11823818
6	1.08566078	-4.30139023	0.29420189
1	1.87842284	-3.72547021	-0.21222434
1	0.26685212	-4.43755099	-0.42888768
50	0.10477524	-0.42095503	0.33572198
7	0.95656195	1.53439153	1.64043019
6	2.03853814	1.05841949	2.53927091
1	2.52654692	1.91938650	3.02924459
1	2.77220110	0.47951941	1.97222744
1	1.61006573	0.38970361	3.29478956
7	1.38037603	0.61849320	-1.03894554
6	1.51506635	2.41629259	0.57691634
1	2.16136203	3.18962255	1.03460584
1	0.67245987	2.90268043	0.07160289
6	2.28394487	1.60483234	-0.46599916
1	2.62751296	2.31036659	-1.24446062
1	3.20260180	1.18856489	-0.00586241
6	1.65650731	0.09418616	-2.32671364
6	2.90480686	-0.49310026	-2.66895718
6	3.11362222	-0.96601942	-3.97182219
6	2.12262377	-0.91307087	-4.95624089
6	0.88789601	-0.35866174	-4.60043566
6	0.63827591	0.14521319	-3.31922297
7	-2.00519774	2.13863543	0.95664065
6	-0.04851301	2.22652527	2.50266091
1	0.48341378	2.95166050	3.14777007
1	-0.46454488	1.45431756	3.16892678
6	-1.18453093	2.98953814	1.82458430
1	-1.77706986	3.43987052	2.64663881
1	-0.78332460	3.83167017	1.24556256
6	-3.24775983	2.65281126	0.49039407
6	-3.29489386	3.75208742	-0.39708255
6	-4.54042898	4.20822125	-0.84853861

6	-5.74239146	3.59978934	-0.47532229
6	-5.67005432	2.48532516	0.36899590
6	-4.45253204	2.00499300	0.86052577
6	3.99305329	-0.68809417	-1.64065785
1	4.08124039	-1.41533821	-4.21306783
6	2.36014420	-1.46879030	-6.34021336
1	0.09452263	-0.29685379	-5.35045208
6	-0.70574362	0.75966211	-3.01626865
6	-2.03881542	4.40212251	-0.92234863
1	-4.56290677	5.05451980	-1.53988685
6	-7.07137425	4.12885425	-0.95775826
1	-6.59060604	1.97356081	0.66062520
6	-4.43455775	0.79424012	1.76478655
1	4.70717579	-1.44862305	-1.98400385
1	3.56672041	-1.01375995	-0.68012886
1	4.56666616	0.23362724	-1.45229770
1	-1.33255008	0.10143534	-2.39195989
1	-1.26004498	0.95651662	-3.94351275
1	-0.59397434	1.69630567	-2.45353355
1	3.42757890	-1.45638663	-6.59959023
1	1.81601194	-0.89294489	-7.10213562
1	2.01645993	-2.51300878	-6.41686083
1	-2.24200060	4.91614806	-1.87061109
1	-1.25535815	3.65103161	-1.09907418
1	-1.63039376	5.15435423	-0.22825146
1	-3.89273300	-0.05389275	1.31451620
1	-5.45691558	0.45363920	1.96990355
1	-3.95652863	1.00731167	2.73469045
1	-6.96323796	4.68064829	-1.90129395
1	-7.51539594	4.81971681	-0.22333531
1	-7.79365266	3.31631853	-1.11685131
1	-2.15718193	1.23842251	1.41272008

Energy = -7584.958176 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 35

Atomic N.	X	Y	Z
8	1.49296939	-1.29752840	0.70721100
6	1.27990493	-2.06515384	1.78803049
8	2.29938717	-1.88199604	2.82473299
6	3.62054330	-2.22132559	2.41912496
1	3.86866708	-1.78031169	1.43955383
1	3.77641159	-3.31335346	2.37048568
1	4.29695417	-1.80884732	3.17956808
8	0.05993885	-1.54565450	2.41690456
6	1.12920165	-3.55750302	1.42459078
1	0.42437315	-3.59018782	0.57922065
1	2.09821713	-3.89036676	1.02180836
6	0.65142329	-4.51878468	2.52278213
1	1.27018081	-4.40974993	3.42860197
1	0.82034209	-5.54572973	2.16159851
6	-0.84257891	-4.36300741	2.85578202
1	-1.38430362	-4.22713573	1.90622522
1	-1.22577936	-5.29979393	3.28917293
6	-1.20065407	-3.20411455	3.80969876
1	-1.17477569	-3.55786119	4.85492193
1	-2.23755128	-2.88821370	3.61950735

6	-0.26179372	-1.99743296	3.75229770
1	-0.73231634	-1.13702091	4.25171381
1	0.67959018	-2.20822361	4.27552908
50	-0.33617274	-0.06259940	0.12994250
7	1.33370779	1.73175039	1.16072645
6	2.59394703	1.28356862	1.78255563
1	3.15675596	2.14901537	2.18258015
1	3.22063695	0.75111357	1.06087325
1	2.36820016	0.57796559	2.58907988
7	1.86718399	0.66710717	-1.45239305
6	1.58963259	2.65312283	0.03594237
1	2.12833058	3.55837295	0.38239431
1	0.61367656	2.97068933	-0.35646726
6	2.39596320	2.00118291	-1.09343925
1	2.34198246	2.65493692	-1.97182278
1	3.46343988	1.93501027	-0.82176678
6	2.02704414	0.24730027	-2.81429987
6	2.90246902	-0.81963787	-3.12419947
6	3.01823049	-1.23920308	-4.45353312
6	2.30086444	-0.63053081	-5.49033152
6	1.42586536	0.40706376	-5.15527210
6	1.26445851	0.85257764	-3.83684028
7	-1.47451022	1.59084541	1.03623113
6	0.50211096	2.36076813	2.21495400
1	1.01019085	3.25953032	2.61798128
1	0.42478942	1.61850397	3.02272598
6	-0.89574600	2.72227798	1.73306223
1	-1.48542482	3.00152011	2.62879055
1	-0.85050976	3.64233395	1.11270452
6	-2.85926419	1.67606579	0.72651212
6	-3.36852407	2.61466505	-0.21235994
6	-4.73995182	2.64468522	-0.49568482
6	-5.64620358	1.76940576	0.10988112
6	-5.13729752	0.84720597	1.03029927
6	-3.77546527	0.78528851	1.34836529
6	3.69565994	-1.51612561	-2.04326102
1	3.69379910	-2.06680935	-4.68342770
6	2.47365595	-1.07570039	-6.92228451
1	0.82487116	0.87407835	-5.93938459
6	0.24465896	1.92171817	-3.53485963
6	-2.45785352	3.56631228	-0.94631197
1	-5.10641416	3.36968980	-1.22794769
6	-7.11423927	1.79369351	-0.24176833
1	-5.82381232	0.15766132	1.52915128
6	-3.30609816	-0.21656457	2.37476738
1	4.32080371	-2.30603922	-2.47763554
1	3.04138617	-1.97652580	-1.28563613
1	4.36507889	-0.82010015	-1.51246018
1	-0.29449133	1.69472499	-2.60374153
1	-0.48881105	1.99281286	-4.34783681
1	0.69648964	2.91979972	-3.41752803
1	3.34472270	-0.58717038	-7.38715768
1	1.59370474	-0.82243403	-7.52855846
1	2.63617826	-2.16027478	-6.98872900
1	-2.90740078	3.87838835	-1.89831267
1	-1.48943367	3.09039339	-1.15562904
1	-2.25430536	4.47996044	-0.36518095
1	-2.56874006	0.22856529	3.05589216

1	-2.81335330	-1.08219956	1.90592046
1	-4.15583112	-0.59547838	2.95883401
1	-7.34175818	1.07861276	-1.04863322
1	-7.42785520	2.78790887	-0.58810911
1	-7.73745636	1.51808487	0.62043670
1	2.26808252	-0.03958857	-0.82686275

Energy = -7584.942574 Hartree

Number of imaginary frequencies = 0.

Compound I4b isomer 36

Atomic N.	X	Y	Z
8	0.61920223	-0.99577660	2.15951312
6	0.44590119	-2.16502562	2.83841587
8	1.67057547	-2.49985814	3.55533298
6	2.79195754	-2.79508535	2.73285839
1	2.89003934	-2.07119283	1.90646458
1	2.74861191	-3.81564527	2.31174118
1	3.67923889	-2.72333042	3.37600109
8	-0.51155118	-1.89350997	3.87017618
6	0.00796379	-3.33886279	1.93188861
1	-0.87071282	-2.99307882	1.36297716
1	0.80436406	-3.50068651	1.18882593
6	-0.34561059	-4.66574570	2.62091962
1	0.45209189	-4.95356169	3.32447720
1	-0.36490341	-5.44891604	1.84604161
6	-1.71603887	-4.65416942	3.31789925
1	-2.44450847	-4.22770587	2.61001345
1	-2.04153676	-5.69226363	3.48751380
6	-1.79093158	-3.88073482	4.65759387
1	-1.76456144	-4.58987552	5.50298921
1	-2.75814244	-3.35954584	4.72600216
6	-0.66013230	-2.88290293	4.90601419
1	-0.87815772	-2.31514314	5.82405679
1	0.29625067	-3.39997263	5.06188147
50	0.00454032	-0.28100544	0.24800876
7	1.35266571	1.59677067	1.14756308
6	2.63271611	1.18122804	1.76627018
1	3.11320775	2.03938061	2.26923883
1	3.31415223	0.78668204	1.00429557
1	2.42001985	0.38888128	2.49132908
7	1.72105073	1.43576579	-1.92917761
6	1.56658807	2.71268405	0.18823259
1	2.04921240	3.55120688	0.72545523
1	0.57520574	3.06247881	-0.13210425
6	2.40495055	2.39395428	-1.04828714
1	2.60442691	3.35741999	-1.55832550
1	3.38446861	1.98857433	-0.76652761
6	2.37245066	1.07846605	-3.14709179
6	3.52370022	0.25977075	-3.13202312
6	4.12394463	-0.08972511	-4.34854977
6	3.60979800	0.32120853	-5.58223211
6	2.44315878	1.09514083	-5.57544386
6	1.81960787	1.48442082	-4.38583850
7	-1.40443632	1.22645938	0.81685165
6	0.41946485	2.03835717	2.23278040
1	0.82285652	2.94530091	2.72053792
1	0.39808227	1.21589637	2.95925764

6	-0.99438810	2.29857145	1.71383566
1	-1.65144092	2.35911769	2.60335998
1	-1.05056070	3.29838082	1.23456987
6	-2.76088864	1.24626225	0.38780062
6	-3.22958701	2.21556829	-0.53963577
6	-4.57188356	2.20955995	-0.93870315
6	-5.48550662	1.26669508	-0.45762496
6	-5.01390601	0.31250504	0.44929144
6	-3.68097919	0.28258948	0.87948576
6	4.07963655	-0.29620599	-1.84471459
1	5.01007746	-0.72905074	-4.32611053
6	4.29171325	-0.04931210	-6.87693000
1	2.00467136	1.41163058	-6.52508080
6	0.55611937	2.31245787	-4.43724221
6	-2.29953083	3.23985902	-1.13922603
1	-4.90878937	2.96104319	-1.65820184
6	-6.92117779	1.25722556	-0.92496533
1	-5.70844261	-0.43152060	0.84895984
6	-3.25454769	-0.77787289	1.86454911
1	4.65914499	-1.20769109	-2.03963498
1	3.26769278	-0.54355310	-1.14564156
1	4.75534609	0.41162484	-1.33727709
1	-0.31484297	1.76635902	-4.03811601
1	0.31713649	2.58341775	-5.47297009
1	0.64695471	3.24879900	-3.86414417
1	4.95949163	0.75732475	-7.21895136
1	3.56214543	-0.22822572	-7.67872309
1	4.90367123	-0.95393702	-6.76173238
1	-2.69137118	3.61176254	-2.09505928
1	-1.30716140	2.79811765	-1.31161292
1	-2.15591650	4.11234938	-0.48185117
1	-2.46553512	-0.43111440	2.54224070
1	-2.85546730	-1.66586294	1.34654122
1	-4.11335858	-1.11990470	2.45810453
1	-7.06138458	0.55812999	-1.76489501
1	-7.23763625	2.25098183	-1.26962006
1	-7.60135960	0.93920588	-0.12254496
1	0.79061933	1.79798491	-2.14134679

Energy = -7584.947844 Hartree

Number of imaginary frequencies = 0.

Transition state 3a (TS3a)

Compound TS3a isomer 1

Atomic N.	X	Y	Z
8	2.68562961	-2.48393750	0.79303700
6	3.58573675	-2.50571370	1.70015228
8	4.88413048	-2.26745439	1.39515769
6	5.14333868	-1.60451758	0.13761768
1	4.79134226	-0.56440216	0.18125364
1	4.65173197	-2.13003993	-0.68960035
1	6.23097801	-1.62546492	0.02057235
8	2.98699141	-0.72573048	2.40217662
6	3.49618816	-3.39935708	2.92078543
1	4.45995903	-3.35878873	3.44719768
1	3.41646433	-4.41541481	2.49546528
6	2.33801961	-3.16501451	3.90486741

1	1.43685865	-2.84829760	3.35851312
1	2.10157037	-4.14137650	4.35597229
6	2.64278293	-2.17867756	5.05413246
1	3.68620324	-2.32876825	5.38437223
1	2.01375437	-2.45947337	5.91379786
6	2.39460182	-0.68878371	4.77824640
1	1.32803810	-0.53033125	4.56111288
1	2.61123800	-0.11912018	5.69882345
6	3.22068787	-0.08133506	3.64805698
1	4.30236673	-0.16035222	3.87220120
1	2.98502946	0.99359483	3.55393863
50	1.66350150	-0.42407620	0.73776072
7	0.15755448	-2.33403778	-0.94525307
6	0.92144907	-3.24330926	-1.81076276
1	0.27327558	-4.00487232	-2.28992057
1	1.44277763	-2.67457986	-2.58944750
1	1.67470765	-3.75361753	-1.19886220
7	0.80221444	-0.17074111	-2.82140207
6	-0.88774812	-1.59534097	-1.67347455
1	-1.73829544	-2.26313114	-1.93140411
1	-1.27990055	-0.82106256	-0.99680179
6	-0.44391489	-0.93398035	-2.98162508
1	-1.28373253	-0.29575521	-3.31045365
1	-0.28246826	-1.68328226	-3.76798081
16	1.20237768	0.97965258	-3.98882914
7	-0.24458136	-1.14445937	1.62764227
6	-0.42334846	-3.10075974	0.17484353
1	-1.14818943	-3.85587811	-0.19742820
1	0.40922424	-3.63443136	0.65318984
6	-1.12893844	-2.23481894	1.22064006
1	-1.38752890	-2.88576126	2.07353282
1	-2.08042526	-1.84563053	0.81379646
16	-0.83552670	0.06978757	2.54591751
8	0.30659282	1.05261827	2.52977991
8	-1.39316881	-0.37383318	3.84322524
6	-2.20794582	0.83601570	1.64092171
6	-3.52214575	0.58808643	2.03883600
6	-4.57262754	1.15646994	1.31308520
6	-4.32779694	1.97123170	0.19826058
6	-2.99354339	2.20609784	-0.17911454
6	-1.93537951	1.64485753	0.53351772
1	-3.70926714	-0.03085703	2.91570759
1	-0.90227562	1.84446681	0.24476992
1	-2.77819586	2.83686686	-1.04400337
6	-5.46358109	2.60686922	-0.56395555
1	-5.60162020	0.96373445	1.62218428
8	2.52128124	1.49985981	-3.58831573
8	0.95753157	0.33833903	-5.29451418
6	0.01300148	2.33444118	-3.82096910
6	-1.10663927	2.38357687	-4.65230894
6	-2.01753569	3.43402576	-4.50458622
6	-1.82213974	4.43534565	-3.54279160
6	-0.67948604	4.36372757	-2.72457981
6	0.23644513	3.32218719	-2.85524821
1	-1.24117351	1.62317264	-5.42089701
1	-2.88970780	3.48092699	-5.15910244
6	-2.80586076	5.56754255	-3.38403010
1	-0.50174689	5.14154243	-1.97937000

1	1.13291788	3.28242111	-2.23614120
1	-6.40885687	2.07590795	-0.39343348
1	-5.60921383	3.65152907	-0.24739072
1	-5.26235151	2.62024188	-1.64389527
1	-2.30122685	6.54284859	-3.43601036
1	-3.57846904	5.54011583	-4.16247606
1	-3.30854321	5.52024508	-2.40577626
1	0.99660265	0.17822056	-1.87290561

Energy = -8524.630260 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 2

Atomic N.	X	Y	Z
8	2.36407414	-1.79993247	-0.05283275
6	3.52404280	-1.54894488	0.43378527
8	4.36044565	-0.70236268	-0.17563020
6	3.79853717	0.15650043	-1.21010297
1	3.01570147	0.80615794	-0.79331513
1	3.38365685	-0.45822772	-2.01736903
1	4.64615202	0.74870616	-1.56586277
8	2.64704746	-0.35092509	1.85842032
6	4.27785923	-2.53434291	1.29657169
1	5.21788180	-2.06222269	1.61350513
1	4.56204999	-3.33622695	0.59154081
6	3.53661031	-3.14584987	2.49711303
1	2.46263888	-3.22675752	2.26738817
1	3.90183079	-4.17817590	2.60946621
6	3.74164593	-2.42859826	3.84866860
1	4.80446760	-2.14228694	3.93817918
1	3.56425983	-3.16694736	4.64705272
6	2.85488356	-1.20974259	4.14363677
1	1.79509158	-1.51201706	4.14179710
1	3.07270237	-0.85764054	5.16621661
6	3.01944923	-0.02545754	3.19757457
1	4.07570827	0.30137445	3.16016901
1	2.41847886	0.82653756	3.54788705
50	0.83440637	-0.42894863	0.82748570
7	-0.56021798	-2.30137446	-0.20869393
6	0.09103672	-3.20761770	-1.18391994
1	-0.60180556	-4.01241605	-1.48725754
1	0.41707518	-2.66158192	-2.07479053
1	0.97563190	-3.64873555	-0.71591629
7	-1.47596310	-0.12399986	-2.63832211
6	-1.86892837	-1.76371980	-0.72481465
1	-2.63370318	-2.53567802	-0.51580569
1	-2.12443733	-0.86827428	-0.14213327
6	-2.00860200	-1.43295519	-2.21617493
1	-3.09466767	-1.37666400	-2.38455734
1	-1.64935867	-2.26259262	-2.84988462
16	0.21448681	-0.20186743	-3.12876863
7	-0.49374872	-1.10113483	2.36845943
6	-0.83083007	-3.08883813	1.02874631
1	-1.53040982	-3.91471975	0.80349123
1	0.12627002	-3.53003269	1.34429886
6	-1.39285333	-2.23422207	2.15871212
1	-1.45294338	-2.85548033	3.06670627
1	-2.41988274	-1.90668744	1.91654212

16	-1.01354524	0.09647885	3.40982725
8	0.07341220	1.10579029	3.35651492
8	-1.42623212	-0.51707712	4.69107660
6	-2.49245943	0.83875454	2.67416452
6	-3.72467589	0.68135375	3.31067008
6	-4.85877654	1.27059414	2.74647082
6	-4.77385672	2.00994203	1.55724633
6	-3.51912140	2.14016490	0.93620259
6	-2.37189348	1.56550248	1.48311675
1	-3.78092604	0.11534767	4.23997441
1	-1.40343701	1.66548075	0.97455073
1	-3.43463043	2.70243286	0.00409476
6	-5.99427942	2.67432661	0.97051676
1	-5.82497022	1.15493824	3.24126158
8	0.43354243	1.08675524	-0.22863112
8	0.34922909	-1.10834436	-4.35116273
6	0.24162806	1.51421409	-3.76202010
6	0.31832702	1.69562254	-5.14049045
6	0.37596703	2.99781344	-5.64633504
6	0.37601518	4.10668132	-4.78746018
6	0.31644814	3.88306670	-3.39966983
6	0.25362129	2.59303119	-2.87257527
1	0.33406020	0.82043507	-5.79235088
1	0.42926425	3.15346885	-6.72584111
6	0.46065509	5.51131628	-5.33284110
1	0.32483912	4.73669971	-2.71818600
1	0.22665082	2.39467202	-1.79565323
1	-6.91886971	2.18552763	1.30436236
1	-6.04855544	3.72975084	1.28016189
1	-5.96873959	2.66104197	-0.12749445
1	1.42282467	5.97854133	-5.07310776
1	0.36595560	5.52336432	-6.42625387
1	-0.32937322	6.15025372	-4.91244584
1	-1.98386915	0.18698130	-3.47495537

Energy = -8524.599811 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 3

Atomic N.	X	Y	Z
8	3.13409901	-2.00595713	-0.40796974
6	4.29999733	-1.87897575	0.10006243
8	5.33705950	-1.42828035	-0.64631289
6	5.00217104	-0.73089796	-1.86676621
1	4.53578854	0.23600042	-1.63173091
1	4.32485437	-1.33074903	-2.48610187
1	5.95659351	-0.57017356	-2.37700796
8	3.74139404	-0.22387832	1.08392906
6	4.81143856	-2.77683973	1.20858812
1	5.88392162	-2.57885623	1.34339273
1	4.73380232	-3.79153514	0.77965790
6	4.08532000	-2.73802829	2.56353831
1	3.00806928	-2.57445312	2.40974331
1	4.18767977	-3.74044704	3.00775194
6	4.64371061	-1.71559954	3.57809281
1	5.74442148	-1.68989778	3.48820853
1	4.43513584	-2.09775448	4.59002304
6	4.08333158	-0.28782752	3.50818324

1	3.00236130	-0.30956107	3.71047306
1	4.53814697	0.30933839	4.31776905
6	4.32177353	0.44970807	2.19369817
1	5.40693235	0.55222064	1.99763560
1	3.90489268	1.47024083	2.26111269
50	1.86349225	-0.14243071	0.04461508
7	0.14951684	-2.27588987	-1.07973456
6	0.66682750	-3.04762816	-2.21826911
1	0.01258362	-3.90664077	-2.47082162
1	0.76669627	-2.40170217	-3.09826636
1	1.66257548	-3.42535067	-1.95748162
7	-0.29238510	-0.03633988	-2.92699766
6	-1.19176948	-1.72112036	-1.32785678
1	-1.96340454	-2.52082229	-1.29580820
1	-1.41883159	-1.02180970	-0.50894469
6	-1.37392402	-0.99691010	-2.66495562
1	-2.36397457	-0.50818050	-2.62324023
1	-1.40219975	-1.70988703	-3.49964333
16	-0.53947228	1.16321278	-4.08764124
7	0.55798143	-1.16628301	1.52735364
6	0.15183501	-3.12650180	0.12709574
1	-0.53482687	-3.99085855	0.00234405
1	1.17367697	-3.51558542	0.23324288
6	-0.23717920	-2.38696170	1.40890968
1	-0.05750024	-3.07067537	2.25641394
1	-1.31905627	-2.15919423	1.40411150
16	0.17830858	-0.06709266	2.67370915
8	1.06876969	1.08930194	2.29872847
8	0.22180320	-0.59864712	4.05442476
6	-1.53176641	0.46664080	2.39017773
6	-2.54625869	0.01511127	3.23502064
6	-3.86453223	0.40744662	2.98711705
6	-4.18207693	1.24679220	1.90945947
6	-3.13958359	1.68837965	1.07519388
6	-1.82026887	1.30439043	1.30864120
1	-2.29467654	-0.62275845	4.08168697
1	-1.01441252	1.66421616	0.66699052
1	-3.36258602	2.34189415	0.22936735
6	-5.60201740	1.69235396	1.66402686
1	-4.65997314	0.05524853	3.64646649
8	0.73542976	1.89706516	-4.16838837
8	-1.14902067	0.48781481	-5.24877071
6	-1.77639663	2.29945588	-3.41191244
6	-3.12002420	2.15062094	-3.75795293
6	-4.06272459	3.03046083	-3.21735477
6	-3.68067336	4.05682755	-2.34199667
6	-2.31736112	4.18778467	-2.01860857
6	-1.36510634	3.31730485	-2.54408598
1	-3.41255999	1.37331128	-4.46312666
1	-5.11351299	2.92245984	-3.49199891
6	-4.69797611	5.00779152	-1.76268566
1	-1.99757648	4.98908854	-1.34957886
1	-0.30701318	3.43483114	-2.30927849
1	-6.32356405	1.01376641	2.13676000
1	-5.77234554	2.69781828	2.07974601
1	-5.82507849	1.74337316	0.58954829
1	-4.44307518	6.05163574	-1.99618053
1	-5.70331240	4.80673122	-2.15321398

1 -4.73627186 4.92682791 -0.66570985
 1 0.18387704 0.34151593 -2.09661770
 Energy = -8524.630265 Hartree
 Number of imaginary frequencies = 0.

Compound TS3a isomer 4

Atomic N.	X	Y	Z
8	2.27844691	-4.00995779	-0.34160188
8	2.80964804	-4.40159655	1.97310007
6	2.75007367	-5.04567385	0.26785260
6	1.94307435	-6.33320904	0.29706076
1	2.37874150	-7.03641367	1.02127743
1	2.10426211	-6.77376604	-0.70206296
6	0.44066840	-6.16686821	0.55359489
1	0.08866182	-5.25961494	0.03976174
1	-0.07698612	-7.01460171	0.07864874
6	0.03627525	-6.13186359	2.03360367
1	0.40307623	-7.05009842	2.52721930
1	-1.06332481	-6.18017435	2.08726597
6	0.50001293	-4.91093254	2.83775973
1	0.13825531	-3.98304248	2.37025976
1	0.02107150	-4.94986343	3.83079123
6	2.00340533	-4.80004692	3.09128761
1	2.39256811	-5.76535606	3.46815228
1	2.17926455	-4.04561901	3.87504220
50	3.07216096	-2.38024545	1.02065873
7	-1.12285876	0.41344732	-0.46590924
6	-2.51283789	0.14631696	-0.10130038
1	-2.56400323	-0.66247559	0.63931459
1	-2.95092392	1.04368711	0.35574892
1	-3.13786650	-0.14425920	-0.97500324
7	0.56359506	3.28000808	-2.26792002
6	-1.01503217	1.56764019	-1.36487854
1	-1.17056847	1.28682721	-2.42844605
1	-1.81277847	2.27711248	-1.10195541
6	0.33907819	2.26940846	-1.20852160
1	1.15485966	1.54053402	-1.31480873
1	0.41500005	2.70906138	-0.20425208
16	-0.04489894	4.85975361	-2.01857138
7	1.00349724	-1.51708066	0.87650961
6	-0.47865054	-0.77464998	-1.03257656
1	-1.12490487	-1.24122477	-1.81337714
1	0.45056924	-0.46716511	-1.53387654
6	-0.12135296	-1.85209930	-0.00427262
1	0.18050541	-2.75781298	-0.55376786
1	-1.00110281	-2.12903666	0.59829247
16	0.74022228	-0.99963617	2.40539575
8	2.03185511	-1.45574152	3.07735443
8	-0.55757177	-1.43343580	2.97206950
6	0.79341483	0.80332184	2.52114463
6	-0.36762196	1.50322962	2.84910822
6	-0.31732079	2.89425445	2.94364786
6	0.87460858	3.59883499	2.71039271
6	2.03051400	2.86352468	2.39758754
6	1.99866307	1.47265494	2.30195618
1	-1.28988385	0.95557058	3.03690648
1	2.90648293	0.91234386	2.07563186

1	2.97132921	3.39020205	2.22817850
6	0.90379184	5.10397911	2.76286840
1	-1.22390532	3.44588280	3.19874239
8	-0.39160198	5.06858158	-0.59408766
8	0.92031455	5.73860788	-2.71265364
6	-1.59040546	4.86778450	-2.94924664
6	-1.55080497	4.74838781	-4.34161997
6	-2.74372482	4.79574537	-5.05730534
6	-3.97820306	4.96767187	-4.40414858
6	-3.98363900	5.09121943	-3.00797510
6	-2.79571438	5.04412365	-2.27301502
1	-0.59648389	4.62487221	-4.85235262
1	-2.71963358	4.70051479	-6.14443207
6	-5.25895119	5.03101349	-5.19743443
1	-4.93143940	5.22866583	-2.48464346
1	-2.79490185	5.14384127	-1.18830919
1	0.24750863	5.49054527	3.55433440
1	1.91983199	5.48062563	2.93769717
1	0.55016297	5.52119970	1.80717802
1	-5.29095125	5.93884373	-5.81866407
1	-5.34768820	4.17232656	-5.87821102
1	-6.13768005	5.04117823	-4.54067612
1	1.55465853	3.42244005	-2.47648621
8	4.11709309	-5.18755484	0.06154199
6	4.81514883	-6.21407509	0.78573549
1	4.60950279	-6.13235903	1.86239779
1	5.87950230	-6.03035355	0.60223752
1	4.55483913	-7.21788025	0.41905338

Energy = -8524.619481 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 5

Atomic N.	X	Y	Z
7	-0.77225477	-0.18359834	2.10477710
6	-1.58923638	0.93686402	2.57148266
1	-1.45891321	1.80683982	1.91550291
1	-2.64982343	0.65373111	2.54490209
1	-1.33560491	1.24665165	3.61030316
7	-1.76254022	-3.44656873	1.71903062
6	-1.02902126	-1.36650264	2.94159675
1	-0.51469958	-1.26211011	3.92458844
1	-2.10595202	-1.41300774	3.15417790
6	-0.61790824	-2.70133495	2.29492640
1	-0.19927329	-3.36302781	3.06601357
1	0.16759099	-2.54676700	1.54076397
16	-2.10061049	-3.31724691	0.04323231
7	1.15459502	0.82400662	-0.21022102
6	0.65877128	0.14755012	2.15809560
1	0.92981058	0.48447901	3.18728924
1	1.24306321	-0.76194513	1.96570420
6	1.14557123	1.23843300	1.20175612
1	2.16411018	1.51128185	1.52828848
1	0.53618866	2.14901280	1.32309365
16	1.21131420	2.00950146	-1.32776713
8	1.71207190	1.26119697	-2.54880500
8	1.92513180	3.23063564	-0.88747519
6	-0.47490248	2.52938056	-1.73620152

6	-0.92908168	3.77711797	-1.30890465
6	-2.23495460	4.16870546	-1.61870122
6	-3.08560371	3.33666515	-2.35962892
6	-2.59727693	2.08636951	-2.78115559
6	-1.30331242	1.67581379	-2.47114897
1	-0.25715554	4.43420839	-0.75808871
1	-0.93326902	0.70657390	-2.80642581
1	-3.24301887	1.42355216	-3.36023521
6	-4.48287010	3.77409983	-2.72262883
1	-2.59323931	5.14490032	-1.28653693
8	-0.98191774	-2.64378691	-0.65162694
8	-2.55430484	-4.67073536	-0.34494585
6	-3.52926493	-2.21941447	-0.02479177
6	-4.80993795	-2.77456880	0.02892426
6	-5.91534615	-1.92719090	-0.03186106
6	-5.75739479	-0.53575331	-0.14754267
6	-4.45671368	-0.01162083	-0.20344058
6	-3.33658934	-0.84376729	-0.14909168
1	-4.92836523	-3.85473967	0.10506504
1	-6.91945219	-2.35350752	0.00863811
6	-6.96095943	0.36897731	-0.23936847
1	-4.31184387	1.06657112	-0.29334551
1	-2.32651067	-0.43590638	-0.18331577
1	-4.78758478	4.66004133	-2.15114093
1	-4.54981279	4.02621555	-3.79206610
1	-5.21362066	2.97366285	-2.53743291
1	-7.34149456	0.40915063	-1.27217209
1	-7.78263760	0.00911965	0.39447662
1	-6.71421814	1.39536905	0.06185851
1	-1.69567180	-4.45394993	1.87875736
8	2.94529462	-1.61282587	0.54767835
8	4.09938478	-0.73121840	-1.39679968
6	4.09983921	-1.89299953	0.05728870
6	5.35840893	-1.58814311	0.85061586
1	6.24354839	-1.67913616	0.20516358
1	5.42130470	-2.41111970	1.58416426
6	5.36700010	-0.23991863	1.58115864
1	4.35322189	-0.03085934	1.95537663
1	6.01152372	-0.34233195	2.46798563
6	5.88579035	0.94428307	0.75306129
1	6.89595032	0.70166707	0.37594467
1	6.01736259	1.80136704	1.43338871
6	5.00870323	1.39875400	-0.42061788
1	3.99751091	1.65373826	-0.06942549
1	5.42884874	2.33709502	-0.82079214
6	4.90427446	0.43357840	-1.60236406
1	5.91822720	0.10633636	-1.90528750
1	4.46422911	0.96827340	-2.46085501
50	1.86073244	-0.98918515	-1.38433719
8	4.09255600	-3.08213925	-0.65398878
6	5.27060461	-3.44869614	-1.39220262
1	5.58036375	-2.62395644	-2.04908872
1	4.97787762	-4.31168842	-2.00009561
1	6.09338617	-3.74050260	-0.72314972

Energy = -8524.613383 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 6

Atomic N.	X	Y	Z
8	0.51504230	-0.22923706	0.75196141
6	1.26633978	0.63481909	1.31558490
8	2.15596724	0.27938220	2.27140713
6	2.48572183	-1.12823832	2.39201808
1	2.90825915	-1.51328969	1.45339108
1	1.60518658	-1.71879971	2.66935849
1	3.24133110	-1.17146993	3.18257833
8	2.49033451	0.84217012	-0.32794920
6	0.83257437	2.08125544	1.49796259
1	0.60370862	2.17634988	2.57235122
1	-0.11408406	2.19020987	0.95326936
6	1.78392947	3.22409010	1.08189809
1	1.67650366	3.38214183	0.00004873
1	1.38973379	4.13332224	1.56318700
6	3.28692341	3.08805156	1.41364276
1	3.42904139	2.48324490	2.32220173
1	3.67568541	4.09095669	1.65033543
6	4.14136839	2.52286625	0.26408842
1	3.98074102	3.14084864	-0.63492191
1	5.20992088	2.61901641	0.52129799
6	3.87513590	1.05789173	-0.08151841
1	4.22598886	0.42250970	0.75538242
1	4.45895672	0.77257323	-0.97612023
50	1.66080523	-0.97350377	-1.22311842
7	-1.24237716	-1.88475978	-1.65824258
6	-1.02698195	-2.64960051	-2.89769316
1	-1.96452439	-2.76976585	-3.47845483
1	-0.28172410	-2.16167784	-3.53728938
1	-0.65203029	-3.64715195	-2.63592196
7	0.45206720	0.27409360	-2.64327216
6	-1.77508199	-0.53822207	-1.92874098
1	-2.82636833	-0.59036070	-2.29029822
1	-1.77490008	0.02021339	-0.98212320
6	-0.97910362	0.25133172	-2.96823382
1	-1.39444077	1.27528143	-2.98184752
1	-1.13897288	-0.17536850	-3.97118592
16	1.48664224	0.49762478	-3.89367580
7	-1.47598147	-2.15268636	1.59276688
6	-2.18233204	-2.66238761	-0.82230943
1	-3.14998698	-2.76375365	-1.36451125
1	-1.76983905	-3.67206097	-0.69808710
6	-2.52131987	-2.10565948	0.56606889
1	-3.38371944	-2.67923808	0.93816876
1	-2.86217666	-1.06174707	0.50608420
16	-1.16714537	-3.61738658	2.35881782
8	0.13590297	-3.43155384	3.03568268
8	-1.38847566	-4.77833557	1.46578348
6	-2.46910810	-3.67878580	3.61132479
6	-3.37499785	-4.73777771	3.60463190
6	-4.35105562	-4.80281305	4.60354757
6	-4.42813396	-3.82731891	5.60657358
6	-3.49803615	-2.77114868	5.58742952
6	-2.52038836	-2.69085908	4.59993505
1	-3.30650616	-5.49692726	2.82640600
1	-1.80039644	-1.87306571	4.59038401
1	-3.54247522	-2.00234580	6.36118412

6	-5.47180605	-3.90593600	6.69221783
1	-5.06375933	-5.62937164	4.60164452
8	2.79504395	0.03189588	-3.29638433
8	1.03949332	-0.10511058	-5.17201853
6	1.63661301	2.27394724	-4.19048786
6	1.43721747	2.78288174	-5.47255945
6	1.56579387	4.15930271	-5.68031025
6	1.89006841	5.02532291	-4.62661457
6	2.07964921	4.47943544	-3.34344053
6	1.95461035	3.11106873	-3.11788583
1	1.18749380	2.10490513	-6.28770304
1	1.41150808	4.56576443	-6.68150520
6	2.04661965	6.50753927	-4.85752678
1	2.32907796	5.14021349	-2.51039100
1	2.09777617	2.67963314	-2.12534952
1	-6.19303560	-4.70949507	6.49773121
1	-5.00639677	-4.09958553	7.67050457
1	-6.02567577	-2.96039128	6.78151083
1	3.10060573	6.80999136	-4.76115179
1	1.70560241	6.79564238	-5.85985184
1	1.47661185	7.08905077	-4.11896276
1	-0.60426021	-1.64965200	1.36729562

Energy = -8524.630838 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 7

Atomic N.	X	Y	Z
8	3.14160490	-1.92838049	-0.12710710
6	4.29605532	-1.44919729	0.10860164
8	4.75133514	-0.60658288	-0.86685991
6	5.94942141	0.15769476	-0.62733614
1	6.84017849	-0.48566791	-0.61150694
1	5.85074472	0.71651405	0.31302023
1	6.01923990	0.85499650	-1.46844828
8	3.66819239	-0.00658457	1.35832310
6	5.31649685	-2.21112800	0.92519581
1	6.10867786	-1.53103912	1.26658499
1	5.79040003	-2.89633965	0.19818354
6	4.75345850	-3.01356530	2.10614657
1	3.75634050	-3.39460063	1.83841419
1	5.39794350	-3.89530039	2.24522352
6	4.69072008	-2.25994539	3.44441390
1	5.68673229	-1.83356273	3.66309023
1	4.50549936	-3.00586367	4.23449898
6	3.62896824	-1.15892553	3.57792878
1	2.63320518	-1.56218386	3.33635402
1	3.58435655	-0.85492724	4.63764477
6	3.86225677	0.11809464	2.76641870
1	4.89553547	0.48075008	2.93886161
1	3.17803502	0.90097445	3.13315821
50	1.80157495	-0.06282590	0.18351354
7	0.23069911	-2.17914653	-1.06009960
6	0.84088290	-2.88203144	-2.19815826
1	0.23851030	-3.75614667	-2.51793480
1	0.95903391	-2.19663835	-3.04524374
1	1.83767867	-3.22651243	-1.89897203
7	-0.24639356	0.10367968	-2.87450361

6	-1.12050247	-1.67142987	-1.35662246
1	-1.85714602	-2.50359917	-1.37817156
1	-1.41321528	-1.00443089	-0.53172946
6	-1.28009522	-0.92328411	-2.68267465
1	-2.29795957	-0.49300137	-2.67476034
1	-1.22930908	-1.61455238	-3.53425646
16	-0.49921340	1.29229414	-4.04535580
7	0.44759732	-1.13769698	1.58457494
6	0.20293497	-3.07522893	0.11394353
1	-0.44669038	-3.95576644	-0.07730162
1	1.22992897	-3.43542814	0.25927880
6	-0.27781153	-2.39351916	1.39732373
1	-0.10280769	-3.09081078	2.23464489
1	-1.36827147	-2.21818519	1.34871233
16	-0.07246463	-0.07841741	2.71586895
8	0.80172420	1.11694610	2.45238328
8	-0.14132214	-0.65176940	4.07858849
6	-1.76792061	0.40142787	2.28464818
6	-2.84132719	-0.13734671	2.99510980
6	-4.14471769	0.21034478	2.62908173
6	-4.38991833	1.09153426	1.56618345
6	-3.28964806	1.62252069	0.86953884
6	-1.98438513	1.28338945	1.22139859
1	-2.64806867	-0.80704069	3.83249855
1	-1.13439488	1.71159816	0.68787402
1	-3.45550609	2.31083274	0.03831084
6	-5.79690027	1.48705792	1.19296050
1	-4.98580885	-0.21047495	3.18321705
8	0.72897118	2.10491729	-4.05279684
8	-1.00004339	0.58490163	-5.23902750
6	-1.84097683	2.34915257	-3.44338322
6	-3.15314698	2.10948539	-3.85384631
6	-4.17657375	2.93346357	-3.37584877
6	-3.90583372	3.99478960	-2.50045848
6	-2.57195711	4.21826458	-2.11210895
6	-1.54039729	3.40367770	-2.57416534
1	-3.35900354	1.30691862	-4.56134415
1	-5.20290947	2.75447035	-3.70135379
6	-5.01087189	4.88213921	-1.98443282
1	-2.33847117	5.04872656	-1.44294596
1	-0.50502056	3.59335852	-2.29043007
1	-6.53102875	0.76314199	1.56924736
1	-6.05227137	2.46965837	1.61961579
1	-5.91400385	1.56610930	0.10338912
1	-4.78392076	5.94322205	-2.16090059
1	-5.96894264	4.65201426	-2.46698356
1	-5.14089251	4.75985909	-0.89810759
1	0.16313075	0.50015825	-2.01879287

Energy = -8524.624279 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 8

Atomic N.	X	Y	Z
8	0.95261723	-0.34340042	0.67327452
6	2.07389116	-0.27901205	1.27996290
8	2.73070335	-1.47121584	1.33758748
6	4.05782652	-1.51840460	1.89787030

1	4.03361320	-1.33123696	2.97950220
1	4.70593309	-0.79679382	1.38200223
1	4.41098785	-2.53768063	1.71270680
8	3.12224722	0.39558139	-0.30964547
6	2.32914639	0.72521687	2.37909937
1	3.40934992	0.89079785	2.49162102
1	1.99248493	0.20681565	3.29590845
6	1.59036791	2.05811262	2.23272848
1	0.57009244	1.86568522	1.86763096
1	1.48555636	2.49099207	3.23979330
6	2.27972126	3.09742069	1.33810675
1	3.29982829	3.28561568	1.71869111
1	1.73491597	4.04823351	1.45865059
6	2.35882688	2.77669430	-0.16302951
1	1.37288880	2.44117093	-0.52492732
1	2.59473467	3.71508074	-0.69469005
6	3.42034721	1.75599670	-0.59720451
1	4.38308954	2.01295733	-0.11115790
1	3.57695580	1.84607685	-1.68589413
50	1.82122588	-1.01233506	-1.45812941
7	-0.96744692	-1.90213645	-1.49192119
6	-0.87723798	-2.62998223	-2.76955271
1	-1.87932706	-2.81506085	-3.20671201
1	-0.27271822	-2.07988644	-3.50163198
1	-0.39438185	-3.59942651	-2.58964610
7	0.41796023	0.44481307	-2.57613897
6	-1.64249420	-0.60246682	-1.64397871
1	-2.72176671	-0.72937053	-1.88287306
1	-1.57406175	-0.07231594	-0.68396020
6	-1.03885889	0.27812204	-2.73968697
1	-1.54724133	1.25714803	-2.67917800
1	-1.27295554	-0.14656231	-3.72908092
16	1.25138891	0.64385200	-3.97743320
7	-1.18150365	-1.82483137	1.80169153
6	-1.67308104	-2.79819918	-0.53860646
1	-2.58039069	-3.19843817	-1.04311013
1	-1.01361239	-3.65231061	-0.32938436
6	-2.17086267	-2.20970726	0.78702950
1	-2.82996559	-2.97045517	1.23142934
1	-2.81313586	-1.33449900	0.60619694
16	-0.63651693	-3.02395916	2.85530758
8	0.51291418	-2.41979194	3.56357026
8	-0.50108218	-4.34532118	2.19699574
6	-2.02364874	-3.16378236	4.00825834
6	-2.65575051	-4.39496565	4.17102289
6	-3.69143558	-4.50933743	5.10341644
6	-4.09901953	-3.41111422	5.87240744
6	-3.43918967	-2.18166304	5.68785095
6	-2.40573168	-2.05096245	4.76443768
1	-2.33069515	-5.24646235	3.57416916
1	-1.89375937	-1.09912145	4.62633896
1	-3.74070525	-1.31621635	6.28115940
6	-5.21798801	-3.53365970	6.87612867
1	-4.18920612	-5.47172928	5.23480797
8	2.67733097	0.44442898	-3.53212309
8	0.76116914	-0.18804787	-5.10735083
6	1.06478834	2.36055303	-4.53066254
6	1.00420082	2.61717653	-5.90240574

6	0.88967192	3.93626070	-6.34227037
6	0.82749516	5.00388050	-5.43265295
6	0.87266791	4.71330404	-4.05971670
6	0.99369437	3.40039468	-3.60288811
1	1.03546679	1.78610814	-6.60563660
1	0.84138101	4.13979101	-7.41370392
6	0.73371261	6.42841625	-5.91873932
1	0.80896521	5.52812672	-3.33586121
1	1.01915288	3.18042278	-2.53676534
1	-5.59428692	-4.56264448	6.93319750
1	-4.88307476	-3.23585868	7.88049746
1	-6.06070280	-2.87782955	6.61094522
1	1.73798811	6.85295630	-6.07418728
1	0.20117676	6.49160147	-6.87689638
1	0.21744944	7.06830454	-5.19104052
1	-0.36209062	-1.29991353	1.43847966

Energy = -8524.621130 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 9

Atomic N.	X	Y	Z
8	3.50428391	0.41259390	2.06569982
6	4.34262466	-0.04647584	1.16957724
8	4.70906305	-1.35587001	1.20960641
6	3.74269938	-2.28783536	1.75840771
1	2.90896130	-2.41391587	1.05702972
1	3.36107063	-1.93296862	2.72119570
1	4.29268789	-3.22718120	1.87654400
8	3.22144866	0.08758817	-0.21736197
6	5.58700275	0.76703787	0.80494654
1	6.25137711	0.12721252	0.20644122
1	6.08915710	0.91534919	1.77436709
6	5.39500809	2.12000656	0.10901596
1	4.49836636	2.63298202	0.50135344
1	6.24332809	2.76168418	0.39360139
6	5.35339165	2.05611181	-1.42886400
1	6.21648073	1.45846295	-1.77125418
1	5.51335001	3.07216430	-1.82427013
6	4.07142448	1.49827921	-2.06089330
1	3.23019624	2.18962216	-1.88691282
1	4.20453548	1.45445168	-3.15523243
6	3.64954638	0.11076132	-1.58337724
1	4.47676468	-0.61522174	-1.67953753
1	2.81131148	-0.25911689	-2.19413090
50	1.90536880	1.43658006	0.93545473
7	-1.24884248	2.83376431	1.72103941
6	-0.72098571	4.05582190	2.31825447
1	-1.47741246	4.59547377	2.92876887
1	0.13543934	3.82175875	2.96538067
1	-0.36379090	4.73024035	1.52783155
7	0.11802830	0.24110994	1.78579342
6	-1.56291974	1.81517649	2.73220158
1	-1.92675781	2.27353477	3.67592549
1	-2.37080717	1.16848218	2.36368775
6	-0.34076425	0.93241203	3.02001357
1	-0.57378620	0.21160920	3.81827927
1	0.47685692	1.55619216	3.42689013

16	0.07649962	-1.42439997	1.86270666
7	-1.66216528	1.03728151	-0.50616634
6	-2.31883764	3.12636590	0.76920706
1	-3.22761202	3.54976773	1.25698948
1	-1.93461251	3.89445496	0.08168741
6	-2.75841641	1.90306640	-0.05678658
1	-3.32567549	2.25392675	-0.92876995
1	-3.43635416	1.25975227	0.52482200
16	-0.77940696	1.44074333	-1.86627698
8	0.66136080	1.28592491	-1.49326813
8	-1.27745819	2.70483303	-2.44738960
6	-1.12068546	0.11526462	-3.03921103
6	-1.86028409	0.39335033	-4.18712759
6	-2.11401200	-0.64039975	-5.09295845
6	-1.63824511	-1.93885636	-4.86285877
6	-0.89530247	-2.18430233	-3.69338536
6	-0.62749106	-1.16832304	-2.77885604
1	-2.22052217	1.40562069	-4.36648178
1	-0.05098621	-1.37038612	-1.87378001
1	-0.51838005	-3.18956947	-3.49575353
6	-1.89552414	-3.04798818	-5.85169268
1	-2.69058156	-0.43046129	-5.99557924
8	0.53663975	-1.88484931	0.52703071
8	0.72735125	-1.95431578	3.08710384
6	-1.67919517	-1.87774777	2.02645564
6	-2.18100929	-2.21596217	3.28548765
6	-3.52427626	-2.57578325	3.41376257
6	-4.37421274	-2.61724043	2.29820633
6	-3.84035945	-2.28539777	1.04150701
6	-2.50210309	-1.91887915	0.89758158
1	-1.51268220	-2.21678829	4.14591980
1	-3.91636825	-2.83838248	4.39828396
6	-5.81438684	-3.04393673	2.43643546
1	-4.48233843	-2.31975532	0.15891749
1	-2.09784698	-1.66784322	-0.08172987
1	-2.65714097	-2.76146889	-6.58784437
1	-0.97645366	-3.30240679	-6.40159225
1	-2.23028445	-3.96399927	-5.34507895
1	-5.92128754	-4.12377357	2.24832749
1	-6.19577503	-2.84841800	3.44718599
1	-6.45843983	-2.52331448	1.71507668
1	-1.00884557	0.76671767	0.26442054

Energy = -8524.621619 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 10

Atomic N.	X	Y	Z
8	4.63341713	1.38985872	-2.37532139
6	4.47861052	2.63410234	-2.08529377
8	3.33446550	3.16532063	-2.60901546
6	3.02028036	4.54108858	-2.33459210
1	3.71829367	5.22635555	-2.83632588
1	3.01273322	4.72548866	-1.25085306
1	2.01441908	4.69510794	-2.73952365
8	3.91734338	2.42728424	-0.26528811
6	5.69383049	3.54251528	-2.00614047
1	5.42989302	4.50037193	-1.53714931

1	5.92363691	3.76821971	-3.06281352
6	6.93081903	2.93866134	-1.32735944
1	6.95313215	1.85476351	-1.51777899
1	7.82248640	3.35499978	-1.82003069
6	7.05027342	3.22688532	0.17644086
1	6.99431038	4.31864548	0.33656630
1	8.05933666	2.92735362	0.50244850
6	6.03028774	2.53958035	1.09276891
1	6.11505270	1.44299090	0.99962842
1	6.29186821	2.77656221	2.13855076
6	4.56358671	2.94124913	0.89562672
1	4.48231840	4.04615927	0.89375025
1	3.98649478	2.58986735	1.77328825
50	3.87839913	0.17084385	-0.71749312
7	-0.18893319	0.85713637	1.43175387
6	0.07398251	1.04223013	2.85879946
1	-0.27850622	2.02711010	3.24024963
1	-0.40803891	0.24876416	3.44302011
1	1.15567756	0.97520566	3.03402877
7	-2.13201785	-1.33853507	1.89177167
6	-1.61338937	0.97005928	1.12008929
1	-1.98014760	2.01415443	1.27309430
1	-1.75118148	0.74614882	0.05100405
6	-2.54632926	0.07202225	1.93462539
1	-3.56558347	0.22215088	1.53273857
1	-2.56367517	0.37439755	2.98949265
16	-3.12921143	-2.45538974	2.67902040
7	1.68391132	0.39375797	-1.07087600
6	0.58141792	1.82449841	0.64118367
1	0.13493033	2.84423614	0.71823192
1	1.58776927	1.89440060	1.07867169
6	0.74108785	1.49713373	-0.84666049
1	1.10568094	2.40569329	-1.35077477
1	-0.23098414	1.25921476	-1.30638266
16	1.44452202	-0.60785258	-2.33472395
8	2.82872343	-1.22183073	-2.47517395
8	0.80771559	0.00262681	-3.52113986
6	0.36475682	-1.97058964	-1.82471037
6	-0.52930212	-2.50271297	-2.75489330
6	-1.29662359	-3.61500263	-2.40006876
6	-1.18413103	-4.20080614	-1.12998462
6	-0.29598397	-3.62396097	-0.20326950
6	0.48008466	-2.51614618	-0.54337752
1	-0.61233574	-2.04769540	-3.74117374
1	1.15583241	-2.06648421	0.18409637
1	-0.22644608	-4.04126692	0.80211425
6	-1.97195244	-5.43328667	-0.76411533
1	-1.99016249	-4.03964806	-3.12856269
8	-2.56087375	-3.77994967	2.35941982
8	-3.27306938	-1.97619832	4.06596756
6	-4.76330614	-2.35066485	1.90623772
6	-5.78959846	-1.66468263	2.55655980
6	-7.04364681	-1.57950926	1.94625759
6	-7.28499985	-2.16843319	0.69676328
6	-6.23054123	-2.85068035	0.06381376
6	-4.97449493	-2.94729757	0.65898150
1	-5.60363579	-1.22032118	3.53368425
1	-7.84993124	-1.04689789	2.45372248

6	-8.64722919	-2.09803963	0.05424999
1	-6.39994907	-3.31778884	-0.90818292
1	-4.16674900	-3.49070978	0.16863948
1	-2.84109735	-5.56531048	-1.42228889
1	-1.34567976	-6.33373070	-0.86293787
1	-2.31362724	-5.38939476	0.27895305
1	-9.18256187	-3.05312109	0.17028178
1	-9.26546288	-1.31369126	0.50884777
1	-8.57160187	-1.89932680	-1.02366066
1	-1.87839174	-1.68825996	0.96250224

Energy = -8524.616624 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 11

Atomic N.	X	Y	Z
8	3.08626819	-0.58829570	1.14798462
6	4.19592476	-0.16895100	0.70795017
8	4.91793013	-0.87816715	-0.19444197
6	4.29408121	-2.05194306	-0.77241963
1	3.61879826	-1.76304281	-1.59116817
1	3.73351955	-2.60807657	-0.01162075
1	5.12247801	-2.64522886	-1.17257559
8	3.19035959	1.24435222	-0.56129187
6	5.10300350	0.76558125	1.49639249
1	6.02434254	0.19414796	1.69043386
1	4.61174393	0.92688632	2.46535611
6	5.48662472	2.13225698	0.89056998
1	4.62484503	2.80983090	0.96719551
1	6.26304150	2.54322147	1.55589533
6	6.00241184	2.15223479	-0.56697512
1	6.44210291	1.17749751	-0.83076382
1	6.82265663	2.88393998	-0.63293195
6	4.94348764	2.54373693	-1.61380029
1	4.49955034	3.51218367	-1.32461941
1	5.43331766	2.69820476	-2.59054017
6	3.82519436	1.51439905	-1.79114890
1	4.26071596	0.59265012	-2.23172760
1	3.09856224	1.89239538	-2.54495120
50	1.38374841	-0.19390576	-0.38286942
7	0.59677780	1.83427942	0.94098538
6	1.53936315	2.00573993	2.07265997
1	1.15642571	2.76336575	2.77977943
1	1.68705189	1.05382740	2.59146976
1	2.50403237	2.33190775	1.67013478
7	-0.04144778	-0.82228988	1.29267395
6	-0.75090963	1.46735585	1.44187844
1	-1.13992047	2.25587344	2.11411428
1	-1.41988730	1.38373435	0.57552683
6	-0.72813314	0.11979384	2.16640759
1	-1.78023410	-0.17062688	2.34669709
1	-0.24621557	0.20469846	3.15543604
16	0.14912684	-2.36510801	1.80749774
7	-0.20140800	2.17544746	-1.97771168
6	0.59871113	3.10958695	0.17481951
1	0.40066832	3.94927001	0.86900526
1	1.62450051	3.22648168	-0.20676088
6	-0.40107009	3.23217821	-0.97182846

1	-0.29635611	4.24258614	-1.40034699
1	-1.43347549	3.15280747	-0.60362524
16	-1.36942220	2.14647508	-3.24941397
8	-0.74791539	1.31073904	-4.29302406
8	-1.84866476	3.51318693	-3.55246735
6	-2.71795249	1.25796080	-2.45290947
6	-3.94775605	1.89484322	-2.29006124
6	-4.99473238	1.19367790	-1.68575811
6	-4.82242632	-0.12536596	-1.24179447
6	-3.56883383	-0.73941541	-1.42198360
6	-2.51650357	-0.05965517	-2.02928329
1	-4.07305145	2.92062759	-2.63511848
1	-1.54618478	-0.53839862	-2.16607165
1	-3.41196179	-1.76053917	-1.07001281
6	-5.95168400	-0.88237888	-0.58994514
1	-5.96068335	1.68418932	-1.55442548
8	1.09138632	-2.97370124	0.82454485
8	0.42185125	-2.45301962	3.26294088
6	-1.45285487	-3.18454194	1.55000043
6	-2.38769865	-3.22714329	2.58521223
6	-3.62380219	-3.84387016	2.36698818
6	-3.93321061	-4.43473816	1.13384557
6	-2.96663928	-4.39086342	0.11273945
6	-1.73543286	-3.76770234	0.31100476
1	-2.13456631	-2.80490756	3.55744958
1	-4.35507631	-3.87903666	3.17700529
6	-5.25555086	-5.12596512	0.90928984
1	-3.18149161	-4.85892296	-0.85059136
1	-0.98047239	-3.74618578	-0.47504804
1	-6.81150055	-0.23042369	-0.39153266
1	-6.29324532	-1.70600677	-1.23503423
1	-5.62898350	-1.33110464	0.36033031
1	-5.11897516	-6.21217442	0.79654622
1	-5.94190264	-4.96013737	1.74939239
1	-5.74404669	-4.76817274	-0.00887620
1	0.70767683	2.24585390	-2.45068312

Energy = -8524.617853 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 12

Atomic N.	X	Y	Z
8	3.56028414	0.88814795	0.71614999
6	4.59547329	0.92017436	-0.03333074
8	5.55397749	-0.03248129	0.06661408
6	5.17970514	-1.26176393	0.72744572
1	4.46026468	-1.81722510	0.10973359
1	4.74554205	-1.05867767	1.71356034
1	6.10875988	-1.83202279	0.82113302
8	3.53441000	0.28483185	-1.60732961
6	5.20360994	2.21546960	-0.53258884
1	6.17041636	1.98274589	-1.00027061
1	5.43177748	2.77126551	0.39401239
6	4.35764170	3.09960866	-1.46374190
1	3.29584193	3.03728151	-1.18153024
1	4.66759491	4.14052248	-1.28195357
6	4.52893162	2.81524181	-2.97250628
1	5.58939886	2.57883596	-3.17202044

1	4.32354069	3.75083661	-3.51658368
6	3.63091159	1.72945321	-3.58242369
1	2.57696748	2.02668905	-3.47859025
1	3.83183479	1.67366350	-4.66658545
6	3.80492449	0.32859427	-3.00278234
1	4.84082699	-0.03047450	-3.15917253
1	3.13385010	-0.37460685	-3.52711725
50	1.81641960	-0.12783374	-0.38555267
7	0.82970870	1.13579297	2.10033250
6	1.64233804	0.99324429	3.31644106
1	1.25795412	1.61627734	4.14936161
1	1.66601980	-0.05561027	3.63409925
1	2.66853833	1.30332315	3.08631134
7	0.03324711	-1.66916251	2.42773485
6	-0.57496572	0.74285573	2.30266380
1	-1.11698067	1.50477529	2.90403080
1	-1.05675614	0.71102190	1.31368995
6	-0.79364729	-0.60010195	3.00590682
1	-1.87348092	-0.82112777	2.92946267
1	-0.55498713	-0.52912450	4.07542276
16	-0.38682610	-3.27387667	2.73592138
7	0.66761708	1.75269926	-0.69044679
6	0.92245042	2.52628827	1.61250448
1	0.49574736	3.23438764	2.35457897
1	1.99283946	2.74902201	1.50525272
6	0.22603443	2.76158786	0.27055916
1	0.48416248	3.78067017	-0.06537287
1	-0.87155122	2.73484945	0.40072203
16	-0.09427821	1.62399578	-2.12903333
8	0.50564981	0.35778221	-2.68350434
8	-0.05776885	2.86061430	-2.94157624
6	-1.84582090	1.28402627	-1.80340910
6	-2.79176188	2.29151249	-1.99184418
6	-4.13497686	2.02714348	-1.70758605
6	-4.54461288	0.77071679	-1.24014938
6	-3.56981134	-0.22824745	-1.06303430
6	-2.22741103	0.02047567	-1.34037352
1	-2.47357631	3.26168060	-2.37196732
1	-1.47998118	-0.76467651	-1.21686375
1	-3.86517620	-1.21592188	-0.70287234
6	-5.99604368	0.48221910	-0.94804555
1	-4.87744761	2.81342745	-1.85566151
8	0.66810554	-4.08223772	2.10018229
8	-0.69184607	-3.34652114	4.17734861
6	-1.92732167	-3.59452677	1.84048867
6	-3.15010905	-3.50754523	2.50703430
6	-4.33001900	-3.75063682	1.79720080
6	-4.30324793	-4.08363676	0.43559611
6	-3.05478430	-4.17009544	-0.20810452
6	-1.86958468	-3.92751646	0.48251212
1	-3.16861796	-3.27945900	3.57225013
1	-5.28814459	-3.69107437	2.31658149
6	-5.57575893	-4.35808706	-0.32612711
1	-3.01205206	-4.43892336	-1.26539481
1	-0.90277827	-4.01760626	-0.01316646
1	-6.60435057	1.39396286	-0.99787295
1	-6.40729809	-0.23658565	-1.67307568
1	-6.12029648	0.03940864	0.05056443

1 -5.59056091 -5.38801193 -0.71214187
 1 -6.46057892 -4.22170067 0.30802068
 1 -5.67067480 -3.69039083 -1.19540036
 1 0.31256977 -1.53963196 1.44567919
 Energy = -8524.630262 Hartree
 Number of imaginary frequencies = 0.

Compound TS3a isomer 13

Atomic N.	X	Y	Z
8	3.00710988	-0.43046829	1.31710398
6	4.08156919	-0.29310125	0.66798711
8	4.24653006	-1.19132721	-0.34611744
6	5.49637079	-1.33841038	-1.04751170
1	6.23174429	-1.85765231	-0.41648695
1	5.89768648	-0.37705636	-1.38705897
1	5.26275730	-1.96210551	-1.91671228
8	3.14764738	1.27723384	-0.43638444
6	5.29587650	0.38001120	1.29117906
1	6.21070528	-0.14448678	0.98003411
1	5.17817307	0.19683143	2.36977935
6	5.49701929	1.89561725	1.08288622
1	4.59266186	2.42662644	1.40792394
1	6.29653263	2.17966032	1.78629565
6	5.90293837	2.37582922	-0.33132809
1	6.48398209	1.58935940	-0.84277362
1	6.60647345	3.21494579	-0.21091785
6	4.76578856	2.86596775	-1.24534142
1	4.25255632	3.70427632	-0.74342030
1	5.20134974	3.27258444	-2.17460990
6	3.71743965	1.80713046	-1.60138881
1	4.17761040	1.01657176	-2.23499846
1	2.94892049	2.28361487	-2.25473690
50	1.33222556	-0.25874290	-0.25129199
7	0.44208521	1.84233356	0.93758678
6	1.33711994	2.08100295	2.09410930
1	0.93268311	2.88580060	2.73473883
1	1.45402515	1.16480005	2.68028569
1	2.32247710	2.36691189	1.71128881
7	-0.16057685	-0.80086523	1.39837146
6	-0.91938311	1.47854364	1.39821982
1	-1.35005260	2.29152298	2.01437473
1	-1.54907560	1.34221768	0.50939381
6	-0.91032851	0.16776955	2.18698311
1	-1.96499968	-0.13574292	2.32679224
1	-0.48296186	0.30919531	3.19447756
16	0.02320884	-2.31420851	1.99428308
7	-0.25814164	2.02726460	-2.02077079
6	0.45454663	3.07815862	0.11236201
1	0.21460997	3.94753647	0.75588715
1	1.49274731	3.19882631	-0.23126857
6	-0.50125617	3.13111353	-1.07727706
1	-0.38853431	4.11966181	-1.55246150
1	-1.54603350	3.06106257	-0.74368250
16	-1.36986089	1.92844784	-3.33547282
8	-0.69390702	1.06134796	-4.31838083
8	-1.85812879	3.27286744	-3.71544814
6	-2.73773837	1.04976177	-2.56075954

6	-3.99079657	1.65866160	-2.50395727
6	-5.05233288	0.96244973	-1.91943061
6	-4.87172031	-0.32354021	-1.39025021
6	-3.59428239	-0.90993810	-1.46373272
6	-2.52704024	-0.23521794	-2.05016732
1	-4.12223291	2.65970159	-2.91331244
1	-1.53838658	-0.69248915	-2.10416818
1	-3.43074751	-1.90415585	-1.04411304
6	-6.01606035	-1.07442856	-0.75773430
1	-6.03659582	1.43129492	-1.87087452
8	1.03211534	-2.94453216	1.09668982
8	0.20853677	-2.33052874	3.46644998
6	-1.54805791	-3.17449617	1.68212116
6	-2.54546309	-3.18273187	2.65834999
6	-3.75816536	-3.82705736	2.39399529
6	-3.98269749	-4.48021317	1.17381454
6	-2.95474958	-4.47031546	0.21380071
6	-1.74568796	-3.82010126	0.45780405
1	-2.35892248	-2.71020103	3.62249470
1	-4.53875589	-3.83381200	3.15747619
6	-5.27862930	-5.20456505	0.90382564
1	-3.10390735	-4.98522711	-0.73797768
1	-0.94339257	-3.82365394	-0.28030491
1	-6.90965271	-0.44433784	-0.66721404
1	-6.28303671	-1.95745742	-1.35768831
1	-5.74366951	-1.43712223	0.24373804
1	-5.13449764	-6.29543161	0.93642604
1	-6.04381084	-4.94766855	1.64759123
1	-5.67295456	-4.96341848	-0.09383686
1	0.67140442	2.07229328	-2.45555830

Energy = -8524.606278 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 14

Atomic N.	X	Y	Z
8	3.42723346	1.19353306	0.66862947
6	4.46603870	0.79517251	0.05212472
8	4.82901382	-0.48700276	0.35773486
6	5.86186886	-1.12517262	-0.41871166
1	6.84686995	-0.68027616	-0.22006497
1	5.61192513	-1.06723607	-1.48663568
1	5.86254883	-2.17048335	-0.09328630
8	3.52593350	0.34391764	-1.66526234
6	5.55056143	1.75951433	-0.37521791
1	6.19077969	1.29227138	-1.13576829
1	6.17955732	1.87898338	0.52630424
6	5.06321764	3.13328552	-0.85542619
1	4.16666985	3.41623139	-0.28333351
1	5.84165430	3.86896539	-0.60051328
6	4.78588343	3.24376893	-2.36327648
1	5.67712736	2.89845562	-2.91834450
1	4.68229723	4.31490088	-2.60179329
6	3.54333520	2.51910257	-2.90033221
1	2.65073705	2.83057380	-2.33577013
1	3.37684321	2.85144329	-3.93918324
6	3.60550666	0.98977405	-2.93516660
1	4.54822445	0.67038137	-3.42319465

1	2.77529860	0.61524498	-3.55643916
50	1.77339268	-0.04584772	-0.38228866
7	0.66454780	1.21206200	2.00084949
6	1.45547462	1.11335170	3.23626614
1	1.03106320	1.73294973	4.05184078
1	1.50914288	0.06986666	3.56723404
1	2.47528577	1.45455301	3.02335262
7	-0.07804168	-1.62244439	2.38538337
6	-0.73168057	0.77502078	2.17693186
1	-1.31370687	1.53653705	2.73991132
1	-1.18475521	0.69894755	1.17693496
6	-0.93166125	-0.55036873	2.91640568
1	-2.00638652	-0.79323334	2.83118153
1	-0.70965165	-0.44270039	3.98633385
16	-0.45453218	-3.22013211	2.77716041
7	0.53429425	1.75610709	-0.79362291
6	0.71463287	2.59869099	1.49401498
1	0.23658386	3.29853201	2.21208620
1	1.77646089	2.86642218	1.41388547
6	0.04540766	2.77949953	0.12934001
1	0.28292954	3.79557753	-0.23000935
1	-1.05374146	2.72563052	0.23511025
16	-0.22536761	1.54657352	-2.22579026
8	0.44802016	0.31273910	-2.76114941
8	-0.27881604	2.77201509	-3.05402327
6	-1.94836915	1.09891582	-1.87685275
6	-2.95661998	2.04994965	-2.03798485
6	-4.27570105	1.70418596	-1.73081970
6	-4.60130072	0.42088482	-1.26896489
6	-3.56601000	-0.51918542	-1.11901677
6	-2.24581194	-0.18846653	-1.41906929
1	-2.70410490	3.04053259	-2.41486168
1	-1.44939041	-0.92723602	-1.31692016
1	-3.79501820	-1.52505887	-0.76120275
6	-6.02969217	0.04256924	-0.96580309
1	-5.06590271	2.44683123	-1.85584819
8	0.61268985	-4.03548098	2.17294359
8	-0.74593884	-3.22455573	4.22323084
6	-1.99540973	-3.62532330	1.91625345
6	-3.21645594	-3.50442100	2.58120823
6	-4.39611435	-3.81790805	1.89937115
6	-4.37118912	-4.25556087	0.56748629
6	-3.12454605	-4.37764597	-0.07353650
6	-1.93952823	-4.06411362	0.58877367
1	-3.23341417	-3.19810700	3.62663698
1	-5.35236931	-3.73284292	2.41868877
6	-5.64471674	-4.59157848	-0.16736352
1	-3.08265948	-4.73137903	-1.10556829
1	-0.97349066	-4.18202353	0.09748349
1	-6.65709114	0.93029243	-0.81474513
1	-6.46561241	-0.53396899	-1.79662323
1	-6.09431839	-0.58536631	-0.06647662
1	-5.59108925	-5.59237432	-0.61902380
1	-6.51362562	-4.56378698	0.50192511
1	-5.82667255	-3.88026428	-0.98771060
1	0.20145290	-1.53321159	1.39997816

Energy = -8524.624277 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 15

Atomic N.	X	Y	Z
8	3.36084723	-1.64441133	-0.00329949
6	4.35154629	-1.56804693	0.80070031
8	5.46907711	-0.88090068	0.46182719
6	5.34290791	0.06927197	-0.61950481
1	4.71861982	0.91707891	-0.30460998
1	4.90760279	-0.40470791	-1.50720263
1	6.36222649	0.41178778	-0.82143724
8	3.37791228	-0.24554053	1.94906271
6	4.69976282	-2.67339969	1.77711475
1	5.67606354	-2.44106555	2.22482371
1	4.85614252	-3.55431151	1.12968183
6	3.67649007	-3.01863217	2.87178230
1	2.65380764	-2.89355016	2.48521376
1	3.79673743	-4.09061289	3.09317183
6	3.84722304	-2.24348712	4.19706869
1	4.92594624	-2.12527704	4.40365362
1	3.45462298	-2.87555575	5.00941753
6	3.14597249	-0.88167673	4.30267429
1	2.05909681	-1.02218711	4.20836210
1	3.31905484	-0.47357422	5.31380224
6	3.59385610	0.17009118	3.29176211
1	4.67350149	0.38679162	3.40957022
1	3.05011487	1.11391079	3.47437215
50	1.79999173	-0.03387681	0.50723886
7	0.67610371	-1.93403912	-1.46310580
6	1.54055548	-2.37038183	-2.56846428
1	1.07573974	-3.18118286	-3.16538024
1	1.76691782	-1.52419603	-3.22745109
1	2.48421741	-2.73674798	-2.14725637
7	0.41553843	0.65604693	-2.81882954
6	-0.62518060	-1.42249846	-1.92473412
1	-1.27631545	-2.25321722	-2.27394176
1	-1.12708116	-0.96216661	-1.06020486
6	-0.57084560	-0.40473253	-3.06800175
1	-1.59476435	-0.00443663	-3.17896366
1	-0.31079805	-0.89104515	-4.01756954
16	0.31475326	2.07983208	-3.71866512
7	0.31882390	-1.47079110	1.34051871
6	0.49637902	-3.05095124	-0.51442677
1	-0.03028373	-3.90042257	-0.99942029
1	1.50373924	-3.38912368	-0.23565012
6	-0.27193913	-2.67208719	0.75344771
1	-0.21652114	-3.52964640	1.44592249
1	-1.34135091	-2.51722169	0.51958621
16	-0.45390138	-0.70944780	2.56118488
8	0.35432056	0.55511802	2.69662142
8	-0.67953765	-1.55815208	3.75259995
6	-2.09770942	-0.22553776	1.96605372
6	-3.22330260	-0.92969668	2.39467478
6	-4.48135996	-0.56670725	1.90567231
6	-4.63002968	0.49141842	0.99762285
6	-3.47865987	1.18523586	0.58396918
6	-2.21735597	0.83395845	1.06143439
1	-3.10726404	-1.73984146	3.11384177

1	-1.33039701	1.38763440	0.74942189
1	-3.56950665	2.01280713	-0.12258583
6	-5.99259615	0.89891738	0.49525285
1	-5.36355305	-1.11595047	2.23964095
8	1.46598315	2.89399338	-3.29168987
8	0.10398472	1.66393876	-5.11817217
6	-1.18538749	2.93707848	-3.17784071
6	-2.36873436	2.79213405	-3.90295339
6	-3.51986527	3.45404506	-3.46494055
6	-3.50227499	4.26073265	-2.31838870
6	-2.29232669	4.39417887	-1.61227357
6	-1.13695455	3.73860025	-2.03178310
1	-2.37435770	2.19077086	-4.81146049
1	-4.44553995	3.34936786	-4.03362274
6	-4.74274158	4.98019266	-1.85101914
1	-2.25470495	5.02799559	-0.72409922
1	-0.19563083	3.86207199	-1.49586225
1	-6.72842455	0.09660050	0.63403809
1	-6.36016798	1.78343010	1.03852308
1	-5.96312904	1.16253138	-0.57093221
1	-4.57981920	6.06721020	-1.81414700
1	-5.59356546	4.78654718	-2.51603007
1	-5.02483797	4.66545010	-0.83497965
1	0.62253594	0.85426497	-1.83042693

Energy = -8524.630258 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 16

Atomic N.	X	Y	Z
8	1.69223559	-1.14926016	0.47290325
6	2.78289533	-1.09755516	1.13811624
8	3.89976072	-1.69728231	0.68194306
6	3.94465303	-1.98158967	-0.73602968
1	3.75546169	-1.06397831	-1.30720830
1	3.20939660	-2.75434756	-0.99165022
1	4.95947170	-2.34653807	-0.92093539
8	3.13126969	0.80523551	0.52819037
6	2.82504773	-1.00120461	2.65018916
1	3.87558770	-1.04357457	2.96865487
1	2.35982275	-1.94657385	2.98102212
6	2.10766745	0.18070357	3.32044935
1	1.19957745	0.44732159	2.75388265
1	1.74921942	-0.17573881	4.29870319
6	2.97701597	1.43005395	3.57586884
1	3.95854259	1.10029459	3.95976377
1	2.51196837	1.99968517	4.39679146
6	3.19498873	2.40057874	2.40566945
1	2.22472739	2.82581687	2.09310603
1	3.79695702	3.25261760	2.76614404
6	3.88880515	1.81994724	1.17282259
1	4.86397839	1.38045204	1.45724165
1	4.09382296	2.62608743	0.44649181
50	1.11925042	1.01320696	-0.22500163
7	-0.51306802	-1.20249081	-1.71969974
6	0.09006662	-2.54475212	-1.77407384
1	-0.41139168	-3.17838264	-2.53341079
1	1.15465510	-2.47055936	-2.01853466

1	0.00880411	-3.04443336	-0.80455303
7	1.59185266	0.75164855	-2.38606763
6	-0.40857661	-0.54710388	-3.03470254
1	-0.81253105	-1.19451213	-3.84349298
1	-1.01296735	0.37162080	-3.00422096
6	1.03125000	-0.15693963	-3.38865829
1	1.01063466	0.31987369	-4.38274145
1	1.66566324	-1.05177724	-3.49372458
16	2.24662161	2.17193365	-2.85474610
7	-1.24128473	-1.69248652	1.20505631
6	-1.91395342	-1.29192519	-1.24516630
1	-2.52482724	-0.55974895	-1.79651141
1	-2.33044600	-2.29205394	-1.45519733
6	-2.07881331	-0.95878643	0.24823676
1	-3.13316011	-1.10707521	0.52742589
1	-1.85127461	0.10777215	0.40178868
16	-1.68274379	-3.24881244	1.67880273
8	-0.43279082	-3.86464834	2.17303944
8	-2.50556755	-3.91055179	0.63969368
6	-2.77422404	-2.94756269	3.08689213
6	-4.13028622	-3.25142646	2.98288488
6	-4.96003246	-3.04025793	4.08828211
6	-4.44989300	-2.53646374	5.29221153
6	-3.07512951	-2.24481201	5.36782837
6	-2.23537874	-2.44724703	4.27646875
1	-4.51992702	-3.65598059	2.04954791
1	-1.16962695	-2.22952127	4.34166622
1	-2.65904975	-1.85628963	6.29933786
6	-5.34247971	-2.32252526	6.48877144
1	-6.02283096	-3.27666712	4.01209211
8	2.35183072	2.89977813	-1.53427494
8	3.44912696	2.04798675	-3.70556021
6	1.01998198	3.06462908	-3.85070920
6	1.24806762	3.26210928	-5.21262360
6	0.29256895	3.94287181	-5.97227097
6	-0.88325638	4.43505144	-5.38838911
6	-1.08532596	4.22373486	-4.01248169
6	-0.14516310	3.54203820	-3.24299836
1	2.17133212	2.89428973	-5.65899515
1	0.46822903	4.09747267	-7.03842926
6	-1.89618587	5.19864082	-6.20394278
1	-1.99225724	4.60398149	-3.53833055
1	-0.30374229	3.39479136	-2.17339635
1	-6.39680815	-2.49395943	6.23834133
1	-5.07374477	-3.00761867	7.30696678
1	-5.24422312	-1.29997253	6.88088322
1	-1.79764247	6.28190756	-6.03292751
1	-1.76343596	5.01958227	-7.27847576
1	-2.92323232	4.92066479	-5.93001509
1	-0.22553600	-1.64939308	1.03597438

Energy = -8524.629864 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 17

Atomic N.	X	Y	Z
8	2.20507813	-1.01538789	3.13033867
6	3.13424373	-1.81792009	2.73329997

8	2.67878795	-3.09895730	2.52516556
6	3.61011147	-4.08362055	2.05216408
1	4.35442972	-4.34399557	2.81901956
1	4.11318684	-3.73455763	1.13820589
1	3.00848436	-4.97037411	1.82411110
8	3.25800109	-1.28284514	0.95452195
6	4.53042459	-1.68463838	3.32519484
1	5.26587868	-2.21065211	2.69981003
1	4.47307110	-2.24433994	4.27515316
6	4.98804665	-0.24906604	3.60607362
1	4.12468004	0.33629090	3.95629978
1	5.70483732	-0.27955949	4.44097185
6	5.66697073	0.45436373	2.42482066
1	6.54583359	-0.13663857	2.10956669
1	6.06451273	1.41806948	2.78151202
6	4.78941202	0.72230691	1.19625175
1	3.90927768	1.32567286	1.47671318
1	5.36521196	1.34606719	0.49166751
6	4.33091068	-0.50885606	0.40425736
1	5.19588375	-1.17881191	0.23445711
1	3.99065685	-0.16682974	-0.58894563
50	1.26246858	-0.19782262	1.32453644
7	1.07179546	-1.36818826	-1.52451241
6	2.18315077	-1.33623743	-2.48317409
1	1.95546281	-1.91499519	-3.40229869
1	2.41810083	-0.30226874	-2.76256776
1	3.06952000	-1.77960265	-2.01279926
7	0.65585411	1.47007000	-1.95476294
6	-0.17945556	-0.86602062	-2.11400080
1	-0.57352972	-1.57008815	-2.87928057
1	-0.92534482	-0.80964816	-1.30796766
6	-0.07186189	0.50436240	-2.79167962
1	-1.10427690	0.83220637	-3.00955749
1	0.45342642	0.43208048	-3.75318980
16	0.51896316	3.11461258	-2.31695628
7	-0.11197956	-1.88818228	1.01901495
6	0.91560245	-2.74888492	-1.02461994
1	0.72917330	-3.45422316	-1.86318982
1	1.87391770	-3.01937461	-0.55869150
6	-0.20646843	-2.92515469	-0.00106921
1	-0.10718959	-3.93408442	0.43469554
1	-1.18925238	-2.88887239	-0.50731260
16	-1.29502594	-1.75623083	2.14107513
8	-0.84960496	-0.54446924	2.91248775
8	-1.60286593	-3.01878929	2.84463143
6	-2.81101274	-1.29176044	1.25737536
6	-3.81610489	-2.23992324	1.06257701
6	-4.96336794	-1.88179135	0.34930164
6	-5.12209463	-0.58818293	-0.16850936
6	-4.09491730	0.34825310	0.04458841
6	-2.94394851	0.00500493	0.75209153
1	-3.69776702	-3.23871970	1.48151278
1	-2.15906286	0.74199873	0.92823899
1	-4.19624281	1.36138785	-0.34996575
6	-6.37685013	-0.19747683	-0.90906197
1	-5.75044203	-2.62246680	0.19552736
8	1.40309381	3.79812837	-1.35701120
8	0.68771011	3.22541022	-3.77824283

6	-1.18163240	3.59589505	-1.92708766
6	-2.13660002	3.65963316	-2.94232392
6	-3.44774413	4.02267408	-2.61967778
6	-3.81412148	4.32528973	-1.30060196
6	-2.82793140	4.25679398	-0.29906794
6	-1.51732635	3.89492917	-0.60179514
1	-1.84424758	3.45175982	-3.97114038
1	-4.19647837	4.08063126	-3.41173005
6	-5.22498178	4.73197222	-0.95593882
1	-3.09125209	4.49728107	0.73273760
1	-0.75076020	3.86471391	0.17286332
1	-6.86792850	-1.07136703	-1.35648644
1	-7.10162115	0.27369124	-0.22669186
1	-6.16188526	0.52698535	-1.70613813
1	-5.25754881	5.76891232	-0.58978873
1	-5.88762474	4.66101933	-1.82750046
1	-5.63777399	4.09847260	-0.15716290
1	0.58995324	1.31493568	-0.94033265

Energy = -8524.618548 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 18

Atomic N.	X	Y	Z
8	2.16439462	-2.12943554	1.42568016
6	3.40516782	-1.83071816	1.26723826
8	4.03334522	-2.71842337	0.38313317
6	5.40071106	-2.49675655	0.00949895
1	6.09083748	-2.64428949	0.85334378
1	5.53865862	-1.49495578	-0.42114499
1	5.62166166	-3.24726272	-0.75867540
8	3.24311233	-0.33918351	0.29645476
6	4.24000216	-1.45045733	2.48790884
1	5.26838017	-1.19372118	2.19709492
1	4.30431843	-2.39320302	3.05640125
6	3.66254449	-0.33810580	3.37459373
1	2.56198621	-0.36003995	3.32201576
1	3.91849184	-0.56631780	4.42021275
6	4.19961500	1.06393397	3.04878688
1	5.30363417	1.03011119	3.07442141
1	3.90060186	1.75186765	3.85590982
6	3.74589419	1.66571534	1.71439397
1	2.66395569	1.87475395	1.73310757
1	4.22991610	2.64822793	1.58312201
6	4.05108547	0.84613675	0.46142575
1	5.11386395	0.54644918	0.44680905
1	3.86674166	1.46798861	-0.42766392
50	0.96547282	-0.29504672	0.48614353
7	0.69811523	-2.10498500	-1.32125759
6	1.96355009	-2.20274448	-2.09028292
1	1.81154084	-2.80537844	-3.00431561
1	2.31281710	-1.20228314	-2.36508656
1	2.72403908	-2.67039657	-1.45683503
7	0.50497687	0.59245992	-1.57804990
6	-0.37878695	-1.55520999	-2.18153238
1	-0.58212358	-2.24133301	-3.02585173
1	-1.29039824	-1.47433197	-1.57278585
6	-0.00704919	-0.16756786	-2.70992851

1	-0.92091781	0.28470728	-3.13705683
1	0.72712952	-0.24327317	-3.53024578
16	0.90154618	2.15738201	-1.78843975
7	-0.67898631	-2.81823754	1.30952668
6	0.37230393	-3.46868229	-0.82535619
1	0.22545117	-4.14191294	-1.69201672
1	1.25772023	-3.81454349	-0.27505744
6	-0.85175318	-3.60116911	0.07607006
1	-0.99142337	-4.67450333	0.28525865
1	-1.76512194	-3.25458074	-0.42923304
16	-1.91831005	-2.98021293	2.48307657
8	-1.29133165	-2.57258201	3.75373149
8	-2.59375572	-4.28808832	2.33462811
6	-3.08682513	-1.70889640	1.96381116
6	-4.27225733	-2.08143878	1.32918811
6	-5.17455101	-1.08734119	0.94376653
6	-4.90679836	0.26839176	1.18663585
6	-3.71014547	0.60924226	1.84102225
6	-2.79689455	-0.36819500	2.23084259
1	-4.48510218	-3.13676167	1.16180253
1	-1.87375998	-0.10195083	2.74454403
1	-3.49376702	1.65778601	2.05371857
6	-5.87051964	1.33872473	0.74071068
1	-6.10676479	-1.37207413	0.45273733
8	1.45299387	2.56593752	-0.46070036
8	1.70168161	2.40267324	-3.01468182
6	-0.65816242	3.05998302	-2.01558256
6	-0.92627144	3.69100666	-3.22899818
6	-2.13152623	4.38305712	-3.38794160
6	-3.06910610	4.45509195	-2.34937787
6	-2.77214837	3.80801606	-1.13536990
6	-1.57843578	3.11154556	-0.96375209
1	-0.18756592	3.64447927	-4.02852583
1	-2.34246635	4.87986183	-4.33688021
6	-4.36018276	5.21789026	-2.51460814
1	-3.48769784	3.85934258	-0.31162331
1	-1.35001123	2.61780953	-0.01839773
1	-6.89643717	0.95393598	0.67509919
1	-5.86361694	2.19591665	1.42704690
1	-5.59622383	1.71548486	-0.25738627
1	-4.38566160	6.09786177	-1.85412610
1	-4.48848629	5.56869268	-3.54634333
1	-5.22869205	4.59546852	-2.25401449
1	0.22177707	-2.99134278	1.77821195

Energy = -8524.623932 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 19

Atomic N.	X	Y	Z
8	2.42742777	-2.85084820	-0.63760632
6	3.47222447	-3.21006632	0.02568273
8	4.54599714	-3.69613075	-0.64287472
6	4.68383741	-3.25374818	-2.01075935
1	4.78775215	-2.16065049	-2.03839684
1	3.81712270	-3.55969858	-2.60884976
1	5.59643126	-3.73374891	-2.37796283
8	3.96251631	-1.40298688	0.45702019

6	3.33350110	-3.83224344	1.40178907
1	2.64836717	-3.19159436	1.97394896
1	2.80696344	-4.78748655	1.22258353
6	4.61825657	-4.11047983	2.19021034
1	5.33154964	-4.65120459	1.54923284
1	4.35245991	-4.80284500	3.00517678
6	5.31119537	-2.88998914	2.81656599
1	4.59698296	-2.35387802	3.46457887
1	6.10031366	-3.27345896	3.48345256
6	5.94883776	-1.89200199	1.83391321
1	6.44328976	-2.43451715	1.01177084
1	6.74109507	-1.33194780	2.35883236
6	4.99422216	-0.84081984	1.27016950
1	4.53579807	-0.27979854	2.10210514
1	5.57291937	-0.12337029	0.65797108
50	2.03080297	-0.63956052	-0.25779942
7	-0.66084039	-2.02268362	-0.70705998
6	-0.56813568	-2.88152242	-1.89452589
1	-1.41275465	-3.59988332	-1.95332336
1	-0.56425571	-2.27244449	-2.80692124
1	0.37547392	-3.43854785	-1.85866034
7	-1.11385190	0.97468698	-1.41717315
6	-1.91341007	-1.25489664	-0.70692241
1	-2.78013372	-1.93482924	-0.86518347
1	-2.04628325	-0.80689114	0.28850839
6	-2.01018548	-0.13881551	-1.75056314
1	-3.06800842	0.17876582	-1.80142152
1	-1.72652364	-0.50097382	-2.74690676
16	-0.82929057	2.16161561	-2.59217548
7	0.83635318	-1.12710381	1.58742499
6	-0.55509979	-2.84158301	0.51552510
1	-1.46478939	-3.46156311	0.66896653
1	0.29365647	-3.52094150	0.36515012
6	-0.30715209	-2.01788306	1.78270733
1	-0.12806766	-2.72600102	2.61071825
1	-1.21594858	-1.44747746	2.05350471
16	1.13871479	0.01147286	2.71534872
8	2.31036782	0.74950689	2.13583159
8	1.20903146	-0.52751219	4.09299612
6	-0.25052437	1.18135178	2.70179415
6	-1.30892205	1.01845872	3.59777308
6	-2.38994098	1.90391254	3.54907775
6	-2.42183852	2.96138048	2.62859941
6	-1.33705544	3.10893083	1.74514079
6	-0.25631309	2.22695041	1.77219331
1	-1.26897526	0.22092935	4.33927250
1	0.58523208	2.35915399	1.09136021
1	-1.32583618	3.93721890	1.03360009
6	-3.56657267	3.94352961	2.61247969
1	-3.21768022	1.77654719	4.24942780
8	-0.00861724	3.17825842	-1.90766990
8	-0.37517110	1.44440293	-3.79720688
6	-2.42442203	2.91990471	-2.99135518
6	-3.19582152	2.39874649	-4.03234196
6	-4.43262053	2.98021221	-4.31916332
6	-4.90707922	4.07866716	-3.58625031
6	-4.10606289	4.58596468	-2.54869461
6	-2.87005520	4.01594019	-2.24700999

1	-2.81683779	1.56400526	-4.62102604
1	-5.03663492	2.57754827	-5.13426304
6	-6.22626781	4.72534370	-3.92540526
1	-4.45265579	5.44797802	-1.97539663
1	-2.23711371	4.42809820	-1.46159220
1	-4.47225809	3.51266909	3.05854607
1	-3.31247234	4.84731913	3.18799305
1	-3.80311871	4.26817465	1.58987737
1	-6.07361794	5.60307837	-4.57258081
1	-6.88738298	4.03224373	-4.46114874
1	-6.74586773	5.07451344	-3.02299929
1	-1.31622708	1.42714703	-0.51963162

Energy = -8524.631485 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 20

Atomic N.	X	Y	Z
8	0.60049313	-0.32494193	0.59818774
6	1.64991486	0.39628872	0.78128934
8	2.55095673	0.08314916	1.73738194
6	2.61853504	-1.30140233	2.15822244
1	2.86467648	-1.94305015	1.30006433
1	1.67966914	-1.63074183	2.61694002
1	3.43125391	-1.33432746	2.89055347
8	2.48327971	-0.14814617	-0.90582502
6	1.61396325	1.88739347	0.51323146
1	1.11659479	2.01899743	-0.45637506
1	0.93556350	2.30544472	1.27876246
6	2.95103931	2.63806391	0.57071698
1	3.41814446	2.46505713	1.55255294
1	2.71557045	3.71403289	0.53160179
6	3.98355293	2.33897471	-0.53290898
1	3.53005314	2.50524879	-1.52432883
1	4.77864361	3.09558225	-0.43564212
6	4.63895178	0.94479287	-0.49117929
1	4.79552555	0.65110266	0.55745202
1	5.63833284	0.99611616	-0.95378649
6	3.86908102	-0.14871766	-1.23986137
1	3.95588136	0.01958331	-2.32866931
1	4.33142662	-1.13194752	-1.02665401
50	0.98852408	-1.71968293	-1.24272382
7	-2.00337029	-1.78867054	-0.96463972
6	-2.26973224	-2.80248761	-1.99949491
1	-3.31879401	-2.76172018	-2.35655975
1	-1.60306644	-2.67097497	-2.86033416
1	-2.08660746	-3.79748464	-1.57443726
7	-0.12450573	-0.40971968	-2.69529009
6	-2.26140666	-0.42323297	-1.45621872
1	-3.35014296	-0.25449103	-1.61031890
1	-1.91816092	0.28121531	-0.68593550
6	-1.55666912	-0.09631636	-2.77203894
1	-1.71316421	0.98093557	-2.96301723
1	-2.03004622	-0.64337349	-3.60287142
16	0.63939047	-0.67794049	-4.11971426
7	-1.55476451	-1.33298540	2.24868250
6	-2.87442684	-2.10545850	0.18961249
1	-3.93665504	-2.06150866	-0.14174597

1	-2.67137361	-3.14068413	0.49338630
6	-2.76322865	-1.20848155	1.42851138
1	-3.62825680	-1.44049621	2.06776071
1	-2.86482453	-0.14578007	1.16458249
16	-1.44360387	-2.62978745	3.31344342
8	-0.01089873	-2.71644592	3.67331839
8	-2.16725969	-3.82234550	2.81520844
6	-2.36483479	-2.03515196	4.75051069
6	-3.49548960	-2.73066711	5.17458534
6	-4.17692757	-2.28943944	6.31301498
6	-3.73956013	-1.16839921	7.03086185
6	-2.59281015	-0.48862901	6.57912636
6	-1.90327823	-0.91373253	5.44731951
1	-3.82646084	-3.60656166	4.61791563
1	-1.01337504	-0.38711831	5.10369301
1	-2.23607159	0.38567272	7.12692928
6	-4.46734858	-0.70025468	8.26587391
1	-5.06347513	-2.83037639	6.64852333
8	1.90781534	-1.36212587	-3.67504287
8	-0.19957188	-1.34140658	-5.14682961
6	1.10448897	0.93049026	-4.80518007
6	0.81406146	1.22597706	-6.13612127
6	1.19138086	2.46927834	-6.65120697
6	1.85164070	3.41535521	-5.85442257
6	2.12339497	3.08929944	-4.51308727
6	1.75485861	1.85478890	-3.98372173
1	0.29804036	0.48851946	-6.74962664
1	0.96611631	2.70749474	-7.69235945
6	2.27723074	4.74726343	-6.41983652
1	2.63097835	3.81707692	-3.87635279
1	1.95818532	1.59846342	-2.94277263
1	-5.38636303	-1.27592182	8.43219280
1	-3.83430886	-0.80780327	9.15949917
1	-4.73725653	0.36301708	8.18969631
1	3.36617851	4.77425528	-6.57975578
1	1.79387391	4.94652748	-7.38462639
1	2.03191876	5.57003498	-5.73372126
1	-0.66109091	-1.15456319	1.76402938

Energy = -8524.635096 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 21

Atomic N.	X	Y	Z
8	2.42322111	-2.77628040	-0.67966622
6	3.55629396	-3.09413624	-0.16326764
8	4.48244858	-3.39694762	-1.10997701
6	5.69801569	-4.08818579	-0.78530031
1	5.49970579	-5.02449036	-0.24559473
1	6.37644243	-3.45281744	-0.20021082
1	6.16035557	-4.31812525	-1.75123978
8	3.92771912	-1.27841544	0.40426835
6	3.54212642	-3.78427148	1.20064187
1	2.63269329	-3.39427996	1.67717004
1	3.33901024	-4.84871721	0.97322750
6	4.68654299	-3.71776772	2.23011041
1	5.60687447	-4.17831707	1.84257936
1	4.35969305	-4.37404251	3.05364347

6	5.03260994	-2.34591103	2.83537316
1	4.11269951	-1.83338106	3.15808153
1	5.61597586	-2.54011703	3.74933100
6	5.85240936	-1.42183030	1.91982627
1	6.56498051	-2.02604055	1.33181202
1	6.47047758	-0.74166495	2.52850151
6	5.00019836	-0.55188531	0.99423611
1	4.55670881	0.26648024	1.58695281
1	5.63960791	-0.10077908	0.21180464
50	1.99752450	-0.57904810	-0.37361103
7	-0.63665652	-2.01121020	-0.82442838
6	-0.50674659	-2.88147879	-2.00122523
1	-1.32747865	-3.62715745	-2.05523682
1	-0.51898026	-2.28287649	-2.92042327
1	0.45554459	-3.40448880	-1.95545745
7	-1.17923057	1.00746965	-1.48736191
6	-1.90640414	-1.27128148	-0.85753089
1	-2.74945736	-1.97078121	-1.05160046
1	-2.08376527	-0.83918154	0.13808852
6	-1.99554718	-0.14486606	-1.89076924
1	-3.06294727	0.12121038	-2.00194836
1	-1.63345599	-0.47573322	-2.87254548
16	-0.95145279	2.25872135	-2.60862136
7	0.81399387	-1.07246363	1.48087823
6	-0.53941137	-2.81533217	0.40951526
1	-1.44344044	-3.44545078	0.55437338
1	0.32125300	-3.48386860	0.28041625
6	-0.32279578	-1.97248518	1.66987348
1	-0.15103348	-2.66808605	2.51020813
1	-1.24296212	-1.40898478	1.91721046
16	1.10814083	0.05680372	2.61861539
8	2.26029539	0.82598180	2.04222393
8	1.20262372	-0.49829617	3.98952794
6	-0.30336094	1.20033932	2.63493276
6	-1.34389007	1.01437724	3.54746914
6	-2.44085145	1.88068795	3.52116728
6	-2.50687432	2.94139123	2.60584259
6	-1.44096339	3.11119294	1.70405734
6	-0.34436852	2.24836302	1.70946622
1	-1.27774882	0.21330766	4.28329897
1	0.48101282	2.39723897	1.01256633
1	-1.45577037	3.94016147	0.99339527
6	-3.66908455	3.90306640	2.61569262
1	-3.25456476	1.73550916	4.23448992
8	-0.23530088	3.30873823	-1.85976779
8	-0.40550148	1.62907588	-3.82383204
6	-2.58959937	2.90456414	-3.03269744
6	-3.27387595	2.38208246	-4.13230848
6	-4.54387999	2.87444019	-4.43975019
6	-5.13798809	3.88529897	-3.66886711
6	-4.42363262	4.39578676	-2.57144046
6	-3.15572691	3.91388583	-2.24888206
1	-2.80274630	1.61634350	-4.74766302
1	-5.07996702	2.47054338	-5.30050278
6	-6.49347782	4.43861389	-4.02945805
1	-4.86465597	5.19051170	-1.96670234
1	-2.59213209	4.32953787	-1.41401672
1	-4.57307100	3.43703437	3.02906513

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1 -3.44040632  4.78424215  3.23534560
1 -3.89697790  4.26907778  1.60533953
1 -6.39147520  5.34082603 -4.65257883
1 -7.08553314  3.71108413 -4.59945965
1 -7.06156921  4.72470856 -3.13425469
1 -1.44044018  1.41277635 -0.58242142
Energy = -8524.614329 Hartree
Number of imaginary frequencies = 0.

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Compound TS3a isomer 22

Atomic N.	X	Y	Z
8	0.32228309	0.01493965	0.22787666
6	1.45898688	0.36611298	0.70867610
8	1.93720579	-0.51763654	1.62154949
6	2.85171223	-0.16622733	2.67468262
1	2.58823466	0.79778731	3.12888789
1	3.88828230	-0.14484002	2.31212783
1	2.73042679	-0.96289247	3.41573596
8	2.38759422	-0.11145940	-0.99688762
6	1.79292297	1.84816074	0.74887270
1	1.25521898	2.26208019	-0.11385281
1	1.27400231	2.23906469	1.64490092
6	3.23789954	2.38175774	0.75300354
1	3.76782990	2.07904172	1.66746676
1	3.13777757	3.47718859	0.82699668
6	4.13653040	2.07062006	-0.45790365
1	3.60760403	2.31573820	-1.39264977
1	4.99325085	2.76064491	-0.39944047
6	4.67424345	0.62943190	-0.52462465
1	4.86007547	0.26571310	0.49940819
1	5.65486240	0.61953396	-1.02711797
6	3.76356888	-0.34563911	-1.27793622
1	3.90622115	-0.21161105	-2.36577964
1	4.05783987	-1.38611758	-1.03989899
50	0.85122716	-1.69255447	-1.28288317
7	-2.02726316	-1.88789189	-1.03147376
6	-2.26113129	-2.97902846	-1.99372029
1	-3.32336712	-3.02907133	-2.30605507
1	-1.63897932	-2.85117888	-2.88780904
1	-1.99099982	-3.93237805	-1.52218437
7	-0.26421717	-0.53351235	-2.83202457
6	-2.39412427	-0.57663459	-1.59876204
1	-3.49195147	-0.50426191	-1.75909472
1	-2.10519195	0.19464073	-0.87280655
6	-1.70435810	-0.27800363	-2.93233347
1	-1.90576637	0.78221047	-3.17064428
1	-2.15078568	-0.88026774	-3.73978353
16	0.56543326	-0.74262005	-4.22508669
7	-1.47493815	-1.19094396	2.13752913
6	-2.81771779	-2.19696569	0.18264154
1	-3.89378023	-2.25222206	-0.09647655
1	-2.51947427	-3.19477582	0.53073508
6	-2.72237372	-1.22413671	1.36548209
1	-3.53819656	-1.48580837	2.05644870
1	-2.92353821	-0.19078518	1.04703963
16	-1.18477428	-2.42463708	3.24697900
8	0.22172773	-2.25764537	3.66772032

8	-1.66973257	-3.74238038	2.77151012
6	-2.26630688	-1.94707847	4.61744356
6	-3.24986076	-2.83356500	5.05296755
6	-4.04716063	-2.48138332	6.14579964
6	-3.87055993	-1.25886214	6.80825615
6	-2.87030005	-0.38440233	6.34505367
6	-2.06720972	-0.72043657	5.25831032
1	-3.37978506	-3.78413510	4.53687191
1	-1.29235816	-0.04171861	4.90314913
1	-2.72057867	0.57351941	6.84685135
6	-4.71516609	-0.89187485	8.00248814
1	-4.82036257	-3.17146468	6.48825169
8	1.82657778	-1.41577351	-3.74978423
8	-0.21955875	-1.37805283	-5.31067562
6	1.03464365	0.90098643	-4.82193327
6	0.78203690	1.25686920	-6.14515686
6	1.16195047	2.52702141	-6.58980560
6	1.78705275	3.43961072	-5.72929907
6	2.02348948	3.05118775	-4.39742136
6	1.65196598	1.79036474	-3.93688154
1	0.29442468	0.54390413	-6.80901337
1	0.96747404	2.81199408	-7.62547302
6	2.20353723	4.80676889	-6.21219778
1	2.50656414	3.75222397	-3.71308231
1	1.82856143	1.48445070	-2.90287614
1	-5.05080605	0.15316074	7.94959259
1	-5.60031128	-1.53569305	8.08091545
1	-4.14039612	-0.99991667	8.93529415
1	1.88372946	4.98064756	-7.24730253
1	1.77269065	5.59954309	-5.58327341
1	3.29704475	4.92339516	-6.17205667
1	-0.63132328	-0.96183020	1.58594537

Energy = -8524.619768 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 23

Atomic N.	X	Y	Z
8	3.63368416	-0.08057832	-1.07111180
6	4.15843248	1.08426738	-1.36264026
8	4.42808723	1.34835112	-2.67110467
6	3.59890175	0.67138380	-3.64412951
1	2.57271504	1.05911672	-3.59820056
1	3.59294581	-0.41010776	-3.47069526
1	4.04728508	0.90950328	-4.61389160
8	2.69954705	2.09273148	-0.99804336
6	5.28321886	1.60216737	-0.47447211
1	4.91790295	1.62011039	0.56348348
1	6.03183937	0.79398841	-0.51590401
6	5.94204760	2.93037987	-0.86864221
1	6.08197689	2.94764209	-1.95921278
1	6.95080471	2.95205975	-0.42741728
6	5.20085812	4.19339895	-0.41388702
1	5.19664907	4.23056316	0.68977404
1	5.78005219	5.07095480	-0.74359989
6	3.75433493	4.34316111	-0.90443581
1	3.70155120	4.27964115	-2.00325513
1	3.40352869	5.35220766	-0.63134253

6	2.76402521	3.34459019	-0.30002031
1	3.00186062	3.18972635	0.77043486
1	1.74710143	3.76740026	-0.33932409
50	1.76809144	0.25283185	-0.03683917
7	-0.89930922	2.12052369	-0.72502643
6	-1.11229694	3.54583526	-0.45032966
1	-2.05413389	3.92160559	-0.90277892
1	-1.13694143	3.72843838	0.63067263
1	-0.28331056	4.12499142	-0.87737006
7	-1.20309150	1.50326514	2.05849266
6	-2.03581738	1.30792010	-0.27063495
1	-2.95344281	1.51937485	-0.86361223
1	-1.77455962	0.25267920	-0.43307483
6	-2.40105963	1.50646281	1.20518327
1	-3.10519171	0.69974500	1.47452414
1	-2.92851019	2.45736480	1.36018884
16	-1.36669064	1.12888968	3.69483638
7	0.46187517	-0.23239069	-1.76782608
6	-0.63316375	1.94450164	-2.16420245
1	-1.44654012	2.39202070	-2.77759123
1	0.29188865	2.49804258	-2.38599634
6	-0.47353667	0.49375638	-2.62328005
1	-0.13027021	0.51994628	-3.67262459
1	-1.45973611	-0.00583092	-2.62503314
16	0.65237284	-1.83851123	-1.99399793
8	1.56628716	-2.18756747	-0.84375596
8	1.03560102	-2.22271752	-3.37045693
6	-0.94219434	-2.63491821	-1.67094207
6	-1.67828548	-3.15832424	-2.73428464
6	-2.92070365	-3.74474978	-2.47857738
6	-3.43476033	-3.81776357	-1.17599928
6	-2.66985416	-3.28386188	-0.12323573
6	-1.42987239	-2.69417286	-0.36187527
1	-1.26867330	-3.11403418	-3.74277735
1	-0.83781880	-2.29674935	0.46324706
1	-3.05004454	-3.32885718	0.89931470
6	-4.76296520	-4.47721815	-0.90132731
1	-3.49923873	-4.15481997	-3.30836868
8	-0.01922515	1.29247057	4.26756477
8	-2.53736544	1.88850081	4.17306900
6	-1.78542840	-0.62977791	3.79246211
6	-3.10896158	-1.01986134	3.99765658
6	-3.41242743	-2.38330793	4.06741238
6	-2.41307282	-3.35786128	3.93591213
6	-1.08656859	-2.93369436	3.73311210
6	-0.76612729	-1.58014667	3.66185832
1	-3.88007092	-0.26085225	4.12559366
1	-4.44530821	-2.69282699	4.23749876
6	-2.73919487	-4.82797003	4.01976299
1	-0.29260650	-3.67664838	3.63652396
1	0.26624879	-1.25603461	3.52752781
1	-5.37274313	-4.54624557	-1.81113124
1	-4.61877108	-5.50029039	-0.52047187
1	-5.33379030	-3.92660213	-0.14114049
1	-2.19322443	-5.30717230	4.84553289
1	-3.81190467	-4.99282694	4.18087530
1	-2.44645691	-5.35206842	3.09770799
1	-0.37645411	1.04484713	1.65566909

Energy = -8524.626045 Hartree
 Number of imaginary frequencies = 0.

Compound TS3a isomer 24

Atomic N.	X	Y	Z
8	2.26778531	2.86702371	-0.59085023
6	3.25897884	3.07586646	0.20059080
8	2.85743260	3.31126785	1.48327959
6	3.79759264	3.40042973	2.56858397
1	4.37718582	4.33346224	2.52067518
1	4.45595407	2.52337193	2.57271099
1	3.18579793	3.39671230	3.47697353
8	3.81678271	1.21505940	0.46957335
6	4.47005701	3.80855823	-0.37245655
1	4.44046354	3.60868096	-1.45293784
1	4.19475460	4.87295914	-0.25978124
6	5.91178226	3.61704707	0.13817899
1	5.95889187	3.62073660	1.23408031
1	6.46485758	4.51389837	-0.18488228
6	6.67076969	2.39505553	-0.40004221
1	6.59062529	2.37727189	-1.50131226
1	7.74003458	2.54429960	-0.17828114
6	6.25090456	1.02755749	0.15190025
1	6.31080484	1.01667082	1.25291359
1	6.97128439	0.27308318	-0.20666181
6	4.85894775	0.56626958	-0.26475424
1	4.73923779	0.71590185	-1.35895503
1	4.76117134	-0.51958996	-0.07673008
50	1.81936431	0.65672618	-0.34885046
7	-1.51270139	2.27569771	-0.19518887
6	-1.11260450	3.62621999	-0.60635573
1	-1.81964684	4.40190315	-0.24183547
1	-0.10832286	3.85616755	-0.23087089
1	-1.07368171	3.67531157	-1.70204186
7	0.64595193	1.00642633	1.48274350
6	-1.55890346	2.15268779	1.26967442
1	-2.14904404	2.98705077	1.71293294
1	-2.08015800	1.21854830	1.52119017
6	-0.17785504	2.12639546	1.93594849
1	-0.31566012	2.08098459	3.02901387
1	0.37249652	3.05718780	1.73548627
16	1.03811884	-0.21936707	2.47787380
7	-1.94403684	-0.28389943	-1.62946892
6	-2.80558801	1.91300881	-0.79669785
1	-3.65746498	2.37049890	-0.24667431
1	-2.83082604	2.30906534	-1.82146668
6	-3.00811291	0.39664468	-0.87005889
1	-3.97603798	0.18734729	-1.34452569
1	-3.03485370	-0.05087743	0.13539334
16	-2.17637777	-0.48823327	-3.30517530
8	-0.82214624	-0.43188223	-3.89175463
8	-3.27093387	0.38171670	-3.79406881
6	-2.77317357	-2.19008255	-3.41076803
6	-4.10550404	-2.43260098	-3.74045730
6	-4.54946089	-3.75419140	-3.84036827
6	-3.67827010	-4.83049297	-3.62148762
6	-2.33828139	-4.55260992	-3.29500127

6	-1.87926459	-3.24194765	-3.19038987
1	-4.77523375	-1.59357285	-3.92552185
1	-0.83768564	-3.02943420	-2.95025778
1	-1.64439082	-5.37801647	-3.12506795
6	-4.15293550	-6.25525999	-3.75989652
1	-5.59166956	-3.95016575	-4.09875345
8	1.97169411	-1.01375794	1.58929622
8	1.49010897	0.19684622	3.82455611
6	-0.42296857	-1.25964499	2.74169040
6	-0.96916080	-1.36564803	4.02015638
6	-2.10217500	-2.16190243	4.21296835
6	-2.69196248	-2.85518718	3.14731693
6	-2.11428332	-2.73510933	1.86967552
6	-0.98923010	-1.94187236	1.65972722
1	-0.49773398	-0.83895546	4.84897327
1	-2.53048396	-2.24892902	5.21320391
6	-3.91856790	-3.70797396	3.35486412
1	-2.55390406	-3.27123904	1.02619028
1	-0.55261505	-1.85805595	0.66390127
1	-5.24823761	-6.31792068	-3.73369575
1	-3.81767583	-6.68691540	-4.71568155
1	-3.74945402	-6.89136028	-2.95999646
1	-3.77191067	-4.71967363	2.95027256
1	-4.16940832	-3.79691553	4.41925287
1	-4.78937721	-3.27823997	2.83683348
1	-1.03985703	0.19390635	-1.50857282

Energy = -8524.618682 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 25

Atomic N.	X	Y	Z
8	0.80057967	1.32126510	0.37372166
6	2.03657269	0.92227823	0.21195997
8	2.15187526	-0.41607401	0.47213182
6	3.36063123	-0.98147446	1.00753105
1	3.71535850	-0.41461375	1.87777650
1	4.14804173	-1.05309069	0.24404642
1	3.08120394	-1.99061465	1.32958472
8	1.97141898	1.04353023	-1.60059226
6	3.11535525	1.90772557	0.66129416
1	2.70279264	2.89483786	0.40540919
1	3.08084750	1.85302007	1.76462448
6	4.57675505	1.85505712	0.19299720
1	5.06904173	0.92631340	0.51340544
1	5.08955336	2.65952682	0.74457794
6	4.83557177	2.06269097	-1.30534005
1	4.35421038	2.99686170	-1.64270461
1	5.91882849	2.21350408	-1.43409884
6	4.38501930	0.90177238	-2.20524716
1	4.57548475	-0.06202815	-1.70335269
1	4.99415159	0.88509363	-3.12412190
6	2.93416977	0.97664601	-2.66309524
1	2.80828834	1.87722206	-3.29178119
1	2.69570899	0.10281963	-3.29280853
50	0.15769719	2.34106684	-1.50368822
7	-2.32516026	2.71986771	0.26433188
6	-2.66793227	4.13449383	0.05190376

8	2.87438893	1.93011749	1.00907528
6	4.11357641	1.79726017	0.61115319
8	5.08627796	1.69586110	1.55836678
6	4.69377756	1.06162786	2.79609227
1	4.27605009	0.06624081	2.59709883
1	3.96066689	1.68000126	3.32919502
1	5.61550856	0.97878939	3.38101053
8	3.91898489	0.11955629	-0.02876775
6	4.59353971	2.63685513	-0.56475747
1	3.90007687	2.46353149	-1.40129077
1	4.42936420	3.67811680	-0.23955211
6	6.05239725	2.46565413	-1.00085962
1	6.70016956	2.52399135	-0.11341185
1	6.31355524	3.33118892	-1.63032758
6	6.37587786	1.19110632	-1.79270256
1	5.78324175	1.17965305	-2.72477078
1	7.43028402	1.25426185	-2.10661483
6	6.16571522	-0.14331217	-1.05901909
1	6.60710192	-0.10570774	-0.05049082
1	6.70822573	-0.93183261	-1.60678566
6	4.71752405	-0.61686498	-0.96930891
1	4.25836468	-0.56218350	-1.97508991
1	4.68651438	-1.66936350	-0.64402252
50	1.72835827	0.35429645	-0.02831699
7	-0.47066030	1.67564833	1.88347208
6	0.18505023	2.88411975	2.40853643
1	-0.36539534	3.30510950	3.27525687
1	1.21379256	2.65976524	2.70976973
1	0.23317790	3.64325976	1.61808681
7	1.38929904	-0.63875490	1.89844811
6	-0.50336128	0.61227071	2.90544343
1	-0.87511033	1.01551831	3.87305880
1	-1.21361113	-0.15890080	2.57727075
6	0.85720205	-0.05997327	3.12854838
1	0.74884832	-0.83230114	3.90753150
1	1.58570528	0.66788918	3.51988864
16	1.50366735	-2.25296140	1.68678701
7	-1.88547206	0.95164120	-0.85198480
6	-1.84052408	2.02195549	1.44976401
1	-2.50529122	2.14115644	2.33318734
1	-1.80559850	2.99538469	0.94290239
6	-2.47958446	1.01076138	0.49243316
1	-3.54263353	1.26597822	0.38359359
1	-2.44240689	-0.00786046	0.90825105
16	-2.38654852	2.10091472	-2.00138259
8	-1.21512485	2.30732417	-2.87657285
8	-3.07189631	3.23318553	-1.33691597
6	-3.64563179	1.20681643	-2.93820715
6	-4.99028873	1.53673184	-2.77297187
6	-5.95283318	0.85124391	-3.51863432
6	-5.58723021	-0.15066642	-4.42911720
6	-4.22241163	-0.45691130	-4.57614946
6	-3.24953175	0.21530637	-3.84001184
1	-5.26911259	2.32825017	-2.07840824
1	-2.19182277	-0.01467889	-3.96575022
1	-3.91886997	-1.23122942	-5.28314257
6	-6.62698984	-0.86196661	-5.25800276
1	-7.00695229	1.10556424	-3.39374971

8	1.99642992	-2.33406758	0.26715145
8	2.24384761	-2.93399787	2.77201176
6	-0.16332980	-2.96921849	1.69962418
6	-0.60035151	-3.67811418	2.81962395
6	-1.89706039	-4.19841480	2.83448148
6	-2.76002717	-4.03001976	1.74178338
6	-2.29054213	-3.31817484	0.62366754
6	-1.00212288	-2.78714943	0.59581375
1	0.07943450	-3.82918024	3.65751362
1	-2.24111652	-4.75201607	3.71020722
6	-4.14551497	-4.62608433	1.74796677
1	-2.94466090	-3.17921042	-0.23934729
1	-0.64415246	-2.24509859	-0.28030998
1	-7.61768913	-0.81317776	-4.78805733
1	-6.71125317	-0.40147331	-6.25476265
1	-6.36545229	-1.91775501	-5.41035509
1	-4.15168524	-5.60309553	1.23990691
1	-4.50943232	-4.78541374	2.77123189
1	-4.86156273	-3.98197317	1.22003484
1	-0.85514897	0.93519956	-0.85531813

Energy = -8524.632921 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 27

Atomic N.	X	Y	Z
8	3.98977208	1.94582546	-3.07874489
6	4.51021004	2.97269416	-2.45108128
8	3.89210320	4.17819548	-2.60093641
6	2.47306895	4.14039516	-2.87747741
1	1.92167079	3.82008696	-1.98332894
1	2.25246835	3.46070671	-3.70714927
1	2.20531106	5.17076206	-3.13238764
8	4.11199093	2.43341208	-0.78772318
6	6.02575541	3.14506912	-2.49434161
1	6.48200130	2.23138046	-2.08266687
1	6.25922585	3.14380813	-3.57180381
6	6.61036348	4.40635109	-1.84901285
1	6.01473379	5.27516174	-2.16517806
1	7.62064028	4.55801773	-2.26079774
6	6.72116184	4.38053560	-0.31976968
1	7.43291140	3.59072042	-0.02029518
1	7.17211199	5.33205605	0.00509240
6	5.41087484	4.16874027	0.45238605
1	4.63730049	4.87691259	0.11550234
1	5.59852028	4.39185905	1.51589704
6	4.85199022	2.74535513	0.39933226
1	5.68315506	2.02568746	0.54033619
1	4.15359449	2.60489011	1.24370432
50	3.81664276	0.32247168	-1.65942895
7	0.35600060	-0.04943829	1.78148007
6	0.83577341	-0.50942934	3.08567500
1	0.70033562	0.24961905	3.88877344
1	0.31916970	-1.43002939	3.38214397
1	1.90713263	-0.73747557	3.01007104
7	-1.81537485	-2.07070255	1.82133222
6	-1.06355226	0.30467427	1.80791318
1	-1.23778367	1.24427021	2.38649726

1	-1.38910258	0.51018214	0.77641749
6	-1.99796462	-0.74139577	2.42066813
1	-3.02957726	-0.36238456	2.29836202
1	-1.81252956	-0.84683228	3.49718285
16	-2.71966267	-3.34463549	2.46965599
7	1.65296435	0.54709363	-1.05618632
6	1.15909064	1.09130967	1.33116364
1	0.94314611	1.99580193	1.94959152
1	2.21594477	0.83746326	1.50626266
6	1.01187229	1.49655974	-0.14028680
1	1.49738252	2.48193336	-0.24408644
1	-0.04349730	1.64414382	-0.41628784
16	0.91577220	0.12239274	-2.44177818
8	2.10796142	-0.40664363	-3.23219776
8	0.06394293	1.16345954	-3.06092930
6	-0.14909860	-1.31638801	-2.18021488
6	-1.32164216	-1.42516220	-2.92959380
6	-2.09581327	-2.58193469	-2.81267095
6	-1.71570873	-3.62830067	-1.95825350
6	-0.54517734	-3.47470188	-1.19188535
6	0.24162601	-2.32853341	-1.29957151
1	-1.61152005	-0.61396503	-3.59619975
1	1.13946724	-2.20933247	-0.69391185
1	-0.25738576	-4.25980091	-0.49146381
6	-2.52222443	-4.89887762	-1.87146521
1	-3.00777960	-2.67622948	-3.40527749
8	-2.42167759	-4.50832129	1.61168897
8	-2.44707680	-3.34500718	3.91878915
6	-4.46774054	-2.92948413	2.25459695
6	-5.17589426	-2.36455321	3.31645226
6	-6.52020979	-2.03014374	3.13550305
6	-7.16598749	-2.25320196	1.91075230
6	-6.42707062	-2.82399487	0.85924023
6	-5.08564281	-3.16390395	1.02207601
1	-4.67906904	-2.21007562	4.27358055
1	-7.07820511	-1.59189177	3.96484780
6	-8.62466335	-1.91783583	1.72861016
1	-6.91414547	-3.01057935	-0.09972410
1	-4.52336931	-3.62316966	0.20918220
1	-2.02276969	-5.71054268	-2.42293358
1	-2.62520242	-5.23042631	-0.82917756
1	-3.52134204	-4.77068090	-2.30856991
1	-9.24212456	-2.82835317	1.77215731
1	-8.98100758	-1.23716903	2.51202607
1	-8.80857372	-1.44949341	0.75192267
1	-1.84799337	-2.09897757	0.79792327

Energy = -8524.625148 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 28

Atomic N.	X	Y	Z
8	2.79376483	0.11459851	1.63732362
6	3.91736698	0.41005799	1.12204087
8	4.44081163	-0.57887667	0.34497228
6	5.84367514	-0.68355858	0.05322206
1	6.45380783	-0.52204961	0.95172542
1	6.14514351	0.01348725	-0.73993170

1	5.98138952	-1.71195149	-0.29720059
8	2.95826459	1.63695168	-0.23825409
6	4.79301548	1.43766475	1.81957936
1	4.08054924	2.06251025	2.37279058
1	5.35467005	0.87408376	2.58862567
6	5.78420925	2.34809375	1.06734550
1	6.60678244	1.76205719	0.63294339
1	6.25409937	2.96304154	1.85251081
6	5.23769999	3.29982257	-0.01357290
1	4.35938787	3.84052849	0.37427253
1	6.01751184	4.05833578	-0.18724796
6	4.88858747	2.63879132	-1.36051881
1	5.56970119	1.79074693	-1.53749096
1	5.07201338	3.34514546	-2.18644190
6	3.42775035	2.16649771	-1.45226014
1	2.81379080	3.05746531	-1.72408235
1	3.33016562	1.44887328	-2.29538655
50	1.31484497	-0.09886967	-0.05646686
7	0.05616034	1.98576760	0.82414013
6	0.79022437	2.43449807	2.03016472
1	0.22800121	3.23221421	2.54948568
1	0.95512193	1.59405661	2.71048403
1	1.76884556	2.81234193	1.71398330
7	-0.28060293	-0.67134482	1.47513890
6	-1.29266787	1.48957813	1.18767726
1	-1.88005447	2.28918648	1.67972577
1	-1.80438948	1.20078397	0.26012713
6	-1.21175218	0.26151174	2.09568787
1	-2.23301601	-0.15742666	2.16928005
1	-0.90672451	0.54002607	3.11891484
16	0.01921214	-2.09107947	2.23315477
7	-0.26107588	1.85376608	-2.20864820
6	-0.00025661	3.14336133	-0.10477182
1	-0.44225812	4.01164484	0.42337149
1	1.04390097	3.39900970	-0.33588734
6	-0.78968328	2.96408844	-1.39948797
1	-0.76428628	3.92454004	-1.94071555
1	-1.84687340	2.75086021	-1.18812859
16	-1.15376186	1.50386143	-3.64150238
8	-0.23669127	0.67855132	-4.44928551
8	-1.76069450	2.73372197	-4.19797277
6	-2.48565006	0.49211848	-2.97387385
6	-3.80385613	0.92355824	-3.11645508
6	-4.83279514	0.12480948	-2.61004162
6	-4.55687046	-1.08806074	-1.96253395
6	-3.21547651	-1.49511087	-1.83610833
6	-2.17780042	-0.71691173	-2.34176731
1	-4.00992489	1.86901677	-3.61704874
1	-1.13937461	-1.03469610	-2.24088073
1	-2.98112011	-2.42868328	-1.32170045
6	-5.66640663	-1.94866419	-1.41334260
1	-5.86752367	0.45463464	-2.71730065
8	1.18032789	-2.66252899	1.49331760
8	0.05849436	-1.95430040	3.71000433
6	-1.39976072	-3.16857624	1.87194645
6	-2.47650552	-3.22514868	2.75797701
6	-3.57107258	-4.04123211	2.45531917
6	-3.59774184	-4.81687689	1.28773355

6	-2.49238491	-4.75326824	0.42015776
6	-1.40019834	-3.93370914	0.70170492
1	-2.44099116	-2.65395617	3.68539047
1	-4.41363621	-4.08609056	3.14834237
6	-4.76453066	-5.72272110	0.97939670
1	-2.48616195	-5.36192322	-0.48696956
1	-0.53657067	-3.89540315	0.03747706
1	-6.63901377	-1.44636583	-1.48724461
1	-5.73298979	-2.89943767	-1.96336234
1	-5.48517132	-2.20031166	-0.35853168
1	-4.48591518	-6.78043890	1.10302484
1	-5.61427593	-5.52178907	1.64431632
1	-5.10391951	-5.60036707	-0.05936018
1	0.70313561	2.01546764	-2.52301884

Energy = -8524.604564 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 29

Atomic N.	X	Y	Z
8	3.50596762	-1.09151185	-0.42738974
6	4.24706268	-0.09865928	-0.81091255
8	4.30077648	0.03822409	-2.18647122
6	5.49987745	0.42847896	-2.87234092
1	6.39020348	-0.06583421	-2.45995307
1	5.64664412	1.51827538	-2.86652327
1	5.35540915	0.09727368	-3.90700054
8	3.13220310	1.21081305	-0.30753252
6	5.49810839	0.20540647	0.01321663
1	5.24550772	-0.12316973	1.03040922
1	6.28124475	-0.48785338	-0.33841264
6	6.06753492	1.63742709	0.08148202
1	6.33778572	2.01720953	-0.91483408
1	7.02042770	1.55233610	0.62732750
6	5.18656874	2.66786742	0.81659573
1	4.66892290	2.15833974	1.64325917
1	5.83907509	3.42365885	1.28119183
6	4.14703846	3.41475916	-0.03898280
1	4.65269947	4.14043713	-0.69768834
1	3.50983596	4.00518036	0.63917011
6	3.27801228	2.49260092	-0.91094935
1	2.27886891	2.92136502	-1.08271885
1	3.71993279	2.34824944	-1.91013968
50	1.48657393	-0.23632573	-0.00660021
7	-0.28288096	2.14393520	1.70101547
6	0.24570245	2.83052254	2.88341832
1	-0.42655453	3.63764405	3.24500251
1	0.41058418	2.11405325	3.69702625
1	1.21491539	3.28028607	2.62992859
7	-0.53580374	-0.31913498	3.23268700
6	-1.59285891	1.52718377	1.94602442
1	-2.38795781	2.29800963	2.06454420
1	-1.84916234	0.93031603	1.05765450
6	-1.66123247	0.62717003	3.18197322
1	-2.63288546	0.10568391	3.14630437
1	-1.65677047	1.22340274	4.10504913
16	-0.76884103	-1.81153274	3.98300385
7	0.08026842	1.31559360	-1.06443834

6	-0.34856647	3.08724141	0.57430333
1	-1.05401361	3.92083049	0.79260874
1	0.65300000	3.52946091	0.46656328
6	-0.76184058	2.47007322	-0.76464921
1	-0.65584135	3.26061177	-1.52860796
1	-1.83167887	2.19157434	-0.73903239
16	0.03657427	0.63032514	-2.51868796
8	0.99060833	-0.55073214	-2.27164769
8	0.31832072	1.48838890	-3.69039035
6	-1.60223842	-0.09105585	-2.79729462
6	-2.31777859	0.25049838	-3.94455576
6	-3.58931875	-0.29467061	-4.14006519
6	-4.15421534	-1.17406702	-3.20519209
6	-3.41191959	-1.49502850	-2.05455112
6	-2.14274764	-0.95983696	-1.84507346
1	-1.87305653	0.93186927	-4.66876316
1	-1.57581031	-1.21980703	-0.94918031
1	-3.83521414	-2.17115688	-1.30904686
6	-5.51566935	-1.78101218	-3.43392968
1	-4.15216875	-0.02961473	-5.03692389
8	0.54434419	-2.47743201	3.94783139
8	-1.49206245	-1.53093123	5.23804665
6	-1.88482559	-2.76245546	2.91944718
6	-3.24580741	-2.83212829	3.22313595
6	-4.09294081	-3.56121898	2.38452363
6	-3.59823561	-4.22558212	1.25212562
6	-2.22319293	-4.13765478	0.97163779
6	-1.36388528	-3.41352153	1.79666996
1	-3.62315226	-2.33959723	4.11878300
1	-5.15671015	-3.62285686	2.62183571
6	-4.51054525	-5.04948807	0.37774006
1	-1.81823897	-4.65143967	0.09764304
1	-0.29452616	-3.36676073	1.58900225
1	-5.42419004	-2.80449939	-3.82986736
1	-6.08770466	-1.84531081	-2.49831486
1	-6.09878922	-1.19787598	-4.15800238
1	-4.51861000	-6.10086060	0.70502418
1	-5.54561043	-4.68564892	0.42147559
1	-4.18026638	-5.03965187	-0.66975451
1	-0.01427910	-0.42665949	2.35173678

Energy = -8524.604464 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 30

Atomic N.	X	Y	Z
8	2.99868178	0.39436740	2.30274677
6	4.14313412	0.00264486	1.79905522
8	4.69786596	-1.13699734	2.29692006
6	3.77670598	-2.11417198	2.83478189
1	3.17706943	-2.55109072	2.02546620
1	3.11512280	-1.66109788	3.58096647
1	4.41083145	-2.88199425	3.28922296
8	3.52355504	-0.48247540	0.16712300
6	5.21782064	1.05709553	1.56407869
1	4.79023218	1.84375191	0.92421985
1	5.34579420	1.51497650	2.55871320
6	6.57876968	0.57721502	1.04310215

1	6.85420561	-0.34832364	1.56916511
1	7.33310461	1.32854784	1.32460213
6	6.66659546	0.36588493	-0.47319040
1	6.52991152	1.33705997	-0.98070830
1	7.69027996	0.03900487	-0.71715814
6	5.67126799	-0.63465416	-1.07625830
1	5.74724579	-1.61518466	-0.57925969
1	5.94556713	-0.79569739	-2.13201618
6	4.21012831	-0.17879143	-1.05546093
1	4.15709972	0.90399200	-1.28182721
1	3.65291929	-0.69515139	-1.85369098
50	1.56265342	0.54144967	0.69675571
7	0.64856142	-1.56697512	-1.71013069
6	1.28550243	-1.80117941	-3.01079226
1	0.82157373	-2.65036106	-3.55546284
1	1.22635937	-0.90111643	-3.63442874
1	2.34506965	-2.04328609	-2.85696006
7	-0.34568739	0.96859097	-2.61194944
6	-0.79761988	-1.34910333	-1.84941018
1	-1.31891406	-2.26934075	-2.19560480
1	-1.19298089	-1.10147548	-0.85411489
6	-1.17411304	-0.22801460	-2.82507777
1	-2.24883938	-0.02093818	-2.67894387
1	-1.04836094	-0.54905504	-3.86792994
16	-0.92609733	2.46424413	-3.13296843
7	0.48289338	-1.33799601	1.18855560
6	0.95442957	-2.69865918	-0.81637490
1	0.65900284	-3.66520619	-1.28174007
1	2.04710889	-2.71370292	-0.68559426
6	0.28488034	-2.64084697	0.55798787
1	0.71544725	-3.45691562	1.16482878
1	-0.79414314	-2.85812092	0.45471290
16	-0.28146365	-1.02026343	2.59629416
8	0.08037537	0.43122715	2.80242252
8	-0.01262912	-1.99742639	3.67423677
6	-2.06470633	-1.08739495	2.28455520
6	-2.81372690	-2.14762354	2.79561162
6	-4.18363237	-2.20562553	2.52555513
6	-4.81425667	-1.21793807	1.75545478
6	-4.03463030	-0.15953074	1.25500262
6	-2.66717196	-0.08817382	1.51409483
1	-2.32323670	-2.90485096	3.40621209
1	-2.07448268	0.74476063	1.13414705
1	-4.50373316	0.62073272	0.65224439
6	-6.29804945	-1.26953340	1.49055040
1	-4.77237034	-3.03409982	2.92358875
8	0.15333486	3.42331958	-2.84054732
8	-1.45636797	2.24615073	-4.49219513
6	-2.32746816	2.88498020	-2.06666446
6	-3.63136554	2.69004774	-2.52252245
6	-4.70079660	3.01818419	-1.68310773
6	-4.48388147	3.53726411	-0.39887947
6	-3.15743780	3.72512913	0.03224855
6	-2.08041286	3.40452051	-0.79063624
1	-3.79824924	2.31076431	-3.53017569
1	-5.72283792	2.87625527	-2.03929949
6	-5.63747978	3.90080547	0.50204563
1	-2.96728802	4.13547182	1.02581012

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1 -1.05487978 3.57335591 -0.46089143
1 -6.69989347 -2.27788258 1.65205169
1 -6.83815575 -0.58568859 2.16372299
1 -6.53202868 -0.96267295 0.46195433
1 -5.61754751 4.97067070 0.75651145
1 -6.60213804 3.68317485 0.02672952
1 -5.58964396 3.34656525 1.45122266
1 0.08761716 1.04442275 -1.68329918
Energy = -8524.626032 Hartree
Number of imaginary frequencies = 0.

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Compound TS3a isomer 31

Atomic N.	X	Y	Z
8	2.69297409	-1.59286475	0.51939625
6	3.72297812	-0.76143295	0.52418494
8	4.95189476	-1.25369096	0.09194790
6	4.91494083	-2.17891097	-1.00008214
1	4.46760225	-1.71640444	-1.89292109
1	4.35784960	-3.08737779	-0.73047811
1	5.96048450	-2.43596506	-1.20473695
8	3.17530727	0.29736122	-0.61428517
6	3.95288420	0.00489673	1.83410811
1	3.02895975	0.56711799	2.04691839
1	4.01993608	-0.77721184	2.60661006
6	5.17382956	0.92169923	1.92853761
1	6.08201551	0.33422798	1.72366285
1	5.25335360	1.26104140	2.97379088
6	5.15038204	2.15249944	1.01400781
1	4.25951719	2.76635695	1.23451936
1	6.02286720	2.77752018	1.26244617
6	5.18796587	1.83152556	-0.48761168
1	5.92320347	1.03627217	-0.68181765
1	5.53590012	2.72108245	-1.03940678
6	3.84453464	1.48772681	-1.12054396
1	3.14345694	2.32554054	-0.99357104
1	3.98084402	1.32888043	-2.20266247
50	0.98777151	-0.10180590	-0.01101636
7	0.42698544	-2.32815385	-1.27301121
6	1.46973169	-2.56285930	-2.29689264
1	1.17088687	-3.37504673	-2.98536634
1	1.64615083	-1.64669979	-2.87039232
1	2.39756179	-2.83472490	-1.78722405
7	0.02083043	0.24048378	-2.04537511
6	-0.86275434	-2.00089812	-1.92396319
1	-1.21725273	-2.85507417	-2.53315544
1	-1.60207498	-1.81073487	-1.13259566
6	-0.73207384	-0.75171411	-2.80227685
1	-1.75234282	-0.40313730	-3.04342008
1	-0.24646707	-0.99913502	-3.76213384
16	-0.01768036	1.80015934	-2.52514267
7	0.10848983	-2.48137021	1.77224314
6	0.33701628	-3.55011439	-0.43403935
1	-0.06771580	-4.38334131	-1.04119861
1	1.36788809	-3.81303000	-0.15813348
6	-0.48981708	-3.45278788	0.84426939
1	-0.53600413	-4.46295404	1.28356206
1	-1.52543056	-3.14465880	0.63436067

16	-0.47803655	-2.49232554	3.37969589
8	0.58080018	-1.83481467	4.16799545
8	-0.98460722	-3.83725715	3.73130631
6	-1.90480042	-1.39542067	3.26700711
6	-3.19131732	-1.93448639	3.31959891
6	-4.28836584	-1.07395434	3.25165200
6	-4.11503649	0.31409174	3.13291907
6	-2.80705929	0.82607579	3.09403324
6	-1.69935620	-0.01801581	3.15979552
1	-3.31987858	-3.01050472	3.43150187
1	-0.68678087	0.38321388	3.13799953
1	-2.65318727	1.90399849	3.01758504
6	-5.30746126	1.23197126	3.03443861
1	-5.29699230	-1.48829067	3.30039692
8	0.77785945	2.50878358	-1.47661948
8	0.32790154	1.98359108	-3.95542884
6	-1.74083889	2.35107136	-2.34942436
6	-2.46426082	2.73972654	-3.47592306
6	-3.78785753	3.16498470	-3.32487917
6	-4.39599705	3.20945215	-2.06296873
6	-3.64342713	2.80758548	-0.94425082
6	-2.32482696	2.37900281	-1.07934332
1	-1.98294973	2.71377349	-4.45309210
1	-4.35592794	3.47009587	-4.20577526
6	-5.81366777	3.69828558	-1.89867628
1	-4.09927607	2.83676052	0.04790832
1	-1.74555385	2.07473326	-0.20598017
1	-6.13316631	0.88610590	3.67059374
1	-5.05004549	2.25791931	3.32731724
1	-5.68725824	1.26670444	2.00095749
1	-5.83022451	4.72101164	-1.49120593
1	-6.34575224	3.71503758	-2.85833931
1	-6.37865448	3.06395769	-1.20126152
1	1.13862276	-2.51515722	1.80935490

Energy = -8524.624960 Hartree

Number of imaginary frequencies = 0.

Compound TS3a isomer 32

Atomic N.	X	Y	Z
8	2.90832472	-1.83205962	1.33742726
6	4.03175116	-1.39158571	0.89473212
8	4.60175419	-2.27226186	0.02497919
6	5.94319820	-2.08390379	-0.44498172
1	6.66508484	-2.07027030	0.38356742
1	6.02963924	-1.16293442	-1.03847909
1	6.14782095	-2.94889855	-1.08503366
8	3.19095778	-0.08641689	-0.26561826
6	4.88887501	-0.57028586	1.85939276
1	4.16122389	-0.12211658	2.55074930
1	5.41694880	-1.33854067	2.45556021
6	5.90100765	0.51138151	1.44946253
1	6.68842459	0.10806894	0.79736644
1	6.41298580	0.79055715	2.38518906
6	5.34160614	1.79508388	0.81851125
1	4.49581051	2.16940451	1.42066050
1	6.12990236	2.56132579	0.89005071
6	4.90928745	1.67184877	-0.64998055

1	5.61621094	1.02142382	-1.19434667
1	4.97175694	2.65952206	-1.13652158
6	3.48066092	1.17664671	-0.85488385
1	2.79081011	1.93887258	-0.43711635
1	3.27976894	1.12371755	-1.94255900
50	1.28429174	-0.36037385	1.02390146
7	0.45075974	-1.68409538	-1.03149605
6	1.32606053	-1.57575893	-2.21554041
1	0.95793402	-2.21675205	-3.03849649
1	1.38206887	-0.53719771	-2.55796814
1	2.33641648	-1.88696957	-1.92954314
7	-0.53800422	1.12048233	-1.48555076
6	-0.95696336	-1.32893288	-1.33658135
1	-1.42808378	-2.14160109	-1.92468846
1	-1.49389851	-1.26658595	-0.37818941
6	-1.16500175	-0.03900362	-2.13372827
1	-2.25445223	0.08816234	-2.26746035
1	-0.71837121	-0.12557539	-3.13210082
16	-0.29004538	2.52148986	-2.42232227
7	-0.03778314	-2.11146164	1.63216579
6	0.51706386	-3.07953358	-0.50770479
1	0.16947663	-3.78780079	-1.28449345
1	1.57550800	-3.27875090	-0.29298568
6	-0.29612771	-3.26166677	0.77444518
1	0.02391237	-4.20509338	1.24625945
1	-1.37378085	-3.36249542	0.53975719
16	-0.15079501	-2.29485440	3.25395751
8	0.59190273	-1.12523150	3.80997968
8	0.17323487	-3.67143893	3.70180535
6	-1.90031254	-2.03390217	3.67371511
6	-2.72331166	-3.13100863	3.92863774
6	-4.07390642	-2.92027831	4.22202969
6	-4.61241150	-1.62695813	4.27367163
6	-3.75909448	-0.53879273	4.01818657
6	-2.41178012	-0.73363984	3.71908450
1	-2.29771471	-4.13402462	3.91326022
1	-1.74736726	0.11234768	3.54016519
1	-4.15748215	0.47718403	4.06391430
6	-6.06116581	-1.40143907	4.63031387
1	-4.71833754	-3.77832627	4.42411757
8	0.30140907	3.49651742	-1.49054706
8	0.39931595	2.06444287	-3.64409399
6	-1.91957605	3.13240933	-2.90789986
6	-2.46942091	2.74157357	-4.13046646
6	-3.73838997	3.20624661	-4.48203421
6	-4.46184540	4.05733919	-3.63269401
6	-3.87994504	4.43615532	-2.41029429
6	-2.61481094	3.98210979	-2.04181528
1	-1.89787805	2.10136485	-4.80154037
1	-4.17112064	2.90741110	-5.43838215
6	-5.81668758	4.58324194	-4.03345776
1	-4.42383766	5.10507965	-1.74088740
1	-2.15486813	4.29766846	-1.10543394
1	-6.65783358	-2.31013274	4.47735691
1	-6.16430807	-1.11224270	5.68794346
1	-6.50208187	-0.59307492	4.03054476
1	-5.73049307	5.59745598	-4.45348644
1	-6.28448820	3.94856477	-4.79676104

1 -6.49330664 4.64670944 -3.17067051
 1 -0.94608372 1.38245881 -0.58402568
 Energy = -8524.609145 Hartree
 Number of imaginary frequencies = 0.

Compound TS3a isomer 33

Atomic N.	X	Y	Z
8	2.70882773	-1.58020401	1.07400012
6	3.77268195	-0.98896432	0.64587843
8	4.53393269	-1.81404269	-0.19383432
6	5.96328211	-1.71062934	-0.26269007
1	6.42329788	-1.67787313	0.73507148
1	6.29286385	-0.83890462	-0.84608191
1	6.29503393	-2.62232566	-0.77371997
8	2.99393535	0.12758404	-0.47054780
6	4.52426529	-0.08503818	1.63293242
1	3.75241256	0.23907821	2.34551191
1	5.18900108	-0.75146699	2.20902181
6	5.30554438	1.15892148	1.16806781
1	6.07423592	0.90809500	0.42176801
1	5.86148262	1.51027739	2.05185437
6	4.42571354	2.31608558	0.65558058
1	3.48087978	2.31437230	1.22168207
1	4.91508722	3.27334285	0.89322156
6	4.10771275	2.31371689	-0.84886724
1	4.98671627	2.66085243	-1.41803384
1	3.29848194	3.03362274	-1.03529179
6	3.70411181	0.94350421	-1.40810978
1	3.06986046	1.06915367	-2.29987240
1	4.58818054	0.36511731	-1.72496164
50	0.94345105	-0.09507916	0.34048742
7	0.59356904	-2.28355145	-0.98948675
6	1.68004322	-2.38583374	-1.99353027
1	1.47873664	-3.21655083	-2.69478846
1	1.76106107	-1.44970882	-2.55466723
1	2.62869239	-2.55895901	-1.47519577
7	-0.13246962	0.26092288	-1.63998067
6	-0.71073765	-2.07126522	-1.66336501
1	-0.95069224	-2.93159842	-2.31733990
1	-1.48452246	-2.00254226	-0.88573444
6	-0.71117300	-0.77679634	-2.48226547
1	-1.75849032	-0.55451757	-2.75729442
1	-0.15329500	-0.90847772	-3.42515564
16	-0.04141635	1.78962171	-2.19218159
7	0.08546696	-2.58292675	2.01742816
6	0.60804349	-3.53888822	-0.19317456
1	0.34829235	-4.38943577	-0.85284269
1	1.64538693	-3.67574716	0.14115193
6	-0.30819803	-3.59546542	1.02555287
1	-0.24872597	-4.61720991	1.43516183
1	-1.35959530	-3.42219615	0.75171906
16	-0.71721983	-2.65057802	3.52905154
8	0.18155076	-1.95152152	4.46596670
8	-1.19519901	-4.02584791	3.79233122
6	-2.16987920	-1.62628579	3.22514224
6	-3.41721201	-2.23149776	3.06760645
6	-4.53670168	-1.42621040	2.84671068

6	-4.42346191	-0.02900846	2.78308392
6	-3.15482426	0.55018795	2.95924830
6	-2.02616382	-0.23714700	3.17884231
1	-3.50263000	-3.31534219	3.13790298
1	-1.04544234	0.21509233	3.32175756
1	-3.05045819	1.63635123	2.92880607
6	-5.63167620	0.83212560	2.51405454
1	-5.51655579	-1.89251351	2.72971630
8	0.70268226	2.50699973	-1.11098695
8	0.44603184	1.88377786	-3.59212089
6	-1.73520362	2.44226789	-2.20041895
6	-2.32339716	2.83678412	-3.40102339
6	-3.62848377	3.33893347	-3.38947511
6	-4.35102844	3.45399237	-2.19421482
6	-3.73339462	3.04475498	-0.99808401
6	-2.43513989	2.54005432	-0.99381739
1	-1.75358307	2.75465155	-4.32601023
1	-4.09108686	3.64897275	-4.32846117
6	-5.74746037	4.02455807	-2.18004632
1	-4.28005838	3.12899899	-0.05621039
1	-1.96002638	2.22848630	-0.06271246
1	-6.55346346	0.35336408	2.86923218
1	-5.54053783	1.81354225	2.99790144
1	-5.74959707	1.00820768	1.43300819
1	-5.74540281	5.05575752	-1.79411864
1	-6.18096876	4.04839849	-3.18796134
1	-6.41375828	3.43881154	-1.53122175
1	1.09878027	-2.55718827	2.19944263

Energy = -8524.616763 Hartree

Number of imaginary frequencies = 0.

Transition state 3b (TS3b)

Compound TS3b isomer 1

Atomic N.	X	Y	Z
8	2.02003813	-1.86166406	-2.09768295
6	2.36910558	-0.62884039	-2.20462918
8	2.41468358	-0.05560033	-3.45782971
6	1.70500648	-0.75355542	-4.49987364
1	0.62053704	-0.76825565	-4.31056023
1	2.06536150	-1.78595400	-4.58751106
1	1.91273117	-0.19012821	-5.41594601
8	0.81749302	0.13152900	-1.41986537
6	3.48019767	-0.04818590	-1.33342707
1	4.37206650	-0.02258299	-1.98012972
1	3.67181301	-0.78779233	-0.54567164
6	3.28064632	1.33667493	-0.68567747
1	2.67507625	1.21358132	0.22374704
1	4.27689886	1.66218948	-0.34580955
6	2.65084124	2.45517373	-1.54383683
1	2.94065928	2.34061861	-2.59997964
1	3.06747055	3.41960979	-1.21262050
6	1.11926448	2.54841900	-1.42388046
1	0.85728616	2.66995668	-0.35986239
1	0.76132888	3.45567226	-1.93961310
6	0.35814604	1.35533404	-1.99698830
1	0.49311379	1.33403981	-3.09372282

1	-0.72366983	1.45569921	-1.80106914
50	-0.19301154	-1.87799680	-1.54716086
7	-2.61145377	-2.08104396	0.01449283
6	-3.05071545	-3.33841753	-0.60321242
1	-3.84926295	-3.82933164	-0.01125057
1	-2.21124077	-4.03817987	-0.70406169
1	-3.43444371	-3.13157725	-1.61121273
7	0.28991196	-2.51991820	0.43458465
6	-2.03530502	-2.30238891	1.34672296
1	-2.75384474	-2.81946874	2.02016973
1	-1.81033409	-1.32131803	1.78701890
6	-0.73313606	-3.10636878	1.30360365
1	-0.35736462	-3.14483953	2.34054494
1	-0.95780247	-4.16269016	1.04329348
6	1.62127507	-2.74498844	0.90605468
6	2.39687657	-3.83445406	0.44191524
6	3.68910861	-4.02623510	0.94841170
6	4.25057268	-3.16971779	1.90135431
6	3.47062516	-2.10140610	2.35758328
6	2.17256570	-1.87786746	1.88160980
7	-2.51241708	1.04165864	0.18777324
6	-3.75542998	-1.14638221	-0.00120407
1	-4.64634943	-1.64060903	0.44642845
1	-3.98780751	-0.95021939	-1.05948639
6	-3.59001446	0.19017296	0.71912944
1	-4.53959417	0.72542828	0.58575213
1	-3.49229980	0.03287757	1.81044507
6	-2.68288326	2.44680595	0.38361320
6	-1.94436026	3.14819813	1.36546457
6	-2.11401749	4.53145838	1.49259245
6	-3.00653315	5.24663877	0.68531340
6	-3.72978210	4.53406906	-0.27687308
6	-3.57853270	3.15270662	-0.45231631
6	1.86765134	-4.78952503	-0.59924972
1	4.27475548	-4.87442255	0.58401835
6	5.66207123	-3.37385225	2.39766979
1	3.88415790	-1.41641474	3.10277486
6	1.37659061	-0.70727283	2.39914751
6	-0.98218328	2.42452788	2.27735567
1	-1.53952694	5.06251621	2.25588584
6	-3.15435410	6.74276638	0.82540739
1	-4.42112923	5.07077360	-0.93154603
6	-4.33791494	2.44796062	-1.54883325
1	2.42326236	-5.73649311	-0.57440257
1	1.98124599	-4.36318445	-1.60776007
1	0.80126125	-5.00832510	-0.45338139
1	0.89208865	-0.18002278	1.56619716
1	2.02084374	-0.00555547	2.94541764
1	0.57665437	-1.02589810	3.08735514
1	5.78864956	-2.98933935	3.41897655
1	6.38732195	-2.84640741	1.75753498
1	5.93869591	-4.43715763	2.39364076
1	-0.60527956	3.10186839	3.05388761
1	-0.10637558	2.03672671	1.73315048
1	-1.45426357	1.56752229	2.78122234
1	-5.24387026	1.94403923	-1.17474234
1	-3.71171355	1.67564666	-2.01762795
1	-4.66069841	3.16304326	-2.31660080

1 -2.39173555 7.27414036 0.23417895
 1 -3.03451157 7.06120062 1.87023807
 1 -4.13742685 7.08318329 0.47357610
 1 -1.61336184 0.73742002 0.56185508
 Energy = -7584.944896 Hartree
 Number of imaginary frequencies = 0.

Compound TS3b isomer 2

Atomic N.	X	Y	Z
8	0.67668414	0.10223893	-0.35965651
6	1.33649158	1.02413177	-0.94214588
8	2.25004268	0.72252786	-1.90975034
6	2.19839907	-0.61146653	-2.46128821
1	1.27436292	-0.76319993	-3.03855801
1	2.25323296	-1.36396110	-1.66517353
1	3.06791115	-0.67978352	-3.12287116
8	-0.24280061	1.64441621	-2.06902385
6	1.72408915	2.32198906	-0.24031164
1	2.82500768	2.31969357	-0.19368321
1	1.35182881	2.23377037	0.78900230
6	1.25071955	3.66983414	-0.81946391
1	0.17159876	3.76909733	-0.64547163
1	1.73862278	4.44219732	-0.20272726
6	1.55593956	3.94708538	-2.30916333
1	2.44929886	3.38634706	-2.62988043
1	1.81089246	5.01293707	-2.41817999
6	0.38496399	3.64861584	-3.26219869
1	-0.50260383	4.20706749	-2.92247295
1	0.63017237	4.01319838	-4.27464294
6	0.03238996	2.16595483	-3.35760665
1	0.87700409	1.62189841	-3.82713270
1	-0.84370667	2.02486849	-4.02197599
50	-1.31816435	-0.21729577	-1.63043928
7	-2.21102118	-2.14310408	0.16845240
6	-2.34537888	-3.43912721	-0.50411046
1	-2.99072909	-4.14145708	0.06052305
1	-1.35685241	-3.88904548	-0.64682573
1	-2.78934026	-3.27811265	-1.49585760
7	0.72520316	-2.76953220	0.79916590
6	-1.62228787	-2.25495291	1.51865137
1	-2.38521242	-2.64147353	2.22892618
1	-1.36099935	-1.23942649	1.85052490
6	-0.39880118	-3.16108322	1.66071045
1	-0.12564526	-3.13468885	2.73543429
1	-0.67551196	-4.20413923	1.44595098
6	1.97537851	-3.38933396	1.09691608
6	2.21379423	-4.72480440	0.69625819
6	3.45231318	-5.31491375	0.97853172
6	4.47643757	-4.62177277	1.63201463
6	4.23075962	-3.29416943	2.00066710
6	3.00177979	-2.66990924	1.75659180
7	-2.54028392	0.76769823	-0.19536445
6	-3.52378726	-1.46952605	0.22664656
1	-4.20985031	-2.00931573	0.91283768
1	-3.95687699	-1.52488458	-0.78556770
6	-3.44954467	-0.00384423	0.64711374
1	-4.48102713	0.39372954	0.57743508

1	-3.18309069	0.06114082	1.72090113
6	-2.55938601	2.16953087	0.05326015
6	-2.00013924	2.72037649	1.23407519
6	-2.06525922	4.10385084	1.45146036
6	-2.66087556	4.97452974	0.53469747
6	-3.20608616	4.41900444	-0.62885821
6	-3.16672015	3.04353571	-0.88437152
6	1.17937815	-5.50196362	-0.07780686
1	3.62595320	-6.34427309	0.65414160
6	5.79322577	-5.28914547	1.94886255
1	5.01518536	-2.72594380	2.50726509
6	2.78808928	-1.24248946	2.20257115
6	-1.30520761	1.85105860	2.25288582
1	-1.62105787	4.51189041	2.36366606
6	-2.68357801	6.46575546	0.77060497
1	-3.68413401	5.07613134	-1.36032784
6	-3.78245783	2.51055098	-2.15444517
1	1.64226747	-6.34868002	-0.60107279
1	0.68715572	-4.85394382	-0.81713825
1	0.39038536	-5.91343164	0.57214534
1	2.66667056	-0.55476302	1.35191643
1	3.64455509	-0.89362419	2.79310989
1	1.88466251	-1.13767505	2.82261944
1	5.77283764	-5.75354147	2.94777226
1	6.62141562	-4.56737518	1.94289744
1	6.02434349	-6.08298588	1.22545981
1	-0.58759224	2.44058847	2.83948565
1	-0.76776189	1.03060114	1.75726151
1	-2.01480603	1.40406156	2.96808505
1	-4.38619900	1.61218786	-1.96668518
1	-3.01142120	2.22446680	-2.88771319
1	-4.41672468	3.27221632	-2.62720013
1	-1.84544790	6.96192646	0.25548944
1	-2.59885430	6.70416975	1.83936536
1	-3.61000657	6.91853189	0.39027578
1	0.81578863	-1.75124419	0.77453375

Energy = -7584.951507 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 3

Atomic N.	X	Y	Z
8	1.90490901	-1.03397393	-2.37519670
6	2.00047898	0.23018600	-2.52777719
8	1.27713358	0.70873779	-3.60229063
6	1.18401933	2.13190985	-3.78578830
1	2.13890958	2.55811310	-4.12602139
1	0.85627979	2.61406994	-2.85424972
1	0.42653000	2.27820659	-4.56378078
8	0.73648083	0.75044078	-1.15914536
6	3.29312897	0.95440149	-2.20406294
1	3.10731101	2.03350759	-2.10863447
1	3.90953779	0.82415861	-3.11186194
6	4.05333376	0.43027607	-0.98108137
1	3.94377136	-0.66348529	-0.93130946
1	5.12400532	0.63355803	-1.13841414
6	3.63739491	1.06483912	0.35242736
1	3.73373270	2.16355228	0.27866757

1	4.36558056	0.74832028	1.11672843
6	2.23289275	0.71265906	0.85921639
1	2.11485171	-0.38071176	0.87807369
1	2.15187335	1.05582011	1.90557444
6	1.05007541	1.32960176	0.10662327
1	1.23038137	2.41342759	-0.04012452
1	0.14386006	1.24258900	0.73198336
50	-0.28432640	-1.21694660	-1.70283747
7	-2.88588691	-1.76803756	-0.17795981
6	-3.48404455	-2.66076708	-1.17597127
1	-4.25729847	-3.32249331	-0.73352289
1	-2.71525002	-3.29022837	-1.64170635
1	-3.94509602	-2.06056499	-1.97144163
7	0.12353220	-2.55506825	-0.07663879
6	-2.22196937	-2.52231336	0.89634877
1	-2.94385600	-3.21880221	1.38009560
1	-1.88955593	-1.80236459	1.65616083
6	-1.00505340	-3.33887410	0.45093909
1	-0.66982037	-3.89185286	1.34288144
1	-1.32739210	-4.12512493	-0.26163885
6	1.39711487	-3.04141688	0.34529489
6	2.23196554	-3.78233290	-0.53048354
6	3.48533154	-4.22140074	-0.08160549
6	3.94797587	-3.96695089	1.21272457
6	3.09761214	-3.27476811	2.08145118
6	1.83618271	-2.81936598	1.67949855
7	-2.51492476	1.15616846	0.42472109
6	-3.93462539	-0.87695986	0.35299894
1	-4.65993118	-1.45409679	0.96856421
1	-4.49145126	-0.48203668	-0.51128507
6	-3.43708754	0.30372962	1.18595779
1	-4.32999420	0.87642914	1.48682499
1	-2.96865416	-0.05553509	2.11689615
6	-2.64930391	2.55951405	0.44886503
6	-2.63613963	3.27067709	1.67324603
6	-2.75991535	4.66576624	1.65194833
6	-2.86245155	5.39272165	0.46157670
6	-2.81634426	4.67465162	-0.73959595
6	-2.71593046	3.28049779	-0.77052534
6	1.79899335	-4.15026188	-1.92913771
1	4.11532116	-4.79237413	-0.76896095
6	5.32245111	-4.41069269	1.65274072
1	3.42468429	-3.07729387	3.10597706
6	0.96679085	-2.09829688	2.68042493
6	-2.39857626	2.56800747	2.98890305
1	-2.74438834	5.20169353	2.60469842
6	-3.02614760	6.89364529	0.47120401
1	-2.87103295	5.21465158	-1.68852484
6	-2.67222357	2.55499125	-2.09335232
1	2.08091640	-3.37216282	-2.65307379
1	0.70987231	-4.28108740	-1.99429095
1	2.27927923	-5.08700943	-2.24286127
1	0.40419930	-1.28441668	2.20370460
1	1.57418334	-1.68135655	3.49457955
1	0.22748514	-2.77474165	3.13981438
1	5.35277891	-4.61570835	2.73167968
1	6.07491016	-3.63270879	1.44652069
1	5.63976860	-5.31824303	1.12091088

1	-2.10185266	3.29216146	3.75853348
1	-1.59704220	1.82016873	2.89131284
1	-3.28812385	2.03859830	3.36301684
1	-3.49912190	1.83315730	-2.19705701
1	-1.73453224	1.98921371	-2.22423482
1	-2.74873710	3.26601815	-2.92566109
1	-2.55772352	7.35503054	-0.40921119
1	-2.57768989	7.33937693	1.36979079
1	-4.09003115	7.18062353	0.46150851
1	-2.39429402	0.79695922	-0.52029228

Energy = -7584.938027 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 4

Atomic N.	X	Y	Z
8	2.10460973	-1.80654597	-2.17785430
6	2.18407464	-0.71425492	-2.82990408
8	1.54600871	-0.76015079	-4.05561924
6	1.39673829	0.46011683	-4.79944992
1	2.35910225	0.81477952	-5.19700575
1	0.92919403	1.23118150	-4.17148638
1	0.73196959	0.21409191	-5.63490582
8	0.82649958	0.25457516	-1.87519586
6	3.43263268	0.14438348	-2.74280500
1	3.23574853	1.14761746	-3.14672804
1	4.13901949	-0.33756310	-3.44211483
6	4.06426764	0.23889565	-1.34799361
1	3.91750407	-0.71687937	-0.82308817
1	5.15062952	0.36330402	-1.47665834
6	3.55466652	1.40419388	-0.48853981
1	3.68817639	2.34991050	-1.04502285
1	4.20602417	1.48092103	0.39718178
6	2.10263753	1.30904102	-0.00254639
1	1.96095550	0.36745065	0.54829335
1	1.92978203	2.12950277	0.71653807
6	1.01658952	1.41345191	-1.07878613
1	1.23791206	2.27351809	-1.74357557
1	0.04940000	1.64711666	-0.59788924
50	-0.13730489	-1.81011760	-1.58785367
7	-2.66917539	-2.09489918	-0.11792234
6	-3.02659106	-3.35859823	-0.77003431
1	-3.82487750	-3.89599562	-0.21822461
1	-2.15359783	-4.01925516	-0.84975892
1	-3.37926793	-3.15293765	-1.78967071
7	0.27467915	-2.38411093	0.45487845
6	-2.13260579	-2.30903888	1.22943211
1	-2.84374404	-2.88075733	1.86711478
1	-1.98476875	-1.32733703	1.70041108
6	-0.78731686	-3.04099917	1.23285151
1	-0.47794318	-3.10961103	2.28898478
1	-0.93948281	-4.09323502	0.91479981
6	1.56783807	-2.55815768	1.03755021
6	2.47718477	-3.53063154	0.54901838
6	3.74481320	-3.64592648	1.13666606
6	4.15165615	-2.83979273	2.20373774
6	3.22818327	-1.91889167	2.71010041
6	1.94831192	-1.77538979	2.16130924

7	-2.66281080	1.00638855	0.11742837
6	-3.84519649	-1.20603371	-0.17376745
1	-4.73838663	-1.73433065	0.23014747
1	-4.03820133	-1.00827134	-1.23965943
6	-3.75896883	0.12925710	0.56379819
1	-4.70803261	0.64690208	0.37052688
1	-3.73177195	-0.03505419	1.65798414
6	-2.89097023	2.40938950	0.24274233
6	-2.26719165	3.16948700	1.25988460
6	-2.48859811	4.55049849	1.31723678
6	-3.32247138	5.20639563	0.40430602
6	-3.93062925	4.43637943	-0.59329593
6	-3.72320294	3.05580401	-0.70054138
6	2.11386275	-4.47629690	-0.57009250
1	4.43391848	-4.40004969	0.74702793
6	5.54191780	-2.95087624	2.78202224
1	3.50856805	-1.29216194	3.56121516
6	0.98802817	-0.79636586	2.79029036
6	-1.37351096	2.51135731	2.28493476
1	-2.00449920	5.12721491	2.10959864
6	-3.52791166	6.70083237	0.47190869
1	-4.57221079	4.92651224	-1.33008766
6	-4.34654236	2.28681254	-1.83866811
1	2.38810134	-4.05645084	-1.54843104
1	1.03521466	-4.68323612	-0.59242195
1	2.64698648	-5.42955494	-0.45245370
1	0.34718144	-0.33296379	2.02894354
1	1.52731371	-0.00847138	3.33271694
1	0.31938943	-1.29183686	3.51349497
1	5.55170727	-2.71420074	3.85497928
1	6.23438025	-2.25098610	2.28737688
1	5.95135689	-3.96162724	2.64895487
1	-1.10311007	3.22459245	3.07363701
1	-0.43150964	2.14624000	1.84451926
1	-1.85993648	1.64950144	2.76642394
1	-5.25504446	1.74395442	-1.53139412
1	-3.64192796	1.53816843	-2.22804880
1	-4.63552904	2.96580482	-2.65132356
1	-2.76202893	7.23442841	-0.11321376
1	-3.46143889	7.06766224	1.50539780
1	-4.50743628	6.98982143	0.06757344
1	-1.79899096	0.74238974	0.59009546

Energy = -7584.932803 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 5

Atomic N.	X	Y	Z
8	0.56155545	0.10471481	-0.09736459
6	1.41812336	0.74026746	-0.79228193
8	2.02326083	-0.03562184	-1.74985862
6	3.04589248	0.51163286	-2.60376835
1	4.01961422	0.51161015	-2.09223294
1	2.79955959	1.52380574	-2.94380236
1	3.09347439	-0.15894814	-3.46885562
8	-0.00725180	1.65995729	-1.84919357
6	2.20284462	1.89745438	-0.18260539
1	3.18311977	1.99129164	-0.67075956

1	2.39957023	1.55852699	0.84752768
6	1.54085779	3.28561783	-0.11934077
1	0.50801820	3.18425846	0.23797864
1	2.09144568	3.84626222	0.65327048
6	1.56612575	4.11454105	-1.42533350
1	2.47147799	3.86432624	-2.00768375
1	1.68072844	5.17511845	-1.15055573
6	0.31964210	4.00439835	-2.31781507
1	-0.56584740	4.29537582	-1.73131859
1	0.40505287	4.72279263	-3.15182281
6	0.07908900	2.61060691	-2.89317346
1	0.88427037	2.34667039	-3.61020112
1	-0.85988909	2.61084056	-3.48073649
50	-1.24982965	-0.17639250	-1.59145701
7	-2.13571620	-2.01976085	0.16943675
6	-2.26403904	-3.33496881	-0.47254518
1	-2.87027431	-4.03850079	0.13044743
1	-1.26897407	-3.75891685	-0.64449149
1	-2.75247812	-3.20214820	-1.44724274
7	0.77640992	-2.94080591	0.72354800
6	-1.46364915	-2.07071948	1.49214840
1	-2.21412420	-2.30663586	2.27502298
1	-1.07780969	-1.06382322	1.70827007
6	-0.34277260	-3.09786010	1.66394484
1	-0.00926366	-3.00054860	2.71716905
1	-0.75529814	-4.11293602	1.57001936
6	1.94847107	-3.68990231	1.03168333
6	1.96478510	-5.09439564	0.84951240
6	3.12624836	-5.81420803	1.15654957
6	4.28980970	-5.19380713	1.62219286
6	4.26721001	-3.80244875	1.76416731
6	3.12416887	-3.04350090	1.48678374
7	-2.60682368	0.84104455	-0.27850774
6	-3.47147846	-1.39466774	0.28712657
1	-4.08876896	-1.94577110	1.02654982
1	-3.95770192	-1.49019933	-0.69670874
6	-3.42030239	0.08087487	0.66393667
1	-4.46614742	0.44398603	0.66039050
1	-3.07562304	0.18039492	1.71367419
6	-2.73831129	2.25137663	-0.18688014
6	-2.27319074	2.97678280	0.94110024
6	-2.44534636	4.36698103	0.99099720
6	-3.06255031	5.08059216	-0.04093550
6	-3.51826406	4.35542536	-1.14808285
6	-3.37021303	2.96614289	-1.23842919
6	0.78192651	-5.82635975	0.26705420
1	3.12356281	-6.89629650	1.00098419
6	5.51744747	-5.99818897	1.97621942
1	5.16493130	-3.28604984	2.11416316
6	3.17250538	-1.54485404	1.66096878
6	-1.55627024	2.28497291	2.07433343
1	-2.06944203	4.90917206	1.86333609
6	-3.19971418	6.58325768	0.01775509
1	-4.01523638	4.88579845	-1.96498358
6	-3.91205645	2.24375916	-2.44832444
1	1.09292769	-6.79862022	-0.13671558
1	0.32656750	-5.24014091	-0.54345131
1	-0.00556393	-6.02158356	1.01252174

1	3.17051792	-1.02845061	0.68855959
1	4.08734035	-1.24986506	2.19071054
1	2.31052732	-1.16201305	2.22717190
1	5.49647093	-6.31236792	3.03208375
1	6.43666744	-5.41512680	1.82803071
1	5.58794880	-6.91017199	1.36745656
1	-0.90684474	2.99170232	2.60880303
1	-0.94109458	1.45756996	1.69300961
1	-2.25750709	1.86730731	2.81470108
1	-4.46668577	1.33992743	-2.16124058
1	-3.11038446	1.91013825	-3.12783194
1	-4.57442999	2.90128589	-3.02724266
1	-2.34407449	7.08036852	-0.46722338
1	-3.24120355	6.94277048	1.05493474
1	-4.10742569	6.92342281	-0.49987140
1	0.97970557	-1.94754744	0.58462375

Energy = -7584.940641 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 6

Atomic N.	X	Y	Z
8	-1.49317944	-2.81956434	-1.66979837
6	-2.52072692	-2.04175615	-1.57840312
8	-3.52042365	-2.34288049	-0.70311368
6	-3.18836689	-3.23660064	0.38248667
1	-2.43695617	-2.78361344	1.03860056
1	-2.81380701	-4.19059896	-0.00564950
1	-4.12923145	-3.38491416	0.92301190
8	-1.58434868	-0.63421786	-0.75266641
6	-3.17519474	-1.41710961	-2.81096363
1	-4.10492516	-0.92571336	-2.48991227
1	-3.48270035	-2.29780602	-3.39959908
6	-2.35947180	-0.46890226	-3.69815469
1	-1.30353022	-0.78678381	-3.73736739
1	-2.73684478	-0.57692176	-4.72710419
6	-2.46550822	1.01906240	-3.31923413
1	-3.53504515	1.27104616	-3.20669365
1	-2.10225534	1.62019086	-4.16870022
6	-1.71040583	1.47088349	-2.06285381
1	-0.62262321	1.39512122	-2.22778440
1	-1.91781151	2.54053402	-1.89088881
6	-2.04720664	0.71301597	-0.77877867
1	-3.14121938	0.69773126	-0.61214405
1	-1.60776484	1.24766946	0.08296240
50	0.35173333	-1.50604200	-1.52569902
7	3.04696488	-0.32375884	-0.79955477
6	3.71243834	0.04719384	-2.04800773
1	4.81974792	0.01290347	-1.96298850
1	3.41852856	1.05720484	-2.35715032
1	3.39955974	-0.64511657	-2.84174895
7	1.46184921	2.16075039	0.07935148
6	3.38697791	0.59119809	0.29613936
1	4.48902893	0.60940307	0.46049425
1	2.94079590	0.19067243	1.21868479
6	2.92849517	2.04009962	0.12643568
1	3.36034250	2.61316061	0.97172207
1	3.35487223	2.47643733	-0.78618985

6	0.92980772	3.48165083	0.08260469
6	1.04264855	4.29661131	-1.06831932
6	0.47969425	5.57865238	-1.05471027
6	-0.21033901	6.08170986	0.05323621
6	-0.33588472	5.25001144	1.17170548
6	0.22565067	3.96884298	1.21100557
7	1.06010091	-2.35768270	0.29313785
6	3.37825394	-1.71513546	-0.45098415
1	4.43711376	-1.80367827	-0.12043535
1	3.28055120	-2.30937767	-1.37452006
6	2.48753572	-2.34065294	0.62158346
1	2.86685610	-3.37247324	0.76453549
1	2.66302991	-1.84011364	1.59608114
6	0.31120905	-3.07488942	1.27363908
6	-0.18414693	-2.41633677	2.42536926
6	-0.86800051	-3.15036654	3.40315652
6	-1.08098054	-4.52823877	3.27921104
6	-0.58901316	-5.16503954	2.13419461
6	0.09590059	-4.46703720	1.13060701
6	1.70690536	3.79240537	-2.32504559
1	0.56534040	6.19362068	-1.95442986
6	-0.78289944	7.47869444	0.04909588
1	-0.87944794	5.61078501	2.04859567
6	0.06533993	3.12165332	2.45210505
6	-0.01456985	-0.92692238	2.59127426
1	-1.24888980	-2.62741089	4.28452492
6	-1.84500098	-5.29601431	4.33164263
1	-0.74432641	-6.24062300	2.01420331
6	0.56489629	-5.19957495	-0.10172701
1	1.32238710	4.32547474	-3.20443726
1	1.52398491	2.71648669	-2.45642805
1	2.79872656	3.94244409	-2.30888534
1	-0.57760024	2.24294257	2.27854323
1	-0.39964589	3.70494580	3.25664282
1	1.03079200	2.74759507	2.82680917
1	-0.04827199	8.21074772	0.42085633
1	-1.66990411	7.55122948	0.69301045
1	-1.06856108	7.79121590	-0.96470237
1	-0.56048751	-0.56959772	3.47422409
1	-0.39399299	-0.40105730	1.70352542
1	1.04275954	-0.64461291	2.71417785
1	1.60955191	-4.96631145	-0.34962183
1	-0.04200293	-4.91318464	-0.97405201
1	0.47460425	-6.28518915	0.03541986
1	-2.92813063	-5.27637577	4.13069963
1	-1.69265544	-4.86646700	5.33132172
1	-1.53808308	-6.35035181	4.35971165
1	1.06740737	1.62501812	0.85310811

Energy = -7584.948813 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 7

Atomic N.	X	Y	Z
8	-0.50785905	-0.97589785	-1.33579886
6	-1.71196926	-0.72665614	-1.65203083
8	-2.65798545	-0.50109327	-0.71829003
6	-2.19699430	-0.03479687	0.57300806

1	-1.82722735	0.99167496	0.46061534
1	-1.40396690	-0.68226779	0.96353334
1	-3.07868290	-0.06286675	1.22039783
8	-1.23848069	1.25703549	-2.15383291
6	-2.36701536	-1.23677349	-2.92293239
1	-3.40597486	-0.88026839	-2.94123673
1	-2.42014647	-2.32878852	-2.76435971
6	-1.67556775	-0.95402509	-4.26581097
1	-0.58269566	-0.90355539	-4.12864828
1	-1.85444725	-1.82519126	-4.91484737
6	-2.18952966	0.29031581	-5.01741409
1	-3.29364848	0.28402475	-4.98520565
1	-1.92157233	0.17650042	-6.08061218
6	-1.68493974	1.66509295	-4.55492592
1	-0.59755820	1.73645759	-4.73265600
1	-2.15129018	2.43567801	-5.19335222
6	-1.96415997	2.02754998	-3.09216380
1	-3.04419637	1.89788866	-2.87860417
1	-1.75164890	3.10340405	-2.93695784
50	0.89838850	0.74904293	-2.18369198
7	2.93128276	-0.50297648	-0.77679020
6	4.00998640	-0.16761746	-1.71734071
1	5.00642538	-0.38594854	-1.28562737
1	3.96983504	0.89433390	-1.99224472
1	3.88566923	-0.75189835	-2.63934278
7	1.31646574	1.92388976	-0.44242376
6	2.99620795	0.30761603	0.45017862
1	4.00300026	0.26369637	0.91626745
1	2.26094389	-0.10757368	1.15059841
6	2.62896419	1.77218330	0.18899132
1	2.64256239	2.28262901	1.16554391
1	3.43224096	2.26187158	-0.40129834
6	0.55846542	3.04767442	-0.01600980
6	0.35447636	4.15983772	-0.87445384
6	-0.43046939	5.23721266	-0.44588783
6	-1.02198350	5.26958799	0.82166177
6	-0.78415835	4.18736219	1.67416525
6	-0.00703406	3.08777118	1.28732753
7	0.99837512	-2.26898980	1.01440275
6	2.94517708	-1.97626507	-0.56692386
1	3.99007249	-2.33849835	-0.63605082
1	2.39864516	-2.42962217	-1.41155672
6	2.41810346	-2.53679824	0.75378811
1	2.62138319	-3.62551808	0.71023601
1	3.02859950	-2.14858341	1.58371663
6	0.36055505	-3.09982157	1.97683370
6	0.67584991	-2.96524858	3.35006666
6	0.02428369	-3.77817178	4.28641129
6	-0.94720393	-4.71317101	3.91627622
6	-1.26345587	-4.81562233	2.55671883
6	-0.62543130	-4.03888416	1.58298433
6	1.00700939	4.23094654	-2.23518252
1	-0.57175756	6.08560514	-1.12113059
6	-1.90058303	6.42243814	1.24419904
1	-1.22541082	4.18951893	2.67483425
6	0.20435420	1.96031868	2.26776695
6	1.65622032	-1.92482424	3.83121109
1	0.27139288	-3.65470171	5.34410429

6	-1.61692131	-5.59509659	4.94258881
1	-2.02356482	-5.53320551	2.23707795
6	-0.99888021	-4.21511364	0.13023460
1	1.04267025	5.26993418	-2.59008408
1	0.45762190	3.65513563	-2.99777961
1	2.03114581	3.83375597	-2.21212840
1	0.27837285	0.99501121	1.74996471
1	-0.61808670	1.91539562	2.99457645
1	1.13488698	2.08886862	2.84494162
1	-1.57032466	7.36634350	0.78844398
1	-1.89938807	6.54929209	2.33538389
1	-2.94552660	6.26027870	0.93455201
1	1.47404766	-1.68301105	4.88643312
1	1.56751812	-1.00291455	3.23910570
1	2.70118475	-2.26526928	3.75181556
1	-0.11456262	-4.36418200	-0.50779462
1	-1.53330004	-3.33878851	-0.26738647
1	-1.65583575	-5.08539724	0.00741099
1	-2.66269112	-5.80061817	4.67531538
1	-1.60244226	-5.13166189	5.93841887
1	-1.10558403	-6.56741571	5.02659178
1	0.46976861	-2.20758224	0.14211489

Energy = -7584.949441 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 8

Atomic N.	X	Y	Z
8	-0.71648151	-1.16851115	0.37944344
6	-1.51228607	-0.44516352	1.06153095
8	-1.00526881	0.77998668	1.38154173
6	-1.86223483	1.75133669	2.00879717
1	-2.11319327	1.46594954	3.04061389
1	-2.77059889	1.89520204	1.40947902
1	-1.28563619	2.68216252	2.02259064
8	-2.71374846	0.09791892	-0.43075773
6	-2.49479437	-1.07301426	2.03377128
1	-3.24866605	-0.33814913	2.34660554
1	-1.88404524	-1.28445196	2.93067718
6	-3.17477870	-2.36326075	1.55056000
1	-2.51143432	-2.87507892	0.83633196
1	-3.27603102	-3.03748631	2.41472149
6	-4.57386684	-2.17011857	0.94351578
1	-5.19444609	-1.59727025	1.65607214
1	-5.04957390	-3.16113639	0.86232448
6	-4.64512300	-1.49359977	-0.43158594
1	-4.10443449	-2.10090184	-1.17782342
1	-5.70112324	-1.47841060	-0.75353456
6	-4.12319517	-0.05254092	-0.50338960
1	-4.58902407	0.54467380	0.30617887
1	-4.47184086	0.40168595	-1.45121610
50	-1.30326366	-0.92725295	-1.85836601
7	1.32597423	-1.23785520	-2.42133617
6	1.23488951	-1.90345216	-3.73100638
1	2.22504663	-1.96921921	-4.22046518
1	0.55017889	-1.35810041	-4.39274645
1	0.83568555	-2.91747308	-3.59576654
7	-0.53893131	0.99274135	-2.41286588

6	1.78878534	0.15713227	-2.55748272
1	2.71551871	0.20856814	-3.16566205
1	2.01040602	0.53553635	-1.55226624
6	0.71097320	1.05506468	-3.16749167
1	1.10732579	2.08407092	-3.16768599
1	0.57203341	0.80147022	-4.24059916
6	-1.27337980	2.21040487	-2.36198735
6	-2.45292425	2.38961554	-3.12702632
6	-3.16473079	3.59349871	-3.03877878
6	-2.74242401	4.64779520	-2.22275162
6	-1.56914067	4.46584034	-1.48220599
6	-0.83032435	3.27762318	-1.53671110
7	2.94034815	-2.52280688	0.73484588
6	2.18097854	-2.06083465	-1.53537822
1	3.13469625	-2.30653811	-2.04429007
1	1.64863467	-3.01459503	-1.38661826
6	2.48313498	-1.44509137	-0.16606531
1	3.28754663	-0.70470876	-0.24854565
1	1.58527660	-0.93544841	0.22300620
6	3.47392750	-2.13055444	1.99423063
6	2.77338004	-2.42485762	3.18923426
6	3.34075665	-2.08267665	4.42125225
6	4.58172798	-1.44138491	4.51381493
6	5.26694155	-1.17775834	3.32313800
6	4.74638224	-1.51773179	2.06828260
6	-2.95321178	1.31179821	-4.06001568
1	-4.07158852	3.71323586	-3.63794565
6	-3.50495100	5.95038557	-2.17081547
1	-1.21997035	5.27128172	-0.82972199
6	0.41213614	3.13725114	-0.69369507
6	1.43098080	-3.11750722	3.14391136
1	2.78964090	-2.31702614	5.33576918
6	5.15410376	-1.03764832	5.85147953
1	6.25503826	-0.71209276	3.36779547
6	5.57468081	-1.28208852	0.82945555
1	-3.64480925	1.73385525	-4.80181074
1	-3.50155139	0.51723105	-3.52749395
1	-2.12604880	0.82134795	-4.59117842
1	0.44982025	2.14598298	-0.22206469
1	0.44143841	3.90939808	0.08712861
1	1.33156538	3.25103354	-1.29087722
1	-3.14077473	6.65653896	-2.93423772
1	-3.39226294	6.44188166	-1.19448161
1	-4.57693195	5.79603815	-2.35556364
1	0.97556746	-3.13741755	4.14215040
1	1.51795435	-4.16515112	2.80852222
1	0.72884190	-2.61631536	2.45926261
1	5.33157349	-0.32606906	0.33795235
1	5.40619230	-2.07986021	0.09205670
1	6.64295912	-1.25178242	1.08145940
1	6.25106192	-0.98726070	5.81832981
1	4.86757565	-1.74551177	6.64156008
1	4.79076815	-0.04357069	6.15777826
1	2.15659618	-3.15880108	0.88513744

Energy = -7584.947871 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 9

Atomic N.	X	Y	Z
8	-0.85618144	-0.26590437	0.23572649
6	-1.92558193	0.34216928	-0.12043736
8	-2.19224024	1.45011544	0.63334471
6	-3.27589822	2.31309152	0.25146064
1	-4.25438833	1.85024881	0.44938472
1	-3.18587685	2.59355998	-0.80634797
1	-3.16417646	3.20999908	0.87000954
8	-1.24087894	1.17055905	-1.72267592
6	-3.12331653	-0.45187318	-0.61805552
1	-3.87806702	0.21829320	-1.05243957
1	-3.56855679	-0.85706139	0.30808553
6	-2.80956364	-1.60098326	-1.58616936
1	-1.80176461	-1.98833430	-1.37088335
1	-3.50533438	-2.42623186	-1.37207246
6	-2.94819021	-1.24269068	-3.07369304
1	-3.94716811	-0.80117756	-3.24166465
1	-2.93251109	-2.17801690	-3.65688419
6	-1.88457859	-0.30221480	-3.65298343
1	-0.88968062	-0.77479637	-3.58733344
1	-2.09024262	-0.16606914	-4.72929096
6	-1.80130875	1.09645331	-3.02705717
1	-2.81160259	1.55194843	-3.01198936
1	-1.18909633	1.73557436	-3.69377804
50	0.79387629	0.23957223	-1.22591913
7	3.49916911	-0.27100322	-0.13522863
6	4.40533257	-0.01172668	-1.25684381
1	5.45937777	0.10574334	-0.92968172
1	4.10523510	0.90170801	-1.78519523
1	4.34908867	-0.84424585	-1.97093952
7	1.48371136	1.98881185	-0.20775689
6	3.47613049	0.84684300	0.81839287
1	4.50348616	1.07129800	1.18415511
1	2.86869979	0.54060817	1.68169522
6	2.87016368	2.12716317	0.24598154
1	2.91822243	2.87716055	1.05418038
1	3.53264570	2.52811003	-0.55033714
6	0.72905403	3.18839860	-0.02549668
6	0.50416255	4.07600069	-1.10420775
6	-0.21500006	5.25958061	-0.88991249
6	-0.71634668	5.60410261	0.36978874
6	-0.48272112	4.71942806	1.42892289
6	0.22645222	3.52403212	1.25665998
7	1.57588851	-2.48208427	0.57520479
6	3.85636568	-1.54145253	0.51777530
1	4.77074289	-1.42330050	1.13873065
1	4.11254549	-2.25870228	-0.27928877
6	2.75998545	-2.15728474	1.38470030
1	3.18755627	-3.05910611	1.86347997
1	2.48460102	-1.47222316	2.19791675
6	0.65165430	-3.45004463	1.04103744
6	-0.03972526	-3.28145719	2.26420021
6	-0.95718825	-4.26126289	2.66442513
6	-1.24358022	-5.38901043	1.88838732
6	-0.58541268	-5.51118994	0.65951526
6	0.35498238	-4.57139206	0.22590365
6	1.03844404	3.77460933	-2.48280525

1	-0.37786156	5.93654680	-1.73299503
6	-1.45375502	6.90426350	0.58785874
1	-0.87253159	4.96017313	2.42217636
6	0.42994490	2.59945512	2.42961526
6	0.12493762	-2.03889799	3.10375190
1	-1.48776805	-4.11565351	3.60904408
6	-2.21729517	-6.44060278	2.36348271
1	-0.80181623	-6.36933088	0.01797739
6	1.03338802	-4.75665903	-1.11168647
1	0.98860449	4.66668749	-3.12136626
1	0.45626065	2.98056650	-2.97434759
1	2.08033514	3.42748284	-2.44763136
1	0.23357794	1.55989766	2.13699102
1	-0.23931378	2.86902618	3.25711727
1	1.46240592	2.64587164	2.81357861
1	-0.76292670	7.70958233	0.88494754
1	-2.20418668	6.81129885	1.38542664
1	-1.96429110	7.23488140	-0.32713500
1	-0.71687651	-1.93926334	3.80118370
1	0.14921232	-1.14513993	2.46416354
1	1.04612350	-2.05470371	3.70752406
1	2.13048625	-4.81409502	-1.01809013
1	0.80833852	-3.93353629	-1.81063044
1	0.69685709	-5.68650627	-1.58685923
1	-2.72837734	-6.92537022	1.52018976
1	-2.98156953	-6.00874996	3.02427435
1	-1.70462322	-7.23269224	2.93269420
1	1.87132502	-2.70887446	-0.37295282

Energy = -7584.941849 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 10

Atomic N.	X	Y	Z
8	-0.93028069	-2.16388297	-1.41374242
6	0.17426033	-2.82563186	-1.39173698
8	0.97310048	-2.82107878	-2.51621270
6	0.73131692	-1.75375223	-3.45484281
1	0.94920969	-0.77023178	-3.01108766
1	-0.31087646	-1.76942134	-3.79647708
1	1.41623461	-1.94337702	-4.28818178
8	1.09972870	-1.72988677	-0.18313770
6	0.25099438	-4.19411469	-0.71348506
1	0.23805372	-4.92865705	-1.53427804
1	-0.68954557	-4.31172752	-0.15977049
6	1.43141150	-4.50515270	0.22761391
1	1.23948216	-4.03508425	1.20305717
1	1.40367019	-5.59251881	0.40312177
6	2.84982395	-4.10775948	-0.23490626
1	2.93382287	-4.18761969	-1.33035171
1	3.56572270	-4.83309364	0.18273365
6	3.28820348	-2.70515466	0.22227007
1	3.19399166	-2.64394927	1.31996655
1	4.35511637	-2.55382133	-0.01578751
6	2.49687457	-1.56454945	-0.41285643
1	2.70385027	-1.53866696	-1.49788666
1	2.81698990	-0.59162843	-0.00017458
50	-0.57095641	-0.22985491	-0.29547191

7	0.33658746	1.00192916	1.98034608
6	1.77555275	0.96080810	2.27997422
1	2.01461315	1.45053160	3.24425673
1	2.33662486	1.45296729	1.47645426
1	2.09223008	-0.08760453	2.33622456
7	1.01837528	3.08009195	-0.16600169
6	-0.18664423	2.39031839	1.92564189
1	-0.34577799	2.76409769	2.95750022
1	-1.17715073	2.35514712	1.44369328
6	0.68414885	3.43198085	1.22056973
1	0.12266763	4.38513422	1.27536583
1	1.60628796	3.58820868	1.79937959
6	1.42102671	4.12450266	-1.04051554
6	2.63105989	4.82368279	-0.82183397
6	3.00759459	5.83491087	-1.71577024
6	2.24151850	6.16620731	-2.83702135
6	1.06696534	5.43660021	-3.05743051
6	0.63995212	4.43234777	-2.18292856
7	-1.77427804	-0.97564882	1.29914379
6	-0.41396621	0.21418177	2.98693323
1	-0.47048795	0.77434033	3.94297934
1	0.15478800	-0.70937943	3.16120028
6	-1.81523609	-0.17645651	2.52135205
1	-2.27900481	-0.75220686	3.33852267
1	-2.44616961	0.73197955	2.41501451
6	-2.71545315	-2.03892207	1.22373462
6	-3.81333494	-1.98920119	0.32732865
6	-4.72812557	-3.04839468	0.28886208
6	-4.59967804	-4.17497301	1.10816479
6	-3.51049590	-4.21813774	1.98399293
6	-2.57041168	-3.18209791	2.05409884
6	3.55934310	4.45929861	0.31053883
1	3.94895220	6.36133146	-1.53768170
6	2.65731478	7.27724409	-3.77087402
1	0.45394397	5.66106176	-3.93408084
6	-0.64331424	3.68877840	-2.46799326
6	-4.01970005	-0.81244546	-0.59391785
1	-5.57307196	-2.98627687	-0.40226299
6	-5.58144760	-5.31906557	1.02158070
1	-3.37477064	-5.09348106	2.62535954
6	-1.38961005	-3.32251811	2.98214507
1	4.57852411	4.80688858	0.09710620
1	3.58719873	3.36945271	0.45653033
1	3.25594687	4.91113138	1.26838529
1	-0.47628069	2.61264992	-2.63708735
1	-1.12981868	4.09189510	-3.36501026
1	-1.35950243	3.76814198	-1.63451409
1	2.14277411	8.21962166	-3.52379346
1	2.41133833	7.03853655	-4.81497383
1	3.73718739	7.46833372	-3.70872426
1	-5.05613995	-0.77985215	-0.95598936
1	-3.36864996	-0.88120043	-1.48049808
1	-3.79280305	0.14013383	-0.09488649
1	-1.52672136	-2.76977921	3.92604017
1	-0.48007524	-2.92772436	2.50760341
1	-1.22655416	-4.37585020	3.24628997
1	-5.28672981	-6.03801394	0.24036019
1	-6.59029865	-4.96310329	0.77019751

1 -5.63883257 -5.87171888 1.96927214
 1 0.26781937 2.52019978 -0.57672894
 Energy = -7584.949149 Hartree
 Number of imaginary frequencies = 0.

Compound TS3b isomer 11

Atomic N.	X	Y	Z
8	2.34148169	-1.46091413	0.98980486
6	3.13559914	-1.72227240	0.03028381
8	3.12413192	-2.94971251	-0.57432121
6	1.97577834	-3.78247285	-0.31875375
1	1.06462634	-3.34289265	-0.75078666
1	1.83295548	-3.92053628	0.76054955
1	2.19821596	-4.73725986	-0.80649781
8	2.11244392	-0.60726708	-1.32236111
6	4.53007936	-1.10926557	-0.06770414
1	5.23616600	-1.95144737	0.00857707
1	4.65380669	-0.49637052	0.83545864
6	4.89856195	-0.25828546	-1.29834652
1	4.34709930	0.68997449	-1.25395143
1	5.96532297	-0.00851381	-1.17632282
6	4.68611860	-0.89963627	-2.68898058
1	4.74430227	-1.99830425	-2.61750722
1	5.51731348	-0.59303492	-3.34322119
6	3.37301302	-0.49091023	-3.37966275
1	3.32089186	0.60893166	-3.42852807
1	3.37063789	-0.86272359	-4.41887712
6	2.12120938	-1.01439309	-2.67852426
1	2.09897351	-2.12109995	-2.75306535
1	1.21469283	-0.64197147	-3.19530940
50	0.39434189	-0.50463897	0.04935525
7	-0.17922778	-0.01936954	2.62631488
6	1.06404459	-0.06980994	3.41357183
1	0.92164278	0.38366050	4.41389608
1	1.86801744	0.45049778	2.88461947
1	1.37265551	-1.11531126	3.53412366
7	0.81797475	1.54985070	0.43317220
6	-0.65211117	1.36369753	2.42395258
1	-0.86975676	1.85877347	3.39286447
1	-1.58426929	1.30447006	1.84362459
6	0.35765463	2.21233511	1.65073895
1	-0.15291212	3.16409039	1.40951562
1	1.19387138	2.48736882	2.32425761
6	1.52727485	2.38500595	-0.47364491
6	2.80714130	2.90811157	-0.15742557
6	3.46363664	3.74177599	-1.07340980
6	2.90505433	4.07665586	-2.30963469
6	1.64367366	3.55143166	-2.61391068
6	0.94982600	2.72080898	-1.72670937
7	-2.88969207	-0.96245724	1.45282376
6	-1.17901170	-0.89680421	3.28753304
1	-1.14468050	-0.72145522	4.38199949
1	-0.85051721	-1.93594694	3.12102604
6	-2.64463472	-0.74459213	2.88341427
1	-3.20478177	-1.47138667	3.50249553
1	-3.00262785	0.25156644	3.18444586
6	-4.16979885	-1.40388799	1.03517652

6	-5.31859303	-0.60809278	1.25466347
6	-6.56522274	-1.07321894	0.81558764
6	-6.71632290	-2.28728676	0.13931935
6	-5.56090164	-3.03864717	-0.10794733
6	-4.29835176	-2.62657022	0.32888964
6	3.50544095	2.54519629	1.12945175
1	4.45495176	4.12436342	-0.81478226
6	3.64662766	4.94490147	-3.29773641
1	1.17763889	3.80373144	-3.57033324
6	-0.41540661	2.20881271	-2.11775303
6	-5.22013044	0.76206839	1.87944674
1	-7.44301462	-0.44453618	0.98654777
6	-8.07519341	-2.77692986	-0.30013788
1	-5.64302063	-3.98351979	-0.65130353
6	-3.08846593	-3.48343015	0.03952413
1	4.59499359	2.62295604	1.01379919
1	3.25448537	1.51695895	1.42523837
1	3.21925926	3.20856547	1.96140826
1	-0.38623920	1.15241218	-2.43423414
1	-0.81656241	2.78354192	-2.96325040
1	-1.12411141	2.26353955	-1.28037226
1	2.96467662	5.62932682	-3.82205749
1	4.14636755	4.33470917	-4.06702948
1	4.42001534	5.54611158	-2.80119872
1	-6.10841703	1.35836625	1.63390362
1	-4.33161974	1.29533243	1.50977874
1	-5.14633322	0.72435755	2.97777128
1	-2.55802083	-3.77131081	0.96177417
1	-2.35604143	-2.96612096	-0.60178483
1	-3.38577938	-4.40527153	-0.47587779
1	-8.01951694	-3.31257749	-1.25805283
1	-8.78222847	-1.94411469	-0.41453922
1	-8.50608063	-3.47350025	0.43685424
1	-2.14509344	-1.52418673	1.03829253

Energy = -7584.948447 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 12

Atomic N.	X	Y	Z
8	-0.72618163	-2.07942986	-1.49294865
6	0.49491879	-2.19530702	-1.86754405
8	0.88516885	-1.19094884	-2.74772215
6	2.26988316	-1.11851394	-3.12688112
1	2.54969311	-1.94774806	-3.79344440
1	2.90952802	-1.10918903	-2.23339844
1	2.37848520	-0.17109799	-3.66647911
8	1.35074317	-1.51670849	-0.36143392
6	1.07931507	-3.57251978	-2.14454532
1	2.17790627	-3.53073764	-2.11855507
1	0.79937130	-3.78101110	-3.19186020
6	0.55562365	-4.69138908	-1.24021244
1	-0.52213532	-4.54042435	-1.07914221
1	0.66740996	-5.64559507	-1.77825916
6	1.27466989	-4.80983973	0.10751079
1	2.34808731	-5.00750828	-0.06705781
1	0.88287020	-5.69935179	0.62653852
6	1.13335168	-3.60360122	1.04477072

1	0.07131711	-3.34329820	1.16441560
1	1.50073040	-3.90271330	2.04154897
6	1.91753507	-2.34462023	0.65160131
1	2.94047618	-2.63301229	0.33641684
1	2.03565526	-1.71213174	1.55037987
50	-0.52571732	-0.16685438	-0.23609188
7	0.36461589	1.28270137	1.99417722
6	1.79538357	1.34506190	2.32152581
1	1.99352133	1.94287181	3.23344493
1	2.34858942	1.77394700	1.47740543
1	2.16610932	0.32692161	2.49264860
7	0.99901259	3.18630743	-0.31792784
6	-0.22498174	2.62895942	1.80067301
1	-0.43176851	3.08782411	2.78962779
1	-1.19869852	2.49965715	1.29999757
6	0.61152261	3.64634109	1.02179861
1	0.00187297	4.56996632	0.97507614
1	1.50809383	3.90214467	1.60488188
6	1.38302290	4.15690184	-1.27887785
6	2.53891850	4.95044947	-1.08636296
6	2.89698076	5.88667059	-2.06521964
6	2.16764736	6.05164862	-3.24638414
6	1.05251932	5.22725868	-3.43821907
6	0.64377052	4.29255772	-2.48145175
7	-1.59587502	-0.95489663	1.45286334
6	-0.38284788	0.54401410	3.03547549
1	-0.53367472	1.18620420	3.92842174
1	0.23650400	-0.31256104	3.33556557
6	-1.73179400	0.00599360	2.55357122
1	-2.21611977	-0.47430298	3.41724062
1	-2.39722943	0.85353768	2.28649116
6	-2.46892381	-2.07602620	1.50161600
6	-3.49001312	-2.25826359	0.52922308
6	-4.31763935	-3.38607764	0.59155083
6	-4.18912411	-4.35604811	1.59050024
6	-3.20045829	-4.15650368	2.55781984
6	-2.34762740	-3.04539490	2.53757215
6	3.43751431	4.76085711	0.11118800
1	3.79622626	6.48726320	-1.90451753
6	2.55950236	7.08825254	-4.27172041
1	0.47132897	5.31881475	-4.35939455
6	-0.57263124	3.43727922	-2.74434900
6	-3.73833108	-1.24863327	-0.56491041
1	-5.09949160	-3.50114179	-0.16397192
6	-5.07069445	-5.58157825	1.60857284
1	-3.07760739	-4.89392757	3.35596037
6	-1.30793738	-2.92402577	3.62541366
1	4.44158077	5.15170431	-0.09933826
1	3.52683067	3.69476271	0.36698070
1	3.06678057	5.28364420	1.00719237
1	-0.32705963	2.36448717	-2.80190897
1	-1.04173028	3.71879578	-3.69544554
1	-1.33137405	3.54381204	-1.95259619
1	2.01650500	8.03346252	-4.11110449
1	2.32955909	6.75175381	-5.29213095
1	3.63292861	7.31631994	-4.22003078
1	-4.76741076	-1.33509994	-0.93906873
1	-3.06633973	-1.40486598	-1.42272305

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1 -3.58953238 -0.21914247 -0.20697755
1 -0.38894978 -2.45895600 3.24584985
1 -1.05705428 -3.91336274 4.03082800
1 -1.65889513 -2.30927038 4.47035217
1 -4.65916014 -6.37782383 0.96771955
1 -6.07925510 -5.35514975 1.23519015
1 -5.16477060 -5.99355125 2.62258172
1 0.28945327 2.55100632 -0.68997329
Energy = -7584.939436 Hartree
Number of imaginary frequencies = 0.

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Compound TS3b isomer 13

Atomic N.	X	Y	Z
8	2.30811429	-1.37981761	1.07684135
6	2.73506284	-2.18672967	0.20144445
8	1.96169221	-3.31316781	0.05787501
6	2.18555617	-4.18231535	-1.06617665
1	3.12849569	-4.73926115	-0.96934623
1	2.16835308	-3.60277081	-1.99848640
1	1.34837782	-4.88882685	-1.05784142
8	2.01628280	-1.13413846	-1.37303662
6	4.20714521	-2.29121995	-0.13203047
1	4.35472679	-2.93491769	-1.00950360
1	4.63767481	-2.83831811	0.72681999
6	4.94525099	-0.95725811	-0.32699502
1	4.45549107	-0.18427806	0.28331175
1	5.96181393	-1.07759154	0.07830933
6	5.07504559	-0.48974159	-1.78904045
1	5.40382957	-1.34464002	-2.40819049
1	5.89773560	0.24261834	-1.83376300
6	3.84119177	0.16234942	-2.42841673
1	3.54946613	1.05086732	-1.84956801
1	4.12382603	0.52321202	-3.43330407
6	2.61307740	-0.73401749	-2.59261441
1	2.89532018	-1.63656032	-3.17671442
1	1.86317801	-0.19746432	-3.20569062
50	0.36147907	-0.52178276	0.04211382
7	-0.18389504	0.11409851	2.57468200
6	1.05779374	0.09330168	3.36712527
1	0.91536605	0.59916800	4.34198713
1	1.86943591	0.57809991	2.81652808
1	1.35548437	-0.94744527	3.54092336
7	0.81143951	1.57388294	0.28985918
6	-0.64586908	1.48835683	2.30261755
1	-0.86090726	2.03389549	3.24485040
1	-1.57681382	1.40910792	1.72261548
6	0.37715077	2.28452206	1.49430799
1	-0.11264709	3.23807216	1.22152281
1	1.21948242	2.56301498	2.15726733
6	1.45522678	2.38779998	-0.67646080
6	2.68329000	3.04793692	-0.39832434
6	3.26778698	3.87165880	-1.37001932
6	2.69562626	4.06112909	-2.63073683
6	1.49374902	3.39680147	-2.90071487
6	0.86539817	2.57632089	-1.95665991
7	-2.91763043	-0.85642910	1.46363890
6	-1.18922472	-0.72518033	3.27806520

1	-1.14423084	-0.50437862	4.36367464
1	-0.87245762	-1.77343309	3.15204525
6	-2.65633535	-0.57248771	2.87960052
1	-3.21995759	-1.26108193	3.53796601
1	-2.99829769	0.44187349	3.13508749
6	-4.20595169	-1.30094731	1.07705140
6	-5.34468937	-0.48452061	1.27157128
6	-6.59986210	-0.95516098	0.86347896
6	-6.76912165	-2.19545126	0.24147168
6	-5.62332582	-2.96856165	0.01689040
6	-4.35276365	-2.55146527	0.42456499
6	3.41916847	2.82462049	0.89980841
1	4.21799374	4.36020851	-1.13672447
6	3.36590981	4.91818333	-3.67755675
1	1.01619029	3.53514266	-3.87455368
6	-0.45029891	1.92811608	-2.31509471
6	-5.22743320	0.91069829	1.83487856
1	-7.46977425	-0.31066167	1.01480043
6	-8.13663292	-2.68928289	-0.16548169
1	-5.71957064	-3.93508697	-0.48450133
6	-3.15400481	-3.43194604	0.16215017
1	4.49626255	2.99199080	0.76443630
1	3.26505256	1.79647624	1.25767159
1	3.08296132	3.50600100	1.69750595
1	-0.33528492	0.86082029	-2.57026386
1	-0.89484632	2.41633177	-3.19269252
1	-1.16324580	1.97558331	-1.48051059
1	2.62732172	5.45073080	-4.29310560
1	3.97681522	4.30677700	-4.36099911
1	4.03154612	5.66254997	-3.22014189
1	-6.11303473	1.50384700	1.57241642
1	-4.33835030	1.41924119	1.43305302
1	-5.14203453	0.92063063	2.93296194
1	-2.61910272	-3.68821669	1.09093690
1	-2.41943836	-2.95032191	-0.50384355
1	-3.46478391	-4.37073517	-0.31330287
1	-8.09742260	-3.25093865	-1.10931873
1	-8.84068394	-1.85578299	-0.29272023
1	-8.56083012	-3.36347032	0.59581786
1	-2.18388510	-1.44823503	1.07189882

Energy = -7584.939741 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 14

Atomic N.	X	Y	Z
8	0.61233336	-1.19227147	2.43274045
6	1.81807160	-1.57440484	2.17910004
8	2.19011045	-2.85890698	2.44796586
6	1.12472284	-3.83420610	2.46477342
1	0.71225244	-3.94600296	1.45520556
1	0.33043638	-3.53323317	3.15686727
1	1.59478593	-4.76781130	2.79129958
8	1.62481689	-1.55805957	0.31093791
6	3.01747537	-0.67490876	2.46833372
1	3.93543339	-1.25258601	2.28760314
1	2.95972347	-0.52447712	3.55927801
6	3.09588528	0.68678653	1.76617956

1	2.08468628	1.10191905	1.61708987
1	3.60378456	1.38477767	2.44949818
6	3.87995124	0.68369687	0.44201654
1	4.85133791	0.18692583	0.61417657
1	4.11599827	1.72682953	0.17620280
6	3.18993640	0.02984871	-0.76246417
1	2.30361962	0.62421948	-1.04391944
1	3.88072252	0.05913190	-1.62378669
6	2.73772979	-1.41883373	-0.55986226
1	3.56855464	-2.03069568	-0.15854807
1	2.47266483	-1.86187983	-1.53867185
50	-0.24806966	-0.28774026	0.54374081
7	-0.92145491	-0.60406739	-2.15856695
6	-0.43222708	-1.87681365	-2.70930862
1	-1.03103554	-2.20926428	-3.58129287
1	-0.46405914	-2.65119028	-1.93550777
1	0.61036825	-1.75546455	-3.02931714
7	-1.75884211	-1.83100379	0.38624591
6	-2.34474134	-0.70915586	-1.77005243
1	-2.97552991	-0.86539966	-2.67098761
1	-2.63834977	0.25233278	-1.32136512
6	-2.63676906	-1.83844018	-0.78173798
1	-3.69644356	-1.71496797	-0.48194918
1	-2.59990859	-2.80035424	-1.33036649
6	-2.17130375	-2.72125721	1.41546619
6	-2.14213490	-4.13054514	1.22943676
6	-2.58011270	-4.98120928	2.25327229
6	-3.04855251	-4.49584484	3.47704625
6	-3.05999041	-3.10863042	3.65756583
6	-2.63938737	-2.22013497	2.66062999
7	0.42887896	2.37000084	-2.10897946
6	-0.74841297	0.45949575	-3.17509460
1	-1.49779809	0.31113473	-3.98036146
1	0.23808993	0.30932710	-3.64260936
6	-0.84167588	1.91138601	-2.69636440
1	-1.12336504	2.52952313	-3.57127500
1	-1.65005004	2.02269316	-1.96235287
6	0.62457174	3.76584959	-1.92667758
6	-0.18304069	4.50998640	-1.03615940
6	0.06717324	5.87958574	-0.87584937
6	1.10661769	6.53825331	-1.53883803
6	1.91499329	5.77683592	-2.39130759
6	1.69184101	4.41281557	-2.60069323
6	-1.58431518	-4.74974537	-0.02843716
1	-2.53434038	-6.06178904	2.09020734
6	-3.54321861	-5.42981529	4.55538034
1	-3.41655326	-2.69799376	4.60601950
6	-2.69755459	-0.73916578	2.94320250
6	-1.26683760	3.85765648	-0.21396168
1	-0.56446087	6.44219637	-0.18350658
6	1.37684751	8.00659943	-1.31348836
1	2.74053645	6.25996923	-2.92036295
6	2.59336114	3.64546418	-3.54045320
1	-1.21603668	-5.76502180	0.17182818
1	-0.75269836	-4.14657974	-0.42039028
1	-2.33785176	-4.83125496	-0.82827842
1	-1.70773947	-0.34459847	3.22351837
1	-3.37628508	-0.53207749	3.78151560

1	-3.04063201	-0.17252795	2.06598854
1	-4.63944244	-5.53469706	4.52062893
1	-3.28504658	-5.06000090	5.55755854
1	-3.11535883	-6.43509150	4.44037485
1	-1.48378885	4.46067572	0.67744964
1	-0.96344316	2.85163879	0.11380290
1	-2.21206331	3.75491929	-0.77162105
1	2.03006053	3.15597820	-4.35171890
1	3.16830182	2.85994768	-3.02111602
1	3.32201195	4.31938648	-4.00769377
1	2.18613529	8.15626049	-0.58123213
1	0.48678055	8.52222443	-0.92903465
1	1.68589985	8.50521851	-2.24308395
1	1.19341981	1.99863052	-2.67150092

Energy = -7584.945944 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 15

Atomic N.	X	Y	Z
8	2.06663966	-1.56128311	-0.88139969
6	3.27016926	-1.26103556	-0.58450115
8	4.20988989	-1.20016086	-1.56058550
6	3.71215320	-1.19133854	-2.91731572
1	2.93298864	-0.43017131	-3.03728747
1	3.31217527	-2.18030548	-3.17898107
1	4.58050299	-0.95622927	-3.54120636
8	2.82316995	0.68143189	-0.26642334
6	3.93434095	-1.63694906	0.72639453
1	4.95340347	-1.22509146	0.72448021
1	4.05084085	-2.73258281	0.64646888
6	3.20734549	-1.29372931	2.03424358
1	2.11666155	-1.29508245	1.87276816
1	3.40288973	-2.11195445	2.74423027
6	3.65749145	0.01721664	2.70682526
1	4.76181412	0.04037801	2.72087312
1	3.34551048	-0.01790721	3.76332760
6	3.13573670	1.32927132	2.10619116
1	2.03980637	1.38048100	2.22652817
1	3.54858160	2.16999173	2.69038105
6	3.46990705	1.56972301	0.63136071
1	4.56367302	1.48338282	0.47493482
1	3.19712639	2.60876822	0.36394957
50	0.66049945	0.17230769	-0.30893555
7	-0.85896194	-1.37077141	-1.86825967
6	-0.54249060	-2.80849528	-1.91143036
1	-1.18595433	-3.34697843	-2.63365936
1	-0.66655684	-3.24342561	-0.91298902
1	0.50601095	-2.92608142	-2.20384955
7	-2.14161539	-1.90935552	0.86695802
6	-2.27898860	-1.12023747	-1.50992012
1	-2.91441894	-1.27412498	-2.40526867
1	-2.37161589	-0.05855072	-1.23276114
6	-2.87781596	-1.98701465	-0.40128964
1	-3.92566919	-1.64804327	-0.28400269
1	-2.93048167	-3.03113699	-0.74248827
6	-2.81906366	-2.25826144	2.06347752
6	-3.28002262	-3.57887006	2.27583075

6	-3.93106031	-3.89058924	3.47684360
6	-4.12107277	-2.94897342	4.49230576
6	-3.61979914	-1.65884161	4.28067207
6	-2.98184323	-1.29463947	3.09088016
7	0.42786342	1.25592494	-2.16413522
6	-0.54824024	-0.74488980	-3.17778373
1	-1.26052701	-1.10080659	-3.94936252
1	0.46036208	-1.08119154	-3.45698047
6	-0.55554283	0.77934605	-3.12817836
1	-0.29730609	1.13389707	-4.14561749
1	-1.58948529	1.14200127	-2.94625759
6	0.59225547	2.67704535	-2.11098862
6	-0.40387756	3.54580212	-1.58784556
6	-0.17374258	4.92923689	-1.55125022
6	1.01249170	5.49995327	-2.01737571
6	1.98252940	4.63854408	-2.54285192
6	1.79598165	3.25288606	-2.59921908
6	-3.02049112	-4.67585564	1.27268887
1	-4.27560234	-4.91684294	3.62909222
6	-4.84928513	-3.30483246	5.76610613
1	-3.73663521	-0.90411472	5.06264925
6	-2.47172880	0.11608729	2.91668010
6	-1.72261643	3.03382254	-1.05915511
1	-0.95010960	5.57746792	-1.13556385
6	1.25383365	6.98794603	-1.93403804
1	2.91543031	5.05761576	-2.92964506
6	2.87558770	2.38702488	-3.19447041
1	-3.08785319	-5.65923023	1.75600159
1	-2.01722980	-4.57259226	0.83358681
1	-3.74424314	-4.67158937	0.44220880
1	-1.37801719	0.15302679	2.78543162
1	-2.71932173	0.72526103	3.79499388
1	-2.91210008	0.60767078	2.03428531
1	-5.91104174	-3.01524138	5.71300840
1	-4.41631508	-2.78937769	6.63472700
1	-4.81466103	-4.38594055	5.95749664
1	-2.15650392	3.74765301	-0.34660870
1	-1.60529029	2.06845522	-0.54495353
1	-2.45830965	2.88856435	-1.86641109
1	2.46984577	1.73049867	-3.97762966
1	3.31660509	1.73742282	-2.42529416
1	3.66852546	3.00631762	-3.63498378
1	1.86386967	7.24272394	-1.05275440
1	0.30983636	7.54323769	-1.85212529
1	1.79391325	7.35654306	-2.81757474
1	-1.67475116	-1.00421226	0.95272821

Energy = -7584.951760 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 16

Atomic N.	X	Y	Z
8	1.93501401	-1.23409438	-0.72404724
6	3.05172133	-0.62809259	-0.62838596
8	3.55239892	-0.21241884	-1.82793033
6	4.72089911	0.62677163	-1.84651804
1	5.62297106	0.07714916	-1.54111040
1	4.56389189	1.50633240	-1.20857346

1	4.83105230	0.94891459	-2.88748217
8	2.34500504	1.09985352	0.05496338
6	4.04862356	-0.99752206	0.45537660
1	4.84589481	-0.24474820	0.51786548
1	4.52568436	-1.91806889	0.07210821
6	3.45585227	-1.26020873	1.84842074
1	2.41779184	-1.61104870	1.74136865
1	4.01421595	-2.09322476	2.30192566
6	3.52913451	-0.06863807	2.81781721
1	4.56840134	0.30617943	2.84081388
1	3.32392454	-0.44308028	3.83388424
6	2.58168387	1.10670877	2.54509258
1	1.53422737	0.76767975	2.62228084
1	2.72214317	1.85699916	3.34278941
6	2.76335073	1.82469368	1.20205259
1	3.82865310	2.10596442	1.07959831
1	2.19969273	2.77759290	1.23090422
50	0.27547491	0.24064964	-0.15745012
7	-1.05465460	-1.38738787	-1.78405643
6	-0.57710367	-2.78001428	-1.82658017
1	-1.12369800	-3.37855577	-2.58028364
1	-0.69318897	-3.24047828	-0.83835661
1	0.48979065	-2.77174568	-2.07471395
7	-2.35518384	-2.10771942	0.91222268
6	-2.50022078	-1.28703463	-1.45608521
1	-3.09612060	-1.48352695	-2.36983323
1	-2.70492530	-0.24529034	-1.16043150
6	-3.03744984	-2.23373580	-0.38206902
1	-4.11797237	-2.00857496	-0.29285666
1	-2.97023511	-3.26970434	-0.74564409
6	-3.04146576	-2.52347517	2.08109784
6	-3.40680838	-3.87848783	2.26238441
6	-4.07217073	-4.25603199	3.43615150
6	-4.36773825	-3.34609103	4.45530844
6	-3.95934963	-2.01892924	4.27652168
6	-3.31125236	-1.58997834	3.11385036
7	0.04924920	1.33163190	-1.98088872
6	-0.77876019	-0.71242893	-3.07558823
1	-1.46749055	-1.09283459	-3.85714436
1	0.25018173	-0.97464693	-3.35799265
6	-0.87538189	0.80795211	-2.98065281
1	-0.64040166	1.20958781	-3.97968864
1	-1.92657065	1.11198092	-2.78701758
6	0.59964609	2.61419058	-2.23620534
6	0.27363199	3.72476888	-1.41467595
6	0.84189636	4.97888613	-1.67458260
6	1.72770727	5.18887997	-2.73550105
6	2.03548288	4.09151173	-3.54695582
6	1.49890864	2.81864548	-3.31941795
6	-3.02937222	-4.93820190	1.25653958
1	-4.34184694	-5.30768013	3.56435513
6	-5.11003733	-3.77434111	5.69834709
1	-4.16001606	-1.28899312	5.06375313
6	-2.90417385	-0.14250799	2.97442198
6	-0.70315373	3.59452009	-0.26991183
1	0.56867439	5.82192516	-1.03389442
6	2.35164595	6.54227972	-2.97942972
1	2.73203945	4.22329235	-4.38005066

6	1.92325377	1.67667902	-4.20915699
1	-3.03971362	-5.93075514	1.72547853
1	-2.02166486	-4.75372458	0.85588694
1	-3.72085261	-4.97593403	0.39986500
1	-1.81217134	-0.02172244	2.88692927
1	-3.23160338	0.43473071	3.84818101
1	-3.34475636	0.32530895	2.07932377
1	-6.19180250	-3.58872294	5.60122681
1	-4.76483488	-3.22210550	6.58345938
1	-4.97940302	-4.84771347	5.89224243
1	-1.09736013	4.57955885	0.01506161
1	-0.23773606	3.16442537	0.63295472
1	-1.54562414	2.93948722	-0.53166932
1	1.19368601	1.47494423	-5.01043463
1	2.03757858	0.75366008	-3.62481499
1	2.87755442	1.90790176	-4.70216703
1	3.33488607	6.62330437	-2.48851538
1	1.72202075	7.35029602	-2.58221889
1	2.50852156	6.72577095	-4.05151987
1	-1.95979178	-1.17139018	1.01967859

Energy = -7584.948204 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 17

Atomic N.	X	Y	Z
8	1.47064745	-1.89480150	1.12205863
6	2.03292108	-2.56340027	0.13109531
8	2.11106062	-3.93318224	0.27155200
6	1.01379251	-4.55609226	0.96998864
1	0.10301858	-4.51406050	0.35727832
1	0.83366656	-4.06635571	1.93332148
1	1.31893849	-5.59818840	1.11529899
8	0.87541693	-2.26409268	-1.06949174
6	3.38792801	-2.04114604	-0.36407980
1	3.23266673	-1.02433908	-0.75974494
1	3.97948503	-1.92420256	0.55747008
6	4.16209078	-2.91536784	-1.35571802
1	4.19671297	-3.94318438	-0.96625209
1	5.20393038	-2.55787516	-1.38362765
6	3.62007785	-2.92470360	-2.78929496
1	3.73421359	-1.91791296	-3.22957134
1	4.25276995	-3.59392166	-3.39443469
6	2.15483785	-3.35617185	-2.94328356
1	1.97114623	-4.31173801	-2.42866015
1	1.95565963	-3.53038001	-4.01400805
6	1.12738502	-2.31982136	-2.48366141
1	1.43661296	-1.32112741	-2.85170388
1	0.15292509	-2.55557036	-2.94476175
50	0.27142030	-0.33752525	0.15046269
7	-1.94735646	0.44897413	-1.42267954
6	-2.44484878	-0.72092158	-2.15567374
1	-3.49947810	-0.59221232	-2.47358513
1	-2.36461949	-1.61945474	-1.53393543
1	-1.83229244	-0.86845636	-3.05553269
7	-1.51694226	-1.02541900	1.07822597
6	-2.74219441	0.73772323	-0.21719292
1	-3.78056192	1.03288043	-0.48015064

8	0.55146307	-1.21458483	-1.87002444
6	1.83698320	-1.41331327	-1.83239269
8	2.52967715	-1.42870033	-3.00731850
6	2.02409410	-0.56117773	-4.04253054
1	2.07417941	0.48265344	-3.70632339
1	0.99044549	-0.82338524	-4.29933167
1	2.68509436	-0.71998423	-4.90111732
8	2.24673343	0.20277800	-1.07177627
6	2.38621259	-2.46985912	-0.87965590
1	2.01508975	-2.23223257	0.12919366
1	1.87383461	-3.39849997	-1.18376052
6	3.89969444	-2.70509839	-0.87755883
1	4.24664164	-2.81374693	-1.91601622
1	4.08484888	-3.67447901	-0.38754958
6	4.74378920	-1.64322090	-0.16118807
1	4.45304060	-1.60293710	0.90376085
1	5.79176235	-1.98425269	-0.17576659
6	4.68447399	-0.22143567	-0.74089122
1	4.80224991	-0.24433695	-1.83589005
1	5.54105759	0.35106483	-0.34690434
6	3.43659759	0.58365917	-0.37640885
1	3.27795124	0.50902516	0.71956831
1	3.61808610	1.64707410	-0.61411113
50	0.14411192	0.24027520	-0.21755707
7	-2.34767580	-0.24401055	-0.91104066
6	-2.59644079	-1.61088634	-1.40233016
1	-3.63928843	-1.73976433	-1.74904728
1	-2.38295984	-2.33261466	-0.60514307
1	-1.91082275	-1.81050134	-2.23324776
7	-2.28298688	-1.48329830	1.91072106
6	-3.22748470	0.12567121	0.22996698
1	-4.21757555	0.43419641	-0.16023906
1	-2.78730440	1.01057172	0.71751851
6	-3.49809599	-0.95176315	1.28086460
1	-4.17030191	-0.48398536	2.02649093
1	-4.07314825	-1.76937568	0.82211763
6	-2.39858556	-2.10015702	3.18327928
6	-3.14789104	-3.28886485	3.34666896
6	-3.22610354	-3.87815642	4.61560583
6	-2.56717253	-3.34921408	5.72905970
6	-1.79666221	-2.19579792	5.53779221
6	-1.70449257	-1.56039476	4.29567337
7	-0.42237881	1.90891933	-1.43798065
6	-2.51060224	0.73790336	-2.01240158
1	-3.58683395	0.88115758	-2.23642421
1	-2.02540326	0.30602160	-2.89845657
6	-1.84594333	2.07887006	-1.70880330
1	-2.00489235	2.72595692	-2.58631229
1	-2.37871575	2.58585215	-0.87565148
6	0.44403908	2.94479322	-1.86551619
6	1.17386639	3.72128582	-0.92607927
6	2.05051112	4.71869373	-1.37268651
6	2.23382807	4.99763489	-2.73037767
6	1.49910259	4.24067545	-3.64896011
6	0.61797380	3.22869539	-3.24999046
6	-3.80246139	-3.97692657	2.17389417
1	-3.80309629	-4.80020952	4.72482491
6	-2.68854165	-3.99032664	7.09055948

1	-1.25494766	-1.76732087	6.38496447
6	-0.86503798	-0.31302920	4.15347958
6	1.00199556	3.51957130	0.56062829
1	2.59567928	5.30797195	-0.63019949
6	3.20825076	6.05576086	-3.18947840
1	1.62675035	4.42970324	-4.71867514
6	-0.09968301	2.43153024	-4.31164169
1	-3.98548198	-5.03438616	2.40493917
1	-3.16092205	-3.92258763	1.28202903
1	-4.77338791	-3.52961946	1.90785515
1	-0.02494770	-0.45130566	3.45360136
1	-0.44214651	-0.02222511	5.12323570
1	-1.45308185	0.53889102	3.77579737
1	-3.45798349	-3.49026632	7.70035458
1	-1.74401486	-3.93065810	7.64917183
1	-2.97196651	-5.04849195	7.00994778
1	1.34314382	4.40649176	1.11177611
1	1.58615148	2.66481709	0.94067895
1	-0.04767607	3.32446814	0.82064009
1	-0.24248926	1.39274251	-3.98491073
1	0.47213411	2.43438840	-5.24958849
1	-1.09593046	2.84222198	-4.54350853
1	4.18305397	5.61390114	-3.45143771
1	3.38840604	6.80106115	-2.40281677
1	2.84090042	6.58163118	-4.08178759
1	-1.54034054	-0.78119797	1.90214670

Energy = -7584.954843 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 19

Atomic N.	X	Y	Z
8	1.75278449	-1.92463017	1.07072747
6	1.75582147	-2.90014291	0.24058050
8	0.67128605	-3.73144841	0.38447046
6	0.52943683	-4.88107634	-0.45770535
1	1.33386350	-5.61201048	-0.28794256
1	0.49622896	-4.58733654	-1.51646399
1	-0.42657262	-5.33544731	-0.17373960
8	1.13552690	-1.99796903	-1.34457064
6	3.12040138	-3.51891589	-0.09109389
1	3.85194898	-2.73224759	0.14123225
1	3.24992013	-4.28285789	0.69595271
6	3.47772241	-4.14882565	-1.45263743
1	2.67518783	-4.79727936	-1.82554162
1	4.33540344	-4.81484509	-1.26310384
6	3.89072680	-3.17204046	-2.56191254
1	4.66922665	-2.49255681	-2.17260551
1	4.37034559	-3.75354147	-3.36628938
6	2.76143146	-2.33536053	-3.17122221
1	1.98695004	-2.98996830	-3.60536194
1	3.17663288	-1.74235046	-4.00406075
6	2.09146571	-1.37109089	-2.19391203
1	2.87418056	-0.84571677	-1.60555553
1	1.56630409	-0.57996029	-2.76809072
50	0.44104874	-0.30892110	0.15276960
7	-1.54927659	0.06039160	-1.51881075
6	-1.83472502	-1.21909499	-2.19466043

1	-2.83025908	-1.20017779	-2.67853785
1	-1.78988886	-2.04220772	-1.47440958
1	-1.06815267	-1.40296543	-2.95671463
7	-1.33670294	-1.02831745	1.12568069
6	-2.56827593	0.38490543	-0.49765843
1	-3.56807542	0.50901490	-0.96134508
1	-2.27097344	1.33915389	-0.03917184
6	-2.65140247	-0.69006133	0.58419758
1	-3.30683255	-0.28768301	1.37915981
1	-3.18983483	-1.56555915	0.17188357
6	-1.35177588	-1.72873139	2.36222148
6	-1.98247433	-2.99499345	2.49458241
6	-2.01171350	-3.63569665	3.74031091
6	-1.42404127	-3.08144498	4.87958622
6	-0.78385502	-1.84625196	4.73575783
6	-0.73813522	-1.16494107	3.51433730
7	-0.45403028	2.92779469	-1.11638176
6	-1.41174221	1.11344922	-2.56025553
1	-2.22324228	0.98763239	-3.30479336
1	-0.46312714	0.92335910	-3.08815527
6	-1.47136319	2.57292604	-2.11205578
1	-1.36108994	3.17525554	-3.03442574
1	-2.47710013	2.79239988	-1.72336209
6	-0.03490505	4.27834320	-1.01632547
6	-0.94637561	5.29609680	-0.65067995
6	-0.48944879	6.61696005	-0.55037248
6	0.84589714	6.96669054	-0.77054429
6	1.74128580	5.93739080	-1.08633471
6	1.32911301	4.60805988	-1.21832645
6	-2.57772946	-3.71175838	1.30835617
1	-2.49417496	-4.61479425	3.81166768
6	-1.49308527	-3.77653337	6.21821070
1	-0.30883816	-1.38705862	5.60694265
6	-0.03502141	0.16902545	3.46321058
6	-2.37767911	4.98107290	-0.29053780
1	-1.20356023	7.39222431	-0.26066178
6	1.30665708	8.40149307	-0.67924505
1	2.79632282	6.17531157	-1.24432743
6	2.33904886	3.54041266	-1.56694055
1	-2.57466507	-4.79735279	1.47864711
1	-1.99826443	-3.49568486	0.40080905
1	-3.62272692	-3.41843963	1.11760938
1	0.97654349	0.08206176	3.03179717
1	0.08843855	0.57923007	4.47464323
1	-0.58792329	0.89834875	2.85435677
1	-2.31159973	-3.37385559	6.83645439
1	-0.56268620	-3.64509106	6.78847885
1	-1.67246437	-4.85394287	6.09971571
1	-2.80849934	5.79437590	0.30761614
1	-2.43630576	4.05191565	0.29571056
1	-3.02058887	4.85212040	-1.17563307
1	2.06868529	3.00418758	-2.49125981
1	2.43484426	2.78142023	-0.77327973
1	3.33059216	3.98486829	-1.71859920
1	2.31496239	8.47356224	-0.24817105
1	0.62619364	9.00079250	-0.05930894
1	1.34477389	8.87312317	-1.67428541
1	0.34400073	2.29380751	-1.17029607

Energy = -7584.935161 Hartree
 Number of imaginary frequencies = 0.

Compound TS3b isomer 20

Atomic N.	X	Y	Z
8	0.51835912	-1.45242345	-1.99705684
6	1.78354990	-1.47679830	-2.27533960
8	1.99857831	-1.17916298	-3.59672785
6	3.24938536	-1.46453118	-4.23330498
1	3.51039290	-2.53022099	-4.16000128
1	4.06434536	-0.85070252	-3.82403755
1	3.10089016	-1.20434952	-5.28720903
8	2.19908857	0.03001151	-1.31732941
6	2.60005713	-2.57866335	-1.58502185
1	2.08331013	-2.71991587	-0.62525493
1	2.38539982	-3.49028158	-2.17313528
6	4.11213589	-2.51384997	-1.31346190
1	4.69084024	-2.48618150	-2.24822617
1	4.36229467	-3.48001671	-0.84487134
6	4.61454248	-1.39284706	-0.39009255
1	3.99086094	-1.34750104	0.51865816
1	5.62734365	-1.67043090	-0.05800423
6	4.67313766	-0.00737828	-1.04941189
1	5.00052214	-0.11532773	-2.09751773
1	5.44281673	0.61286718	-0.56097025
6	3.36549377	0.77963465	-0.98410290
1	3.23060465	1.13930809	0.05499472
1	3.43372512	1.67212868	-1.63168395
50	0.17588726	-0.02672541	-0.30820334
7	-2.24174404	-0.55891889	-1.03619599
6	-2.49960518	-1.96990156	-1.37870121
1	-3.52684712	-2.11287475	-1.76300013
1	-2.34864521	-2.59831595	-0.49294990
1	-1.77979672	-2.27461720	-2.14609909
7	-2.37729073	-1.44356668	1.90722489
6	-3.18336892	-0.03629753	-0.00899990
1	-4.13899803	0.23510754	-0.49888986
1	-2.75117564	0.89464450	0.39073178
6	-3.54145575	-0.97301173	1.14535892
1	-4.24308872	-0.40674287	1.78801274
1	-4.10854101	-1.83059072	0.75449800
6	-2.56768489	-1.86654472	3.24720526
6	-3.37959933	-2.98592281	3.54604197
6	-3.53037643	-3.38368130	4.88116837
6	-2.88452339	-2.73078489	5.93493509
6	-2.05140901	-1.65206254	5.61424637
6	-1.88533819	-1.20516932	4.29982281
7	-0.47872111	1.67436552	-1.42910779
6	-2.31145525	0.27795732	-2.26382351
1	-3.35212970	0.30187568	-2.64407372
1	-1.67071080	-0.21147290	-3.01022291
6	-1.80129445	1.69673169	-2.03280926
1	-1.79024625	2.19387913	-3.01928830
1	-2.53480530	2.27177167	-1.42564595
6	0.35045445	2.80510187	-1.63967037
6	0.68062788	3.66973281	-0.56364328
6	1.53013921	4.76323986	-0.78083515

6	2.07119608	5.04459190	-2.03888345
6	1.73767102	4.18855190	-3.09505129
6	0.90018564	3.08018327	-2.92273140
6	-4.02406645	-3.80677152	2.45597219
1	-4.15551901	-4.25449848	5.09553623
6	-3.08432341	-3.16456103	7.36723089
1	-1.51805329	-1.13147342	6.41380787
6	-0.97960186	-0.03015961	4.01733732
6	0.11644221	3.44534469	0.81997746
1	1.76359189	5.42286634	0.05953509
6	3.00683069	6.21180344	-2.24627972
1	2.15830302	4.37683249	-4.08707905
6	0.63584834	2.16682363	-4.09301424
1	-4.27407837	-4.80831289	2.82953882
1	-3.34521914	-3.91613913	1.59725666
1	-4.95703697	-3.35708332	2.08083439
1	-0.12338816	-0.30555910	3.38018680
1	-0.57672268	0.37761781	4.95289803
1	-1.51015639	0.78443396	3.49849749
1	-3.85484600	-2.55479312	7.86572838
1	-2.15996432	-3.05928612	7.95223141
1	-3.40856028	-4.21246719	7.42574024
1	0.16837832	4.36910152	1.41218865
1	0.67183727	2.67117238	1.37425935
1	-0.92791080	3.10807467	0.77545410
1	0.60078382	1.11831307	-3.76828289
1	1.42219639	2.27686596	-4.85195446
1	-0.32271856	2.39224291	-4.58869839
1	4.06049395	5.89238691	-2.20097589
1	2.86480784	6.97990465	-1.47386956
1	2.85352325	6.68097687	-3.22826743
1	-1.60585582	-0.77755636	1.83289766

Energy = -7584.939139 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 21

Atomic N.	X	Y	Z
8	2.50449228	-1.98794651	0.06132614
6	3.06768274	-0.81148851	-0.11530357
8	3.72721124	-0.59579438	-1.30234766
6	3.19110751	-1.27180374	-2.45825028
1	2.17735624	-0.91446507	-2.67817760
1	3.17145705	-2.35632992	-2.30323195
1	3.86926651	-1.01318741	-3.27910972
8	1.62647498	0.13086770	-0.17590329
6	3.92652464	-0.26914597	1.03416479
1	3.27641320	-0.15357769	1.91647196
1	4.61363363	-1.09874070	1.26563990
6	4.73904991	1.00242400	0.76889116
1	5.28514624	0.88018006	-0.17786852
1	5.50233078	1.08845699	1.55908251
6	3.93428302	2.30674267	0.73637390
1	3.51513934	2.50195146	1.73949683
1	4.63095379	3.13580060	0.53142613
6	2.78660131	2.36023402	-0.28243208
1	3.13610578	2.06421614	-1.28353512
1	2.44497871	3.40551949	-0.36276349

6	1.55158496	1.54269457	0.09895356
1	1.32720125	1.70761049	1.16918349
1	0.68671185	1.91331208	-0.47624528
50	0.61654383	-1.52923691	1.12652779
7	-2.22662044	-1.81019950	2.06762886
6	-2.23251867	-1.98067153	3.51960993
1	-3.14640689	-2.49990177	3.87941122
1	-2.16668010	-1.00846577	4.02285385
1	-1.35365224	-2.56748104	3.82048988
7	-2.01373053	1.14796233	1.23870921
6	-3.31701946	-0.94010270	1.61685133
1	-4.29173946	-1.27838445	2.03587961
1	-3.39908600	-1.03578591	0.52362663
6	-3.14604092	0.54040122	1.96011329
1	-4.10281038	1.04796195	1.72335100
1	-2.98940563	0.67197090	3.03831577
6	-1.80534291	2.54161835	1.45391560
6	-1.26428604	2.99507737	2.67933536
6	-1.03357506	4.36510468	2.85586429
6	-1.30214047	5.30479240	1.85496175
6	-1.80959451	4.83206701	0.63916391
6	-2.07324076	3.47483301	0.42321050
7	-0.53739172	-2.53697395	-0.34531119
6	-2.25088644	-3.12001228	1.40067005
1	-3.24696279	-3.60708261	1.49703562
1	-1.52591074	-3.76169896	1.92767930
6	-1.86890209	-3.08376527	-0.07668207
1	-1.92453992	-4.13149881	-0.43080893
1	-2.65093136	-2.55025530	-0.65718412
6	-0.13738991	-2.78576803	-1.69534349
6	-0.49487469	-1.89024556	-2.72938633
6	-0.14687140	-2.18801379	-4.05443478
6	0.55273509	-3.35115361	-4.39109325
6	0.90599829	-4.22465372	-3.35503507
6	0.57970023	-3.96342468	-2.01883006
6	-0.88005936	2.02909875	3.77263451
1	-0.60582823	4.70257664	3.80349231
6	-1.06976783	6.77892208	2.08377671
1	-2.01710773	5.54115629	-0.16623244
6	-2.62647748	3.02316165	-0.90887153
6	-1.21286047	-0.59991908	-2.41938233
1	-0.42918178	-1.48679554	-4.84434557
6	0.93649632	-3.64816833	-5.82129192
1	1.45753527	-5.13852596	-3.59197879
6	1.02093017	-4.91994047	-0.93988049
1	-0.08960440	2.45693588	4.40323496
1	-0.51917559	1.08058786	3.34901953
1	-1.72811496	1.79392076	4.43646145
1	-1.90161228	2.41809726	-1.47850001
1	-2.88046312	3.88961220	-1.53211319
1	-3.53818774	2.41618800	-0.79583704
1	-1.97920787	7.26987028	2.46532369
1	-0.78974897	7.29104996	1.15309381
1	-0.27413705	6.94873857	2.82187963
1	-1.37486815	-0.01657318	-3.33536530
1	-0.62048155	0.00752128	-1.71897423
1	-2.19445920	-0.77458119	-1.95282483
1	0.19984207	-5.18188286	-0.25803244

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1  1.81420767 -4.46509695 -0.32788557
1  1.41467118 -5.84533644 -1.38040996
1  2.00864124 -3.46334434 -5.99312353
1  0.37542325 -3.01842022 -6.52442932
1  0.74677837 -4.70038223 -6.07742691
1 -2.13131452  0.96698499  0.24105199
Energy = -7584.950330 Hartree
Number of imaginary frequencies = 0.

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Compound TS3b isomer 22

Atomic N.	X	Y	Z
8	0.21884981	-0.48665440	0.32735431
6	1.16383410	-1.02297854	1.03622413
8	1.94661796	-1.97955108	0.47312599
6	2.16147876	-1.86203897	-0.95076692
1	2.62808156	-0.89451373	-1.17575133
1	1.21481311	-1.96052074	-1.49530017
1	2.83669519	-2.68515038	-1.20673621
8	2.23966694	0.51394701	1.03492701
6	0.91239405	-1.32499313	2.50767946
1	0.54481524	-0.40024576	2.97806668
1	0.05714388	-2.02315950	2.50074267
6	2.05911565	-1.94324529	3.31270671
1	2.48143649	-2.78760695	2.74746633
1	1.62418437	-2.37321234	4.22909737
6	3.18438911	-0.98586553	3.72613764
1	2.76645494	-0.18104491	4.35682297
1	3.87654281	-1.54837382	4.37359381
6	3.99329972	-0.34985217	2.58470631
1	4.26412868	-1.10900080	1.83378839
1	4.94254732	0.02913566	2.99972296
6	3.33186865	0.84319347	1.89280581
1	3.00208187	1.56079268	2.67368507
1	4.09202147	1.35315287	1.27321517
50	0.35210481	1.73927057	0.81301987
7	-2.02857590	2.32907033	-0.43858904
6	-2.20575619	3.68489099	0.11121538
1	-2.99249339	4.24299717	-0.43274969
1	-1.26933920	4.25327253	0.04932073
1	-2.48668718	3.61180615	1.16952825
7	0.81083727	2.31049895	-1.19813788
6	-1.58968651	2.38891912	-1.84709072
1	-2.31510997	2.97244215	-2.45308924
1	-1.56993425	1.36141670	-2.23395371
6	-0.19425577	2.99169803	-2.00986171
1	0.06147317	2.91421652	-3.07983899
1	-0.23257697	4.08306026	-1.80535805
6	2.11808801	2.27913380	-1.75517404
6	3.16091108	3.08048248	-1.22350466
6	4.44543171	3.00852752	-1.77759457
6	4.74389410	2.17253160	-2.85887766
6	3.70282006	1.40600598	-3.39268565
6	2.40470695	1.44325733	-2.86795807
7	-2.79549670	-0.74386513	0.44518122
6	-3.32325196	1.61622655	-0.29445502
1	-4.07136774	2.12123179	-0.94349605
1	-3.64832377	1.74820018	0.74702871

6	-3.36041927	0.11710494	-0.60481089
1	-4.42143536	-0.14326622	-0.72136551
1	-2.90032768	-0.09021623	-1.58898485
6	-3.48795271	-1.95769465	0.71279025
6	-2.95994020	-3.21432400	0.32959715
6	-3.65985656	-4.38286257	0.65800714
6	-4.88106346	-4.35426664	1.33881056
6	-5.38673306	-3.10386729	1.71293104
6	-4.71382570	-1.91171420	1.42337990
6	2.90611219	4.04319954	-0.08768188
1	5.23461485	3.63846469	-1.35811508
6	6.14549637	2.08290410	-3.41332245
1	3.90689468	0.74540251	-4.24002218
6	1.33571911	0.57376665	-3.48233557
6	-1.65841281	-3.32217836	-0.42890522
1	-3.24005318	-5.34565878	0.35490382
6	-5.63947201	-5.62435770	1.64162922
1	-6.32465887	-3.05205202	2.27221155
6	-5.26733637	-0.60217100	1.92725277
1	3.69775081	4.80329943	-0.04226041
1	2.88917851	3.54034853	0.89288414
1	1.93821704	4.55050516	-0.19953063
1	0.65311557	0.19626541	-2.70879984
1	1.78303909	-0.27664208	-4.01453924
1	0.72457224	1.12559509	-4.21515560
1	6.69053268	3.02751088	-3.27956080
1	6.13918972	1.83889759	-4.48447704
1	6.72532892	1.29719555	-2.90280485
1	-1.56164432	-4.31761217	-0.88134253
1	-0.78421301	-3.17366505	0.22341293
1	-1.58474553	-2.57286119	-1.22999620
1	-5.75530720	-0.01428658	1.13329399
1	-4.45956707	0.02239697	2.33593583
1	-6.01719046	-0.77494287	2.71016264
1	-6.16912317	-5.55557728	2.60219574
1	-4.96765757	-6.49231529	1.68240833
1	-6.39667225	-5.83152008	0.86852652
1	-1.79202604	-0.88630962	0.30748382

Energy = -7584.953673 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 23

Atomic N.	X	Y	Z
8	0.49888337	0.43930900	-0.49564299
6	1.80000663	0.51596886	-0.45696342
8	2.39073443	1.68973112	-0.82577252
6	1.63054967	2.88732672	-0.55786532
1	1.41840649	2.96983886	0.51503748
1	0.69106901	2.88436508	-1.12329495
1	2.27146649	3.71264768	-0.88658279
8	1.93127763	0.45754862	1.34797215
6	2.61217833	-0.66564792	-0.98451596
1	2.29802680	-1.56220508	-0.42718819
1	2.24825764	-0.80256450	-2.01634240
6	4.13721275	-0.52812594	-0.99730510
1	4.40406752	0.44071984	-1.44498718
1	4.53732061	-1.30128312	-1.67283249

6	4.83071041	-0.67637503	0.36216107
1	4.64846659	-1.69228733	0.75630462
1	5.91826296	-0.60608315	0.19680452
6	4.43151855	0.34439683	1.43834424
1	4.45360279	1.36691642	1.02972746
1	5.18541241	0.31198660	2.24306059
6	3.08124590	0.09275269	2.11410522
1	3.02440763	-0.97696638	2.40583515
1	3.04649782	0.68737978	3.04531741
50	-0.05884894	-0.73965287	1.31012952
7	-2.82665610	-1.76347291	1.37209332
6	-2.92424321	-2.51868939	2.62449670
1	-3.97462702	-2.75435233	2.89346123
1	-2.47842693	-1.94748223	3.44819593
1	-2.36443734	-3.45869946	2.52934074
7	-1.37478125	0.80510396	1.98589134
6	-3.48180795	-0.45125005	1.47573435
1	-4.53165388	-0.56475455	1.82734478
1	-3.50712228	-0.00713357	0.47068194
6	-2.74891949	0.52025974	2.40117407
1	-3.33541632	1.45517421	2.39748049
1	-2.80929613	0.15221080	3.44767475
6	-0.96570647	2.14458418	2.25691128
6	-0.19560705	2.45225048	3.40526557
6	0.18195067	3.77860975	3.65132117
6	-0.18713512	4.82574463	2.79911613
6	-0.96551639	4.51178551	1.67982304
6	-1.35803795	3.19776678	1.39324391
7	-1.42441225	-2.29662561	-1.23973572
6	-3.36618447	-2.55915999	0.25578108
1	-4.47711182	-2.54895830	0.26255229
1	-3.06462526	-3.60637546	0.42199898
6	-2.88301325	-2.13424230	-1.12963152
1	-3.41993833	-2.75364256	-1.87308359
1	-3.16218019	-1.09074485	-1.32862115
6	-0.82083869	-2.42111778	-2.51667905
6	-0.93915135	-1.40488458	-3.49411607
6	-0.29664159	-1.57365513	-4.72750187
6	0.48496515	-2.69442368	-5.02482367
6	0.62755239	-3.66470003	-4.02647924
6	-0.01040046	-3.55274963	-2.78726363
6	0.20048812	1.37431705	4.38494349
1	0.77299345	4.00073624	4.54391909
6	0.26148045	6.24262285	3.06652474
1	-1.27073824	5.31213522	1.00008607
6	-2.17710757	2.91402030	0.15971252
6	-1.66819060	-0.11392168	-3.21508980
1	-0.39085865	-0.77769446	-5.47067499
6	1.14258897	-2.85631537	-6.37411928
1	1.24953425	-4.54301786	-4.21708155
6	0.18211570	-4.63379526	-1.74892628
1	0.58237427	1.81736326	5.31435728
1	0.99003619	0.72521812	3.97803617
1	-0.64786541	0.72156149	4.63265657
1	-1.77524745	2.04216647	-0.37431058
1	-2.17944527	3.78040504	-0.51497734
1	-3.22706699	2.68778157	0.40653011
1	0.33156723	6.44492865	4.14437246

1	-0.43006486	6.97248888	2.62415671
1	1.25769341	6.43217611	2.63561273
1	-1.37305701	0.65188658	-3.94399476
1	-1.41951025	0.25593632	-2.21019578
1	-2.76219416	-0.22216734	-3.28171897
1	-0.77293813	-5.09473085	-1.44642079
1	0.66438675	-4.25247955	-0.83314842
1	0.82163900	-5.43367577	-2.14243436
1	2.09082627	-3.40589547	-6.29574728
1	1.34928250	-1.88189912	-6.83749580
1	0.49749804	-3.41769767	-7.06893015
1	-1.13153291	-3.06852627	-0.64279622

Energy = -7584.949646 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 24

Atomic N.	X	Y	Z
8	2.14780569	-2.45232725	-0.69452560
6	2.46757269	-1.22654092	-0.89941883
8	1.83925414	-0.68454534	-1.98181796
6	2.15738082	0.63239259	-2.44528985
1	3.21898508	0.72174513	-2.71815896
1	1.89480853	1.38857353	-1.69239867
1	1.54322112	0.77606618	-3.34123206
8	1.33652413	-0.39128393	0.47888088
6	3.91192770	-0.82402164	-0.59376448
1	4.27829313	-1.58428240	0.10978729
1	4.43751001	-1.02538061	-1.54462683
6	4.32030392	0.57303590	-0.08483439
1	3.77385926	1.37090182	-0.60331345
1	5.37891674	0.70383590	-0.36251894
6	4.20575094	0.78900468	1.43029940
1	4.69799471	-0.05108167	1.95130086
1	4.78610182	1.68926620	1.69084477
6	2.78336883	0.95351535	1.97394383
1	2.29605293	1.82706034	1.51152146
1	2.84539151	1.17136490	3.05342913
6	1.88110757	-0.26601011	1.79951108
1	2.44540572	-1.17986250	2.08384156
1	1.02992046	-0.19289859	2.50144744
50	0.23689276	-2.46343064	0.50004309
7	-2.35887384	-1.72610509	1.34201527
6	-2.53983974	-2.07650518	2.75362825
1	-3.60944176	-2.17545915	3.02871633
1	-2.07303286	-1.31727636	3.39184642
1	-2.03797603	-3.03402591	2.94833207
7	-1.29858875	1.05586588	1.95581710
6	-3.02244425	-0.45988455	0.98102421
1	-4.12586164	-0.59974265	0.97575039
1	-2.72474480	-0.21632066	-0.04899381
6	-2.73132205	0.73952740	1.87958896
1	-3.31779099	1.58401418	1.46580267
1	-3.12467575	0.56215912	2.89177227
6	-0.96138179	2.35895085	2.42063522
6	-1.07886815	2.67538118	3.79318094
6	-0.71805084	3.95582771	4.23235798
6	-0.22462988	4.93212700	3.36078644

6	-0.09254026	4.59143639	2.00906515
6	-0.46094301	3.33259082	1.52245939
7	-1.05500221	-2.42082286	-1.20668125
6	-2.84992075	-2.81886840	0.48095614
1	-3.95242214	-2.92260599	0.56682283
1	-2.40256476	-3.75253224	0.86032730
6	-2.48334312	-2.65419078	-0.99412328
1	-2.81067586	-3.58536530	-1.49860573
1	-3.10262108	-1.85121131	-1.44250607
6	-0.70098424	-2.42361736	-2.58820033
6	-0.97564584	-1.30136156	-3.40823746
6	-0.65418994	-1.34053004	-4.77123213
6	-0.05894948	-2.46029782	-5.36029434
6	0.20801111	-3.56196904	-4.53994465
6	-0.09817605	-3.56486678	-3.17351627
6	-1.53450656	1.64311731	4.79344463
1	-0.80446839	4.18525743	5.29760504
6	0.13499629	6.31238031	3.85612416
1	0.29798496	5.33183861	1.30614984
6	-0.32506147	3.02163148	0.05071450
6	-1.57185316	-0.04440943	-2.82666397
1	-0.86989832	-0.46346006	-5.38829660
6	0.30638728	-2.47433162	-6.82570553
1	0.66623980	-4.45345116	-4.97675133
6	0.22758868	-4.78563356	-2.34918642
1	-1.20427656	1.91159606	5.80531931
1	-1.12737107	0.65379298	4.53861380
1	-2.63173723	1.54707241	4.82359171
1	0.36135218	2.17827797	-0.12996446
1	0.06200303	3.89302349	-0.49265352
1	-1.29211318	2.74747539	-0.39933276
1	-0.71561539	7.00533915	3.75558853
1	0.97084045	6.73933125	3.28497386
1	0.41798747	6.29551077	4.91742229
1	-1.39809620	0.81442958	-3.48913503
1	-1.12896574	0.16783021	-1.84351742
1	-2.66184616	-0.12626818	-2.68441939
1	-0.58240169	-5.03427744	-1.64942348
1	1.13630664	-4.62185287	-1.74933088
1	0.41020983	-5.65297794	-2.99753857
1	1.38134360	-2.28204584	-6.97123337
1	-0.24460334	-1.70460486	-7.38280249
1	0.08943832	-3.44967079	-7.28425074
1	-0.84672379	0.86566144	1.05915761

Energy = -7584.936985 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 25

Atomic N.	X	Y	Z
8	0.16592441	-0.54071808	0.27564207
6	1.01892388	-1.22520411	0.97339332
8	1.80852044	-2.13217640	0.34198439
6	2.15640807	-1.82269776	-1.02572048
1	2.68404460	-0.86115110	-1.06448007
1	1.25953913	-1.78696406	-1.65558064
1	2.81478596	-2.63747883	-1.34447563
8	2.15451813	0.23434637	1.29089475

6	0.62244600	-1.72167253	2.35756850
1	0.25308278	-0.85545301	2.92742848
1	-0.25734380	-2.36346817	2.17584848
6	1.66419148	-2.51145864	3.15520382
1	2.09967518	-3.28812599	2.50870824
1	1.13011873	-3.04362965	3.95855546
6	2.78713655	-1.68694162	3.79780650
1	2.34844494	-0.95823771	4.50257874
1	3.39264083	-2.37370491	4.41132021
6	3.72316289	-0.94097054	2.83390665
1	4.02681589	-1.59902048	2.00427723
1	4.64691067	-0.67986423	3.37746453
6	3.18047500	0.37453562	2.27317119
1	2.81619716	0.99185985	3.12149501
1	4.01495838	0.92252392	1.79867232
50	0.34916297	1.58127022	1.09555185
7	-1.87785554	2.47318602	-0.25759029
6	-2.05391312	3.74088335	0.47311974
1	-2.76347375	4.41321993	-0.04729939
1	-1.09460306	4.26244497	0.58027649
1	-2.43637514	3.52788758	1.47941864
7	1.01814771	2.41302514	-0.75957197
6	-1.30502522	2.71667480	-1.59654009
1	-1.94561338	3.42181993	-2.16784787
1	-1.29039431	1.75815952	-2.13208652
6	0.12277780	3.26019979	-1.54302335
1	0.47537154	3.32774305	-2.58577800
1	0.10956427	4.30986261	-1.17913508
6	2.36926174	2.39157152	-1.20039570
6	3.39028263	3.04907441	-0.46694446
6	4.71660709	2.98884988	-0.91312689
6	5.07970524	2.30413818	-2.07800221
6	4.06228733	1.68109393	-2.80781388
6	2.72351789	1.71204972	-2.39677906
7	-2.85495400	-0.65146244	0.08968011
6	-3.20721745	1.81641912	-0.33942124
1	-3.86780739	2.44864964	-0.97173762
1	-3.62755585	1.81374180	0.67597061
6	-3.27138257	0.38154879	-0.87100661
1	-4.32351637	0.19888595	-1.12930787
1	-2.71815133	0.29253307	-1.82447326
6	-3.62317538	-1.84893537	0.10701763
6	-3.11268926	-3.06692839	-0.40357336
6	-3.89363551	-4.22739124	-0.32156536
6	-5.17764711	-4.22487116	0.23234668
6	-5.66500235	-3.01317811	0.73579955
6	-4.91393661	-1.83337188	0.69322300
6	3.07053256	3.84844136	0.77427441
1	5.48858738	3.50723410	-0.33786088
6	6.52198458	2.22127652	-2.51719975
1	4.31701660	1.14068270	-3.72381806
6	1.68154836	1.00035107	-3.22378111
6	-1.74413371	-3.14183640	-1.03786480
1	-3.48631310	-5.16002560	-0.72078568
6	-6.01865911	-5.47848654	0.26758331
1	-6.65360785	-2.98676181	1.20179045
6	-5.45988274	-0.57924157	1.32904649
1	3.88553429	4.54877901	1.00185370

1	2.94053102	3.20958924	1.66288066
1	2.13950133	4.41942072	0.65655518
1	0.91316622	0.55543047	-2.57694936
1	2.14064884	0.21062219	-3.83380008
1	1.16696167	1.68412876	-3.91854072
1	6.60394239	2.09988451	-3.60591149
1	7.03029823	1.36099088	-2.05281210
1	7.08117914	3.12232637	-2.22925401
1	-1.64360380	-4.06663942	-1.62060308
1	-0.93828070	-3.13957334	-0.28791741
1	-1.55316079	-2.29169393	-1.70823956
1	-5.83339357	0.14480399	0.58722925
1	-4.67388296	-0.06900821	1.90481043
1	-6.29625130	-0.81791258	1.99881434
1	-6.64214468	-5.51744270	1.17184067
1	-5.39363289	-6.38132763	0.24354637
1	-6.69909716	-5.52706385	-0.59764153
1	-1.84972620	-0.83007121	0.02770654

Energy = -7584.953685 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 26

Atomic N.	X	Y	Z
8	0.54367775	0.44941387	-0.46217695
6	1.84334219	0.49321899	-0.36689293
8	2.47811794	1.65447044	-0.69797921
6	1.73626256	2.86871457	-0.45273623
1	1.48223364	2.94890428	0.61113691
1	0.82132584	2.89199233	-1.05636203
1	2.41011524	3.68016553	-0.74840307
8	1.89526463	0.41934651	1.44549882
6	2.64883566	-0.70444053	-0.86677480
1	2.28867269	-1.59681201	-0.33106259
1	2.32737064	-0.82579863	-1.91453004
6	4.17594194	-0.60348332	-0.81173921
1	4.48450565	0.36502096	-1.23241329
1	4.58689356	-1.37615919	-1.48123038
6	4.80613804	-0.78872073	0.57375497
1	4.58482218	-1.80660129	0.94192916
1	5.90117359	-0.74028105	0.45690936
6	4.38284969	0.22194432	1.65021789
1	4.45289087	1.25163162	1.26569760
1	5.09567738	0.15182801	2.48927855
6	2.99448371	-0.00468299	2.25409603
1	2.89055514	-1.07959569	2.51204038
1	2.93311524	0.56421673	3.19998550
50	-0.12679052	-0.71535045	1.31293905
7	-2.92833447	-1.68560648	1.27313530
6	-3.09576702	-2.43800378	2.51943302
1	-4.16175079	-2.64878917	2.74459839
1	-2.67133069	-1.87711751	3.36140871
1	-2.55484247	-3.39106536	2.44735765
7	-1.43765581	0.86163294	1.91890848
6	-3.55377650	-0.35732591	1.35153580
1	-4.61696911	-0.44399020	1.66943395
1	-3.53671241	0.08303059	0.34469983
6	-2.82795334	0.60117686	2.29654479

1	-3.39632869	1.54686451	2.27686310
1	-2.92331028	0.23448513	3.34068346
6	-1.02020097	2.20254946	2.16970372
6	-0.28477585	2.52946162	3.33515239
6	0.10349094	3.85662293	3.55994058
6	-0.22188424	4.88628387	2.66959691
6	-0.96789789	4.55414391	1.53352880
6	-1.36883700	3.23848033	1.26723576
7	-1.42058218	-2.26627946	-1.26631367
6	-3.44009423	-2.46599221	0.13341369
1	-4.54921770	-2.42051148	0.08715342
1	-3.18028092	-3.52205062	0.31341666
6	-2.87740350	-2.05784988	-1.22692990
1	-3.39589119	-2.66094089	-1.99614811
1	-3.11391377	-1.00606251	-1.43818772
6	-0.76373976	-2.43554497	-2.51138592
6	-0.80547744	-1.43581975	-3.51182961
6	-0.11407510	-1.64919245	-4.71134996
6	0.64356875	-2.79975629	-4.95188332
6	0.71014071	-3.75375962	-3.93020415
6	0.02131327	-3.59702706	-2.72343469
6	0.06018719	1.47244680	4.35584688
1	0.66815537	4.09359121	4.46568108
6	0.23949572	6.30309677	2.91475296
1	-1.23970366	5.34072733	0.82418025
6	-2.15049529	2.93420458	0.01458896
6	-1.50391209	-0.11734664	-3.28878784
1	-0.14923656	-0.86577046	-5.47277451
6	1.35494030	-3.00920439	-6.26694393
1	1.31120217	-4.65491533	-4.07598495
6	0.13206755	-4.66249323	-1.65736032
1	0.46242771	1.93263829	5.26813650
1	0.81651551	0.77073133	3.97506976
1	-0.81877083	0.87172616	4.62864685
1	-1.73370731	2.05296445	-0.49198699
1	-2.13089108	3.78860927	-0.67489564
1	-3.20750809	2.71262884	0.23344906
1	-0.44541949	7.03253412	2.46125865
1	1.23687220	6.47647953	2.47972894
1	0.31214154	6.52127123	3.98920488
1	-1.15758979	0.62248546	-4.02195930
1	-1.28203523	0.26705149	-2.28292847
1	-2.59745002	-0.19352856	-3.39462924
1	-0.84975439	-5.08684492	-1.38950968
1	0.58593088	-4.27867699	-0.72820753
1	0.76119792	-5.49049759	-2.00676775
1	2.27526331	-3.59521317	-6.13712692
1	1.62226844	-2.05132937	-6.73384047
1	0.71966505	-3.55490565	-6.98296642
1	-1.17884278	-3.03344965	-0.64113528

Energy = -7584.949642 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 27

Atomic N.	X	Y	Z
8	0.20934039	-1.69207621	-2.02072263
6	0.91820598	-2.68944335	-1.58393323

8	2.23242760	-2.79090452	-1.99336481
6	2.85770392	-1.56347787	-2.40853596
1	2.94604754	-0.85984159	-1.56583297
1	2.28907466	-1.08741236	-3.21699643
1	3.85674310	-1.84914112	-2.75500441
8	0.95598847	-2.22775769	0.15190874
6	0.27352214	-4.06438351	-1.51461351
1	-0.67647165	-3.93643427	-0.98048258
1	0.01537045	-4.31798792	-2.55658889
6	1.10259712	-5.20227337	-0.90901285
1	2.01632357	-5.34806108	-1.50669956
1	0.51214218	-6.12583780	-1.02103472
6	1.49734855	-5.05728197	0.57127118
1	0.59949803	-4.86299992	1.18218708
1	1.89238667	-6.02991676	0.90510583
6	2.56338882	-3.98188472	0.84633994
1	3.29034209	-3.97794747	0.02169002
1	3.12530017	-4.23577690	1.76043379
6	2.00365233	-2.57070208	1.05970585
1	1.56873310	-2.51583242	2.07553625
1	2.82876468	-1.83399034	1.01417100
50	0.03051279	-0.20412987	-0.36986861
7	-0.60764188	0.73285687	2.31298065
6	0.37219030	0.32449657	3.32752967
1	0.02658434	0.55430317	4.35618114
1	1.33120549	0.83154064	3.16477609
1	0.54285437	-0.75656104	3.25145435
7	0.59986240	3.29091644	0.80460137
6	-0.93072385	2.17432117	2.43800259
1	-1.34130847	2.35518193	3.45502353
1	-1.72559714	2.40659022	1.71507633
6	0.21177571	3.16449904	2.21578741
1	-0.15809615	4.14015865	2.55879307
1	1.07282400	2.92454171	2.87056279
6	1.51912212	4.33103609	0.48952433
6	2.84286165	4.03300667	0.08340733
6	3.70953751	5.07656097	-0.25931257
6	3.31520271	6.41851139	-0.20320666
6	1.99826610	6.69223642	0.17946440
6	1.09053540	5.67978239	0.51494080
7	-1.96428251	-0.77812892	0.06067459
6	-1.84942186	-0.06049253	2.44691610
1	-2.47291350	0.33574021	3.27625322
1	-1.55921555	-1.08833730	2.70483518
6	-2.67109513	-0.11268361	1.15774262
1	-3.60022831	-0.65985715	1.38476694
1	-2.99845147	0.91012973	0.87959594
6	-2.74904275	-1.67612875	-0.71766460
6	-3.12597179	-1.35100293	-2.04530382
6	-3.91074920	-2.24751973	-2.78058076
6	-4.33825350	-3.47093296	-2.25335097
6	-3.95551896	-3.78364205	-0.94526333
6	-3.17121530	-2.91698503	-0.17303665
6	3.32511449	2.60410476	-0.00004643
1	4.72736549	4.83067083	-0.57298732
6	4.28132439	7.53065300	-0.53380585
1	1.65077794	7.72864676	0.19330327
6	-0.33975944	6.04143524	0.83180183

6	-2.69738436	-0.05515746	-2.68804646
1	-4.20115757	-1.97582936	-3.79894853
6	-5.15558529	-4.43316555	-3.08183026
1	-4.26381159	-4.73912334	-0.51210821
6	-2.74788022	-3.34203553	1.21120000
1	4.39797735	2.57251930	-0.22888114
1	2.79982448	2.03687024	-0.78530777
1	3.16450119	2.05762291	0.94266200
1	-1.02548301	5.26054049	0.47369698
1	-0.60846186	6.99445009	0.35737062
1	-0.51385087	6.16140890	1.91364014
1	4.87371540	7.81985903	0.34904239
1	3.75311375	8.42929077	-0.88051921
1	4.99121761	7.22734404	-1.31567168
1	-3.34662485	0.18818934	-3.53969502
1	-1.66804707	-0.12938684	-3.07341957
1	-2.72264910	0.78174502	-1.97682035
1	-1.68784857	-3.10113811	1.37939870
1	-2.89285684	-4.42209721	1.34596574
1	-3.32363081	-2.83500338	2.00218654
1	-4.51016665	-5.04510593	-3.73205400
1	-5.86076403	-3.90083623	-3.73547506
1	-5.72912645	-5.12195969	-2.44699454
1	0.91811818	2.38684511	0.44551331

Energy = -7584.950465 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 28

Atomic N.	X	Y	Z
8	1.40161514	-1.99186587	1.47895384
6	2.53006721	-2.23903775	0.91661006
8	2.69421434	-3.39294338	0.19893287
6	1.49011517	-4.02364016	-0.27379873
1	0.97471035	-3.37958169	-1.00240195
1	0.81080860	-4.24362612	0.55958986
1	1.81833863	-4.94854355	-0.75970387
8	2.40223908	-0.83645660	-0.37556490
6	3.82679248	-1.82126188	1.58384073
1	3.70035052	-0.77216810	1.87669516
1	3.87949967	-2.41430831	2.51440573
6	5.12539482	-2.01303005	0.79149246
1	5.22023439	-3.06880999	0.49270779
1	5.95619583	-1.81665421	1.48855019
6	5.31877375	-1.11814785	-0.44597721
1	5.18379450	-0.06015739	-0.16481447
1	6.36952591	-1.22319305	-0.76064742
6	4.41493130	-1.45291519	-1.64744365
1	4.26873732	-2.54219723	-1.70218372
1	4.91640139	-1.15525436	-2.58335376
6	3.06146002	-0.73640692	-1.63207185
1	3.23281288	0.33746380	-1.83749163
1	2.42628169	-1.13529515	-2.44901633
50	0.24562076	-0.54153478	0.11505193
7	-1.35943973	-0.36125937	2.21315455
6	-0.62792861	-0.79467440	3.41678882
1	-1.16284633	-0.49140334	4.33735085
1	0.38061532	-0.37076393	3.41848397

1	-0.52513415	-1.88631630	3.40267467
7	0.68755633	1.30328393	1.10519314
6	-1.53817737	1.10448861	2.17207885
1	-2.12060666	1.46023130	3.04637957
1	-2.10223985	1.33469486	1.25668335
6	-0.20055579	1.84446180	2.12915039
1	-0.43584719	2.90669942	1.92559195
1	0.25390902	1.83039236	3.14011097
6	1.81780601	2.10206938	0.78569317
6	2.85992861	2.33113647	1.72256184
6	3.95655227	3.12580132	1.36377835
6	4.07335615	3.70995164	0.09913840
6	3.03894162	3.48365664	-0.81535578
6	1.92159283	2.70186329	-0.49802533
7	-3.33421564	-0.50857937	-0.17864685
6	-2.63900232	-1.11677551	2.15559196
1	-3.08410430	-1.14544582	3.17036772
1	-2.38339114	-2.15562582	1.88984632
6	-3.73809123	-0.59814495	1.22936022
1	-4.59180021	-1.29067540	1.35947311
1	-4.08360052	0.38238239	1.59039712
6	-4.32788420	-0.59789836	-1.18504524
6	-5.36007690	0.36527568	-1.27301478
6	-6.31657934	0.24969134	-2.29046559
6	-6.27498674	-0.76978874	-3.24589014
6	-5.21959257	-1.68682528	-3.16830254
6	-4.25365591	-1.62531042	-2.15947676
6	2.83618665	1.70202994	3.09359956
1	4.75368690	3.27767730	2.09708261
6	5.28474665	4.52859306	-0.27802700
1	3.09454703	3.94142222	-1.80681503
6	0.83273274	2.53009129	-1.53009474
6	-5.40919018	1.55517626	-0.34603935
1	-7.10469055	1.00490534	-2.34965158
6	-7.33290100	-0.88544124	-4.31681633
1	-5.14800119	-2.48462987	-3.91202784
6	-3.14247823	-2.64768767	-2.12247181
1	3.85593200	1.58855295	3.48583078
1	2.36098242	0.71171087	3.05756736
1	2.27459645	2.31041551	3.82066536
1	0.88082945	1.54683852	-2.02840996
1	0.92493165	3.28921461	-2.31845355
1	-0.16621037	2.60278368	-1.07929575
1	5.02554464	5.32179356	-0.99306971
1	6.05664015	3.90221071	-0.75346583
1	5.74270105	4.99784994	0.60337073
1	-6.02167606	2.35444474	-0.78301579
1	-4.39854956	1.95150387	-0.16717286
1	-5.84408092	1.31138909	0.63613695
1	-3.11900473	-3.19568849	-1.16645181
1	-2.14879489	-2.18780899	-2.25036454
1	-3.27178216	-3.38388777	-2.92568064
1	-6.90574741	-1.22977638	-5.26902199
1	-7.82940388	0.07829663	-4.49349499
1	-8.11321926	-1.60880041	-4.03074169
1	-2.54774570	-1.13020658	-0.37165776

Energy = -7584.951485 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 29

Atomic N.	X	Y	Z
8	0.02089463	-1.87057173	-1.90218270
6	0.97459835	-2.63812852	-1.54379916
8	2.22257519	-2.19853926	-1.94399214
6	3.27900314	-3.10572624	-2.30320644
1	2.89929390	-3.97882843	-2.85010099
1	3.85222435	-3.43665457	-1.42618299
1	3.93814874	-2.52992439	-2.96348715
8	0.94597685	-2.09913182	0.33004436
6	0.71214503	-4.12892199	-1.38861299
1	-0.35457551	-4.19610023	-1.13746071
1	0.80866796	-4.56434441	-2.39979410
6	1.51963985	-4.98684406	-0.39043954
1	2.59864092	-4.94863129	-0.59845698
1	1.22327650	-6.02731133	-0.59831679
6	1.26360321	-4.71298265	1.10531104
1	0.20593888	-4.44170809	1.23543978
1	1.41118836	-5.65328979	1.66034400
6	2.14058614	-3.64115739	1.77814198
1	3.17706680	-4.00702810	1.87386179
1	1.76642942	-3.50105214	2.80525041
6	2.15582466	-2.28969955	1.03640580
1	2.32065463	-1.46299171	1.75222969
1	3.00655222	-2.24168754	0.33130589
50	-0.01649515	-0.18000585	-0.38261083
7	-0.60876483	0.70878613	2.22358322
6	0.37591299	0.26844171	3.22218513
1	0.05336266	0.51336193	4.25418234
1	1.34806156	0.74345309	3.04253626
1	0.50459224	-0.81784010	3.14321399
7	0.59399861	3.29768801	0.67767823
6	-0.88165909	2.16302633	2.35587978
1	-1.25684023	2.34981298	3.38450408
1	-1.69045579	2.41944218	1.65717316
6	0.28166491	3.12271881	2.10241890
1	-0.03380602	4.09555960	2.50260210
1	1.16969383	2.83055902	2.69714022
6	1.49803579	4.34793901	0.35128391
6	2.79889321	4.06284761	-0.13135332
6	3.64825463	5.11764574	-0.48266715
6	3.25917506	6.45711660	-0.36236918
6	1.96381330	6.71823597	0.09505571
6	1.07290554	5.69469500	0.44243431
7	-2.03272772	-0.72894293	0.02266215
6	-1.87582469	-0.04157921	2.39777350
1	-2.45795679	0.38211578	3.24234557
1	-1.61143756	-1.07741010	2.65097690
6	-2.72523952	-0.07058068	1.12840533
1	-3.65355372	-0.61438686	1.36904287
1	-3.05237722	0.95861441	0.86903000
6	-2.84199882	-1.56921339	-0.79224592
6	-3.19716406	-1.18753743	-2.11119866
6	-4.01035309	-2.02710533	-2.88089395
6	-4.48698711	-3.25118899	-2.39742923
6	-4.12204742	-3.62297845	-1.10028601

6	-3.31059766	-2.81225443	-0.29503575
6	3.27345848	2.63742876	-0.28627327
1	4.64846611	4.88242388	-0.85564405
6	4.20933723	7.57916784	-0.70576626
1	1.61893487	7.75357437	0.16030671
6	-0.33981588	6.04460907	0.84106749
6	-2.70825386	0.10930471	-2.70747638
1	-4.28284359	-1.71058178	-3.89143515
6	-5.34217262	-4.14831781	-3.26047087
1	-4.46779823	-4.58097029	-0.70187300
6	-2.91302514	-3.29567003	1.07723343
1	4.33444309	2.61329627	-0.56584060
1	2.71301723	2.09454179	-1.06399775
1	3.15638399	2.05942535	0.64388233
1	-1.04184735	5.27320719	0.49420342
1	-0.63211811	7.01086664	0.40917039
1	-0.46064824	6.13182688	1.93333411
1	4.86876154	7.81797266	0.14403369
1	3.66575909	8.49776936	-0.96532840
1	4.85642338	7.31301737	-1.55310047
1	-3.32719374	0.39902571	-3.56725550
1	-1.67231584	0.01325074	-3.07098985
1	-2.72072291	0.92678112	-1.97369587
1	-3.50378299	-2.82095122	1.87774074
1	-1.85708904	-3.06001401	1.27424562
1	-3.06216335	-4.38019276	1.16569006
1	-4.73788309	-4.66053581	-4.02593517
1	-6.11566496	-3.57551050	-3.79228210
1	-5.84160757	-4.92144823	-2.66133118
1	0.89153028	2.40692186	0.26946780

Energy = -7584.934848 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 30

Atomic N.	X	Y	Z
8	1.63738286	-1.79263520	2.24935746
6	2.33543038	-2.66310287	1.66091859
8	1.61202896	-3.68432689	1.11328924
6	2.24418616	-4.64328861	0.24590521
1	3.02359271	-5.20973921	0.77474010
1	2.65623522	-4.12865210	-0.63138229
1	1.44317603	-5.32530355	-0.05885740
8	2.41323376	-1.59331989	-0.21168363
6	3.77474523	-2.90411019	2.09349370
1	4.00704908	-2.07870483	2.78031850
1	3.71986604	-3.81682968	2.71508694
6	4.94264984	-3.06909251	1.09796298
1	4.69136620	-3.77551866	0.29653516
1	5.74857998	-3.54831767	1.67771709
6	5.51664877	-1.78370190	0.47900653
1	5.59292316	-1.00592411	1.25900376
1	6.55243635	-2.00505829	0.17310321
6	4.77662897	-1.20815408	-0.73526520
1	4.66530895	-1.98232150	-1.51384985
1	5.40359068	-0.41217232	-1.17240298
6	3.40529943	-0.60328984	-0.44135666
1	3.49679470	0.08444281	0.42269063

1	3.10468602	0.01943207	-1.30539048
50	0.31978714	-1.01749694	0.42631420
7	-1.45379245	-0.45858431	2.50881410
6	-0.94398367	-1.09205067	3.73723340
1	-1.53502858	-0.77833521	4.62081337
1	0.10752440	-0.83804554	3.89580917
1	-1.00902426	-2.18343067	3.63732839
7	0.67716432	1.02186763	1.04829168
6	-1.29342473	1.00777221	2.55142093
1	-1.68147540	1.41913021	3.50845122
1	-1.87344444	1.43683445	1.72508276
6	0.16575782	1.42793131	2.35999656
1	0.18982515	2.52718472	2.43836379
1	0.77221757	1.04692459	3.20385551
6	1.41184402	1.98801637	0.32776013
6	2.49255347	2.70390630	0.92103118
6	3.16428995	3.68851137	0.18609889
6	2.83493495	3.99210072	-1.13840854
6	1.80313611	3.25319815	-1.72667420
6	1.09116042	2.26951218	-1.03059375
7	-3.11543512	-0.36359122	-0.09116665
6	-2.85944653	-0.89926428	2.33742380
1	-3.41007710	-0.75140423	3.29036713
1	-2.82740235	-1.98683286	2.15812874
6	-3.69845200	-0.23195598	1.24939120
1	-4.69778395	-0.70623058	1.30511761
1	-3.85279417	0.82870221	1.49519312
6	-3.96509886	-0.25379601	-1.22109520
6	-4.64592171	0.95370615	-1.50284410
6	-5.46205235	1.02718604	-2.63943219
6	-5.60936069	-0.04255469	-3.52719307
6	-4.89212227	-1.21373653	-3.25433135
6	-4.08151388	-1.34215975	-2.12241721
6	3.00927472	2.35303140	2.29678655
1	3.99663043	4.21525049	0.66181535
6	3.55198073	5.08337545	-1.89632201
1	1.52618146	3.45840597	-2.76438355
6	-0.01657591	1.53551197	-1.74544048
6	-4.45582247	2.18425298	-0.65040821
1	-5.97677803	1.96871722	-2.84808207
6	-6.51532412	0.05586593	-4.73093796
1	-4.97077751	-2.06168509	-3.93958116
6	-3.33575583	-2.63266993	-1.87703037
1	4.04393291	2.70266414	2.41243172
1	2.98861861	1.26429021	2.45392489
1	2.41932654	2.80367136	3.10991979
1	0.30697346	0.54317385	-2.10757661
1	-0.34453031	2.09572721	-2.63147330
1	-0.88477093	1.36819315	-1.09146380
1	3.04912686	6.05607224	-1.77109146
1	3.58355117	4.87068987	-2.97393608
1	4.58498526	5.20495653	-1.54123032
1	-4.73510122	3.08487558	-1.21234667
1	-3.40607119	2.28372526	-0.33720407
1	-5.07119513	2.16653252	0.26307946
1	-3.58884621	-3.07649684	-0.90052795
1	-2.24225783	-2.49238539	-1.88968050
1	-3.58124423	-3.37052989	-2.65110540

1 -6.10412264 -0.49264306 -5.58984947
 1 -6.66598034 1.10115325 -5.03309584
 1 -7.50908947 -0.37030241 -4.51907063
 1 -2.54273796 -1.20674932 -0.14319114
 Energy = -7584.936394 Hartree
 Number of imaginary frequencies = 0.

Compound TS3b isomer 31

Atomic N.	X	Y	Z
8	0.94789201	-2.35303593	-0.76032209
6	1.10180449	-3.05470133	0.34850144
8	2.22809267	-3.84599876	0.43160778
6	3.41096544	-3.32394290	-0.20732822
1	3.78990078	-2.45631742	0.34969673
1	3.20193410	-3.03509259	-1.24326158
1	4.14163160	-4.13943338	-0.17154633
8	1.32803190	-1.77239394	1.43315041
6	-0.10997494	-3.87235379	0.81410706
1	-0.92768943	-3.16702271	1.03411007
1	-0.41747928	-4.42654848	-0.08656006
6	0.10400809	-4.85819340	1.96703768
1	0.99391186	-5.46648645	1.74940860
1	-0.75112206	-5.55278778	1.98417222
6	0.23731005	-4.22783136	3.35768890
1	-0.71908349	-3.74951649	3.63521361
1	0.39630389	-5.03559685	4.09019852
6	1.35908997	-3.19133234	3.51302934
1	2.31747150	-3.59319067	3.15010118
1	1.49092543	-2.98180676	4.58782005
6	1.08382154	-1.84113789	2.84822130
1	0.03938588	-1.54086554	3.06594110
1	1.74722564	-1.08148110	3.29607987
50	0.16196913	-0.41534889	-0.10249290
7	0.48885232	2.07297945	1.22212040
6	1.65622604	1.98537874	2.10683990
1	2.06932521	2.98610735	2.34740615
1	2.43912697	1.37657940	1.64131486
1	1.35846221	1.50347519	3.04806089
7	1.78911364	0.63514423	-0.98460633
6	0.79743332	2.74246073	-0.05257018
1	1.06417775	3.80924153	0.10676303
1	-0.11589909	2.70747638	-0.66604042
6	1.94170499	2.08193851	-0.82278681
1	1.97639167	2.58230114	-1.80964494
1	2.90028763	2.33738375	-0.33041304
6	2.74049330	0.06281877	-1.88017774
6	4.11237049	-0.03343953	-1.53190100
6	5.02776909	-0.56187439	-2.45225883
6	4.63637733	-1.01454651	-3.71513605
6	3.27674055	-0.93886822	-4.03706074
6	2.32842970	-0.41256112	-3.15214992
7	-2.49612308	2.05621457	0.45636281
6	-0.61137033	2.72592092	1.96771610
1	-0.22686905	3.64307570	2.46316504
1	-0.91277784	2.03205180	2.76989508
6	-1.84217846	3.15753484	1.17261875
1	-2.53147602	3.61631107	1.90541649

1	-1.55977535	3.96125054	0.47455671
6	-3.90002203	2.07596111	0.28313363
6	-4.52878141	3.13502026	-0.41345370
6	-5.92066383	3.11629701	-0.57244200
6	-6.71596909	2.07130361	-0.09320824
6	-6.06934834	1.01001167	0.55201524
6	-4.68600893	0.99349660	0.75365561
6	4.60659933	0.36154547	-0.16246971
1	6.07907820	-0.63686830	-2.16062045
6	5.64330721	-1.55385137	-4.70252085
1	2.93873549	-1.29914629	-5.01219082
6	0.87916070	-0.38027856	-3.57041144
6	-3.72569847	4.23733139	-1.06020522
1	-6.39134789	3.93814969	-1.11833119
6	-8.21684933	2.08855462	-0.25622177
1	-6.66066408	0.16809823	0.92120457
6	-4.04618883	-0.17470998	1.46505165
1	5.55072784	-0.14934827	0.06929754
1	3.86615252	0.09413711	0.60509479
1	4.79556799	1.44380379	-0.07788194
1	0.31682134	-1.20917034	-3.11040568
1	0.78774631	-0.49358770	-4.65879250
1	0.38797447	0.55583370	-3.27142596
1	5.93068695	-0.78626364	-5.43863535
1	5.23723698	-2.40563917	-5.26601219
1	6.56138611	-1.88320267	-4.19733858
1	-4.32517099	4.74726582	-1.82535386
1	-2.82384992	3.82963538	-1.54109514
1	-3.39381790	5.00260496	-0.34122950
1	-3.48410845	0.14460172	2.35801053
1	-3.33659649	-0.71751279	0.81920666
1	-4.81054115	-0.89118683	1.79103422
1	-8.61316872	1.08042705	-0.44163513
1	-8.52039814	2.73394084	-1.09165800
1	-8.71305084	2.47072792	0.65030617
1	-2.16207647	1.15008080	0.78346366

Energy = -7584.948287 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 32

Atomic N.	X	Y	Z
8	0.90549666	-0.94452906	2.30378151
6	0.42937130	-2.12407851	2.55567598
8	0.17696740	-2.44972944	3.85431433
6	0.01295609	-1.33824754	4.76015282
1	-0.71449029	-0.61957443	4.36596680
1	0.97466940	-0.83516997	4.92594242
1	-0.34958109	-1.77914739	5.69488955
8	-1.24329376	-1.80212855	1.79798579
6	0.96461040	-3.32865977	1.79179525
1	0.86862165	-3.11471510	0.71639425
1	2.04647732	-3.32095027	2.01076746
6	0.38880810	-4.70435858	2.14589024
1	0.34787688	-4.80421495	3.24075103
1	1.10439658	-5.46478462	1.79437196
6	-0.98301208	-5.03547335	1.54410672
1	-0.90471399	-5.03898859	0.44233599

1	-1.23335505	-6.06942034	1.83259690
6	-2.14802861	-4.11836100	1.94641089
1	-2.17545557	-3.98026991	3.03934741
1	-3.09168625	-4.61876345	1.67125809
6	-2.16686797	-2.75144172	1.25993085
1	-1.98694313	-2.89518666	0.17449322
1	-3.17477679	-2.31044650	1.36520672
50	-0.24796435	-0.18648745	0.53073174
7	1.41743410	1.76285172	1.00792480
6	2.74207926	1.37849236	1.52928615
1	3.35366464	2.26722670	1.77503955
1	3.26614904	0.76549596	0.78695899
1	2.59908485	0.77441740	2.43097544
7	2.41983438	0.86784136	-1.74879241
6	1.51963782	2.62366414	-0.20084088
1	1.75218344	3.66134024	0.11083942
1	0.52728242	2.64792848	-0.67652768
6	2.57310891	2.23680997	-1.23981726
1	2.48710966	2.98518658	-2.05179954
1	3.57637286	2.36646771	-0.80896467
6	3.00144601	0.54339081	-3.00202918
6	4.40431786	0.57528847	-3.18005991
6	4.94245911	0.22991796	-4.42697573
6	4.14466763	-0.17315063	-5.50158358
6	2.76166582	-0.23838390	-5.29247236
6	2.17644930	0.11581932	-4.07305908
7	-1.43861341	1.36518109	1.42511964
6	0.64452565	2.46413994	2.06722713
1	1.11147773	3.44364285	2.29180837
1	0.70141584	1.83311343	2.96540761
6	-0.82229960	2.65527034	1.69820654
1	-1.30901909	3.14364338	2.56603599
1	-0.90876573	3.38621187	0.86557394
6	-2.84455514	1.39602816	1.17075777
6	-3.39107180	1.88743639	-0.04483569
6	-4.78049707	1.88343453	-0.23586924
6	-5.66416979	1.41033518	0.73752081
6	-5.11732340	0.93827969	1.93616700
6	-3.73712921	0.92292994	2.16842294
6	5.33775997	0.89995193	-2.03971624
1	6.02872324	0.25260812	-4.54754400
6	4.74870157	-0.51650447	-6.84198570
1	2.11180282	-0.56686538	-6.10762691
6	0.67705041	0.03455561	-3.91018724
6	-2.51716733	2.41758513	-1.15582657
1	-5.18029022	2.25831556	-1.18206191
6	-7.15431690	1.38235366	0.49615234
1	-5.78583241	0.57533395	2.72165680
6	-3.21093178	0.41012803	3.48417592
1	6.34201622	0.50659877	-2.24424219
1	4.97557449	0.45566005	-1.10088563
1	5.44109631	1.98380375	-1.87192833
1	0.37801445	-0.68696499	-3.13240314
1	0.20538747	-0.28011146	-4.84948492
1	0.24066390	1.00603735	-3.62720823
1	4.70104742	0.34045690	-7.53284454
1	4.21569014	-1.34901750	-7.32214594
1	5.80569077	-0.79859859	-6.74331999

1	-3.06138372	2.41914415	-2.10923600
1	-1.61099052	1.80627692	-1.28001261
1	-2.18976545	3.45179963	-0.96293849
1	-2.50148153	1.11917782	3.93382597
1	-2.66557646	-0.53378701	3.33888483
1	-4.03413820	0.23916055	4.19084167
1	-7.48113823	0.39056495	0.14499608
1	-7.45084810	2.11456323	-0.26690322
1	-7.71360588	1.59960258	1.41696417
1	1.43924284	0.58304590	-1.71373868

Energy = -7584.953571 Hartree
Number of imaginary frequencies = 0.

Compound TS3b isomer 33

Atomic N.	X	Y	Z
8	2.33349180	-1.69851840	0.46426457
6	2.07182670	-2.53367448	1.39340794
8	2.89363766	-2.35890961	2.47062731
6	2.82594633	-3.21750140	3.61547637
1	3.13812494	-4.24330711	3.37353826
1	1.81679130	-3.21619606	4.04949141
1	3.53244233	-2.79137278	4.33679628
8	0.41834867	-1.61625814	2.05327535
6	1.61094320	-3.92810559	0.96383357
1	1.06607270	-3.75429845	0.02446398
1	2.55778050	-4.41618586	0.66407722
6	0.80493748	-4.91843081	1.82001114
1	1.27174973	-5.09392643	2.79797912
1	0.87377566	-5.88228941	1.28870857
6	-0.68460643	-4.61111689	2.01999617
1	-1.15462673	-4.42004013	1.03926599
1	-1.15718710	-5.52726078	2.41011405
6	-1.01737022	-3.45119500	2.96720576
1	-0.40406895	-3.51431179	3.88282847
1	-2.06635094	-3.55479741	3.29536414
6	-0.88631284	-2.05507040	2.35471272
1	-1.53085220	-2.03784180	1.44250190
1	-1.34291875	-1.34037125	3.07728148
50	0.52567911	-0.44782937	-0.13989626
7	1.08190382	1.38948083	1.46684909
6	2.22758555	0.92730534	2.29019928
1	2.60486984	1.75795913	2.91333151
1	3.02969146	0.55382788	1.64747250
1	1.89313054	0.09714095	2.92063236
7	1.86157036	0.91361648	-1.19131458
6	1.50212872	2.51090598	0.58727813
1	1.95853615	3.31492090	1.19679081
1	0.60514331	2.90455794	0.09335948
6	2.47101426	2.02853942	-0.49063826
1	2.64576554	2.87859368	-1.17761290
1	3.45609617	1.80937088	-0.02966101
6	2.40711379	0.53258514	-2.44561338
6	3.75399733	0.10534333	-2.60167074
6	4.22369909	-0.25974837	-3.87081480
6	3.40816212	-0.24153791	-5.00562429
6	2.08190060	0.17319256	-4.84115887
6	1.57252109	0.56322324	-3.59745646

7	-2.00078297	1.36605561	0.98810941
6	0.00093661	1.78069913	2.41358399
1	0.40307790	2.53954053	3.11293006
1	-0.22044334	0.88069797	3.00760078
6	-1.29228985	2.34255290	1.82837033
1	-1.90711796	2.66653728	2.69232225
1	-1.09534419	3.24802709	1.24082148
6	-3.28674626	1.75046575	0.50039780
6	-3.40771937	2.74289799	-0.49853557
6	-4.68253803	3.08269072	-0.96953768
6	-5.84396124	2.46021771	-0.50254482
6	-5.69912148	1.45535183	0.46100894
6	-4.44898224	1.09397209	0.97387356
6	4.68716240	-0.01406921	-1.42160141
1	5.26189327	-0.59070027	-3.96580434
6	3.92693782	-0.68416721	-6.35293913
1	1.42328465	0.21374872	-5.71322107
6	0.14739650	1.05348074	-3.50903010
6	-2.19589353	3.40029430	-1.10853875
1	-4.76168776	3.84516573	-1.74859858
6	-7.20716953	2.86449432	-1.00953841
1	-6.58704042	0.93768078	0.83256263
6	-4.35756254	-0.00132935	2.01096368
1	5.52225637	-0.68561590	-1.66227543
1	4.15882969	-0.41455236	-0.54549509
1	5.12345505	0.95691931	-1.13613868
1	-0.50511944	0.34989291	-2.96866131
1	-0.27380502	1.19295537	-4.51374865
1	0.09372046	2.00714397	-2.96561837
1	5.01702929	-0.56617922	-6.42133522
1	3.46800375	-0.10755963	-7.16861820
1	3.69986463	-1.74622512	-6.53987885
1	-2.42570210	3.77043867	-2.11597586
1	-1.36239922	2.68816853	-1.18220413
1	-1.84739518	4.26493788	-0.52018458
1	-3.84044147	-0.89468169	1.62401557
1	-5.36063671	-0.31813142	2.32242060
1	-3.81702614	0.32283589	2.91419744
1	-7.14467430	3.31214356	-2.01052499
1	-7.67315006	3.61001444	-0.34560919
1	-7.88863564	2.00414848	-1.06028998
1	-2.08254623	0.48857290	1.50359631

Energy = -7584.931753 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 34

Atomic N.	X	Y	Z
8	1.79461169	-1.56186008	0.46483323
6	1.63612604	-2.20598841	1.55959857
8	2.66365218	-1.95683956	2.50462890
6	3.23011708	-3.00511670	3.29699588
1	3.39235640	-3.92603803	2.71858573
1	2.62121487	-3.23788691	4.18467569
1	4.20470953	-2.62754226	3.63200474
8	0.27190086	-1.32814920	2.23886323
6	1.10935962	-3.64490223	1.44519222
1	0.43580115	-3.60994983	0.57676035

1	1.96768403	-4.26000118	1.12356460
6	0.37492567	-4.34681082	2.60129213
1	1.00517929	-4.42920160	3.49937987
1	0.20922379	-5.38363600	2.26667452
6	-0.98927957	-3.74115610	2.97581649
1	-1.48629987	-3.39545798	2.05560446
1	-1.63088024	-4.53502226	3.39010286
6	-0.95859134	-2.59490466	3.99702001
1	-0.65309328	-2.98889709	4.98109961
1	-1.98586941	-2.22048211	4.12135315
6	-0.01437196	-1.42884147	3.62839723
1	-0.45674640	-0.47332984	3.95826650
1	0.94973284	-1.52595854	4.15748215
50	-0.34419629	-0.19762927	0.29584828
7	1.28558457	1.58192301	1.12519300
6	2.55767941	1.14551055	1.74021721
1	3.15056539	2.02412057	2.05529022
1	3.13730502	0.53082508	1.04740548
1	2.33953547	0.51686931	2.60829520
7	1.91052151	0.58954465	-1.59742153
6	1.53698242	2.49350262	-0.01913087
1	2.01966476	3.42178464	0.34579340
1	0.56050718	2.76330495	-0.44392526
6	2.41235995	1.88921165	-1.12060976
1	2.41757607	2.59871531	-1.95762956
1	3.46003556	1.81191337	-0.77953821
6	2.11133552	0.27800643	-2.97701907
6	3.01611590	-0.74285382	-3.35490131
6	3.16708779	-1.05043983	-4.71148062
6	2.46077752	-0.37268960	-5.71237183
6	1.55832958	0.61845154	-5.31441450
6	1.35973346	0.94929290	-3.96788311
7	-1.54437447	1.44970357	1.11787891
6	0.47980413	2.26416969	2.17661977
1	1.01051855	3.17283344	2.52046990
1	0.42206970	1.56136882	3.01969862
6	-0.92800009	2.61790466	1.71905673
1	-1.48158491	2.96021056	2.61644125
1	-0.88869882	3.49776626	1.04457474
6	-2.91789937	1.54882038	0.77071756
6	-3.40121484	2.47109056	-0.19890374
6	-4.76841068	2.51294065	-0.50232065
6	-5.69636011	1.66205907	0.10424765
6	-5.21214247	0.74773210	1.04561198
6	-3.85698748	0.67753673	1.38735521
6	3.81002450	-1.50294840	-2.31874609
1	3.86652708	-1.84185648	-4.99266672
6	2.67537189	-0.69450867	-7.17172432
1	0.96493852	1.13701284	-6.07173967
6	0.30557096	1.96188450	-3.59729409
6	-2.47024250	3.38028169	-0.96053493
1	-5.11273193	3.22587180	-1.25689852
6	-7.15824699	1.69905448	-0.27097046
1	-5.91373205	0.07269441	1.54333270
6	-3.41587210	-0.31348327	2.43518734
1	4.47593164	-2.22694016	-2.80491471
1	3.16119504	-2.05159807	-1.61861813
1	4.43614769	-0.83160245	-1.71001983

1	-0.25522211	1.62546110	-2.71343637
1	-0.40057129	2.10364795	-4.42535257
1	0.72788858	2.95135927	-3.35858297
1	3.53628063	-0.14043236	-7.57880354
1	1.79781759	-0.42353305	-7.77419281
1	2.87768149	-1.76403153	-7.32166052
1	-2.91609383	3.67320824	-1.92026734
1	-1.51532435	2.87451696	-1.16224325
1	-2.24159336	4.30668497	-0.40983424
1	-2.74648905	0.15638196	3.16890121
1	-2.85797644	-1.15475452	1.99547553
1	-4.28510857	-0.73308200	2.95953083
1	-7.37864304	0.99008322	-1.08520567
1	-7.45897102	2.69733405	-0.61717623
1	-7.79703999	1.42412555	0.57990521
1	2.26279950	-0.16635980	-1.00280821

Energy = -7584.932310 Hartree

Number of imaginary frequencies = 0.

Compound TS3b isomer 35

Atomic N.	X	Y	Z
8	1.83098745	-1.67523968	0.82700938
6	1.51053715	-2.36693573	1.85046518
8	2.31388378	-2.09161448	2.98446226
6	2.74495530	-3.12482309	3.87583137
1	3.05854583	-4.03285360	3.34101272
1	1.97494698	-3.38842225	4.61761236
1	3.61407948	-2.71402550	4.40540504
8	-0.02305541	-1.56541455	2.26493788
6	1.08931899	-3.82457089	1.61362338
1	0.60195130	-3.80022597	0.62837058
1	2.02441335	-4.39142466	1.46180189
6	0.17635931	-4.58812571	2.58958006
1	0.62299687	-4.67110920	3.59155011
1	0.12685773	-5.62051058	2.20686460
6	-1.26135111	-4.05109072	2.70465398
1	-1.58703482	-3.69811678	1.71361268
1	-1.93174982	-4.88446474	2.96884561
6	-1.48540616	-2.93819475	3.73882079
1	-1.33346319	-3.34567118	4.75261545
1	-2.54135466	-2.63285446	3.68568373
6	-0.57141477	-1.70241821	3.56790471
1	-1.13823938	-0.78522086	3.80288577
1	0.27123088	-1.74013734	4.28111076
50	-0.20650136	-0.37733400	0.28353804
7	1.16704822	1.46102273	1.39393866
6	2.41024423	1.02044535	2.06430435
1	2.90039968	1.88268185	2.55421376
1	3.09154272	0.55838692	1.34565580
1	2.17161751	0.25582021	2.80876684
7	1.56453586	1.28190279	-1.65237665
6	1.46335363	2.57098222	0.45203343
1	1.98722768	3.37683654	1.00174415
1	0.50435096	2.98453999	0.11110822
6	2.30429316	2.19449449	-0.76598471
1	2.57744527	3.13682890	-1.28033161
1	3.24365044	1.72004187	-0.46160337

6	2.18676805	0.87759000	-2.87321997
6	3.34487963	0.06745091	-2.87407136
6	3.89472890	-0.31710914	-4.10473108
6	3.32971215	0.04541543	-5.33074951
6	2.15904045	0.81193686	-5.30360603
6	1.58221149	1.23701370	-4.10318947
7	-1.61086357	1.17208076	1.00494421
6	0.20724076	1.92411864	2.43655729
1	0.62142450	2.80481839	2.96443772
1	0.12522125	1.10081434	3.15920210
6	-1.17314625	2.24936533	1.87268806
1	-1.84879255	2.38653040	2.74205613
1	-1.14717782	3.23923898	1.37077689
6	-2.90435791	1.28968668	0.43206301
6	-3.24381113	2.31379580	-0.49619809
6	-4.53553152	2.37185431	-1.03734076
6	-5.52465868	1.44028258	-0.71383423
6	-5.18131495	0.42571986	0.18655196
6	-3.90815401	0.33587027	0.75907117
6	3.97172761	-0.44349408	-1.60036969
1	4.78674269	-0.94861734	-4.09539461
6	3.96186113	-0.36739668	-6.63800097
1	1.67887390	1.09297347	-6.24423170
6	0.31088915	2.05471110	-4.13545847
6	-2.22858691	3.32251954	-0.96937597
1	-4.76573944	3.16623235	-1.75310731
6	-6.89816427	1.50073707	-1.33751094
1	-5.93438292	-0.31613967	0.46640596
6	-3.62819123	-0.76397413	1.75130880
1	4.57702208	-1.33459425	-1.81192064
1	3.21542025	-0.71926504	-0.85235000
1	4.64849615	0.29740560	-1.14322162
1	-0.53576994	1.52661741	-3.66612864
1	0.02069760	2.26908183	-5.17140007
1	0.42192566	3.02267337	-3.62017393
1	4.59712410	0.43585393	-7.04421473
1	3.20158696	-0.59492302	-7.39812469
1	4.59662580	-1.25471175	-6.51175261
1	-2.51388288	3.73190689	-1.94744468
1	-1.23951375	2.85095882	-1.06340551
1	-2.11756802	4.17317247	-0.27782369
1	-3.17099380	-0.36255956	2.66626906
1	-2.92535830	-1.51137173	1.35269654
1	-4.55565310	-1.28899646	2.01698732
1	-6.98512459	0.79681152	-2.18063664
1	-7.11881351	2.50503778	-1.72354293
1	-7.68018103	1.23321533	-0.61261588
1	0.66830838	1.71647620	-1.87653720

Energy = -7584.928534 Hartree

Number of imaginary frequencies = 0.

Intermediate 5a (I5a)

Compound I5a isomer 1

Atomic N.	X	Y	Z
8	3.91777327	-3.60148368	-0.24090625
6	4.99065602	-3.12241612	0.08444865

8	5.81718120	-2.47464929	-0.78086175
6	5.33275592	-2.39314594	-2.14596465
1	4.42039741	-1.78651031	-2.19555003
1	5.12790661	-3.39727401	-2.53831680
1	6.14053645	-1.91409545	-2.70735401
8	0.67914534	-1.54715351	2.86628740
6	5.61094062	-3.18915939	1.46957730
1	6.17898650	-2.26323117	1.64369972
1	6.35774980	-4.00059849	1.43460150
6	4.59355546	-3.44610315	2.58484676
1	4.00555979	-4.34168234	2.33129571
1	5.14332293	-3.67811717	3.51166089
6	3.64410548	-2.26829937	2.82644935
1	3.09898418	-2.04796835	1.89636348
1	4.23117538	-1.36499585	3.06984847
6	2.62561865	-2.52499735	3.94147788
1	2.14088571	-3.50388240	3.78650247
1	3.13580349	-2.57384632	4.91942553
6	1.52499406	-1.46381875	4.01266636
1	1.99214156	-0.46136098	4.10940472
1	0.91670403	-1.61872612	4.92186490
50	0.06745783	0.12725517	1.84830925
7	-0.52481532	-1.62090957	0.10415444
6	0.61639791	-2.50992626	-0.21012703
1	0.31464941	-3.32050894	-0.89708543
1	1.43651377	-1.94081168	-0.65975483
1	0.97891530	-2.94476674	0.72709190
7	0.77445422	0.53324278	-1.57226451
6	-1.12614372	-1.01176831	-1.10903402
1	-1.73888891	-1.76851759	-1.63727711
1	-1.81234229	-0.21735451	-0.77731010
6	-0.15146999	-0.45091448	-2.14693842
1	-0.76770927	-0.02933116	-2.96276809
1	0.46060276	-1.25333891	-2.57723227
16	2.03853235	1.10347660	-2.56047568
7	-2.11842993	-0.32474137	1.96905574
6	-1.55947194	-2.40220157	0.84495585
1	-1.95695702	-3.20700539	0.19719239
1	-1.04237945	-2.85167182	1.70308130
6	-2.69911501	-1.51933897	1.35857944
1	-3.27142347	-2.10630377	2.09473354
1	-3.39069381	-1.24805757	0.54081992
16	-2.61235120	0.15557824	3.45544027
8	-1.42055307	0.92824224	3.95228547
8	-3.18527624	-0.93940107	4.27167374
6	-3.93802254	1.36850970	3.22318352
6	-5.25552131	1.00863023	3.50623200
6	-6.27532921	1.94182201	3.30174081
6	-5.99541086	3.23089260	2.82626030
6	-4.65736245	3.56635956	2.55368777
6	-3.62925771	2.64629669	2.74858232
1	-5.46832562	0.01373883	3.89587363
1	-2.59152395	2.91600857	2.55207412
1	-4.41862815	4.56769626	2.18964378
6	-7.09511365	4.24714305	2.64398740
1	-7.30728602	1.66362216	3.52420634
8	2.75384108	2.08714579	-1.73184015
8	2.68885566	-0.10357260	-3.10782130

6	1.27512777	1.98559846	-3.94002190
6	1.00874323	1.31121059	-5.13266293
6	0.40360600	2.00589820	-6.18309890
6	0.06510505	3.36117879	-6.05849193
6	0.35208385	4.01469938	-4.84634701
6	0.95426041	3.33883486	-3.78759019
1	1.29540562	0.26563920	-5.23975717
1	0.19922370	1.48562490	-7.12039470
6	-0.57357154	4.11284592	-7.19871459
1	0.10919504	5.07318308	-4.73582840
1	1.20105902	3.85374840	-2.85919154
1	-8.07491493	3.76377343	2.53799013
1	-7.15167860	4.92125249	3.51297593
1	-6.91985528	4.87424491	1.75917758
1	0.09441852	4.90463083	-7.56947029
1	-0.80662277	3.44677200	-8.03856221
1	-1.50492900	4.60237755	-6.87946864
1	0.32604585	1.32678432	-1.10492713

Energy = -8524.654951 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 2

Atomic N.	X	Y	Z
8	3.40886537	-3.16574714	-1.27391387
6	4.35375389	-2.40519323	-1.09644562
8	5.31217092	-2.20323313	-2.04255952
6	5.10111671	-2.90559369	-3.29016509
1	4.17185954	-2.56876985	-3.76733210
1	5.04767587	-3.98807094	-3.11903726
1	5.96524759	-2.65342326	-3.91239601
8	0.95084513	-1.72306993	2.63740209
6	4.58174422	-1.54579947	0.11791243
1	3.98170045	-0.62963262	-0.06165630
1	5.64022708	-1.25698496	0.17543211
6	4.06214451	-2.15943864	1.42093943
1	3.03320141	-2.49960145	1.25440755
1	4.64628794	-3.05489369	1.69272424
6	4.07454621	-1.14795625	2.57785206
1	3.74073341	-0.17205673	2.18786624
1	5.11123630	-1.01346750	2.92785967
6	3.17118775	-1.53846144	3.76275584
1	3.18275545	-2.63147375	3.91663564
1	3.56917598	-1.09339817	4.69126530
6	1.71861638	-1.05770691	3.65452233
1	1.71797500	0.03678868	3.50203685
1	1.20512052	-1.24742490	4.61414916
50	0.49444120	-0.76021288	0.89463483
7	-0.33243732	-2.98259102	0.34792548
6	0.67895023	-4.03322481	0.64439333
1	0.21938191	-5.03168381	0.55300793
1	1.52015634	-3.94804955	-0.05497318
1	1.04705697	-3.87815212	1.66400558
7	-0.02627082	-0.86043261	-1.64758772
6	-0.79195298	-3.09417793	-1.06556053
1	-0.80080640	-4.15561357	-1.36369644
1	-1.82490175	-2.72531577	-1.12934597
6	0.08755134	-2.28905486	-2.01446908

1	-0.20987820	-2.47593021	-3.05732298
1	1.14327306	-2.58449097	-1.90678356
16	1.21975622	0.08533365	-2.61603242
7	-1.65442462	-0.63956770	1.13466888
6	-1.47180416	-3.09150187	1.30612220
1	-2.02710088	-4.02904880	1.12548919
1	-1.02465018	-3.12085968	2.30817936
6	-2.41973699	-1.88775218	1.21151485
1	-3.05328089	-1.89825620	2.11218095
1	-3.08753310	-1.97527951	0.33736443
16	-1.92729111	0.53049625	2.28276299
8	-0.61732628	1.26161502	2.27147541
8	-2.48180867	-0.01101426	3.54304852
6	-3.17830472	1.63321572	1.59101526
6	-4.43158022	1.70317787	2.19843415
6	-5.40266773	2.54679745	1.65244405
6	-5.13502139	3.31909457	0.51351067
6	-3.85992180	3.22790751	-0.07379379
6	-2.87903360	2.39290585	0.45619333
1	-4.63111199	1.10997659	3.08985102
1	-1.88989762	2.34309721	0.00079254
1	-3.62979334	3.82159584	-0.96063306
6	-6.17705395	4.24673472	-0.05902025
1	-6.38485264	2.60681391	2.12465466
8	1.95089960	0.25393090	0.21431178
8	0.93379333	-0.26797931	-4.06701573
6	0.44657262	1.73933519	-2.37761543
6	-0.36202804	2.21511712	-3.40959077
6	-0.88545198	3.50698873	-3.31824536
6	-0.58590496	4.33291306	-2.22313972
6	0.24639636	3.82695797	-1.20927576
6	0.77124487	2.53500738	-1.27437975
1	-0.54794189	1.58031216	-4.27785283
1	-1.52307104	3.88622817	-4.11956580
6	-1.11693054	5.74325964	-2.14563887
1	0.48764437	4.45424310	-0.34846714
1	1.39836276	2.10504448	-0.48464263
1	-7.17585911	4.02136607	0.33554697
1	-5.94758133	5.29388237	0.19203689
1	-6.21341627	4.17897966	-1.15518145
1	-0.31590347	6.47480425	-2.33242692
1	-1.90653502	5.91762621	-2.88813391
1	-1.52289275	5.96297854	-1.14788388
1	-0.93970903	-0.49293856	-1.94754549

Energy = -8524.629380 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 3

Atomic N.	X	Y	Z
8	4.00134999	-2.87889780	-1.97527994
6	5.04146498	-2.24581739	-2.03665608
8	5.37903375	-1.45725069	-3.09291957
6	4.40352497	-1.42032903	-4.16620694
1	3.46505683	-0.97155723	-3.81887268
1	4.20975910	-2.43381134	-4.53981442
1	4.85861735	-0.80001377	-4.94422510
8	1.93878563	-1.46805075	2.27821632

6	6.14563107	-2.24552308	-0.99331777
1	6.60103444	-1.24439010	-0.96623646
1	6.92874524	-2.92419313	-1.37210429
6	5.67709402	-2.69092287	0.39483620
1	5.16927478	-3.66356695	0.30437496
1	6.56535235	-2.85322404	1.02707896
6	4.73577447	-1.68910821	1.07112077
1	3.85161047	-1.53828336	0.43373019
1	5.23738683	-0.70848892	1.15258112
6	4.26775813	-2.13447946	2.46011064
1	3.90497318	-3.17543222	2.41565081
1	5.11402346	-2.12211244	3.16911737
6	3.13868147	-1.26924837	3.02499945
1	3.45743162	-0.20583400	3.01794939
1	2.95539960	-1.53833731	4.08074928
50	0.74997454	0.10416416	1.70389061
7	-0.20350519	-1.67922500	0.16741195
6	0.84753095	-2.35970494	-0.62230899
1	0.42775532	-3.19427409	-1.21163465
1	1.34227196	-1.65316431	-1.29664256
1	1.59918438	-2.74834401	0.07257317
7	0.02709628	0.69931956	-1.68882760
6	-1.30362655	-1.15220622	-0.67901839
1	-1.95451794	-1.98853040	-1.00171616
1	-1.91917801	-0.49012422	-0.05077092
6	-0.89122710	-0.41530567	-1.95513318
1	-1.82635329	-0.08728019	-2.44600003
1	-0.37743441	-1.09529857	-2.64602705
16	0.72361923	1.48699538	-3.02864891
7	-1.13475781	-0.70549667	2.59275046
6	-0.75246914	-2.63673003	1.17297937
1	-1.24589442	-3.48205249	0.65593599
1	0.11180728	-3.01293494	1.73631669
6	-1.72510867	-1.96580258	2.14547391
1	-1.88288758	-2.65529755	2.99024443
1	-2.70740016	-1.79445395	1.66966997
16	-1.08948076	-0.34667142	4.19060877
8	0.07607714	0.60149165	4.27099062
8	-1.14319583	-1.53914149	5.06724393
6	-2.56515773	0.63404541	4.56894569
6	-3.59917260	0.06170461	5.30837533
6	-4.74412330	0.81789905	5.57669864
6	-4.86565722	2.13777982	5.12160203
6	-3.80296992	2.69081865	4.38388127
6	-2.65730378	1.94986335	4.10479976
1	-3.49372805	-0.95724950	5.67917808
1	-1.82886029	2.38792011	3.54792298
1	-3.87393217	3.72153585	4.03035580
6	-6.09339020	2.95888451	5.42831988
1	-5.55399043	0.37386624	6.15858053
8	1.54076049	2.56652652	-2.45184857
8	1.29356458	0.41341492	-3.86655047
6	-0.62738748	2.24462921	-3.95881660
6	-1.22345127	1.54477426	-5.01000768
6	-2.27945648	2.13733588	-5.70550155
6	-2.74375324	3.41801215	-5.36893194
6	-2.12067207	4.09890883	-4.30839360
6	-1.06607766	3.52356992	-3.60183759

1	-0.84708075	0.56105488	-5.28834750
1	-2.74614341	1.59654410	-6.53067129
6	-3.86044585	4.06666690	-6.14670647
1	-2.46181661	5.10000218	-4.03855356
1	-0.56745974	4.06347564	-2.79694403
1	-6.86969987	2.35310007	5.91245764
1	-5.85012083	3.79530842	6.10097469
1	-6.51997205	3.39610016	4.51390492
1	-3.45612505	4.75942006	-6.90107305
1	-4.46821023	3.32132369	-6.67519668
1	-4.51913518	4.65139009	-5.49060194
1	-0.32507557	1.40031445	-1.03025835

Energy = -8524.654968 Hartree
Number of imaginary frequencies = 0.

Compound I5a isomer 4

Atomic N.	X	Y	Z
8	2.00274408	-4.18377697	-0.67320437
8	2.55516489	-4.26251079	2.28496160
6	2.68152330	-5.12837469	-0.29339517
6	2.14064389	-6.48392363	0.10304077
1	2.68330783	-6.83608957	0.99128405
1	2.42065513	-7.17302182	-0.71418014
6	0.62468740	-6.53463506	0.34748324
1	0.13760940	-5.75275429	-0.25397506
1	0.25784280	-7.49801228	-0.03839543
6	0.17158190	-6.42580297	1.81663646
1	0.74996379	-7.14069592	2.42935129
1	-0.86827336	-6.78984938	1.84518649
6	0.18988584	-5.04162744	2.49666393
1	-0.13846556	-4.26930702	1.78380652
1	-0.57043314	-5.05365187	3.29657023
6	1.48862410	-4.58777086	3.17499006
1	1.84780585	-5.40129931	3.83508213
1	1.25275072	-3.73126421	3.83058606
50	2.99082316	-2.40438891	1.51204349
7	-1.13132187	0.46059096	-0.22530743
6	-2.52229582	0.27430992	0.18376314
1	-2.58913206	-0.48195458	0.97672505
1	-2.91466797	1.21666877	0.58882587
1	-3.17734301	-0.04781450	-0.65626297
7	0.60338080	3.12178612	-2.28230033
6	-1.00584275	1.53939809	-1.21168440
1	-1.20849295	1.18683327	-2.24563086
1	-1.76462878	2.30022849	-0.97858663
6	0.37950798	2.19237036	-1.15085747
1	1.16154150	1.42505861	-1.23872520
1	0.51112734	2.69280940	-0.18154456
16	0.06292653	4.73719769	-2.11935835
7	0.93641537	-1.46747220	1.21687522
6	-0.54540346	-0.78946015	-0.71799182
1	-1.22317902	-1.28027154	-1.45571971
1	0.38782148	-0.55822627	-1.25103540
6	-0.21687154	-1.81078823	0.37490959
1	0.03606301	-2.75850050	-0.12525629
1	-1.09795775	-2.01353782	1.00473039
16	0.72608423	-0.83864903	2.70267522

8	2.06271846	-1.25266398	3.34498902
8	-0.52962025	-1.22592768	3.38246493
6	0.79512209	0.96704085	2.70758847
6	-0.33512548	1.69342205	3.08093318
6	-0.27317405	3.08748993	3.08813953
6	0.90022177	3.76748044	2.72637085
6	2.02790271	3.00595161	2.37339353
6	1.98303434	1.61291367	2.35944533
1	-1.24212475	1.16498708	3.37076685
1	2.86829622	1.03391172	2.09484076
1	2.95507799	3.51460617	2.10352249
6	0.94070836	5.27250236	2.68428600
1	-1.15581209	3.65999275	3.37858997
8	-0.25113694	5.04066386	-0.70438082
8	1.04984466	5.53456106	-2.87841263
6	-1.49588270	4.75541607	-3.02736226
6	-1.48036180	4.57997253	-4.41426755
6	-2.68220680	4.63147624	-5.11464517
6	-3.90175797	4.86253916	-4.45183354
6	-3.88300089	5.04158938	-3.06178885
6	-2.68580625	4.99179040	-2.34227237
1	-0.53727584	4.41107918	-4.93281693
1	-2.67691647	4.49277948	-6.19733577
6	-5.19199151	4.93058670	-5.22918547
1	-4.81860697	5.22560059	-2.53091906
1	-2.66622549	5.13566165	-1.26270812
1	0.26255918	5.71300647	3.42709888
1	1.95420498	5.65302213	2.86692837
1	0.62449497	5.62918044	1.69156154
1	-5.21625465	5.82458404	-5.87063054
1	-5.30553524	4.05849498	-5.88877467
1	-6.06129488	4.97248452	-4.56121238
1	1.59083898	3.21023160	-2.53317359
8	4.03566058	-4.95444326	-0.29995301
6	4.90161591	-5.94178437	0.30125961
1	4.69916377	-6.01618022	1.37836016
1	5.91684033	-5.56419428	0.14172729
1	4.79563246	-6.92164516	-0.18337319

Energy = -8524.628126 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 5

Atomic N.	X	Y	Z
7	-0.45153477	-0.17123116	2.05825635
6	-1.23518152	0.62293374	3.00639542
1	-1.38610918	1.63931347	2.61712539
1	-2.22372390	0.16574333	3.14771438
1	-0.74143241	0.70999711	3.99917954
7	-1.30038446	-3.17906091	0.99274993
6	-0.24886350	-1.53509698	2.58148714
1	0.61247277	-1.56434978	3.28102235
1	-1.14158347	-1.82236167	3.15470581
6	-0.03420825	-2.58553949	1.48594753
1	0.55900694	-3.41491131	1.89456312
1	0.54579093	-2.16978292	0.64989386
16	-1.94510496	-2.74720656	-0.52650114
7	0.97483426	1.20773014	-0.56538498

6	0.84745148	0.47554004	1.80520212
1	1.28444459	0.83216470	2.76345210
1	1.55450386	-0.27664671	1.42681063
6	0.80035820	1.65611301	0.82678334
1	1.59842247	2.36707017	1.09609236
1	-0.15958307	2.18910225	0.93819218
16	0.94324371	2.32492752	-1.73952388
8	1.60610661	1.52951674	-2.87747324
8	1.51583851	3.64772741	-1.40775563
6	-0.75937641	2.61036579	-2.27229681
6	-1.21053908	3.92041290	-2.43434883
6	-2.52236938	4.13547387	-2.86358692
6	-3.38224639	3.06083809	-3.13310020
6	-2.89964339	1.75273904	-2.94941993
6	-1.59568172	1.51744611	-2.51931475
1	-0.53715278	4.75066203	-2.22589647
1	-1.24372430	0.49661990	-2.36212717
1	-3.55774980	0.90319416	-3.14019350
6	-4.78751359	3.29598596	-3.62698436
1	-2.88192812	5.15805779	-2.99190023
8	-1.01726154	-1.82093408	-1.21368280
8	-2.36662043	-4.02324819	-1.14654312
6	-3.44653613	-1.82583592	-0.13315462
6	-4.67794557	-2.47978163	-0.20575466
6	-5.84098482	-1.76438104	0.08115458
6	-5.78940265	-0.40649353	0.43529773
6	-4.53462088	0.22114874	0.49722194
6	-3.36022133	-0.47616491	0.21154259
1	-4.71461169	-3.52983418	-0.49283502
1	-6.80675849	-2.27023518	0.02640232
6	-7.05491879	0.36516102	0.71485327
1	-4.47504167	1.27619361	0.77139337
1	-2.38460540	0.00608034	0.27374433
1	-5.11622617	4.32454927	-3.43082936
1	-4.85104251	3.12735753	-4.71325691
1	-5.49863620	2.60550159	-3.15289083
1	-7.49597404	0.74460395	-0.22030278
1	-7.81211433	-0.26733811	1.19723424
1	-6.86196213	1.23065873	1.36187726
1	-1.28743265	-4.19974377	0.98600835
8	3.50923353	-1.81689741	1.98971546
8	3.95830232	-0.00681724	-0.98371315
6	4.13724041	-2.28882098	1.06133420
6	5.61274944	-2.06489376	0.79706541
1	5.74332417	-1.82120653	-0.26723159
1	6.10934375	-3.03844320	0.95479145
6	6.26315818	-0.98842042	1.67880817
1	5.73437767	-0.94854740	2.64271952
1	7.29379652	-1.30829729	1.89719692
6	6.33517205	0.42276258	1.06737800
1	6.84657467	0.36612564	0.09060145
1	7.00247550	1.01053193	1.71740430
6	5.00728054	1.19941222	0.90078110
1	4.24338200	0.79749791	1.58475701
1	5.17312254	2.24766487	1.20209255
6	4.43489429	1.25807585	-0.51900211
1	5.22502633	1.60540630	-1.21185910
1	3.63414039	2.01778989	-0.54694630

50	2.08298294	-0.43932508	-1.68241416
8	3.46036544	-3.13165071	0.21155406
6	4.13761607	-3.73115507	-0.91366183
1	4.48560303	-2.96582957	-1.62097193
1	3.38525599	-4.36014826	-1.40067772
1	4.98065979	-4.35556636	-0.58696703

Energy = -8524.624911 Hartree
Number of imaginary frequencies = 0.

Compound I5a isomer 6

Atomic N.	X	Y	Z
8	0.94524838	-0.31450021	1.46367343
6	1.11187968	0.23998711	2.54607700
8	1.69513032	-0.36052911	3.60531303
6	2.17063813	-1.72006856	3.37868433
1	2.87407857	-1.73323413	2.53737760
1	1.33579897	-2.39830069	3.16622927
1	2.67320876	-1.99964746	4.30907055
8	2.80819058	1.80609223	-0.93453694
6	0.72486653	1.67475269	2.83704548
1	0.97472272	1.92188645	3.87761009
1	-0.36763598	1.74662936	2.71925086
6	1.42018179	2.62544180	1.84592052
1	1.18551201	2.30869888	0.82109281
1	1.00597606	3.63769322	1.97392222
6	2.94583027	2.66362470	2.03031399
1	3.32583571	1.64044256	2.20005136
1	3.18180349	3.22469312	2.94928960
6	3.70726943	3.26210390	0.83642495
1	3.15296379	4.12078189	0.42131421
1	4.68137028	3.65227250	1.17687636
6	3.99427961	2.26013253	-0.28733123
1	4.57596966	1.41566502	0.14230704
1	4.65264923	2.73946440	-1.03733080
50	2.47211606	-0.20793272	-1.26113116
7	-1.31264018	-1.59657759	-1.64534312
6	-1.28319165	-2.24162717	-2.96274442
1	-2.19533966	-2.03230609	-3.56392361
1	-0.40522567	-1.92231116	-3.53560140
1	-1.21563663	-3.32740243	-2.81740363
7	0.84813310	0.30881732	-2.71376644
6	-1.42918578	-0.13324962	-1.72679845
1	-2.48295560	0.16862376	-1.93758377
1	-1.16802812	0.29315376	-0.74521174
6	-0.59444684	0.56020600	-2.80652814
1	-0.80492299	1.64113922	-2.71406819
1	-0.95426723	0.24453860	-3.79877122
16	1.71467212	0.37026759	-4.08920725
7	-1.37134888	-2.27777484	1.44298817
6	-2.43314199	-2.15695021	-0.87914592
1	-3.40737663	-1.83870738	-1.32318668
1	-2.38256421	-3.25090877	-0.95549380
6	-2.47509338	-1.78434252	0.60634860
1	-3.41625801	-2.17014698	1.02579081
1	-2.50697832	-0.69289616	0.74290624
16	-1.38675850	-3.89822574	1.92102005
8	-0.01731923	-4.15640868	2.41955295

8	-1.99429497	-4.79386757	0.91078137
6	-2.52737951	-3.85610326	3.32344352
6	-3.66561272	-4.65968748	3.29764169
6	-4.51759969	-4.66729471	4.40589489
6	-4.24296755	-3.88569479	5.53637487
6	-3.08574425	-3.08495520	5.53288869
6	-2.22667671	-3.06642263	4.43768455
1	-3.87146451	-5.26861372	2.41814188
1	-1.33114400	-2.44565694	4.44200617
1	-2.85606927	-2.46913950	6.40450115
6	-5.15272453	-3.90745834	6.73880976
1	-5.41117998	-5.29360874	4.38924214
8	3.09864778	0.01030329	-3.54297074
8	1.18975520	-0.44453128	-5.20553891
6	1.79849348	2.07248601	-4.69708134
6	1.49466263	2.32974801	-6.03423987
6	1.55712048	3.64540363	-6.49940966
6	1.91510996	4.69933404	-5.64635800
6	2.20595723	4.40505827	-4.30199807
6	2.15151262	3.09991999	-3.81650580
1	1.21529404	1.50753971	-6.69158039
1	1.32193000	3.85488228	-7.54446991
6	2.00238031	6.11596482	-6.15609637
1	2.47937090	5.21543068	-3.62290940
1	2.37590409	2.86840653	-2.76951836
1	-6.08210363	-4.45138825	6.52883357
1	-4.66113034	-4.39789523	7.59274966
1	-5.41395283	-2.88895950	7.05962708
1	3.05212680	6.43685906	-6.24016370
1	1.54222971	6.21570709	-7.14725976
1	1.50560287	6.81788015	-5.47158861
1	-0.43406336	-2.02670683	1.10772431

Energy = -8524.642571 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 7

Atomic N.	X	Y	Z
8	4.47445870	-2.85318053	-0.82236807
6	4.69465131	-1.66668443	-0.67329926
8	4.11096298	-0.79827182	-1.56137121
6	4.34455945	0.62263813	-1.46243357
1	5.41082068	0.86152998	-1.58081836
1	3.97452749	1.02298992	-0.50810744
1	3.77563943	1.07151141	-2.28299197
8	2.60096274	-1.17980860	1.52201419
6	5.60492313	-1.07520393	0.38681375
1	5.06900170	-0.25770731	0.89139957
1	6.44901932	-0.60551351	-0.14742963
6	6.13012041	-2.08676108	1.41597618
1	6.24818993	-3.06546063	0.92732441
1	7.13709183	-1.76169732	1.72138072
6	5.28543556	-2.24275362	2.69391249
1	5.13056972	-1.24727850	3.14482765
1	5.90343998	-2.80207540	3.41397535
6	3.91937506	-2.95814400	2.55824181
1	3.87793253	-3.52274883	1.61450036
1	3.81797930	-3.69512184	3.37267342

6	2.69348549	-2.04917656	2.65469743
1	2.75171671	-1.45295567	3.58438129
1	1.78955902	-2.68159355	2.74478913
50	1.01454985	0.01970923	1.05335668
7	0.06920185	-1.80579844	-0.55016152
6	1.07279200	-2.34870933	-1.49203385
1	0.64460054	-3.16261134	-2.10537119
1	1.45064002	-1.55624840	-2.14533880
1	1.92429254	-2.73872779	-0.92291034
7	-0.00191601	0.68061467	-2.23732561
6	-1.14305723	-1.29573876	-1.23598042
1	-1.77837050	-2.14605693	-1.55519413
1	-1.72518484	-0.71835978	-0.50052215
6	-0.90808587	-0.44614091	-2.48830748
1	-1.90438892	-0.12170798	-2.84226279
1	-0.45425516	-1.04859888	-3.28475047
16	0.52647216	1.59485027	-3.57056525
7	-0.63205510	-1.09324867	2.03382094
6	-0.30638729	-2.86660283	0.42378634
1	-0.80624032	-3.70506839	-0.09932795
1	0.63438299	-3.24105581	0.84904777
6	-1.19916054	-2.34830715	1.55385180
1	-1.21722337	-3.11187181	2.34896256
1	-2.23816592	-2.21266247	1.20173741
16	-0.69058064	-0.67977780	3.61431396
8	0.35303540	0.40062521	3.68344099
8	-0.62650904	-1.84229693	4.52926939
6	-2.28611196	0.12188150	3.91389658
6	-3.28173854	-0.56624261	4.60761165
6	-4.51985909	0.04905570	4.81009376
6	-4.77336293	1.34417010	4.33612152
6	-3.74921994	2.01468801	3.64398633
6	-2.51032039	1.41403660	3.43003421
1	-3.07561347	-1.56377874	4.99399330
1	-1.71342284	1.94475503	2.90871831
1	-3.92500302	3.02690178	3.27434155
6	-6.09812666	2.01873253	4.59075985
1	-5.30027051	-0.48623514	5.35421152
8	1.43338413	2.60520607	-2.99657558
8	0.96766907	0.61348849	-4.57809314
6	-0.91904947	2.45518964	-4.22879364
6	-1.64432598	1.88461642	-5.27597184
6	-2.77208261	2.55162167	-5.76126160
6	-3.18089387	3.77817866	-5.21791607
6	-2.42490342	4.33121385	-4.16843213
6	-1.29817551	3.68081953	-3.67060310
1	-1.31254946	0.94470272	-5.71578550
1	-3.33917557	2.11342538	-6.58428768
6	-4.38862029	4.50407655	-5.75421527
1	-2.71913200	5.29241310	-3.74279869
1	-0.69860894	4.12407769	-2.87556945
1	-6.88695023	1.28628788	4.80520154
1	-6.03105800	2.69542124	5.45695401
1	-6.41193709	2.62525605	3.73024649
1	-4.09605829	5.44871500	-6.23678216
1	-4.92472739	3.89869490	-6.49548516
1	-5.08959119	4.75994550	-4.94677457
1	-0.28297362	1.30594362	-1.47644916

Energy = -8524.639173 Hartree
 Number of imaginary frequencies = 0.

Compound I5a isomer 8

Atomic N.	X	Y	Z
8	1.64371534	-1.33170478	3.20861377
6	2.74859379	-1.15185969	2.71757001
8	3.33439099	-2.21509956	2.09776821
6	4.65070442	-2.09057362	1.51728283
1	5.39322042	-1.79448486	2.27059444
1	4.64971596	-1.37652999	0.68214209
1	4.89253973	-3.08948868	1.14086024
8	1.95249377	0.16830743	-0.03911133
6	3.52507390	0.14508179	2.79470002
1	3.91770722	0.37509907	1.79320100
1	4.40398697	-0.05735252	3.43181003
6	2.73598645	1.34152482	3.34704128
1	2.01299110	0.98295175	4.09457173
1	3.44651124	1.99105257	3.88121863
6	2.01504143	2.20254943	2.29357106
1	2.74787521	2.51823524	1.53143436
1	1.69705099	3.12573064	2.80285715
6	0.78757449	1.57218437	1.59081236
1	0.45376372	0.67749880	2.13689232
1	-0.05331450	2.28521328	1.62176058
6	0.99640515	1.21684653	0.11713800
1	1.33658166	2.12181401	-0.42270621
1	0.02213527	0.93453576	-0.32445022
50	2.40334762	-0.82914994	-1.78675441
7	0.44652760	-2.50783078	-1.86802785
6	0.86106400	-3.42276511	-2.95394592
1	0.04929800	-4.12572008	-3.21061085
1	1.13943450	-2.85521939	-3.85070888
1	1.73660863	-3.99643163	-2.62541882
7	0.74767459	0.03780423	-2.99870398
6	-0.74542211	-1.72102332	-2.27240586
1	-1.57029539	-2.39432130	-2.57437896
1	-1.07711837	-1.14592799	-1.39930022
6	-0.42345068	-0.74433118	-3.40337152
1	-1.30695500	-0.09565258	-3.54235231
1	-0.25866598	-1.27312701	-4.35707089
16	1.45192499	1.01479655	-4.12334014
7	-0.01338809	-3.29786854	1.80803781
6	0.20546070	-3.31182666	-0.63797447
1	-0.57146634	-4.07473999	-0.82741909
1	1.14043441	-3.84325903	-0.41230224
6	-0.17236097	-2.48204756	0.59477569
1	-1.20075569	-2.09704480	0.51532489
1	0.50204424	-1.61688501	0.68101106
16	-1.39922800	-3.97061417	2.48887675
8	-0.93776940	-4.72591387	3.66626011
8	-2.14285095	-4.60666854	1.38005093
6	-2.41808315	-2.59456591	3.08225706
6	-3.60945645	-2.28258560	2.42789842
6	-4.38794945	-1.22130213	2.89978994
6	-3.99016985	-0.46986728	4.01381631
6	-2.78258096	-0.80696824	4.65221519

6	-1.99588899	-1.86183831	4.19709475
1	-3.92224353	-2.87972897	1.57197400
1	-1.06531548	-2.11963389	4.70263908
1	-2.45633411	-0.23339143	5.52192813
6	-4.83825448	0.66428984	4.53286448
1	-5.32404081	-0.97753971	2.39387537
8	2.76068086	1.35183259	-3.46993338
8	1.43732725	0.43339680	-5.48666912
6	0.47348200	2.53253462	-4.19945011
6	-0.48201731	2.67960259	-5.20708793
6	-1.25173990	3.84385570	-5.24851358
6	-1.07201791	4.86732806	-4.30560132
6	-0.09643945	4.69437085	-3.30898453
6	0.67582047	3.53546749	-3.24824847
1	-0.60141844	1.89806090	-5.95660490
1	-1.99986462	3.96257253	-6.03449466
6	-1.87874717	6.13919878	-4.38127791
1	0.06314289	5.48303035	-2.57124988
1	1.44335860	3.41050896	-2.48557087
1	-5.67180903	0.88476267	3.85420948
1	-5.26216604	0.41858012	5.51834906
1	-4.24430528	1.58095893	4.65824696
1	-1.35070336	6.89977848	-4.97758189
1	-2.85328620	5.96901291	-4.85720225
1	-2.04816497	6.56714645	-3.38433588
1	0.57434782	-2.83463221	2.51982522

Energy = -8524.646120 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 9

Atomic N.	X	Y	Z
8	4.81427360	1.46250356	2.12322301
6	5.32508294	0.35774352	2.18406716
8	5.52583504	-0.31645086	3.34768536
6	5.04541454	0.37050045	4.53280792
1	3.95930523	0.50798228	4.46883251
1	5.53562256	1.34691547	4.63403988
1	5.30604716	-0.28490326	5.36929694
8	0.35074276	-0.23917422	-0.13183622
6	5.83116937	-0.43428751	0.98975818
1	5.93016064	-1.49226637	1.26979285
1	6.84574828	-0.06255556	0.77001303
6	4.92874082	-0.25427241	-0.23783179
1	4.82300876	0.82236477	-0.44088948
1	5.42292875	-0.70050917	-1.11570417
6	3.54140570	-0.87577367	-0.04790287
1	3.10725925	-0.48236673	0.88687085
1	3.63720783	-1.96309347	0.11403633
6	2.59527601	-0.62128220	-1.22536299
1	2.59011390	0.44490019	-1.50608752
1	2.96970568	-1.15970537	-2.11299374
6	1.14899581	-1.07033195	-0.99196441
1	1.15035592	-2.09580506	-0.57446067
1	0.64029172	-1.11489094	-1.97049067
50	0.99325932	1.29585838	1.15052047
7	-1.42014370	2.53211882	1.05197808
6	-1.07715554	3.74369305	1.82737261

8	5.31291896	1.49862397	-1.80675334
6	4.78849531	2.38188683	-2.48965780
8	3.66442605	2.06825591	-3.14497493
6	2.95812169	3.03205933	-3.95924193
1	3.59282592	3.39102365	-4.78020868
1	2.60431008	3.87455798	-3.35036226
1	2.10014141	2.47660437	-4.34808933
8	4.09915355	1.77213511	0.98940924
6	5.37001448	3.77637204	-2.59537631
1	4.54510167	4.50568269	-2.57714802
1	5.83057495	3.87266303	-3.59466582
6	6.37665818	4.09510094	-1.48062510
1	7.22507981	3.39964649	-1.55295243
1	6.77935349	5.09875111	-1.68191590
6	5.75284665	4.02701389	-0.06223081
1	4.66453626	3.88403436	-0.15591466
1	5.88970961	4.99103689	0.45000532
6	6.29312593	2.89039945	0.83040087
1	6.71354141	2.09656801	0.19483351
1	7.11625803	3.25231302	1.46928161
6	5.21372156	2.26286270	1.72560123
1	4.83099392	3.02066695	2.43507833
1	5.68417887	1.46659884	2.33679682
50	4.19070548	-0.00390094	-0.08426227
7	-0.00628312	0.47907907	1.89555780
6	0.05239119	0.40062978	3.35605539
1	-0.29374188	1.33516256	3.85307303
1	-0.55348608	-0.43688058	3.72248889
1	1.09212900	0.22203639	3.65913900
7	-2.18966174	-1.54686597	1.86675195
6	-1.35713459	0.75958012	1.41097711
1	-1.65383631	1.81502200	1.62844056
1	-1.36257563	0.65600059	0.31464888
6	-2.47248213	-0.11015574	1.99571349
1	-3.40888228	0.18006438	1.48405790
1	-2.60499493	0.09545076	3.06558150
16	-3.29790582	-2.61863423	2.55806061
7	2.06714842	0.38117127	-0.52985224
6	0.93138251	1.50302379	1.42162216
1	0.55889429	2.52368778	1.68167702
1	1.88381695	1.37474003	1.95306459
6	1.23931949	1.51496664	-0.07956879
1	1.78350841	2.45388106	-0.27238853
1	0.32063804	1.55958906	-0.68380483
16	1.65479327	-0.38267958	-1.92708478
8	2.91744181	-1.08149024	-2.32685798
8	0.97095473	0.51088631	-2.89861631
6	0.46641721	-1.70282632	-1.55765069
6	-0.53020511	-1.98098818	-2.49441820
6	-1.35723031	-3.09045664	-2.30082573
6	-1.20346374	-3.92616783	-1.18431806
6	-0.21634075	-3.59760604	-0.23642885
6	0.61972064	-2.49631958	-0.41801193
1	-0.64175293	-1.33685725	-3.36581662
1	1.37501320	-2.24497168	0.32595239
1	-0.11101543	-4.20945568	0.66055032
6	-2.05144292	-5.16007501	-1.00659331
1	-2.12794267	-3.31783642	-3.04001940

8	-2.83875562	-3.96479104	2.16239141
8	-3.43378763	-2.21891390	3.97102634
6	-4.90015646	-2.32373333	1.76780087
6	-5.84559133	-1.52192298	2.40874765
6	-7.07268764	-1.28528407	1.78395792
6	-7.36807051	-1.83887171	0.52992031
6	-6.39622401	-2.64290532	-0.09182888
6	-5.16736893	-2.88934503	0.51701148
1	-5.62205581	-1.10773294	3.39124714
1	-7.81573902	-0.66160993	2.28418625
6	-8.70376033	-1.60363363	-0.12922676
1	-6.61012931	-3.08752158	-1.06567797
1	-4.42548830	-3.52822386	0.03828917
1	-2.91015400	-5.15853497	-1.69115541
1	-1.46282029	-6.06618092	-1.21799608
1	-2.41605612	-5.24362226	0.02649780
1	-9.34205350	-2.49695313	-0.04767664
1	-9.24003619	-0.76789274	0.33766719
1	-8.58826696	-1.38625003	-1.20015259
1	-1.93078209	-1.86173783	0.92678710

Energy = -8524.625999 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 11

Atomic N.	X	Y	Z
8	3.47127250	-0.47547213	0.86556743
6	4.68372179	-0.66129653	0.96484631
8	5.22322090	-1.87544651	1.15291454
6	4.27385502	-2.98229911	1.25545272
1	3.63988220	-3.02286931	0.36310210
1	3.63319452	-2.85201754	2.13528968
1	4.89856152	-3.87533490	1.34558533
8	2.26455254	2.19743435	-0.96233913
6	5.73539972	0.43005940	0.93942746
1	6.67718636	0.00584381	0.56182723
1	5.92164634	0.69984486	1.99350996
6	5.28695282	1.65323530	0.13937433
1	4.28499594	1.95398819	0.47131936
1	5.96524625	2.49406833	0.35288465
6	5.24449993	1.40190848	-1.37460706
1	4.79510753	0.41309516	-1.57573764
1	6.27615508	1.34919035	-1.75970440
6	4.44309707	2.46403950	-2.14284828
1	4.60729655	3.45911930	-1.69541305
1	4.80624586	2.52490140	-3.18272231
6	2.93639157	2.18559889	-2.22090897
1	2.79846049	1.20628411	-2.73643942
1	2.47728205	2.93889345	-2.88962084
50	1.24301501	0.29197387	-0.49147308
7	0.56226660	2.01146793	1.38615369
6	1.77372620	2.19523901	2.21737608
1	1.55073330	2.81229571	3.10748558
1	2.16107048	1.22288563	2.54053024
1	2.53769409	2.69068757	1.60863401
7	0.26717606	-0.73650131	1.34342136
6	-0.51497614	1.37140460	2.17738633
1	-0.72721537	1.97198132	3.08336186

1	-1.41952333	1.35038344	1.55494554
6	-0.16193319	-0.06108538	2.56184845
1	-1.06923974	-0.52125223	2.99502468
1	0.61108743	-0.08761522	3.34930471
16	0.46104134	-2.36036042	1.44942445
7	-0.47753606	2.58361837	-1.32862867
6	0.13091517	3.35103973	0.90617605
1	-0.22249211	3.95375612	1.76525601
1	1.02386114	3.83635658	0.49069708
6	-0.95676749	3.34443619	-0.16400753
1	-1.17475862	4.39260835	-0.42574608
1	-1.89370475	2.89838010	0.20231625
16	-1.30395440	2.82552473	-2.80699622
8	-0.34042376	2.41777813	-3.84732093
8	-1.94100390	4.16111812	-2.82404610
6	-2.62319522	1.59895595	-2.71962179
6	-3.92836093	2.01176508	-2.44874949
6	-4.94469730	1.05545846	-2.40451989
6	-4.67260682	-0.30283063	-2.62929919
6	-3.34981801	-0.68421546	-2.91266204
6	-2.32198791	0.25618925	-2.95938751
1	-4.13812475	3.07004479	-2.29732689
1	-1.29968886	-0.04090622	-3.19340735
1	-3.12279616	-1.73376412	-3.10867074
6	-5.77314273	-1.33097937	-2.55462069
1	-5.96918309	1.37256283	-2.20149753
8	1.03746335	-2.78465539	0.14423088
8	1.13788508	-2.77501084	2.70851909
6	-1.21854981	-3.05028080	1.54008680
6	-1.65970580	-3.65992439	2.71336829
6	-2.95290425	-4.19105420	2.76368096
6	-3.80755443	-4.12485335	1.65555273
6	-3.33607369	-3.50315896	0.48441983
6	-2.05298942	-2.96540876	0.42116890
1	-0.98614569	-3.72273294	3.56752851
1	-3.30000501	-4.66989787	3.68137005
6	-5.19382880	-4.71847172	1.70262149
1	-3.98541716	-3.44729882	-0.39212529
1	-1.69018438	-2.49126975	-0.49125076
1	-6.73125476	-0.91820486	-2.89710169
1	-5.53871315	-2.21515712	-3.16150789
1	-5.91800033	-1.67067941	-1.51679416
1	-5.26498201	-5.60503936	1.05409374
1	-5.46320112	-5.02631705	2.72086136
1	-5.94857887	-4.00076042	1.34992606
1	0.55305950	2.71900567	-1.47076956

Energy = -8524.637169 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 12

Atomic N.	X	Y	Z
8	3.27588362	-0.20737950	1.02927369
6	4.42469376	-0.61091930	1.15936667
8	4.59590790	-1.85090042	1.66659193
6	5.92125515	-2.38315500	1.87335841
1	6.51948037	-1.73238508	2.52543470
1	6.43812689	-2.53811722	0.91642837

1	5.76383021	-3.34868553	2.36301731
8	2.13040551	2.23020432	-0.93226277
6	5.64448760	0.23071068	0.82660883
1	6.38231064	-0.38038008	0.28202564
1	6.12547682	0.49047122	1.78627514
6	5.27855045	1.48610536	0.03216209
1	4.38734114	1.94761080	0.47759655
1	6.09927053	2.21603405	0.11077828
6	5.00067010	1.19137417	-1.44890300
1	4.38080584	0.28161636	-1.53520475
1	5.95528116	0.95697949	-1.94843881
6	4.28545080	2.34256441	-2.17701643
1	4.55786975	3.30769755	-1.71758167
1	4.62152541	2.38990614	-3.22641045
6	2.75739745	2.20747409	-2.21016509
1	2.51564756	1.26543791	-2.75688759
1	2.35016448	3.02468132	-2.83667356
50	1.10331319	0.32202223	-0.43624913
7	0.37394175	2.07955643	1.38973271
6	1.56552724	2.28687102	2.24380379
1	1.32580910	2.94614551	3.09892114
1	1.93037995	1.32578439	2.62014312
1	2.35194607	2.74390050	1.63281194
7	0.12539932	-0.66891418	1.39439298
6	-0.71666033	1.44167184	2.16387913
1	-0.96015220	2.05455955	3.05382348
1	-1.60386989	1.40111543	1.51770026
6	-0.35918041	0.01893436	2.58306694
1	-1.27622897	-0.44679037	2.98956344
1	0.38392339	0.01475909	3.39910158
16	0.41710299	-2.27891220	1.54712744
7	-0.62554946	2.61069617	-1.35440657
6	-0.05285866	3.40837449	0.87917552
1	-0.42081208	4.02523801	1.72224476
1	0.84615305	3.88813898	0.46989876
6	-1.12384277	3.38420383	-0.20719535
1	-1.34134616	4.42841201	-0.48498143
1	-2.06491390	2.93998171	0.15084999
16	-1.43612662	2.81978822	-2.84373493
8	-0.45871230	2.40614720	-3.86886224
8	-2.08948108	4.14708221	-2.89056395
6	-2.74159369	1.57920442	-2.74701850
6	-4.05520416	1.98008007	-2.50584388
6	-5.05858062	1.00940198	-2.44620251
6	-4.76399159	-0.34974018	-2.62618997
6	-3.43114913	-0.71966588	-2.88104260
6	-2.41769276	0.23358271	-2.94244279
1	-4.28214976	3.03887758	-2.38616238
1	-1.38731644	-0.05473596	-3.15073451
1	-3.18579789	-1.77138253	-3.04018570
6	-5.84539322	-1.39656730	-2.53574564
1	-6.08984312	1.31645240	-2.26346071
8	1.11041607	-2.67448384	0.29158396
8	1.00568545	-2.62534909	2.86528544
6	-1.22141404	-3.07027242	1.51348969
6	-1.75468336	-3.61636210	2.67996071
6	-3.01778602	-4.21674967	2.64040358
6	-3.75152672	-4.28405942	1.44886896

6	-3.18782517	-3.72775835	0.28567859
6	-1.93408529	-3.12175885	0.31150679
1	-1.17148044	-3.58128102	3.59976065
1	-3.43591568	-4.64632332	3.55298740
6	-5.10342731	-4.95269721	1.40136996
1	-3.74019829	-3.77976294	-0.65538733
1	-1.49593481	-2.70111063	-0.59413314
1	-6.84345684	-0.95353277	-2.64446552
1	-5.72169597	-2.16752760	-3.30861328
1	-5.81284670	-1.90617274	-1.55995382
1	-5.06235700	-5.88531478	0.81807046
1	-5.46135198	-5.20325404	2.40806906
1	-5.85340920	-4.30670207	0.92211888
1	0.40641134	2.73925335	-1.48118873

Energy = -8524.621076 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 13

Atomic N.	X	Y	Z
8	4.89448208	1.45750195	1.53994715
6	4.91683405	0.54250768	0.73935330
8	4.25418116	-0.61053300	1.07736018
6	4.26229321	-1.75011423	0.19150384
1	5.28404552	-2.12043059	0.02727517
1	3.79145651	-1.51031381	-0.77223926
1	3.67005012	-2.51961260	0.69735518
8	2.65047464	1.53975502	-1.03669262
6	5.66299005	0.55970979	-0.58180920
1	4.98150545	0.21532181	-1.37352449
1	6.45721234	-0.20330398	-0.50636325
6	6.27193171	1.91967866	-0.95244610
1	6.56341363	2.44374071	-0.02999338
1	7.19926023	1.72995505	-1.51546590
6	5.38731218	2.83999498	-1.81349191
1	5.06652666	2.28939519	-2.71485486
1	6.03808269	3.65103501	-2.17689564
6	4.14744058	3.47218319	-1.13600923
1	4.24967737	3.43106797	-0.04092581
1	4.09741174	4.53975047	-1.40926472
6	2.80012481	2.87086003	-1.53916662
1	2.71587694	2.86905758	-2.64201507
1	1.99288937	3.52950293	-1.16574147
50	0.92694339	0.44177647	-1.03215374
7	0.39999339	1.19893712	1.40488590
6	1.53594372	1.04121471	2.33973673
1	1.28702669	1.44088551	3.33988207
1	1.81579134	-0.01325919	2.42533805
1	2.40419709	1.58027090	1.94388740
7	0.04238490	-1.77993147	1.53396754
6	-0.83320077	0.52767316	1.88346599
1	-1.30102055	1.13253814	2.68580428
1	-1.54606344	0.50110644	1.04426914
6	-0.66041999	-0.88177986	2.45735047
1	-1.67245998	-1.24378516	2.71778435
1	-0.07178091	-0.85269984	3.38257322
16	0.50746685	-3.31254986	2.10493667
7	-0.57926994	2.06766638	-1.03627195

6	0.14125445	2.64960013	1.19688322
1	-0.17862950	3.11991851	2.14715022
1	1.10116610	3.09411674	0.90168130
6	-0.89667392	2.91913191	0.10462265
1	-0.83893814	3.98743475	-0.16176973
1	-1.91848262	2.72633896	0.47965450
16	-0.81193208	2.57831221	-2.57197352
8	0.02756856	1.60097625	-3.34693932
8	-0.61439074	4.03591329	-2.74339343
6	-2.53600899	2.24054606	-3.00959560
6	-3.44612717	3.29525297	-3.08307087
6	-4.78032132	3.02266822	-3.39632248
6	-5.21510113	1.71291411	-3.64487053
6	-4.27419360	0.67072258	-3.56770080
6	-2.94103962	0.92479187	-3.25205116
1	-3.10202540	4.31464363	-2.91199558
1	-2.21142203	0.11582046	-3.21134778
1	-4.59194346	-0.35487311	-3.76595592
6	-6.64779999	1.42841761	-4.02080321
1	-5.49434176	3.84620350	-3.45648731
8	1.21285186	-3.93683551	0.97100797
8	1.15226691	-3.07509276	3.40894592
6	-1.00787603	-4.25092149	2.39991846
6	-1.57000816	-4.26868824	3.67735266
6	-2.75015716	-4.98628539	3.88808809
6	-3.37206115	-5.68536497	2.84333937
6	-2.77535031	-5.65705339	1.56983515
6	-1.59954249	-4.94630529	1.33991968
1	-1.07208273	-3.74927652	4.49540899
1	-3.18914812	-5.01138775	4.88689842
6	-4.64838092	-6.45463636	3.07220322
1	-3.23399147	-6.21175514	0.74911794
1	-1.12349752	-4.94909940	0.35942862
1	-7.31577734	2.23741920	-3.69825609
1	-6.75211823	1.32901223	-5.11255589
1	-7.00071376	0.48823250	-3.57545722
1	-4.56173394	-7.48619201	2.70231627
1	-4.90891157	-6.49244236	4.13713427
1	-5.48901698	-5.99008971	2.53491200
1	-0.37637334	-1.86686156	0.60337607

Energy = -8524.639107 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 14

Atomic N.	X	Y	Z
8	4.71562233	-2.10223406	-1.30643866
6	5.63825315	-1.37906589	-0.97150738
8	6.11364442	-0.36305205	-1.74176008
6	5.44299830	-0.19625480	-3.01749043
1	4.39413825	0.08683025	-2.86744454
1	5.49316544	-1.12577809	-3.59862001
1	5.98681370	0.60760742	-3.52276193
8	1.48456958	-1.74026813	2.40859568
6	6.43678584	-1.49450117	0.31566865
1	6.72998465	-0.48420292	0.63761878
1	7.37462261	-2.01235077	0.05169904
6	5.70228566	-2.25075586	1.42627362

1	5.36876803	-3.22389071	1.03400542
1	6.41864561	-2.46277857	2.23677413
6	4.49626029	-1.48994117	1.98631956
1	3.78789982	-1.28541192	1.16948598
1	4.82559179	-0.50868989	2.37176572
6	3.75888081	-2.24722036	3.09505861
1	3.55888011	-3.28240161	2.77009460
1	4.39198172	-2.31327009	3.99720204
6	2.42109746	-1.60953391	3.47739219
1	2.58988787	-0.54697495	3.75118799
1	2.01450529	-2.10712519	4.37615518
50	0.28522051	-0.18063799	1.82196930
7	-0.02570748	-1.69087066	-0.19640221
6	1.26559873	-2.11579545	-0.78239087
1	1.11394782	-2.84672498	-1.59651363
1	1.81698140	-1.25249765	-1.16901448
1	1.86590136	-2.57451041	0.01015832
7	0.34524712	1.02224030	-1.48491407
6	-0.94090126	-1.09486848	-1.20212989
1	-1.37821465	-1.89925683	-1.82577173
1	-1.77284480	-0.62296273	-0.65700490
6	-0.32480869	-0.08716116	-2.17506918
1	-1.14397693	0.25450279	-2.83491405
1	0.42838691	-0.57146296	-2.80897265
16	1.24714461	2.11368713	-2.43123480
7	-1.64285207	-1.29576108	2.02463228
6	-0.67901975	-2.86952904	0.44660427
1	-0.91847571	-3.63065473	-0.32066806
1	0.06064700	-3.28181522	1.14564182
6	-1.93839746	-2.48419553	1.22605612
1	-2.21011177	-3.33857673	1.86649571
1	-2.78680025	-2.29916059	0.54308020
16	-2.03072698	-1.26552742	3.61615321
8	-1.05045118	-0.26356330	4.16353852
8	-2.14094490	-2.61130621	4.22465105
6	-3.66691262	-0.50150575	3.76395039
6	-4.76810830	-1.29422986	4.08637803
6	-6.03056386	-0.70179949	4.17697883
6	-6.20554047	0.67185914	3.95745688
6	-5.07620600	1.44639969	3.63762150
6	-3.81128415	0.87056306	3.53982567
1	-4.62654750	-2.35743711	4.27727280
1	-2.93598519	1.47766683	3.30840472
1	-5.19112366	2.51923849	3.47019318
6	-7.56381198	1.31361900	4.09384420
1	-6.89404388	-1.31936107	4.43156161
8	1.75020749	3.11661740	-1.47891547
8	2.14038043	1.27740285	-3.25716325
6	0.08525897	2.93512546	-3.54464146
6	-0.13320968	2.41933910	-4.82311293
6	-1.04645178	3.05929217	-5.66486760
6	-1.73939118	4.20523602	-5.24823805
6	-1.49304816	4.70439922	-3.95641284
6	-0.58686587	4.07977656	-3.10252668
1	0.42393734	1.54492252	-5.15752720
1	-1.21613013	2.66451237	-6.66803254
6	-2.71154008	4.90399098	-6.16456486
1	-2.01227526	5.60361923	-3.61965494

1	-0.37654769	4.48388195	-2.11236557
1	-8.36832931	0.57155043	4.01104103
1	-7.66679832	1.80560105	5.07366662
1	-7.72283888	2.08449762	3.32730213
1	-2.34871903	5.90880344	-6.42796619
1	-2.85943655	4.34366067	-7.09595310
1	-3.69073544	5.03298102	-5.68140810
1	-0.24746359	1.54745037	-0.83540129

Energy = -8524.654944 Hartree
Number of imaginary frequencies = 0.

Compound I5a isomer 15

Atomic N.	X	Y	Z
8	1.26577361	-1.80420218	3.22049221
6	2.45257643	-1.76830142	3.53044998
8	3.29672536	-2.81018566	3.36158981
6	2.71410496	-3.99938322	2.76014839
1	2.39026852	-3.78746749	1.73436546
1	1.85209906	-4.34693862	3.34028971
1	3.51582316	-4.74303398	2.76518336
8	1.80231542	1.40865770	0.38309780
6	3.13198835	-0.55954130	4.13033829
1	4.14422956	-0.82848152	4.46159534
1	2.54090014	-0.27412869	5.01354290
6	3.16972381	0.62348882	3.13991406
1	2.16318259	0.80397752	2.73927923
1	3.45581911	1.52646162	3.70245227
6	4.15758395	0.42315453	1.98308289
1	3.92966860	-0.51674645	1.45008574
1	5.16919075	0.29438770	2.40380668
6	4.16515662	1.58078562	0.96808127
1	4.02418869	2.54033954	1.49287366
1	5.15115132	1.63348586	0.47627437
6	3.12401880	1.46464461	-0.14794183
1	3.34078682	0.54419177	-0.72926513
1	3.24548523	2.31704215	-0.83816264
50	0.03308662	1.93762932	-0.49469249
7	-0.26459034	-0.49756515	-1.38125280
6	0.97156756	-1.27686127	-1.15874809
1	0.83500591	-2.32825763	-1.46452541
1	1.79092016	-0.83144180	-1.73331780
1	1.25032198	-1.24114400	-0.10153024
7	0.48179834	1.86480121	-2.66034245
6	-0.50942482	-0.31194170	-2.83676773
1	-0.48800702	-1.28638957	-3.35958460
1	-1.52042366	0.10877139	-2.94292172
6	0.48559407	0.65849472	-3.47734254
1	0.13669518	0.85810776	-4.50615308
1	1.49224470	0.21495515	-3.55975879
16	1.34473679	3.18813864	-3.07087297
7	-0.63479774	-2.56304665	1.15619351
6	-1.45115740	-1.15813063	-0.77454734
1	-2.31430650	-0.51047331	-0.99131239
1	-1.63354592	-2.13661939	-1.25384326
6	-1.38104266	-1.36124627	0.74389002
1	-2.41604445	-1.38802939	1.12429682
1	-0.89911578	-0.49617309	1.22379109

16	-1.50471040	-3.98370098	1.41631129
8	-0.50871681	-4.96412196	1.89074684
8	-2.31747069	-4.21690600	0.20471636
6	-2.65796586	-3.65768443	2.77272591
6	-4.02643077	-3.58538499	2.51360172
6	-4.90634092	-3.33318766	3.57024043
6	-4.43566093	-3.14995202	4.87762413
6	-3.04956005	-3.22517937	5.10763884
6	-2.15901476	-3.47829655	4.06774169
1	-4.38858904	-3.73892127	1.49768443
1	-1.08704098	-3.54013714	4.25628397
1	-2.66489882	-3.08505639	6.11958960
6	-5.38642699	-2.89383024	6.01969996
1	-5.97833971	-3.27912442	3.37245064
8	1.26509046	3.99390296	-1.80164008
8	2.66474490	2.88700229	-3.67143351
6	0.39692993	4.07996976	-4.32745568
6	0.87921753	4.14903091	-5.63409240
6	0.13076514	4.82754618	-6.60028547
6	-1.08701912	5.44130078	-6.27613373
6	-1.54715250	5.35596856	-4.94936687
6	-0.81601356	4.68036390	-3.97570801
1	1.83447041	3.68581805	-5.87832939
1	0.50527121	4.88430303	-7.62402056
6	-1.87673045	6.19950640	-7.31342361
1	-2.49170313	5.83080535	-4.67686700
1	-1.17163940	4.62722781	-2.94662378
1	-6.40443378	-2.70122521	5.65869866
1	-5.42770241	-3.76052889	6.69687355
1	-5.06428340	-2.03129011	6.62018113
1	-1.75487836	7.28568879	-7.18031638
1	-1.54677082	5.95072256	-8.33005652
1	-2.95146098	5.98408644	-7.23538786
1	0.02218920	-2.40450138	1.93610012

Energy = -8524.659062 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 16

Atomic N.	X	Y	Z
8	3.12656710	-0.68248921	3.17722082
6	3.26840506	-1.80133103	3.65329867
8	2.16971010	-2.57584944	3.78286580
6	2.24111282	-3.90948888	4.32480465
1	2.65141299	-3.90592742	5.34413017
1	2.83752103	-4.56861828	3.67860610
1	1.20301187	-4.25586825	4.33770617
8	3.54408192	-1.10682811	0.11663960
6	4.61411902	-2.34728614	4.10016491
1	4.68767361	-3.40685925	3.80991890
1	4.63142063	-2.33692498	5.20435506
6	5.79899039	-1.56629954	3.51697767
1	5.74556636	-0.52237543	3.85795755
1	6.71846402	-1.98978803	3.94825572
6	5.84601432	-1.61663444	1.96853315
1	5.09354486	-2.33854999	1.61311527
1	6.82183351	-2.00314688	1.63696369
6	5.56360788	-0.27211726	1.26939381

1	4.96784654	0.36700698	1.93697296
1	6.50372077	0.26735740	1.06321835
6	4.79289631	-0.43548966	-0.04642597
1	5.39523691	-1.03420245	-0.75713575
1	4.66735057	0.56594119	-0.50670860
50	1.87105937	-0.02156946	0.71348447
7	1.14734094	-0.80255455	-1.73385255
6	2.11753474	-0.41010974	-2.77058990
1	1.88123258	-0.87318901	-3.74749817
1	2.13273526	0.68026012	-2.88178106
1	3.11151354	-0.74269177	-2.44929705
7	0.06194226	1.98351116	-1.69449518
6	-0.24369501	-0.45380861	-2.09355207
1	-0.61228339	-1.13784839	-2.88564950
1	-0.86817296	-0.62346785	-1.20479160
6	-0.47607165	0.96723759	-2.60929612
1	-1.56661549	1.06898876	-2.76304858
1	0.00815535	1.12109483	-3.58189020
16	-0.12610501	3.61511257	-2.13758840
7	0.56051178	-1.79160555	0.81102960
6	1.25816855	-2.26205325	-1.48282241
1	0.97633273	-2.83237099	-2.39007067
1	2.31571256	-2.45166952	-1.25492368
6	0.39480315	-2.72540458	-0.30643623
1	0.70660208	-3.74777442	-0.03491529
1	-0.66508640	-2.78701971	-0.61503379
16	-0.57469595	-1.84818486	2.00638373
8	-0.21739625	-0.76366052	2.95167270
8	-0.78416334	-3.23986524	2.47848320
6	-2.14541336	-1.35052356	1.23111891
6	-3.02921704	-2.30892016	0.73317145
6	-4.20587726	-1.89323596	0.10083610
6	-4.51862486	-0.53314490	-0.03155168
6	-3.61889566	0.41268238	0.49288951
6	-2.43930693	0.01306710	1.11899009
1	-2.80296753	-3.36698515	0.86256301
1	-1.75269392	0.74340153	1.54993791
1	-3.85134128	1.47700845	0.41347575
6	-5.80267234	-0.08857152	-0.68724038
1	-4.89692584	-2.64276311	-0.28988231
8	0.48827104	4.38470732	-1.04363496
8	0.33191525	3.70484636	-3.53658522
6	-1.90320830	3.95309281	-2.11815083
6	-2.64615555	3.83349585	-3.29436678
6	-4.02024103	4.08152177	-3.25734618
6	-4.66102993	4.44651759	-2.06350782
6	-3.88403648	4.57267875	-0.89861622
6	-2.51166013	4.32788027	-0.91626806
1	-2.14410569	3.57822913	-4.22700540
1	-4.60311284	3.99989420	-4.17655592
6	-6.14898669	4.68769192	-2.02531930
1	-4.36030244	4.87972970	0.03444412
1	-1.90666627	4.45288617	-0.01812016
1	-6.25362897	-0.89751471	-1.27612779
1	-6.54036174	0.22488397	0.06765192
1	-5.63474140	0.77106694	-1.35143481
1	-6.40853103	5.48083987	-1.31170518
1	-6.53568722	4.96873642	-3.01325068

1 -6.68332639 3.77789991 -1.70889308
 1 -0.20993620 1.86331277 -0.71386596
 Energy = -8524.631683 Hartree
 Number of imaginary frequencies = 0.

Compound I5a isomer 17

Atomic N.	X	Y	Z
8	2.38185421	-2.89815779	2.45373192
6	3.50900557	-2.87395580	1.98847618
8	3.92242412	-3.98991275	1.30442980
6	5.24078556	-4.03724690	0.71794159
1	6.01970450	-4.03329383	1.49276590
1	5.40342330	-3.20446426	0.02026396
1	5.27915001	-4.98608552	0.17297886
8	2.96822837	0.18123538	0.05277463
6	4.42490483	-1.67680766	2.02549239
1	4.34443920	-1.24171116	1.00990192
1	5.47136111	-1.98132474	2.17175530
6	4.02047412	-0.60890271	3.04644766
1	2.92619753	-0.50657616	3.05064455
1	4.29662177	-0.96185570	4.05210984
6	4.68020803	0.75806735	2.77887133
1	5.71992383	0.60674343	2.43677002
1	4.76121570	1.29252671	3.73881718
6	3.95542468	1.69640353	1.79619600
1	2.94159452	1.91163476	2.17862260
1	4.48577715	2.66481370	1.80620995
6	3.84602329	1.27579574	0.32166137
1	4.85174312	0.98707768	-0.04342778
1	3.53650423	2.16045839	-0.26120273
50	0.93050261	0.23388808	0.48578308
7	0.84066648	-1.80453016	-1.17102054
6	2.08985739	-1.78073040	-1.96700269
1	2.00351328	-2.45157646	-2.84190257
1	2.31508745	-0.76116976	-2.29211038
1	2.92188650	-2.10775860	-1.33536249
7	0.06854821	0.85601072	-1.49561365
6	-0.31683497	-1.44977110	-2.03258842
1	-0.41937883	-2.18637499	-2.85312860
1	-1.22230909	-1.49574324	-1.41254424
6	-0.19865391	-0.03921567	-2.61289865
1	-1.15792628	0.19483049	-3.10948788
1	0.58826062	0.01128136	-3.38370584
16	0.48555804	2.40932717	-1.75141210
7	-0.47972902	-2.66774122	1.50388710
6	0.68950468	-3.18188099	-0.62163009
1	0.64401242	-3.89638271	-1.46747899
1	1.60468714	-3.40966808	-0.05855494
6	-0.51862395	-3.46433762	0.26924975
1	-0.51916683	-4.54784190	0.47520221
1	-1.45993846	-3.24619502	-0.25534338
16	-1.81049727	-2.88730631	2.55615411
8	-1.33765379	-2.43236263	3.87615934
8	-2.40678973	-4.22921041	2.36790884
6	-2.99181042	-1.68642646	1.90721230
6	-4.10386872	-2.13106493	1.19166799
6	-5.02052318	-1.19238735	0.71159027

6	-4.84004691	0.17979128	0.94121517
6	-3.71692689	0.59409608	1.67838593
6	-2.79031554	-0.32731360	2.16176395
1	-4.25075581	-3.19939019	1.03577215
1	-1.92376876	-0.00431274	2.73770897
1	-3.57010072	1.65648957	1.88170756
6	-5.81677803	1.19060614	0.39542428
1	-5.89572169	-1.53420075	0.15610648
8	0.99446246	2.81629668	-0.39366724
8	1.33691705	2.62427173	-2.94536850
6	-1.04281685	3.33881956	-2.03564249
6	-1.26601480	3.93657247	-3.27485817
6	-2.45369289	4.64395148	-3.48585612
6	-3.41587995	4.76463566	-2.47436843
6	-3.16202595	4.15164043	-1.23319799
6	-1.98648593	3.44002001	-1.00850072
1	-0.50842584	3.85338974	-4.05327231
1	-2.63094336	5.11492035	-4.45450975
6	-4.68704277	5.54577639	-2.69589526
1	-3.89755290	4.24058398	-0.43081483
1	-1.79025802	2.97311279	-0.04312397
1	-6.81060859	0.74901557	0.24614288
1	-5.91748367	2.05384886	1.06686366
1	-5.47578467	1.57184638	-0.58010511
1	-4.69484445	6.46419981	-2.08939389
1	-4.79977676	5.83756767	-3.74758352
1	-5.57136604	4.96090482	-2.40450395
1	0.37866914	-2.82726367	2.05430928

Energy = -8524.639672 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 18

Atomic N.	X	Y	Z
8	4.08138548	-2.64732687	-0.48889792
6	4.18637862	-3.81580968	-0.12342400
8	4.87939910	-4.73671425	-0.83495961
6	5.51536561	-4.23924935	-2.03951268
1	6.21225080	-3.42838474	-1.79547384
1	4.76095038	-3.86746206	-2.74378872
1	6.04706552	-5.09843675	-2.45867114
8	4.27993963	-1.82164432	2.68867250
6	3.60491401	-4.39443392	1.13991631
1	2.94183283	-3.63180036	1.55883759
1	3.00680008	-5.28288682	0.88507848
6	4.68912195	-4.78290266	2.17509505
1	5.50590879	-4.04885114	2.14079897
1	5.11006581	-5.75748959	1.88853286
6	4.12852764	-4.84082504	3.61149001
1	3.08195869	-5.19074935	3.58139234
1	4.68337764	-5.60768865	4.17519968
6	4.21067891	-3.52769722	4.41102603
1	5.26964874	-3.27036061	4.57966872
1	3.76728256	-3.70150764	5.40643328
6	3.53099855	-2.29462907	3.80717116
1	2.48813626	-2.54046957	3.52210801
1	3.46475399	-1.50850532	4.57974482
50	3.81931144	-0.34892026	1.36215161

7	0.27174372	-0.58674166	-1.57240881
6	0.96967281	-0.61533257	-2.85864850
1	0.71583782	-1.51087402	-3.46904566
1	0.73095575	0.28265166	-3.44203291
1	2.05136916	-0.62028826	-2.67536011
7	-1.38044692	1.79654971	-2.23177339
6	-1.18042182	-0.63423393	-1.73588676
1	-1.50709845	-1.61365457	-2.16191035
1	-1.64149149	-0.56171925	-0.73790570
6	-1.78626326	0.44186376	-2.63804184
1	-2.88319020	0.30574026	-2.60432903
1	-1.47301940	0.30486331	-3.68080759
16	-2.11711174	3.09046962	-3.03651405
7	1.53456067	-0.55073752	1.33323524
6	0.71749993	-1.69040515	-0.71215401
1	0.20370180	-2.64045439	-0.98771774
1	1.78958710	-1.85137974	-0.89147513
6	0.51782825	-1.46041767	0.79082296
1	0.56639157	-2.44038877	1.29733279
1	-0.49274687	-1.06534608	0.98737548
16	1.17588764	0.36065446	2.62284547
8	2.57602808	0.86845489	2.98648923
8	0.38242377	-0.28122233	3.69423389
6	0.24860594	1.82555821	2.10813837
6	-0.77627491	2.30164940	2.92726869
6	-1.43840586	3.47815746	2.56903170
6	-1.08975718	4.18350876	1.40695980
6	-0.06923868	3.66496618	0.58826437
6	0.60193699	2.49195685	0.93145921
1	-1.03977999	1.75386466	3.83110566
1	1.38064180	2.08763948	0.28443812
1	0.18693412	4.18026752	-0.33822888
6	-1.76812826	5.48110782	1.04786315
1	-2.23626829	3.85818902	3.21000230
8	-1.62825628	4.30475778	-2.35337162
8	-1.90236095	2.85701625	-4.47599211
6	-3.89723631	2.96380799	-2.73265564
6	-4.72884593	2.43702817	-3.72168046
6	-6.09943170	2.33030142	-3.47150357
6	-6.64903579	2.74179593	-2.24882752
6	-5.78601836	3.26730606	-1.27048546
6	-4.41725547	3.38232999	-1.50348740
1	-4.30227701	2.13278589	-4.67681944
1	-6.75348432	1.92214226	-4.24407165
6	-8.13216667	2.65126405	-1.99302382
1	-6.19597130	3.59689244	-0.31393514
1	-3.75720068	3.80613408	-0.74652452
1	-2.75797998	5.56102253	1.51683353
1	-1.16995895	6.33676710	1.39857965
1	-1.87475845	5.58448288	-0.04028956
1	-8.60502070	3.64087168	-2.08943932
1	-8.62271367	1.97805696	-2.70727382
1	-8.34164923	2.29154153	-0.97624703
1	-1.38639489	1.96352311	-1.22100055

Energy = -8524.639723 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 19

Atomic N.	X	Y	Z
8	0.49949841	0.62173291	0.85524967
6	1.29535350	1.52054873	1.13010735
8	1.79404447	1.69552767	2.37071445
6	1.35974740	0.74068690	3.37562053
1	1.571111789	-0.28651671	3.05578172
1	0.28304980	0.85000272	3.55588944
1	1.93087194	0.99621138	4.27303603
8	2.54252178	-0.00176092	-1.49558840
6	1.76275855	2.58163659	0.16034233
1	1.54803520	2.20194368	-0.84588845
1	1.09662939	3.44346421	0.34330555
6	3.22808358	3.04660797	0.28112545
1	3.49587183	3.14079101	1.34367503
1	3.29046656	4.06145760	-0.14185297
6	4.25698891	2.16420218	-0.44767737
1	4.02973542	2.18374965	-1.52548426
1	5.23958045	2.64720755	-0.33145309
6	4.34371345	0.69057273	0.01603502
1	3.77471708	0.54336706	0.94739941
1	5.38698627	0.43056952	0.26048190
6	3.85273530	-0.31041444	-1.03758208
1	4.54346508	-0.28679219	-1.90372770
1	3.91926864	-1.33451566	-0.61520862
50	1.00023061	-1.37464104	-1.30241672
7	-2.30624283	-1.25860207	-0.82416619
6	-2.78565079	-2.12251084	-1.91153961
1	-3.83296181	-1.88781480	-2.19961650
1	-2.15402882	-2.02819718	-2.80152742
1	-2.74793863	-3.16643770	-1.57454680
7	-0.28911582	-0.12478952	-2.64377482
6	-2.31522081	0.16169277	-1.19455845
1	-3.35577307	0.55310462	-1.28299640
1	-1.82148646	0.72658133	-0.39075581
6	-1.62038100	0.48335136	-2.52635610
1	-1.55614152	1.58406738	-2.59393224
1	-2.25220157	0.14275945	-3.36120594
16	0.16037669	-0.69100287	-4.10908692
7	-1.48035759	-1.09798749	2.27110930
6	-3.15246693	-1.51827277	0.35044028
1	-4.20840926	-1.23075171	0.13082046
1	-3.14026473	-2.60132461	0.52902783
6	-2.78259465	-0.80927360	1.65918726
1	-3.56518090	-1.05938468	2.39254752
1	-2.82294637	0.28401879	1.54167182
16	-1.17541719	-2.61066902	2.95307014
8	0.28179966	-2.61103273	3.20797883
8	-1.80831008	-3.71966884	2.20478864
6	-2.05378463	-2.49388002	4.53008983
6	-3.18642871	-3.27829782	4.74238559
6	-3.84274405	-3.20589616	5.97456283
6	-3.37741710	-2.36686652	6.99610870
6	-2.22744215	-1.59250096	6.75502538
6	-1.56397062	-1.65116166	5.53251694
1	-3.53580705	-3.94096667	3.95154681
1	-0.66582857	-1.06053927	5.35516758
1	-1.84670258	-0.93767941	7.54118074

6	-4.07442174	-2.30461169	8.33182932
1	-4.73074083	-3.81735443	6.14406413
8	1.23538466	-1.69214007	-3.71076037
8	-0.95897411	-1.16362726	-4.95638924
6	0.99667602	0.61449125	-5.03995915
6	0.50505790	0.98191475	-6.29232338
6	1.15516080	1.99486702	-7.00189500
6	2.28564117	2.63684602	-6.47635893
6	2.75079542	2.24483469	-5.20801685
6	2.11658308	1.23844011	-4.48218538
1	-0.36874812	0.47454546	-6.69897402
1	0.77690978	2.28814821	-7.98296774
6	3.00524839	3.70467844	-7.26159164
1	3.62809689	2.73783715	-4.78359938
1	2.47100641	0.93053304	-3.49278175
1	-5.03693098	-2.83060523	8.30684681
1	-3.45825646	-2.76818437	9.11725987
1	-4.25724030	-1.26481552	8.63804209
1	3.88775475	3.28624510	-7.77039568
1	2.35770744	4.14226748	-8.03227191
1	3.36191560	4.51220336	-6.60777404
1	-0.66305733	-0.78221938	1.73315477

Energy = -8524.641105 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 20

Atomic N.	X	Y	Z
8	2.29444338	-5.43256283	-0.52392563
6	2.82735867	-4.68042535	-1.31770197
8	2.02536509	-4.07752414	-2.25523014
6	2.57858911	-3.18220626	-3.24602097
1	3.23171493	-3.72456013	-3.94432189
1	3.12787144	-2.35286454	-2.78130026
1	1.71413936	-2.78338509	-3.78768653
8	2.70629419	-1.01266252	1.04788166
6	4.30500829	-4.33711398	-1.28402994
1	4.82370909	-5.22736450	-0.90230201
1	4.68854830	-4.12708079	-2.29142159
6	4.58552587	-3.13081375	-0.35269228
1	3.91964414	-2.29051902	-0.59551304
1	5.61313310	-2.78385628	-0.54872699
6	4.44577213	-3.45788499	1.14088687
1	3.47837796	-3.95108146	1.32773933
1	5.21868596	-4.19763042	1.40861508
6	4.57262526	-2.22217910	2.05053416
1	5.32293031	-1.52497305	1.64077793
1	4.94018100	-2.53024038	3.04396899
6	3.26209165	-1.46531370	2.28254353
1	2.55197325	-2.14999865	2.79147334
1	3.44798508	-0.62256876	2.97055472
50	1.40339083	0.52301393	0.70276652
7	-0.49422169	-1.28441146	0.62805950
6	-0.08630600	-2.48051611	-0.13978615
1	-0.84758222	-3.27910494	-0.08270489
1	0.09026824	-2.22350992	-1.18876493
1	0.85361687	-2.85527832	0.27854182
7	-0.83159109	0.20790711	-1.96626559

6	-1.77409056	-0.71028307	0.15171419
1	-2.61937766	-1.34400647	0.48820115
1	-1.90058439	0.27330828	0.63074951
6	-1.92389979	-0.56747602	-1.36625513
1	-2.91577459	-0.11704021	-1.55257302
1	-1.91509358	-1.55513560	-1.84416661
16	-0.61253073	0.12619380	-3.65157505
7	0.21912073	0.56422447	2.59423280
6	-0.60294111	-1.65100044	2.06664586
1	-1.44063811	-2.35986586	2.21696512
1	0.33115350	-2.16685412	2.32550433
6	-0.76593582	-0.43828467	2.98477684
1	-0.60500319	-0.77797390	4.02113471
1	-1.79240980	-0.03316201	2.92594574
16	1.08953373	1.37790222	3.71010120
8	2.24607685	1.87545732	2.88277554
8	1.34094993	0.60644409	4.94946268
6	0.14311763	2.84108074	4.20086212
6	-0.42492005	2.89759686	5.47349236
6	-1.17338337	4.02081362	5.83538880
6	-1.35516157	5.08973971	4.94640648
6	-0.76778841	5.00575468	3.67136951
6	-0.02208458	3.89138947	3.29331337
1	-0.26543975	2.07485577	6.16948538
1	0.44459248	3.83843978	2.30946465
1	-0.89248011	5.83098188	2.96744335
6	-2.13191211	6.31637095	5.35490050
1	-1.61764974	4.06880151	6.83137192
8	0.49136987	1.05994104	-3.93071143
8	-0.53732682	-1.31253810	-3.97359517
6	-2.11003289	0.77999553	-4.42071709
6	-3.14072542	-0.09069822	-4.78087633
6	-4.29950212	0.43376352	-5.35696091
6	-4.44015215	1.81179392	-5.58189075
6	-3.38335324	2.66199344	-5.21208772
6	-2.21945160	2.15752813	-4.63475234
1	-3.02216707	-1.16319358	-4.63067279
1	-5.10641507	-0.24249743	-5.64444083
6	-5.67895189	2.36743298	-6.23704140
1	-3.47082989	3.73561970	-5.38826620
1	-1.39084236	2.81535884	-4.37295765
1	-2.80362838	6.10432822	6.19665538
1	-1.45085929	7.12232222	5.67003032
1	-2.73192489	6.70750233	4.52188015
1	-5.51055252	2.52486654	-7.31375984
1	-6.53029703	1.68286900	-6.13299761
1	-5.95825633	3.33892510	-5.80765859
1	-0.77108928	1.18312343	-1.66226614

Energy = -8524.640006 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 21

Atomic N.	X	Y	Z
8	0.69527706	0.65472053	0.61465397
6	1.33705465	0.63317689	1.66014238
8	1.67407947	-0.58389125	2.15159842
6	2.35739209	-0.73647424	3.41675187

1	1.82655229	-0.20887393	4.21970632
1	3.39386606	-0.38181627	3.34636488
1	2.33307207	-1.81138334	3.61704517
8	2.73065330	0.65383906	-1.88947667
6	1.77471683	1.90152405	2.36294774
1	1.07698190	2.67530821	2.01900284
1	1.66698243	1.80576904	3.45287508
6	3.22275890	2.34873943	2.02065883
1	3.95040781	1.74318741	2.58386676
1	3.32149088	3.37401548	2.40751820
6	3.56413422	2.30457966	0.51930196
1	2.65661638	2.49111529	-0.07483106
1	4.26817990	3.11762179	0.28288965
6	4.18239831	0.97031088	0.07211190
1	3.69086125	0.12543996	0.58458624
1	5.24442414	0.93141652	0.37195637
6	4.07584769	0.72030842	-1.43759064
1	4.57230461	1.54710739	-1.98117699
1	4.64305036	-0.19893378	-1.68613518
50	1.59452604	-1.05604864	-1.57306442
7	-2.01542136	-1.51284896	-1.06019699
6	-2.37474985	-2.45257023	-2.12954923
1	-3.39897853	-2.27356170	-2.52359479
1	-1.66579599	-2.38925308	-2.96254341
1	-2.33741718	-3.47326690	-1.72764688
7	0.00495282	-0.27503552	-2.92846121
6	-2.06073147	-0.11178057	-1.50637384
1	-3.11549752	0.23458501	-1.61825636
1	-1.59542496	0.51417798	-0.73119701
6	-1.38546482	0.18455573	-2.85030084
1	-1.44195187	1.27884400	-2.99236465
1	-1.96720238	-0.27975167	-3.66204191
16	0.55838945	-0.78326225	-4.37489853
7	-1.35552224	-1.45634156	2.05615616
6	-2.93830442	-1.72515356	0.06428903
1	-3.96934918	-1.40116909	-0.21508240
1	-2.98193993	-2.80335592	0.26841207
6	-2.57707308	-1.00624489	1.36671848
1	-3.41871637	-1.12337619	2.06541241
1	-2.46283090	0.07585784	1.20551278
16	-1.44369304	-2.86862145	2.98866325
8	-0.04101735	-3.18473861	3.33436705
8	-2.31131906	-3.91071595	2.39304032
6	-2.30452194	-2.26578043	4.46161602
6	-3.45243292	-2.93014231	4.89017922
6	-4.08311643	-2.50975206	6.06457458
6	-3.58147224	-1.43671643	6.81363210
6	-2.42229868	-0.78402593	6.35486293
6	-1.78066437	-1.19256569	5.18875028
1	-3.83917154	-3.76263329	4.30356575
1	-0.88510449	-0.68341494	4.83461161
1	-2.01947934	0.05655286	6.92328617
6	-4.25598538	-0.99146653	8.08665864
1	-4.98333519	-3.02631421	6.40196993
8	1.85174270	-1.46740830	-3.95058842
8	-0.41390238	-1.56542987	-5.17175092
6	1.01953512	0.64311255	-5.38865324
6	0.49657360	0.75954370	-6.67620208

6	0.85196925	1.86621805	-7.45204588
6	1.71828873	2.85006933	-6.95544103
6	2.22276736	2.70345173	-5.65024105
6	1.88179501	1.60866020	-4.85890969
1	-0.17495822	-0.00889380	-7.05676458
1	0.44776972	1.96437984	-8.46126344
6	2.11432017	4.03578477	-7.79960035
1	2.89556917	3.46351196	-5.24719292
1	2.27207629	1.49052741	-3.84211241
1	-4.45508925	0.08974886	8.07477832
1	-5.20833565	-1.51412807	8.23955491
1	-3.61714672	-1.19179270	8.96009373
1	1.52687343	4.08386663	-8.72524357
1	1.97335089	4.97923203	-7.25286434
1	3.17784973	3.98163078	-8.07817918
1	-0.53203582	-1.52355719	1.44715180

Energy = -8524.629486 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 22

Atomic N.	X	Y	Z
8	3.76083715	0.02892894	-1.20788868
6	4.62374127	0.82542450	-1.58990242
8	4.93553218	0.97460096	-2.88261755
6	4.10293872	0.21774343	-3.81030834
1	3.06637592	0.56408899	-3.73620349
1	4.14420213	-0.85136813	-3.57642661
1	4.52227747	0.42693866	-4.79840766
8	2.40127822	2.47799258	-1.32952479
6	5.51569400	1.61049211	-0.65865277
1	5.00552729	1.64968189	0.31381317
1	6.39151145	0.95358888	-0.51072030
6	5.99845999	3.00340768	-1.10214190
1	6.13202162	3.01797862	-2.19373684
1	7.00126435	3.15113696	-0.67223877
6	5.13751261	4.20078780	-0.66044388
1	4.93161028	4.11965429	0.42169682
1	5.77557711	5.09250177	-0.77010435
6	3.81803105	4.48895782	-1.40602710
1	3.92138953	4.25372891	-2.47829420
1	3.63726428	5.57623087	-1.34770362
6	2.53945901	3.81679460	-0.88594730
1	2.51781237	3.89999405	0.22218775
1	1.68541747	4.42106791	-1.25891409
50	1.69175469	0.92188007	-0.12545347
7	-0.79792020	2.04622751	-0.57561997
6	-1.03039194	3.42626762	-0.11802514
1	-2.01724785	3.80507826	-0.44800599
1	-0.97269044	3.47542851	0.97550635
1	-0.25453861	4.07794520	-0.53526156
7	-1.09440980	1.13902125	2.22742277
6	-1.87780965	1.13578293	-0.13808123
1	-2.80322145	1.33568951	-0.71735781
1	-1.55898672	0.11104292	-0.37444515
6	-2.26482733	1.21533090	1.34031893
1	-2.97929365	0.39012504	1.51581063
1	-2.79103627	2.15174248	1.56660773

16	-1.37059390	0.84496777	3.87453075
7	0.60635394	-0.05243359	-1.76368351
6	-0.66778746	2.02277907	-2.05212898
1	-1.58769566	2.41479541	-2.53124925
1	0.17054289	2.68668775	-2.30341285
6	-0.38138858	0.62255500	-2.60810490
1	-0.03104112	0.73662806	-3.64834620
1	-1.31782698	0.03670813	-2.64866682
16	0.82463369	-1.67086906	-1.99271229
8	1.73733188	-2.09779069	-0.90242464
8	1.14251663	-1.98319682	-3.40783582
6	-0.78799855	-2.44459127	-1.66409359
6	-1.62654707	-2.80084266	-2.72114916
6	-2.86887935	-3.37869785	-2.44402512
6	-3.28383633	-3.61094343	-1.12462415
6	-2.41759765	-3.24832273	-0.07804718
6	-1.17642102	-2.66919245	-0.33961849
1	-1.29310585	-2.64103668	-3.74618662
1	-0.49728212	-2.41032138	0.47360886
1	-2.71817277	-3.42265181	0.95737293
6	-4.61139996	-4.26535955	-0.83259822
1	-3.52574619	-3.65762123	-3.27025035
8	-0.03807006	0.85884535	4.50045126
8	-2.45195100	1.76546228	4.27288457
6	-2.01558213	-0.84151615	3.99224388
6	-3.39084880	-1.05417316	4.09296367
6	-3.87144910	-2.36503900	4.16701969
6	-2.99801308	-3.46162024	4.14230937
6	-1.61579954	-3.21511600	4.04773620
6	-1.11909964	-1.91598100	3.97245497
1	-4.06649341	-0.20055654	4.13857097
1	-4.94582463	-2.53601323	4.25494384
6	-3.51772986	-4.87522522	4.21856987
1	-0.91849682	-4.05495562	4.04049842
1	-0.04616812	-1.72871096	3.92336128
1	-5.31815521	-4.12681984	-1.66100580
1	-4.48786804	-5.34937897	-0.68283716
1	-5.06477342	-3.86049023	0.08237741
1	-3.03925778	-5.43034472	5.03809249
1	-4.60283936	-4.89603107	4.37896171
1	-3.30073041	-5.42592153	3.29062866
1	-0.32402435	0.55041957	1.88851113

Energy = -8524.637160 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 23

Atomic N.	X	Y	Z
8	2.47105864	3.00013868	-0.70632499
6	3.22564528	3.55574111	0.09410930
8	2.83704917	3.57128596	1.38782054
6	3.73735421	3.89884744	2.46803921
1	4.35800066	4.77436815	2.23845999
1	4.35902234	3.02222107	2.68738584
1	3.09308313	4.11854436	3.32537164
8	3.99762336	0.84064932	0.67312581
6	4.49514791	4.26096443	-0.32669562
1	4.39181109	4.46304025	-1.40055604

1	4.55861291	5.23050946	0.19133278
6	5.78841427	3.45345569	-0.06289970
1	5.81685542	3.14561630	0.99003315
1	6.62777199	4.15276901	-0.19651603
6	5.99420009	2.20723408	-0.95971684
1	5.09788828	2.03697415	-1.57580336
1	6.81382477	2.41165266	-1.66414969
6	6.30448815	0.92222776	-0.16445168
1	6.79734844	1.18616664	0.78605947
1	7.01933577	0.28950123	-0.71618291
6	5.06131820	0.07082252	0.12130625
1	4.76061421	-0.41184004	-0.83756671
1	5.33074005	-0.75339296	0.80863258
50	2.14790509	0.39571665	-0.17453484
7	-1.47726039	2.25214202	-0.03868207
6	-1.07256298	3.60234258	-0.43581012
1	-1.73297372	4.38612073	-0.00499192
1	-0.04178587	3.79855792	-0.11765158
1	-1.10034086	3.68410483	-1.52980349
7	0.79025169	0.88018179	1.54000870
6	-1.42599528	2.07662868	1.41862876
1	-1.97438157	2.90134586	1.93083563
1	-1.94523474	1.14222305	1.67283815
6	-0.00618397	2.02054123	2.00072180
1	-0.08405656	2.00679974	3.10135151
1	0.54710210	2.93536562	1.74960857
16	1.00231798	-0.41150905	2.50844049
7	-1.92550315	-0.22020112	-1.48162522
6	-2.80632178	1.92326182	-0.57280465
1	-3.62415355	2.35526854	0.04504378
1	-2.88864602	2.36279751	-1.57687974
6	-3.00548451	0.40952391	-0.70071484
1	-3.96967511	0.21085911	-1.18686755
1	-3.02844050	-0.07513013	0.28740790
16	-2.16842252	-0.41667532	-3.15481592
8	-0.82702434	-0.28541659	-3.75870835
8	-3.31339697	0.39984420	-3.62074855
6	-2.67765925	-2.14648157	-3.27250047
6	-3.99685686	-2.45507257	-3.59967830
6	-4.37295038	-3.79697196	-3.70716773
6	-3.44727311	-4.82885287	-3.49764761
6	-2.12243828	-4.48479179	-3.17273796
6	-1.73079331	-3.15285441	-3.06125443
1	-4.70929768	-1.65004798	-3.77619356
1	-0.70055631	-2.88925980	-2.82251212
1	-1.38696220	-5.27462080	-3.00880303
6	-3.84904979	-6.27496209	-3.64577201
1	-5.40461899	-4.04433012	-3.96393512
8	1.92617987	-1.25176136	1.64029339
8	1.40334160	-0.09769291	3.89717077
6	-0.54016889	-1.35468395	2.64176303
6	-1.20241258	-1.41280536	3.86804215
6	-2.39243782	-2.13942138	3.96513117
6	-2.92428087	-2.81268859	2.85636647
6	-2.22889788	-2.74408376	1.63521440
6	-1.04610960	-2.01789073	1.51960956
1	-0.77429072	-0.90802993	4.73320857
1	-2.91142453	-2.18960888	4.92408130

6	-4.21402952	-3.58761932	2.95981304
1	-2.62156489	-3.26504328	0.75971567
1	-0.52045717	-1.97038052	0.56596229
1	-4.93814072	-6.39716779	-3.58730153
1	-3.52213962	-6.67258634	-4.61912333
1	-3.38688130	-6.90088138	-2.87010628
1	-4.10635622	-4.59718779	2.53862409
1	-4.54256696	-3.68231212	4.00240465
1	-5.01771573	-3.08897928	2.39668152
1	-1.04813110	0.30687977	-1.36040801

Energy = -8524.625040 Hartree
Number of imaginary frequencies = 0.

Compound I5a isomer 24

Atomic N.	X	Y	Z
8	0.54545714	0.03537517	0.50286783
6	1.59487855	-0.15376551	1.12219815
8	1.52963419	-1.01590590	2.16428464
6	2.64245264	-1.11996021	3.08855759
1	2.77579611	-0.16844797	3.61809310
1	3.56322255	-1.42077096	2.57433572
1	2.34951983	-1.90134975	3.79685553
8	1.99711787	0.81945280	-2.24597046
6	2.91392684	0.45830843	0.73220814
1	2.67647977	1.36273555	0.16262301
1	3.48295030	0.76342616	1.62074277
6	3.75431451	-0.50124608	-0.14850057
1	3.08629677	-1.02975024	-0.84130110
1	4.22893804	-1.25880307	0.49433051
6	4.83370976	0.24821158	-0.95992889
1	5.15464955	1.14562363	-0.40371064
1	5.72732004	-0.39156997	-1.03474063
6	4.42367178	0.64365588	-2.38870072
1	4.24520214	-0.27107172	-2.97909114
1	5.27635176	1.15954052	-2.86278119
6	3.18884547	1.53887225	-2.54008810
1	3.30683181	2.43640589	-1.89248239
1	3.15937172	1.91500794	-3.58157778
50	0.30239924	1.85357969	-1.61967642
7	-2.89633154	1.42516417	-0.25047905
6	-3.51046496	2.74200680	-0.43281355
1	-4.61428560	2.72398020	-0.30246340
1	-3.08664342	3.46096135	0.28011359
1	-3.28713657	3.10762551	-1.44267900
7	-1.21542678	1.74730452	2.22929487
6	-3.20435275	0.85900504	1.06476655
1	-4.30552447	0.75390304	1.20306979
1	-2.78381904	-0.15877130	1.10229446
6	-2.68085240	1.64264814	2.26802320
1	-3.02986957	1.10943533	3.17091449
1	-3.10597155	2.65456009	2.30557811
16	-0.40624249	2.15929858	3.63829200
7	-1.03865547	0.26487820	-2.39529786
6	-3.29371299	0.47812104	-1.30926781
1	-4.15982873	-0.13957683	-0.98931615
1	-3.61621484	1.04389465	-2.19201666
6	-2.14298041	-0.44528649	-1.73893381

1	-2.54741523	-1.22630587	-2.40495323
1	-1.71337707	-0.96315462	-0.86788552
16	-1.20263347	0.68828371	-3.96717469
8	-0.27672564	1.88997805	-4.04528122
8	-2.60079190	0.84364490	-4.43390179
6	-0.46141327	-0.60772333	-4.98927306
6	-1.21534832	-1.18801329	-6.00857708
6	-0.63418684	-2.18831823	-6.79271322
6	0.68458797	-2.60846867	-6.56978372
6	1.41434504	-2.00482544	-5.52937156
6	0.85410288	-1.00719380	-4.73449916
1	-2.23845454	-0.85519305	-6.17854543
1	1.41611032	-0.53701641	-3.92061540
1	2.44089787	-2.32559658	-5.33901510
6	1.31831960	-3.66804075	-7.43637393
1	-1.21806676	-2.64869047	-7.59197015
8	1.02611587	1.91234662	3.35276613
8	-0.88439169	3.48801773	4.06117332
6	-0.93738671	0.99148402	4.92419019
6	-1.51083144	1.48564957	6.09596274
6	-1.90413701	0.58930595	7.09266100
6	-1.74016166	-0.79426755	6.93153998
6	-1.17319884	-1.26429769	5.73390887
6	-0.76865060	-0.38323998	4.73192058
1	-1.64442868	2.56052825	6.21289051
1	-2.35250884	0.97399774	8.01049719
6	-2.14408966	-1.75595321	8.02059132
1	-1.05155906	-2.33889759	5.58360879
1	-0.33203976	-0.76109914	3.80611105
1	0.56187020	-4.24406088	-7.98472358
1	1.99274160	-3.21366026	-8.17891732
1	1.92046898	-4.36666652	-6.83905407
1	-1.27455555	-2.03548350	8.63578400
1	-2.89209408	-1.31261966	8.69030382
1	-2.55789677	-2.68382761	7.60320992
1	-0.73424174	0.98267138	1.73788310

Energy = -8524.636471 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 25

Atomic N.	X	Y	Z
8	3.09283290	2.04092738	0.92593155
6	4.30086502	2.19504837	0.68040272
8	5.24665996	2.07511926	1.61955184
6	4.81166272	1.51262469	2.88440559
1	4.39325213	0.51448581	2.70756471
1	4.06589501	2.16382141	3.35627904
1	5.71631192	1.45556603	3.49659121
8	4.17565809	-0.21290567	-0.02258269
6	4.83599926	2.71884814	-0.63142978
1	4.08460836	2.49030779	-1.40073203
1	4.81558396	3.81801110	-0.51277401
6	6.24676737	2.29538363	-1.07758279
1	6.92377216	2.30365466	-0.21036886
1	6.60972064	3.08803417	-1.75092302
6	6.38406665	0.95773352	-1.83403448
1	5.60348731	0.89916862	-2.61320864

1	7.34024243	1.01412105	-2.37833778
6	6.38692701	-0.35188335	-1.01594088
1	6.83584833	-0.17701483	-0.02413367
1	7.03636384	-1.08485703	-1.52470800
6	5.02277433	-1.01711607	-0.82843120
1	4.58338305	-1.20792954	-1.83154541
1	5.15955646	-2.00593711	-0.35228268
50	2.19108531	0.13711657	-0.52090346
7	-0.70401320	1.82417469	2.05570310
6	-0.00768670	3.04720434	2.46013954
1	-0.28558510	3.37321315	3.48597371
1	1.07823976	2.89610810	2.42349070
1	-0.25346812	3.85529311	1.75934158
7	1.23879594	-0.48891824	1.41211335
6	-0.37619321	0.69631291	2.93745887
1	-0.47505763	0.99383633	4.00702868
1	-1.10565376	-0.10670620	2.76140341
6	1.03386086	0.12745072	2.72593334
1	1.24394874	-0.60269911	3.52561884
1	1.78188124	0.92605548	2.83196537
16	1.26580264	-2.11058997	1.26994294
7	-2.12644725	1.05470016	-0.32033076
6	-2.15403450	2.04186441	1.96374236
1	-2.65375381	1.97377195	2.95458107
1	-2.32295187	3.05812253	1.58100460
6	-2.80531426	1.05385281	0.98856798
1	-3.86280288	1.31615233	0.85372685
1	-2.76820572	0.02500619	1.37847658
16	-2.70384942	2.12801920	-1.50939909
8	-1.51143161	2.51448687	-2.29149384
8	-3.60314766	3.14447519	-0.91520408
6	-3.73246482	1.05367312	-2.53512273
6	-5.11891755	1.19354390	-2.50379276
6	-5.90218154	0.37002970	-3.31733786
6	-5.31676470	-0.58330478	-4.16244134
6	-3.91465550	-0.69712000	-4.17442155
6	-3.11909249	0.11509312	-3.36984205
1	-5.56904008	1.94608688	-1.85737496
1	-2.03244862	0.03416371	-3.39155058
1	-3.44080690	-1.43167218	-4.82829217
6	-6.16340268	-1.44753711	-5.06286259
1	-6.98838928	0.47583676	-3.29746774
8	1.77805686	-2.24888246	-0.15825244
8	1.96592784	-2.82682884	2.35841968
6	-0.42233270	-2.76819559	1.24311385
6	-0.83412115	-3.63242711	2.25788606
6	-2.13869574	-4.13255100	2.23704989
6	-3.03252807	-3.78643378	1.21344535
6	-2.58835674	-2.91359391	0.20384212
6	-1.29286891	-2.40170295	0.21273431
1	-0.13175078	-3.91092923	3.04250844
1	-2.46488888	-4.80771014	3.03030548
6	-4.42970608	-4.35291857	1.17748583
1	-3.26962932	-2.62447340	-0.59874363
1	-0.96653467	-1.71871784	-0.57145530
1	-7.20662116	-1.48001124	-4.72358071
1	-6.16137336	-1.05691046	-6.09233457
1	-5.78007979	-2.47613628	-5.10748847

1	-4.49188272	-5.19219375	0.46736350
1	-4.73606432	-4.72910458	2.16193898
1	-5.15853714	-3.59885691	0.85029778
1	-1.12610573	1.26626937	-0.18462221

Energy = -8524.639773 Hartree
Number of imaginary frequencies = 0.

Compound I5a isomer 26

Atomic N.	X	Y	Z
8	3.97245047	1.94317063	-3.03618006
6	4.42280087	3.09599427	-3.06057036
8	3.94542318	4.00450150	-3.91663019
6	2.84923315	3.54841515	-4.77169999
1	2.03547370	3.13665759	-4.16345512
1	3.21605589	2.77456729	-5.45567793
1	2.53666321	4.44128956	-5.31960659
8	4.27740498	1.73861545	0.04992540
6	5.50066234	3.62647141	-2.15828576
1	6.01589135	2.76030683	-1.72943223
1	6.22435076	4.19645269	-2.75863660
6	4.93554319	4.52854164	-1.02921814
1	3.93335090	4.18045496	-0.74572795
1	4.83051365	5.54937505	-1.42329167
6	5.83884479	4.52143317	0.22059883
1	6.89273015	4.42142406	-0.09155930
1	5.76753586	5.50369380	0.71400232
6	5.50394743	3.44946719	1.27385784
1	4.52399282	3.67943137	1.72434781
1	6.24656496	3.52341252	2.08675650
6	5.45202132	1.98697470	0.81141089
1	6.38009740	1.74026239	0.25024091
1	5.46364580	1.34480173	1.71422561
50	4.12282521	0.19260190	-1.33808357
7	0.51599575	-0.05403001	1.68878232
6	0.98738563	-0.49425024	3.00222911
1	0.85286867	0.27920421	3.79224039
1	0.46462845	-1.40685440	3.31378307
1	2.05775517	-0.72776822	2.93494172
7	-1.71893444	-2.03595773	1.73756448
6	-0.89774686	0.31853752	1.70870045
1	-1.05662761	1.26878088	2.27535334
1	-1.21945685	0.51755731	0.67446183
6	-1.85123754	-0.70067991	2.33650375
1	-2.87384263	-0.29337726	2.23039079
1	-1.65083490	-0.80930388	3.41009639
16	-2.61443906	-3.29046107	2.43056733
7	1.94080401	0.41510917	-1.12564027
6	1.33121989	1.07093863	1.21585326
1	1.07551116	2.00303408	1.77476811
1	2.38428526	0.85554039	1.43981475
6	1.23605692	1.39642519	-0.27864660
1	1.68007272	2.39500226	-0.41788470
1	0.18747759	1.47747088	-0.60383832
16	1.25312794	0.02252456	-2.56826909
8	2.36914263	-0.64985507	-3.30807855
8	0.54330549	1.16000251	-3.21006226
6	-0.00269046	-1.25066757	-2.27772431

6	-1.21055417	-1.17629762	-2.97295776
6	-2.12874938	-2.22267923	-2.85502371
6	-1.85509949	-3.34242879	-2.05471290
6	-0.64373053	-3.37343665	-1.33886102
6	0.28310699	-2.33708362	-1.44704202
1	-1.41416383	-0.31014979	-3.60138480
1	1.21460876	-2.36253858	-0.88275246
1	-0.43347188	-4.21617099	-0.67885475
6	-2.81484498	-4.50309801	-1.98108358
1	-3.07022686	-2.17249294	-3.40563897
8	-2.40780676	-4.45251882	1.54328798
8	-2.25046326	-3.31658022	3.85935834
6	-4.36174648	-2.82516239	2.33846893
6	-4.97315383	-2.22805197	3.44212421
6	-6.31641063	-1.85404049	3.35606623
6	-7.05716190	-2.06970414	2.18491862
6	-6.41533232	-2.67466889	1.08987361
6	-5.07602208	-3.05348965	1.15818437
1	-4.40337198	-2.07949947	4.35867915
1	-6.79835602	-1.39015183	4.21852898
6	-8.51438197	-1.69025299	2.10567340
1	-6.97733075	-2.85746795	0.17197095
1	-4.58951689	-3.54042088	0.31334852
1	-2.49515153	-5.30995521	-2.65901768
1	-2.84978721	-4.92515969	-0.96756833
1	-3.82809454	-4.20618123	-2.28393683
1	-9.15502819	-2.58106543	2.19615190
1	-8.79300540	-0.99759574	2.90983509
1	-8.75293664	-1.21768784	1.14283478
1	-1.79366655	-2.06920799	0.71631212

Energy = -8524.638226 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 27

Atomic N.	X	Y	Z
8	2.93771827	0.60688007	1.37119127
6	4.05251886	0.08403179	1.29947394
8	4.15311186	-1.10734688	0.69059689
6	5.41240404	-1.81741544	0.65613862
1	5.72752199	-2.09014396	1.67137457
1	6.19086286	-1.23028433	0.15237529
1	5.20414062	-2.72554970	0.08342779
8	1.90776553	2.40546189	-0.81835165
6	5.27389054	0.82200971	1.79320861
1	4.92393894	1.46719998	2.60859881
1	6.03325060	0.13924037	2.19680481
6	5.89707058	1.71389791	0.67870429
1	6.47080390	1.08880670	-0.02467113
1	6.63290947	2.35764351	1.18322478
6	4.88072780	2.56871261	-0.10294330
1	4.06549835	2.87815622	0.56798102
1	5.37575210	3.49222409	-0.44151119
6	4.27505953	1.85328188	-1.32237994
1	4.12124335	0.78223497	-1.11032501
1	4.98892282	1.88711479	-2.16393102
6	2.93582486	2.43620869	-1.79956082
1	3.09162203	3.49136654	-2.10047629

1	2.63628900	1.89190745	-2.71884931
50	1.01910156	0.43333800	-0.23899889
7	-0.21525865	2.33207083	1.10325531
6	0.76476031	2.84273718	2.08993685
1	0.29540341	3.59091398	2.75546711
1	1.15768636	2.01835478	2.69291799
1	1.59684310	3.29666195	1.54089645
7	-0.09344975	-0.37141113	1.63381224
6	-1.34820677	1.66950781	1.79091516
1	-1.84148714	2.38029419	2.48241264
1	-2.07612775	1.37172677	1.02352011
6	-0.89958439	0.42391045	2.54999833
1	-1.81070590	-0.11269245	2.87454011
1	-0.34960870	0.69394525	3.46830976
16	0.38353436	-1.84248632	2.16653963
7	-0.65143407	2.33221470	-1.83930678
6	-0.69333243	3.49164113	0.30390625
1	-1.31099193	4.14846617	0.94655853
1	0.20184602	4.05076850	0.00212473
6	-1.49011593	3.14838266	-0.95139916
1	-1.78483787	4.09766908	-1.42837117
1	-2.41568334	2.60100184	-0.71442689
16	-1.11587467	2.20945372	-3.46880447
8	0.10097981	1.76792718	-4.17881805
8	-1.85740729	3.41886684	-3.89289463
6	-2.29644267	0.84427076	-3.43095947
6	-3.65493944	1.10396223	-3.60327829
6	-4.55712610	0.03610460	-3.58080265
6	-4.11673548	-1.28092304	-3.39084375
6	-2.73815165	-1.51075682	-3.22693243
6	-1.82551728	-0.45957288	-3.24634931
1	-3.99066072	2.12776704	-3.76465935
1	-0.75754488	-0.64198092	-3.12544939
1	-2.37532149	-2.53073717	-3.08510581
6	-5.09019624	-2.43262355	-3.36858252
1	-5.62202110	0.23233118	-3.71743962
8	1.28321203	-2.37411358	1.10657257
8	0.85321710	-1.82433063	3.57751319
6	-1.11716299	-2.87214666	2.15635435
6	-1.62465692	-3.38099077	3.35026987
6	-2.77750753	-4.17334913	3.32220406
6	-3.42792599	-4.46476087	2.11609868
6	-2.89489596	-3.93638149	0.92567737
6	-1.74976576	-3.14385655	0.93894588
1	-1.10888807	-3.15949361	4.28422417
1	-3.17610382	-4.57307682	4.25682441
6	-4.66077285	-5.33410579	2.08400211
1	-3.38563550	-4.15582684	-0.02533226
1	-1.33855972	-2.73949604	0.01325961
1	-6.12362193	-2.08692968	-3.49578318
1	-4.87018672	-3.15171441	-4.17143352
1	-5.02944672	-2.98372289	-2.41832312
1	-4.45528509	-6.29210313	1.58237304
1	-5.01993058	-5.55650200	3.09685136
1	-5.47779013	-4.84974342	1.52967126
1	0.37146792	2.57590090	-1.75175941

Energy = -8524.622475 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 28

Atomic N.	X	Y	Z
8	6.67660234	-0.84945190	-0.17226291
6	6.17187372	-0.47217922	-1.21036128
8	5.34477161	-1.34468962	-1.87392315
6	4.75407636	-0.98364911	-3.14107658
1	5.52534907	-0.83273877	-3.91009308
1	4.11356491	-0.09707346	-3.05531913
1	4.13389826	-1.84228566	-3.42010703
8	2.38609439	2.02675226	1.08472897
6	6.39213983	0.91871743	-1.78444350
1	7.38126137	1.23468173	-1.42628482
1	6.42141646	0.89551964	-2.88286475
6	5.33135118	1.94648167	-1.32260544
1	4.33768222	1.64732915	-1.68852923
1	5.56717042	2.90150100	-1.82146598
6	5.29403901	2.16300518	0.19479247
1	4.96251589	1.24467172	0.70148079
1	6.31738460	2.35577639	0.55599402
6	4.39174703	3.32777676	0.62595486
1	4.71209530	4.25705874	0.12088292
1	4.51371992	3.49420856	1.70825295
6	2.89921970	3.13140293	0.34197228
1	2.36641203	4.05782895	0.63934994
1	2.73114449	3.00945470	-0.74290602
50	1.15240701	0.52400219	0.45631037
7	-0.74370748	1.81668339	1.65080675
6	-0.34222386	2.17994922	3.02600294
1	-1.07681423	2.85811686	3.49717581
1	-0.23060213	1.28032757	3.64117876
1	0.63387155	2.67777557	2.97081487
7	-1.20681453	-0.99615477	2.63208356
6	-2.04443049	1.10689557	1.58658536
1	-2.87319350	1.83241465	1.70995619
1	-2.13868889	0.68149613	0.57541025
6	-2.27264319	0.01163065	2.63106116
1	-3.26998470	-0.42076220	2.42994314
1	-2.30103740	0.44432886	3.63913799
16	-1.09696642	-2.03046570	3.98573952
7	-0.04940917	1.67940848	-1.03001777
6	-0.79693794	3.04785579	0.81534404
1	-1.60639257	3.71462238	1.17096378
1	0.16315222	3.56024601	0.95903599
6	-0.98142920	2.74522530	-0.67331456
1	-0.77137620	3.66981864	-1.23555768
1	-2.02674364	2.45772328	-0.88953002
16	0.65701646	1.64279574	-2.50043274
8	1.82679361	0.72644088	-2.26651143
8	0.87766042	2.98761646	-3.08239338
6	-0.45799580	0.77028582	-3.62931290
6	-1.13402449	1.48367820	-4.61844597
6	-2.00866766	0.80340644	-5.47097940
6	-2.21104791	-0.57844034	-5.35197280
6	-1.51243259	-1.27208285	-4.34688392
6	-0.64059468	-0.60897721	-3.48668083
1	-0.95997558	2.55403057	-4.72273186

1	-0.08919664	-1.15407136	-2.72007122
1	-1.64997449	-2.35034809	-4.24375675
6	-3.13331676	-1.31508882	-6.29091746
1	-2.53709400	1.35851743	-6.24823587
8	0.02195086	-2.93395383	3.67676241
8	-1.11157508	-1.13715671	5.15941428
6	-2.61245828	-3.01334447	4.02452791
6	-3.70550441	-2.57365423	4.77397387
6	-4.87373332	-3.33851852	4.78194737
6	-4.96279345	-4.53652688	4.05676305
6	-3.84406396	-4.95522482	3.31526945
6	-2.66968484	-4.20498249	3.29477483
1	-3.62767308	-1.65864790	5.36023342
1	-5.72886264	-3.00246938	5.37097332
6	-6.21379501	-5.37673635	4.09824754
1	-3.89085052	-5.89035398	2.75421537
1	-1.79382122	-4.54581848	2.74281620
1	-2.55985748	-1.93388185	-6.99805614
1	-3.80484353	-1.99155443	-5.74350603
1	-3.74731462	-0.62006440	-6.87737734
1	-6.09657425	-6.21196203	4.80605617
1	-7.08234923	-4.78902844	4.42129145
1	-6.43561212	-5.81471406	3.11567070
1	-1.13329905	-1.55040656	1.77503200

Energy = -8524.638247 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 29

Atomic N.	X	Y	Z
8	3.14379366	0.33543788	2.32582156
6	4.35402853	0.08896884	2.31860226
8	4.86820171	-0.98655299	2.92589133
6	3.88713783	-1.90528521	3.49174645
1	3.26919981	-2.31868416	2.68728479
1	3.24491628	-1.38490835	4.21014403
1	4.48047123	-2.68490192	3.97765132
8	3.54854475	-0.98507295	-0.11353093
6	5.39839383	1.02346267	1.75724738
1	4.88304834	1.68998417	1.05175647
1	5.68026536	1.65765571	2.61676832
6	6.67119647	0.41862471	1.13796209
1	6.94454189	-0.49981836	1.67781753
1	7.48982655	1.13209676	1.31987651
6	6.63601448	0.14870574	-0.37740807
1	6.26070993	1.04802077	-0.89732943
1	7.68654399	0.04591195	-0.69366090
6	5.87868032	-1.09033951	-0.89870784
1	5.97649339	-1.92881747	-0.18938499
1	6.37821710	-1.41593536	-1.82750092
6	4.39325907	-0.92652974	-1.24995868
1	4.26416331	0.01573669	-1.82511891
1	4.13534047	-1.75251774	-1.94626866
50	1.88952518	0.25652798	0.16573268
7	0.65850093	-1.39273453	-1.68813389
6	1.23109813	-1.47273116	-3.04237392
1	0.72116373	-2.24038810	-3.65638725
1	1.15253247	-0.50060083	-3.54275376

1	2.29130120	-1.73984741	-2.96841710
7	-0.50208287	1.22775285	-2.42095355
6	-0.79943497	-1.14713191	-1.72384532
1	-1.33210594	-2.06079789	-2.06043546
1	-1.12216744	-0.94100026	-0.69383812
6	-1.26610037	-0.01065885	-2.63635884
1	-2.34498800	0.12187153	-2.43547424
1	-1.16615735	-0.28165585	-3.69544176
16	-1.13868930	2.66781299	-3.04981740
7	0.68217528	-1.31608151	1.10148776
6	0.95564661	-2.64029104	-0.94470535
1	0.52918983	-3.51860189	-1.47024165
1	2.04943494	-2.73957335	-0.92400296
6	0.42723157	-2.62419673	0.49501020
1	0.92318022	-3.44182396	1.04593043
1	-0.65560016	-2.84583640	0.49914879
16	-0.07747062	-0.97455448	2.52489665
8	0.22886603	0.45293698	2.79450145
8	0.19501541	-2.01057551	3.55129556
6	-1.85922484	-1.07693215	2.17684538
6	-2.57701241	-2.22523982	2.51330336
6	-3.94234573	-2.28916312	2.21941152
6	-4.60246191	-1.21904236	1.59858766
6	-3.85734326	-0.07079609	1.27589276
6	-2.49474033	0.00602958	1.56092810
1	-2.06776474	-3.04672742	3.01653609
1	-1.92486486	0.90673631	1.32963370
1	-4.35094147	0.77657329	0.79509677
6	-6.08225546	-1.28034011	1.31159388
1	-4.50496838	-3.18711795	2.48208634
8	-0.14690197	3.70607406	-2.72418982
8	-1.54878583	2.35799235	-4.43228857
6	-2.63717890	3.02292922	-2.09975845
6	-3.88626734	2.67646037	-2.61573235
6	-5.03139430	2.94664758	-1.86026363
6	-4.94381312	3.55642954	-0.60074483
6	-3.67046710	3.89977331	-0.10973084
6	-2.51895797	3.63839489	-0.84838025
1	-3.95490951	2.22607595	-3.60543153
1	-6.01149595	2.68585535	-2.26361342
6	-6.17930263	3.84548110	0.21426933
1	-3.58196369	4.38602253	0.86356582
1	-1.53648058	3.92763688	-0.47457048
1	-6.44550383	-2.31594313	1.29546120
1	-6.65279144	-0.74163687	2.08419547
1	-6.32254456	-0.81298965	0.34672210
1	-6.23404238	4.90907937	0.48749064
1	-7.09270542	3.58648965	-0.33549904
1	-6.17433807	3.27407493	1.15485126
1	-0.16928484	1.37810960	-1.46079183

Energy = -8524.637134 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 30

Atomic N.	X	Y	Z
8	3.62507456	-2.48114807	1.12886067
6	4.61481409	-1.95869329	1.63296003

8	5.87169290	-2.21405119	1.19412873
6	5.96604698	-3.12100199	0.06898641
1	5.43775391	-2.70646126	-0.79893462
1	5.53434379	-4.09600966	0.32669380
1	7.03635184	-3.21277273	-0.13749049
8	2.41236452	0.49204848	-1.37186030
6	4.60864533	-0.98078806	2.78143722
1	3.61694335	-1.02973026	3.24968402
1	5.35650326	-1.31812362	3.51471307
6	4.93175336	0.47766975	2.37676369
1	5.96655366	0.53586256	2.00484219
1	4.90423636	1.06284299	3.30791551
6	3.96464754	1.09441466	1.34485691
1	2.98106716	0.60204330	1.43243208
1	3.79218789	2.15284218	1.59837872
6	4.45263495	1.02864333	-0.10872524
1	4.76008589	0.00410769	-0.37519242
1	5.35063358	1.66317185	-0.21096132
6	3.40950751	1.48061160	-1.14042039
1	2.97200655	2.44893447	-0.82384035
1	3.91604367	1.67217506	-2.10360715
50	0.58289161	0.52825744	-0.42638933
7	0.43656012	-1.83962687	-1.53003582
6	1.40997375	-1.88019444	-2.64801165
1	1.25714423	-2.79099876	-3.25673110
1	1.30452064	-0.99021800	-3.27489453
1	2.42308482	-1.86423745	-2.23601720
7	-0.83096472	0.54258063	-2.16928984
6	-0.94895744	-1.85453345	-2.06676800
1	-1.11580280	-2.77537710	-2.65841551
1	-1.64076329	-1.86708868	-1.21238386
6	-1.24885952	-0.62538727	-2.93006061
1	-2.33491353	-0.62069481	-3.13581869
1	-0.73439372	-0.69240728	-3.90303672
16	-0.75468730	2.01471948	-2.86436277
7	0.71748663	-2.10335094	1.60584412
6	0.67983549	-3.03617151	-0.67791465
1	0.34094468	-3.93735027	-1.22463801
1	1.76746273	-3.12645478	-0.55036057
6	0.03238954	-3.04855918	0.70583505
1	0.08381451	-4.08176535	1.08781481
1	-1.03279745	-2.77557217	0.65578791
16	0.26083317	-2.20065408	3.24792616
8	1.31914328	-1.46872779	3.97641723
8	-0.09209015	-3.58912221	3.62265037
6	-1.26150077	-1.23595768	3.28560892
6	-2.47999158	-1.88947243	3.47064486
6	-3.65255972	-1.13212316	3.52601922
6	-3.61961206	0.26453368	3.39979401
6	-2.37457536	0.89377618	3.22403153
6	-1.19537895	0.15482037	3.16377251
1	-2.49713831	-2.97261040	3.58634704
1	-0.23304931	0.64648471	3.03041401
1	-2.32873952	1.98038965	3.13178134
6	-4.88963784	1.07674079	3.43323643
1	-4.60868692	-1.63637701	3.67638379
8	0.03140671	2.79593317	-1.84705711
8	-0.31653678	1.99658051	-4.27967981

6	-2.43556409	2.69426927	-2.85761031
6	-3.06785483	2.98603684	-4.06497440
6	-4.36633347	3.50464340	-4.04645747
6	-5.03740261	3.73777362	-2.83853147
6	-4.37450172	3.43219920	-1.63554942
6	-3.08242179	2.91284172	-1.63727668
1	-2.53752317	2.81396122	-5.00095272
1	-4.86384502	3.73537657	-4.99035665
6	-6.42780691	4.32241448	-2.81986083
1	-4.88075536	3.60951327	-0.68429275
1	-2.57045049	2.68374690	-0.70212699
1	-5.71822985	0.50951059	3.87580306
1	-4.75686703	2.00342540	4.00797761
1	-5.19174024	1.36748864	2.41486930
1	-6.40760615	5.37170387	-2.48718319
1	-6.88627511	4.29787943	-3.81657111
1	-7.08253115	3.77712453	-2.12543854
1	1.74996150	-2.21628022	1.57846826

Energy = -8524.652046 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 31

Atomic N.	X	Y	Z
8	3.78301717	-1.33554761	1.92833633
6	4.77696447	-0.90377460	2.48636809
8	5.55671178	-1.80939714	3.14596750
6	6.71481916	-1.38049181	3.89050516
1	6.42493209	-0.76390728	4.75271192
1	7.42935448	-0.83606998	3.25842394
1	7.18061043	-2.30394196	4.24959194
8	3.22392816	-1.67630548	-1.06307640
6	5.20314630	0.54944046	2.43163964
1	4.27599259	1.13645394	2.38810602
1	5.74207518	0.84179454	3.34254127
6	6.06651979	0.88664783	1.18806434
1	7.01427278	0.32387841	1.21525006
1	6.33889407	1.94880369	1.28155238
6	5.35616377	0.65312152	-0.15797644
1	4.28568895	0.89252910	-0.02824105
1	5.72836558	1.38763600	-0.88895702
6	5.51125804	-0.75513248	-0.76255381
1	5.55884611	-1.52923231	0.01700783
1	6.46636033	-0.80230713	-1.31290090
6	4.37009673	-1.14812572	-1.71673696
1	4.11707847	-0.27400683	-2.35451321
1	4.73790228	-1.93681945	-2.39861925
50	1.87033569	-0.56394461	0.04883432
7	0.28627905	-1.67021390	-1.76990285
6	0.77094897	-1.43482300	-3.14122168
1	0.19970326	-2.02593996	-3.88218433
1	0.69611615	-0.37056232	-3.39411731
1	1.82622886	-1.72822425	-3.18082842
7	-0.87248899	1.09589000	-1.55713374
6	-1.15362765	-1.37029563	-1.62018484
1	-1.75468967	-2.14203349	-2.14428709
1	-1.40065007	-1.44050612	-0.55160534
6	-1.62157915	-0.01672106	-2.15645153

1	-2.70701681	0.04729613	-1.95630579
1	-1.48161652	0.04863569	-3.24271467
16	-1.11108329	2.64907541	-2.20722526
7	0.80345569	-2.28790073	0.90689884
6	0.55173837	-3.08142438	-1.38544473
1	-0.03135657	-3.77223512	-2.02574677
1	1.62275897	-3.24971704	-1.56227392
6	0.23140549	-3.35810842	0.08527182
1	0.65599081	-4.33981425	0.35086314
1	-0.86205603	-3.43443026	0.23028958
16	0.22050960	-2.13376074	2.44067532
8	0.99196121	-1.02797980	3.05968071
8	0.09900831	-3.45476114	3.09754390
6	-1.48367723	-1.51175576	2.26229909
6	-2.56025274	-2.39923303	2.21247774
6	-3.85183820	-1.90187496	2.00783558
6	-4.08851449	-0.52712849	1.86800883
6	-2.98965682	0.34833398	1.94200375
6	-1.69548545	-0.13387386	2.13585207
1	-2.38384628	-3.46503432	2.35595875
1	-0.84487715	0.54497386	2.21735107
1	-3.15685057	1.42462093	1.85789673
6	-5.48737139	0.00833271	1.68626762
1	-4.69263184	-2.59728549	1.96694855
8	-0.28278818	3.54141025	-1.37876396
8	-0.92383492	2.50609375	-3.66324570
6	-2.84386965	3.07826787	-1.91643546
6	-3.80349348	2.78627296	-2.88674432
6	-5.14138352	3.10132245	-2.63457811
6	-5.53134958	3.70510704	-1.43044007
6	-4.53983877	3.99790937	-0.47651375
6	-3.20142544	3.68869006	-0.70950473
1	-3.49861506	2.34172217	-3.83353443
1	-5.89468524	2.88092614	-3.39285704
6	-6.97537284	4.04486944	-1.16013244
1	-4.82136307	4.48490313	0.45923686
1	-2.43015965	3.93964214	0.01877307
1	-6.16718433	-0.76645221	1.30875125
1	-5.89589357	0.36993844	2.64283104
1	-5.50403447	0.85578050	0.98665728
1	-7.09729090	5.11743062	-0.95014846
1	-7.61443124	3.79028424	-2.01462640
1	-7.35076589	3.50094713	-0.28046959
1	-0.94049241	1.14211223	-0.53607554

Energy = -8524.627455 Hartree

Number of imaginary frequencies = 0.

Compound I5a isomer 32

Atomic N.	X	Y	Z
8	3.57698339	-2.45012376	1.77492044
6	4.65472978	-2.19580939	1.26374025
8	4.97656481	-2.87810075	0.12166433
6	6.26244042	-2.69623443	-0.51105102
1	7.07347233	-3.05808729	0.13567965
1	6.43546102	-1.64804259	-0.78660638
1	6.22437951	-3.30864923	-1.41769938
8	2.43375857	0.69113835	-0.86040562

6	5.60489027	-1.13985354	1.78690561
1	5.43431638	-1.06737718	2.86896450
1	6.65023658	-1.43544346	1.62580425
6	5.33043471	0.23543050	1.12137376
1	5.28261834	0.11274190	0.02864963
1	6.19215320	0.89095936	1.32447707
6	4.04198327	0.89622439	1.62254801
1	3.22731833	0.15728343	1.60546301
1	4.17170163	1.18186433	2.67901024
6	3.60550862	2.12146357	0.80869487
1	4.38657521	2.90193526	0.83061161
1	2.71836865	2.56146375	1.29564446
6	3.27090054	1.82125972	-0.66582992
1	2.82563039	2.72752362	-1.11622352
1	4.20829593	1.62588169	-1.22080107
50	0.54571215	0.53952673	-0.02728246
7	0.64152505	-1.80940498	-1.15405171
6	1.73035953	-1.79098419	-2.16034415
1	1.67660142	-2.69260702	-2.79854836
1	1.66221539	-0.88986323	-2.77624775
1	2.69319341	-1.75796181	-1.64185010
7	-0.70182240	0.51898327	-1.88903410
6	-0.67633333	-1.88205970	-1.83865990
1	-0.72981874	-2.79988547	-2.45546492
1	-1.45394979	-1.94489752	-1.06429589
6	-0.94936142	-0.65538368	-2.71300485
1	-2.00154461	-0.71408816	-3.04670687
1	-0.32010971	-0.66670010	-3.61839814
16	-0.65498569	2.00936669	-2.54720087
7	0.53925272	-2.13489176	1.99770003
6	0.84624797	-3.00978121	-0.29338604
1	0.62710420	-3.91387626	-0.89358943
1	1.91303512	-3.04727035	-0.03267235
6	0.03397809	-3.09279717	0.99800778
1	0.09624839	-4.13153234	1.36260132
1	-1.03074555	-2.87819466	0.82076469
16	-0.18632375	-2.24772466	3.54608141
8	0.72840867	-1.52163363	4.44708183
8	-0.59836346	-3.64106158	3.83217017
6	-1.69453248	-1.28389026	3.32317492
6	-2.92072025	-1.94192545	3.21997992
6	-4.08457236	-1.18517777	3.06699269
6	-4.03637214	0.21639726	3.01892918
6	-2.78752774	0.84958147	3.13986235
6	-1.61546187	0.11054668	3.28841597
1	-2.95414671	-3.02927891	3.27965440
1	-0.64963495	0.60349221	3.38685689
1	-2.73206068	1.93938801	3.11532410
6	-5.29227080	1.02721265	2.82042816
1	-5.04751974	-1.69339219	2.99129423
8	-0.02341369	2.81712447	-1.44640438
8	-0.08297435	2.05371170	-3.91350917
6	-2.37071146	2.57698417	-2.69121059
6	-2.90380082	2.85225217	-3.94926672
6	-4.23145834	3.27987840	-4.04832608
6	-5.02972965	3.43794150	-2.90752981
6	-4.46478375	3.15130489	-1.65116858
6	-3.14467593	2.72298243	-1.53567972

1	-2.27583040	2.73790964	-4.83214394
1	-4.65170085	3.49726182	-5.03211000
6	-6.45392163	3.92344926	-3.01393417
1	-5.07082904	3.27188253	-0.75059524
1	-2.71019665	2.50695988	-0.55916968
1	-6.18160186	0.48169496	3.16145369
1	-5.24209819	1.98301954	3.35867722
1	-5.43782340	1.26032121	1.75358609
1	-6.54295870	4.96029630	-2.65472010
1	-6.80921390	3.89881070	-4.05188986
1	-7.13233348	3.31158371	-2.40263527
1	1.55563023	-2.23104844	2.14645936

Energy = -8524.640630 Hartree
Number of imaginary frequencies = 0.

Intermediate 5b (I5b)

Compound I5b isomer 1

Atomic N.	X	Y	Z
50	-0.34949555	0.50478340	-0.05052720
7	-0.40861312	1.69788082	-2.26640720
6	-1.07478394	3.00299199	-2.10162207
1	-1.19269400	3.51579485	-3.07406692
1	-0.49114934	3.64036737	-1.42780677
1	-2.06594082	2.85539478	-1.65764477
7	2.30638347	1.93471549	-0.88892261
6	0.91442298	1.84581810	-2.92665871
1	0.77737148	2.33995106	-3.90839172
1	1.28581399	0.82784314	-3.11088235
6	1.97575097	2.61567631	-2.14363978
1	2.85403422	2.70467881	-2.81463123
1	1.64518128	3.64373201	-1.93886833
6	3.40113324	2.42916539	-0.12944011
6	3.31190790	3.67567784	0.53288867
6	4.40063087	4.12589358	1.29017445
6	5.56987172	3.37288459	1.43798406
6	5.62125775	2.12279168	0.81006757
6	4.56676882	1.63979515	0.02779476
7	-2.19314374	-0.16701491	-1.01054330
6	-1.24519730	0.77021689	-3.07678910
1	-0.62094357	-0.10894841	-3.28709265
1	-1.51288531	1.24430323	-4.04115646
6	-2.50518639	0.31811311	-2.34886629
1	-3.24956173	1.14457587	-2.32416307
1	-2.96441726	-0.46138381	-2.98833798
6	-3.31000987	-0.72399425	-0.32368841
6	-3.81666321	-2.00331798	-0.68893880
6	-4.91005291	-2.54812322	-0.00469552
6	-5.54871849	-1.87146918	1.03958041
6	-5.04799056	-0.61533409	1.39212639
6	-3.95424332	-0.03211110	0.73696372
6	2.04357126	4.49205633	0.49978268
1	4.31541087	5.08675625	1.80453716
6	6.73872751	3.89377940	2.23922594
1	6.51388598	1.50254131	0.92525606
6	4.67564213	0.28342467	-0.62797364
6	-3.18077328	-2.81265984	-1.79053714

1	-5.26548009	-3.54117533	-0.29438449
6	-6.74883507	-2.46480932	1.73855910
1	-5.52895686	-0.05869410	2.20131275
6	-3.50453672	1.33674206	1.18778724
1	1.99815583	5.16568637	1.36538298
1	1.16245668	3.83384981	0.52340336
1	1.96927522	5.12096671	-0.40259795
1	3.90464637	-0.41427911	-0.26479256
1	5.65683217	-0.16364728	-0.42436736
1	4.55583226	0.34596572	-1.72117363
1	6.40503159	4.55745475	3.04882315
1	7.42937122	4.47387878	1.60635158
1	7.31700567	3.07312374	2.68526383
1	-3.36268586	-3.88522057	-1.63956181
1	-2.09809931	-2.63466242	-1.82994421
1	-3.58734445	-2.55201053	-2.78141408
1	-3.18526803	1.95867553	0.34022063
1	-2.64779507	1.27912184	1.87711539
1	-4.31810426	1.85409469	1.71449843
1	-6.65472830	-3.55521658	1.84261007
1	-7.67563553	-2.27353115	1.17449124
1	-6.88266884	-2.03491964	2.74063136
1	2.36954653	0.92232098	-1.05065670
8	-0.94590858	-1.75145779	2.07279339
6	-0.56154535	-2.73928597	2.67842350
8	-1.36270101	-3.44883224	3.51596286
6	-2.71417976	-2.93258681	3.64147465
1	-3.21573085	-2.93195172	2.66621661
1	-2.69571723	-1.90884906	4.03504369
1	-3.21407610	-3.61004167	4.34045367
8	1.10162010	-0.72250674	-0.98104963
6	0.84107354	-3.31615391	2.63566816
1	0.77915174	-4.40589708	2.77526491
1	1.36351923	-2.92244994	3.52422608
6	1.59761215	-2.94068168	1.35959168
1	1.55624212	-1.85277660	1.21765778
1	2.65969131	-3.20552752	1.48626519
6	1.04625949	-3.64330067	0.11047717
1	-0.05057435	-3.52807773	0.07826239
1	1.23921624	-4.72572129	0.20182916
6	1.62899596	-3.12534857	-1.21515941
1	2.70622951	-2.91543591	-1.10112078
1	1.54435182	-3.91268584	-1.98425057
6	0.92810424	-1.88050722	-1.77742528
1	-0.14708807	-2.11660220	-1.90540955
1	1.33213599	-1.69428341	-2.79684370

Energy = -7584.977662 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 2

Atomic N.	X	Y	Z
50	-0.83634321	1.15551363	0.08146153
7	-0.77928164	2.15864949	-2.17184395
6	-1.44864294	3.47421818	-2.17452055
1	-1.54665911	3.86462712	-3.20336232
1	-0.87622722	4.18931319	-1.57323751
1	-2.44538705	3.37405545	-1.73093962

7	1.79235530	2.39319229	-0.62741461
6	0.58084790	2.23802601	-2.76593721
1	0.51522205	2.68484397	-3.77603210
1	0.93060673	1.20109556	-2.86754660
6	1.60159353	3.01878270	-1.94236007
1	2.53892975	3.04726370	-2.53229715
1	1.29270859	4.06433264	-1.80715402
6	2.77215967	2.97820676	0.23128480
6	2.51246549	4.20820755	0.87573184
6	3.48598351	4.74958982	1.72573206
6	4.70051644	4.10418603	1.97628012
6	4.92294825	2.87010395	1.35347762
6	3.98806225	2.29892540	0.48402442
7	-2.73161338	0.66105557	-0.83967356
6	-1.57566383	1.15345997	-2.93476894
1	-0.96118614	0.24303269	-2.95691169
1	-1.73350351	1.50819153	-3.97064516
6	-2.91409321	0.83975668	-2.27016776
1	-3.65084246	1.64367202	-2.48741899
1	-3.30881820	-0.06144928	-2.77919416
6	-3.86563360	0.20423374	-0.11243036
6	-4.33073291	-1.13165435	-0.24471714
6	-5.43229246	-1.56473451	0.50500088
6	-6.10497620	-0.72245691	1.39437651
6	-5.63805898	0.59056167	1.52154028
6	-4.54506426	1.06802356	0.78833473
6	1.19285700	4.92089422	0.71413631
1	3.27130830	5.69683360	2.22692072
6	5.74199400	4.71914321	2.87967155
1	5.85583077	2.33393280	1.54492661
6	4.27951357	0.96476907	-0.16129504
6	-3.63596593	-2.11331918	-1.15505264
1	-5.76191651	-2.60221081	0.39957415
6	-7.30610536	-1.20251747	2.17335551
1	-6.14558304	1.27231761	2.20943206
6	-4.12136970	2.50664594	0.96846343
1	1.01041228	5.58938246	1.56531736
1	0.36571150	4.19798471	0.65679313
1	1.16024556	5.54220267	-0.19604208
1	3.57363096	0.18567394	0.16597334
1	5.28977631	0.62523802	0.09883193
1	4.21450217	1.01384561	-1.25934620
1	5.29291077	5.44452827	3.57118120
1	6.50930664	5.25234502	2.29612740
1	6.26058632	3.95403479	3.47382953
1	-3.75257156	-3.13940586	-0.78093812
1	-2.56542745	-1.88263353	-1.23519610
1	-4.05239578	-2.09276215	-2.17550514
1	-3.96131499	3.00277452	0.00072676
1	-3.17705158	2.59281890	1.52788370
1	-4.88790998	3.06570876	1.52151150
1	-7.30971859	-2.29692711	2.26730885
1	-8.24564365	-0.91258915	1.67616326
1	-7.32859029	-0.77145378	3.18404951
1	1.95041676	1.38628504	-0.75006170
8	2.30959773	-5.87649064	2.25908102
6	2.25610701	-6.50125394	1.21650485
8	1.70810213	-7.74836528	1.11633612

6	1.21249030	-8.28868136	2.36460297
1	0.42810781	-7.64218224	2.77759830
1	2.02588297	-8.37458109	3.09625713
1	0.81055660	-9.27511749	2.11395531
8	0.46963167	-0.21299193	-0.88135638
6	2.80653942	-6.04504861	-0.12253179
1	2.19387210	-6.47832239	-0.92667303
1	3.80440283	-6.50661930	-0.21613871
6	2.91212157	-4.52207765	-0.24718665
1	3.44695151	-4.13023860	0.63123248
1	3.52764962	-4.28550660	-1.13001187
6	1.55287178	-3.82446006	-0.37401837
1	0.94121793	-4.05842573	0.51286745
1	1.01465140	-4.23554802	-1.24636537
6	1.67282151	-2.30384752	-0.52031994
1	2.18843353	-1.88512259	0.35963399
1	2.29024932	-2.05754091	-1.40114127
6	0.31719254	-1.60902926	-0.66981735
1	-0.29106269	-1.82851938	0.23336704
1	-0.22520622	-2.06839533	-1.52328803

Energy = -7584.979628 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 3

Atomic N.	X	Y	Z
8	2.56263355	-1.44804408	-2.48758922
6	3.70761403	-1.05586534	-2.32432135
8	4.77714112	-1.63299224	-2.93922887
6	4.46031223	-2.77440966	-3.77078625
1	3.74181141	-2.49432538	-4.55121218
1	4.03502285	-3.58317301	-3.16296883
1	5.41285269	-3.08360256	-4.21180545
8	-0.20191538	0.63767832	-0.75242185
6	4.14964266	0.08551089	-1.43197557
1	4.92867480	0.65529005	-1.96288602
1	4.65103023	-0.37949783	-0.56658700
6	2.99676685	0.97578040	-0.96985182
1	2.21355844	0.35297763	-0.52165734
1	3.36361171	1.63915908	-0.17013001
6	2.38836668	1.82758811	-2.09287155
1	2.19063661	1.19234135	-2.97282520
1	3.13100317	2.57808943	-2.41380195
6	1.08108506	2.53396798	-1.69977354
1	1.17189607	2.96675082	-0.68896219
1	0.90579833	3.38141736	-2.38474952
6	-0.17538869	1.65720829	-1.76016197
1	-0.24396857	1.21677584	-2.77753641
1	-1.06471008	2.30418536	-1.64459486
50	-0.47236322	-1.33746753	-1.39724634
7	-2.56344140	-1.83554360	-0.04245047
6	-2.89062297	-3.18210707	-0.56356752
1	-3.65708194	-3.67258712	0.06285297
1	-1.99305573	-3.81130465	-0.59012586
1	-3.27412211	-3.08667720	-1.58745567
7	0.21298722	-2.19702820	0.44907977
6	-2.05500558	-1.91334912	1.34958005
1	-2.81320709	-2.37171015	2.01432303

8	3.42732213	2.06367008	1.04216239
6	3.46778932	3.11371225	0.42586655
8	4.58915471	3.89620904	0.36673229
6	5.71742935	3.38755649	1.11472619
1	6.02093323	2.40475818	0.73200393
1	5.46421439	3.29254697	2.17851813
1	6.51618506	4.12190798	0.97099282
8	-0.17303016	0.01331120	-1.23477240
6	2.31825743	3.74788986	-0.33064979
1	2.72069442	4.49041028	-1.03500333
1	1.73472706	4.30740817	0.42087342
6	1.40671029	2.73364894	-1.03186652
1	1.04332116	1.99399691	-0.30816459
1	0.51483832	3.26763289	-1.39381310
6	2.08703829	2.02648022	-2.20931024
1	2.95755344	1.45330358	-1.84485767
1	2.48689563	2.79021066	-2.90012887
6	1.17558094	1.07753698	-3.00345362
1	0.26173930	1.60911206	-3.31935494
1	1.70392330	0.78030030	-3.92670044
6	0.76786832	-0.21229639	-2.27852521
1	1.68005223	-0.68583612	-1.86265664
1	0.37012216	-0.91974405	-3.03863265
50	-1.91291080	-1.13164351	-1.21897161
7	-3.36875217	-2.49690542	0.64508568
6	-3.93824706	-3.74490506	0.13055637
1	-4.70032245	-4.16379625	0.81744540
1	-3.15272201	-4.49545148	-0.01782336
1	-4.40637269	-3.55515160	-0.84464385
7	-0.42617323	-2.44991082	0.64655574
6	-2.57050793	-2.70409425	1.86008809
1	-3.10139785	-3.35025623	2.58959549
1	-2.42662405	-1.72692552	2.34269663
6	-1.19961154	-3.31427187	1.56560698
1	-0.66759039	-3.46230878	2.52302042
1	-1.30258160	-4.30465123	1.10641924
6	0.87859144	-2.94151176	0.27889658
6	1.01688785	-4.04582088	-0.58736712
6	2.30703856	-4.47453199	-0.92862730
6	3.45684960	-3.83678126	-0.45397181
6	3.29003113	-2.72315040	0.37746480
6	2.02437643	-2.26423898	0.75610408
7	-2.74527020	0.26664102	0.19293115
6	-4.41414117	-1.47049727	0.79361845
1	-5.14220131	-1.74315373	1.58619829
1	-4.95990731	-1.44523095	-0.16293630
6	-3.84734030	-0.08133914	1.08144255
1	-4.69037996	0.62828456	0.97043288
1	-3.56089098	-0.01667905	2.15327885
6	-2.40453941	1.65005637	0.23591735
6	-1.76554362	2.21629668	1.36729961
6	-1.49294045	3.59132046	1.40088624
6	-1.82748397	4.44126753	0.34447697
6	-2.44938772	3.87119309	-0.77326689
6	-2.73898255	2.50461908	-0.84793262
6	-0.17149368	-4.75348566	-1.19279320
1	2.40870153	-5.32415164	-1.60845693
6	4.83365996	-4.33536754	-0.82057889

1	4.16936769	-2.18546170	0.73915356
6	1.89676029	-1.03830370	1.62754774
6	-1.33841840	1.36443396	2.53602976
1	-0.99229984	4.00420544	2.28129974
6	-1.50237402	5.91542379	0.38607808
1	-2.72415348	4.51216098	-1.61558679
6	-3.40966040	1.96564483	-2.08694998
1	0.11397110	-5.23528869	-2.13687118
1	-0.99333423	-4.05377838	-1.40493796
1	-0.56395975	-5.54571518	-0.53413524
1	1.37366362	-0.22473852	1.10040136
1	2.88340619	-0.64821223	1.90056448
1	1.34993041	-1.24705311	2.56184963
1	5.21065456	-5.04720247	-0.06914518
1	5.55586983	-3.50975886	-0.87770200
1	4.82697601	-4.85481453	-1.78834075
1	-0.44452721	1.78264784	3.01757061
1	-1.10908627	0.34396084	2.20024373
1	-2.12296481	1.29000438	3.30658479
1	-4.21909291	1.26445079	-1.84095604
1	-2.69577936	1.41630531	-2.72317150
1	-3.82143459	2.78400760	-2.69266441
1	-0.61782948	6.14707303	-0.22898250
1	-1.28896122	6.24926577	1.41036185
1	-2.33221751	6.52154566	-0.00501835
1	-0.29564663	-1.53799584	1.09414289

Energy = -7584.975236 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 5

Atomic N.	X	Y	Z
8	5.75228234	-0.70914243	-0.44530798
6	5.36702138	-0.57111286	-1.58639883
8	5.53257395	-1.63108783	-2.44792916
6	5.07661894	-1.54425788	-3.81017526
1	5.54312384	-0.70496993	-4.34539798
1	3.98170759	-1.45755169	-3.86275815
1	5.38464413	-2.48486615	-4.27934349
8	0.17251356	0.711173066	-0.32941334
6	4.76470149	0.70739415	-2.15296536
1	3.86683711	0.46538632	-2.74361596
1	5.49794407	1.09514294	-2.88116899
6	4.44345443	1.77772286	-1.09693765
1	5.14021484	1.65723616	-0.25431822
1	4.63829243	2.76783803	-1.53643522
6	2.99264733	1.75291524	-0.58973336
1	2.30420478	1.92242475	-1.43396555
1	2.85321745	2.60831078	0.09316711
6	2.57862800	0.47148750	0.13934279
1	2.65263544	-0.40250287	-0.52878260
1	3.26974881	0.27717165	0.97661211
6	1.15364353	0.53077762	0.69579175
1	1.07231898	1.38645028	1.39400598
1	0.95497249	-0.38928279	1.27203882
50	-1.03836085	-0.72947216	-1.18508255
7	-2.93255176	-1.10344612	0.49230679
6	-4.03953998	-1.58578866	-0.36313657

1	-4.91217993	-1.87540341	0.24863863
1	-3.71537073	-2.45573607	-0.94833767
1	-4.33443913	-0.79220602	-1.06100372
7	-0.40502278	-2.42273253	-0.01941903
6	-2.43046671	-2.20998797	1.35303112
1	-3.28956008	-2.75594950	1.78788354
1	-1.85888140	-1.76001235	2.17468240
6	-1.50606234	-3.16069085	0.59171983
1	-1.13108847	-3.90679871	1.30948823
1	-2.09386307	-3.74345879	-0.15058397
6	0.86869392	-3.04993204	-0.06727907
6	1.48137777	-3.38349645	-1.30522278
6	2.77966999	-3.90966904	-1.32445383
6	3.51000729	-4.14313560	-0.15600874
6	2.88077647	-3.85730102	1.05943310
6	1.58940388	-3.32261528	1.13036718
7	-1.93380233	2.10986211	1.29441343
6	-3.42348709	0.03534192	1.32271460
1	-4.10829664	-0.37744017	2.08909098
1	-4.02541516	0.68852644	0.67513998
6	-2.32195882	0.88818279	1.99525879
1	-2.66015486	1.13064624	3.01045179
1	-1.40738129	0.28904802	2.11402981
6	-2.86982508	3.13412085	1.03699297
6	-3.58411734	3.76122646	2.09117304
6	-4.49720635	4.78048756	1.79073372
6	-4.70923919	5.24191139	0.48860178
6	-3.94578012	4.66045237	-0.53011238
6	-3.04069757	3.62260843	-0.28634785
6	0.76479260	-3.20334123	-2.62344858
1	3.23204050	-4.15251546	-2.28984018
6	4.93435120	-4.63545930	-0.20492873
1	3.42576182	-4.02636184	1.99184056
6	1.02158884	-3.00409561	2.49205236
6	-3.32209096	3.43234570	3.54111609
1	-5.03431655	5.25291488	2.61764691
6	-5.71937390	6.32399773	0.19242349
1	-4.06052504	5.01921585	-1.55632971
6	-2.25353506	3.04079272	-1.43353443
1	0.82432440	-2.16893989	-3.00498764
1	-0.30328755	-3.45034212	-2.54540568
1	1.21276459	-3.84810726	-3.39211853
1	0.42701607	-2.07996813	2.46690550
1	1.82926725	-2.87821346	3.22472839
1	0.36357653	-3.80296161	2.87112044
1	5.18432643	-5.23251911	0.68282762
1	5.63320979	-3.78505325	-0.24152528
1	5.11635002	-5.24955850	-1.09774532
1	-3.62290636	4.27401401	4.17869635
1	-2.25414504	3.23283338	3.71174802
1	-3.88207323	2.54929005	3.89130125
1	-2.48227135	1.97262309	-1.59145633
1	-1.16515525	3.09811376	-1.27660162
1	-2.48606103	3.56896307	-2.36696703
1	-5.39656246	6.95671279	-0.64602518
1	-5.88095814	6.97042833	1.06602201
1	-6.69695789	5.89548088	-0.08169537
1	-1.29827736	1.89535415	0.51870564

Energy = -7584.960076 Hartree
 Number of imaginary frequencies = 0.

Compound I5b isomer 6

Atomic N.	X	Y	Z
8	3.17494742	-0.93482461	-3.06864794
6	2.41342320	-0.04443536	-3.38921062
8	1.29414578	-0.39370267	-4.10495784
6	0.32101732	0.61036315	-4.45187237
1	0.75590226	1.39180497	-5.09178577
1	-0.11662186	1.05933711	-3.54910496
1	-0.45688110	0.07707391	-5.00895225
8	0.68601457	0.26610508	-0.93045284
6	2.64073426	1.43311908	-3.12186063
1	1.71094106	1.86654881	-2.72789742
1	2.80945356	1.90515118	-4.10570711
6	3.81954422	1.72204871	-2.18023472
1	4.51599347	0.87145464	-2.21899508
1	4.36588953	2.59669408	-2.56643624
6	3.44833850	2.01699369	-0.71642630
1	2.76045622	2.88116765	-0.68310854
1	4.37393713	2.35683386	-0.22376854
6	2.85071816	0.86762010	0.12645219
1	3.22640325	-0.10640726	-0.22165373
1	3.21236850	0.98434337	1.16242267
6	1.31765756	0.80936150	0.21983362
1	0.94446823	1.84284769	0.37839180
1	1.05714453	0.22542760	1.12156875
50	-0.64055495	-1.32144837	-1.07806042
7	-2.92912991	-2.31637901	0.06375098
6	-3.26581034	-3.45316244	-0.80013326
1	-4.16118930	-3.99427287	-0.43655067
1	-2.42712584	-4.15877266	-0.84390200
1	-3.45520184	-3.09318635	-1.82046520
7	-0.11949436	-2.28254763	0.79702563
6	-2.48160816	-2.75183198	1.39546802
1	-3.15760589	-3.52499172	1.81576098
1	-2.50377632	-1.88537680	2.07034042
6	-1.04630104	-3.27540409	1.34677061
1	-0.75818948	-3.53994904	2.37801850
1	-1.01663258	-4.23467748	0.78682666
6	1.21726355	-2.44584667	1.27500584
6	2.23623405	-3.01556923	0.46862859
6	3.53345429	-3.14576038	0.98402666
6	3.86993024	-2.73722243	2.27762164
6	2.85383021	-2.19534392	3.07127059
6	1.54426874	-2.04684755	2.59994545
7	-2.41017114	0.57642857	0.42524149
6	-4.02112920	-1.33712293	0.05698739
1	-4.95261649	-1.76322927	0.48893665
1	-4.22890042	-1.11397528	-1.00026978
6	-3.71687847	-0.02643665	0.78962879
1	-4.51706388	0.68244362	0.53771385
1	-3.77783164	-0.17156712	1.88109171
6	-2.41281310	1.99534447	0.20287621
6	-1.89424590	2.87443565	1.18095657
6	-1.87508963	4.24911794	0.92004798

6	-2.36913271	4.78405743	-0.27516241
6	-2.89219409	3.89570596	-1.22028389
6	-2.91775913	2.51099002	-1.00979955
6	1.97148989	-3.50039873	-0.93622219
1	4.30475442	-3.58534969	0.34644088
6	5.28647340	-2.84951856	2.78762240
1	3.08654350	-1.86686547	4.08800017
6	0.50716259	-1.43795537	3.51076119
6	-1.37426296	2.35760011	2.50202809
1	-1.47045335	4.92145107	1.68052699
6	-2.30900782	6.26780955	-0.54638253
1	-3.27943277	4.28675784	-2.16441062
6	-3.46276572	1.60357979	-2.08373476
1	2.06484334	-2.68920086	-1.67710648
1	0.96853248	-3.93869905	-1.03692532
1	2.70856686	-4.26319019	-1.22181998
1	-0.18036597	-0.79385912	2.94383573
1	0.98330598	-0.84260241	4.30103041
1	-0.11269797	-2.20230690	4.00759382
1	5.31452176	-2.92696748	3.88310924
1	5.87958746	-1.96511610	2.50512972
1	5.79534928	-3.72796337	2.36723943
1	-1.12665947	3.19311318	3.16841955
1	-0.45711015	1.75902176	2.38198292
1	-2.11381062	1.72882624	3.02141451
1	-4.48628500	1.26237943	-1.85874135
1	-2.83934614	0.70387905	-2.19592157
1	-3.50230781	2.12663928	-3.04782893
1	-1.33224282	6.55278429	-0.96823193
1	-2.44635250	6.85001809	0.37518941
1	-3.07930720	6.57575738	-1.26591149
1	-1.73125376	0.35784815	1.15600253

Energy = -7584.952669 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 7

Atomic N.	X	Y	Z
8	1.62713589	0.60575359	0.30068947
6	2.47563114	1.47026593	0.41401066
8	3.46619366	1.25787636	1.34138678
6	4.50476372	2.23684462	1.54124252
1	4.09143861	3.21463035	1.82515426
1	5.13289452	2.34314615	0.64580091
1	5.11335165	1.84799416	2.36421523
8	-1.09957260	1.22650863	-2.48251342
6	2.49770123	2.77723281	-0.35695765
1	3.51330138	2.94946747	-0.75118463
1	2.32822501	3.58182664	0.38039889
6	1.46110348	2.85668298	-1.47927835
1	0.47811747	2.53888507	-1.11077807
1	1.35849372	3.91295594	-1.77590680
6	1.83698501	2.03046435	-2.71653553
1	2.00313224	0.97941603	-2.42562079
1	2.79925500	2.40182413	-3.11046074
6	0.77490501	2.08338318	-3.82783120
1	0.33910259	3.09532131	-3.87812043
1	1.25107133	1.89626563	-4.80577118

6	-0.35603698	1.05843323	-3.67903206
1	0.09021311	0.04033007	-3.74752695
1	-1.03391447	1.16029889	-4.54977559
50	-1.37813225	-0.43606935	-1.26022943
7	-2.75041590	-2.22980075	0.65748530
6	-3.31658145	-3.40897158	0.00098557
1	-4.03808915	-3.94693639	0.65207196
1	-2.52302586	-4.10745385	-0.28928030
1	-3.83776046	-3.09985640	-0.91493095
7	0.33073369	-2.58891042	0.98930634
6	-2.00531806	-2.59088998	1.87290303
1	-2.65345040	-3.18014447	2.56001332
1	-1.75410978	-1.66000682	2.40446785
6	-0.71479163	-3.38217420	1.65393288
1	-0.38888418	-3.74896159	2.64920217
1	-0.90701941	-4.28004884	1.05146197
6	1.56597517	-3.27098620	0.76342855
6	1.67840125	-4.18348870	-0.30948635
6	2.90232471	-4.82710065	-0.53105185
6	4.02653587	-4.58522391	0.26576897
6	3.89987884	-3.66212860	1.31022320
6	2.69172912	-3.00875119	1.57940399
7	-2.55180130	0.73237826	0.07442125
6	-3.80523829	-1.24635680	0.94881749
1	-4.42910706	-1.56745364	1.81266036
1	-4.46199682	-1.20175874	0.06658776
6	-3.27582795	0.16031692	1.21395718
1	-4.15695080	0.78925734	1.43406657
1	-2.67432461	0.16590350	2.14478084
6	-2.56820191	2.16438186	0.06193037
6	-1.81414733	2.91354609	0.99766255
6	-1.86903947	4.31454109	0.96588553
6	-2.65376502	5.00556333	0.03956497
6	-3.40504595	4.25026864	-0.86854275
6	-3.37679022	2.85140080	-0.87792069
6	0.51862118	-4.43900840	-1.23921335
1	2.98175735	-5.52223729	-1.37107191
6	5.32715941	-5.31181191	0.01905146
1	4.76477216	-3.44796799	1.94343870
6	2.60306329	-2.03177775	2.72811647
6	-0.94340914	2.24022956	2.03022486
1	-1.27557842	4.87888737	1.69081320
6	-2.67503646	6.51502066	0.00019959
1	-4.03663924	4.76546251	-1.59708238
6	-4.20526536	2.10251196	-1.88990475
1	0.87693549	-4.76498486	-2.22462080
1	-0.08702198	-3.53002820	-1.36350089
1	-0.14609834	-5.23344789	-0.86043147
1	2.42107670	-1.00385261	2.37757147
1	3.54172695	-2.02333495	3.29664455
1	1.79304996	-2.29396051	3.42701309
1	5.35374629	-6.27405170	0.55518387
1	6.18779506	-4.72261811	0.36382498
1	5.46720626	-5.53156593	-1.04843746
1	-0.14098659	2.91509706	2.35924178
1	-0.48797763	1.32379172	1.63197605
1	-1.51753486	1.96385224	2.92922348
1	-4.76209497	1.27468474	-1.42896154

1	-3.55226970	1.66653083	-2.66055265
1	-4.91953974	2.77761995	-2.37956893
1	-2.02091709	6.90126824	-0.79771414
1	-2.32760514	6.94552351	0.94912488
1	-3.68623176	6.89718776	-0.19957733
1	0.50804121	-1.73691226	1.52383619

Energy = -7584.956052 Hartree
Number of imaginary frequencies = 0.

Compound I5b isomer 8

Atomic N.	X	Y	Z
8	-3.81972982	-1.00612742	-1.50054530
6	-3.96902932	-1.66014611	-0.48445667
8	-3.42818762	-2.89611186	-0.29543855
6	-2.66043675	-3.40965541	-1.41156300
1	-1.84833655	-2.71785095	-1.66830063
1	-3.30756369	-3.54359136	-2.28813618
1	-2.25559694	-4.36642304	-1.06907459
8	-0.46726631	0.89932828	0.55395820
6	-4.80848300	-1.26571221	0.71853249
1	-4.30746408	-1.61757507	1.63270665
1	-5.72915108	-1.86879264	0.63849760
6	-5.16793864	0.22383697	0.79710856
1	-5.33843370	0.59818496	-0.22406354
1	-6.13065027	0.30656667	1.32527287
6	-4.16462673	1.14069157	1.52115623
1	-3.96602628	0.73646484	2.53045264
1	-4.67857334	2.10084620	1.68650320
6	-2.82586173	1.43592821	0.81321080
1	-2.97079436	1.46984599	-0.27777284
1	-2.47808831	2.43467479	1.12209475
6	-1.68869179	0.45970768	1.13359900
1	-1.94863636	-0.56013347	0.79341695
1	-1.57931281	0.39793645	2.23778518
50	0.79724595	-0.38465492	-0.53776262
7	2.62775147	0.28010665	1.05301531
6	3.94332294	0.26307024	0.38063729
1	4.75593385	0.51690690	1.08502425
1	3.95182950	0.97291046	-0.45151196
1	4.12546512	-0.74033177	-0.02253245
7	1.47037153	2.65403563	-0.46396212
6	2.33395554	1.61810541	1.63995940
1	3.05160697	1.81758058	2.45807433
1	1.32334274	1.55915819	2.06865975
6	2.40083179	2.79618613	0.66603683
1	2.19220802	3.70543598	1.26547106
1	3.42164075	2.92065942	0.27840731
6	1.46984023	3.74194428	-1.39595235
6	2.48986914	3.84751309	-2.36876281
6	2.46728166	4.91788438	-3.27166407
6	1.45456256	5.88230220	-3.25888179
6	0.43449800	5.74071121	-2.31196436
6	0.42516842	4.69620994	-1.38015922
7	0.77188394	-1.93003454	0.98645263
6	2.58803306	-0.76977280	2.11850812
1	2.94560951	-0.34047646	3.07242343
1	3.28206733	-1.56677628	1.82091423

6	1.19750988	-1.39570220	2.27539668
1	1.28790439	-2.19303618	3.02904931
1	0.49494147	-0.64535089	2.68538957
6	0.44128520	-3.29817360	0.89342332
6	-0.48839713	-3.90679619	1.78752227
6	-0.77302598	-5.27352121	1.67670797
6	-0.19931023	-6.08537416	0.69397707
6	0.69178699	-5.47631828	-0.19531904
6	1.02299628	-4.11813510	-0.11728630
6	3.56711673	2.80017980	-2.49444680
1	3.25685688	4.98171340	-4.02477034
6	1.46805709	7.04104157	-4.22635753
1	-0.38106691	6.46790845	-2.29097017
6	-0.70909813	4.59060298	-0.38959358
6	-1.23989023	-3.10432056	2.82336400
1	-1.49603907	-5.70955900	2.37175918
6	-0.55726480	-7.54716275	0.57086446
1	1.16672211	-6.08296304	-0.97143302
6	2.02437458	-3.57078615	-1.10308947
1	4.04251205	2.85296801	-3.48230033
1	3.14280656	1.79445727	-2.36291648
1	4.36603243	2.92770258	-1.74549453
1	-1.32826526	3.70007468	-0.57562082
1	-1.36174031	5.47006851	-0.45731608
1	-0.34908627	4.51696069	0.64789504
1	2.04353287	7.88904351	-3.82202902
1	0.45195645	7.40407284	-4.43139986
1	1.93176243	6.75971146	-5.18181016
1	-2.17264859	-3.61683846	3.09303613
1	-1.49083612	-2.10585252	2.44256480
1	-0.66826205	-2.95971799	3.75381249
1	2.73937141	-2.89275888	-0.61295421
1	1.54727634	-2.99046607	-1.90951287
1	2.58547520	-4.38716898	-1.57744665
1	-1.41897306	-7.69550979	-0.10014030
1	-0.82673437	-7.97801074	1.54492563
1	0.27781516	-8.13072104	0.15867782
1	0.52710547	2.47717106	-0.09153218

Energy = -7584.973541 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 9

Atomic N.	X	Y	Z
8	-2.70553106	-3.79832240	-2.31563329
6	-3.66004268	-3.08468701	-2.56867856
8	-4.92954210	-3.35953713	-2.13747433
6	-5.04913873	-4.56840050	-1.35289357
1	-4.44048110	-4.49597596	-0.44241284
1	-4.71971127	-5.43931608	-1.93392396
1	-6.11149162	-4.64821504	-1.10218965
8	-0.19505319	0.26559435	-1.24518235
6	-3.61519757	-1.81073392	-3.38585246
1	-4.63645038	-1.43141752	-3.52919516
1	-3.21174801	-2.08953658	-4.37177406
6	-2.71141670	-0.73167130	-2.75805211
1	-1.70310523	-1.13386604	-2.59821469
1	-2.60625478	0.08625108	-3.48901157

6	-3.26508048	-0.16332525	-1.44493671
1	-3.29914979	-0.95949936	-0.68054703
1	-4.31164435	0.14793035	-1.61024339
6	-2.48299062	1.03366442	-0.87773164
1	-2.34131845	1.79628287	-1.66206014
1	-3.09117279	1.50701241	-0.08709017
6	-1.12051103	0.70480607	-0.25889843
1	-1.26131064	-0.09224241	0.49796800
1	-0.75009785	1.60053001	0.27205905
50	1.85122108	0.31550100	-1.35690236
7	4.14268953	-0.00307222	0.16584740
6	5.23847928	0.07731366	-0.80825622
1	6.23018925	0.06253261	-0.31461550
1	5.15686196	1.00047014	-1.39484874
1	5.17211251	-0.76876447	-1.50523810
7	2.17179763	2.14512762	-0.26173015
6	4.08490527	1.19855325	1.01650037
1	5.09071039	1.44579212	1.41663209
1	3.42350582	0.98454400	1.86636805
6	3.51215891	2.40298500	0.26479206
1	3.49517382	3.24881776	0.97044698
1	4.21948780	2.71200917	-0.53366508
6	1.30737168	3.27517557	-0.28271336
6	0.87029140	3.85136749	-1.50431558
6	0.01501505	4.96158775	-1.48380045
6	-0.43453024	5.53919858	-0.29343554
6	0.00025414	4.96529871	0.90578457
6	0.84982415	3.85410796	0.93524284
7	1.81866110	-1.77647726	0.81849154
6	4.23822014	-1.26312643	0.92267921
1	5.09798633	-1.24164181	1.62473167
1	4.45241441	-2.05968816	0.19125625
6	2.98560021	-1.64182305	1.70988030
1	3.20083092	-2.58669888	2.24382942
1	2.77843747	-0.88955527	2.47823824
6	0.62951129	-2.39218972	1.32131159
6	-0.01392635	-1.94926099	2.49930704
6	-1.17805951	-2.60737968	2.91931213
6	-1.75161144	-3.65905736	2.20060304
6	-1.12922766	-4.04117349	1.00727072
6	0.04380205	-3.43090386	0.55562511
6	1.30513183	3.30782606	-2.84367558
1	-0.30227728	5.39314326	-2.43686634
6	-1.38105385	6.71541203	-0.29993752
1	-0.34809712	5.38214614	1.85491697
6	1.21653655	3.25580797	2.27025166
6	0.44816117	-0.74458152	3.28413889
1	-1.66604906	-2.25633416	3.83221657
6	-3.03196757	-4.31390305	2.66083370
1	-1.57324552	-4.82675483	0.39244146
6	0.64803545	-3.86519145	-0.75855435
1	1.18103026	4.06820327	-3.62674568
1	0.70054278	2.43545210	-3.14182670
1	2.35724901	2.98863207	-2.83374182
1	1.28615430	2.16203471	2.19205361
1	0.46413944	3.51058037	3.02823392
1	2.18871723	3.61564392	2.64483185
1	-1.33248300	7.26172648	-1.25160399

1	-1.15344629	7.42012765	0.51219646
1	-2.42380475	6.38751703	-0.16237674
1	-0.37707172	-0.35850300	3.89627241
1	0.77232585	0.06320970	2.61305216
1	1.28080615	-0.96998278	3.96886053
1	1.66774942	-4.27168419	-0.64131389
1	0.69851506	-3.03086031	-1.47680364
1	0.03157915	-4.64322811	-1.22247220
1	-3.08927524	-5.35915463	2.32737755
1	-3.91354666	-3.79117007	2.25567904
1	-3.12072273	-4.29830079	3.75568732
1	2.11464919	-2.30270871	-0.00578609

Energy = -7584.966717 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 10

Atomic N.	X	Y	Z
8	-0.99136713	-1.98507143	1.38398723
6	-1.68138070	-1.00038024	1.59049508
8	-1.06796492	0.21871703	1.57009247
6	-1.86402621	1.42461076	1.64378390
1	-2.46701185	1.45466822	2.56142606
1	-2.49883829	1.50700809	0.75169187
1	-1.14159155	2.24598423	1.66117060
8	-2.71901227	-0.46231250	-1.09697736
6	-3.14375881	-1.04141767	1.98844138
1	-3.69221244	-0.28605466	1.40987416
1	-3.17785849	-0.69901791	3.03778699
6	-3.79594372	-2.42540493	1.85233162
1	-3.00191264	-3.18433238	1.79417292
1	-4.36740000	-2.63824148	2.76847278
6	-4.75122032	-2.58174939	0.66025076
1	-5.56122574	-1.83432675	0.73904052
1	-5.24272982	-3.56201334	0.77196633
6	-4.15368088	-2.51489251	-0.75853840
1	-3.19979088	-3.06590382	-0.79997248
1	-4.84772538	-3.05497684	-1.42538302
6	-3.95208785	-1.12262749	-1.39185141
1	-4.77869994	-0.45584478	-1.07769523
1	-4.07692293	-1.24960682	-2.48971833
50	-1.30640992	-0.78188927	-2.61404487
7	1.35653027	-1.04451678	-2.38432571
6	1.61125699	-1.74288573	-3.65639869
1	2.69575810	-1.82636285	-3.85404582
1	1.14007008	-1.20778139	-4.49178681
1	1.17636925	-2.75030460	-3.61469836
7	-0.50601754	1.18874083	-2.61813358
6	1.83361009	0.35252620	-2.44022406
1	2.83039846	0.40755039	-2.92094589
1	1.92829636	0.72243445	-1.41508519
6	0.84404835	1.26373609	-3.18333952
1	1.22902268	2.29315862	-3.13447824
1	0.84332604	1.00496642	-4.26152172
6	-1.18286346	2.41314931	-2.38020593
6	-2.38911150	2.72354824	-3.06338874
6	-3.04190945	3.93605775	-2.80972339
6	-2.54636203	4.87703075	-1.90163760

6	-1.36463901	4.55829677	-1.22621815
6	-0.68068205	3.35487150	-1.44012563
7	2.18441096	-2.15272457	1.16709814
6	1.93485732	-1.85167594	-1.27655777
1	2.95928361	-2.16949023	-1.54668505
1	1.32816150	-2.76598403	-1.19424215
6	1.96140177	-1.16488600	0.09601616
1	2.75502426	-0.40942685	0.14303390
1	1.00318383	-0.64613126	0.26486567
6	3.13810305	-1.88237915	2.17793442
6	2.74532547	-1.86492298	3.54133841
6	3.70492864	-1.64192105	4.53417910
6	5.05384429	-1.42135390	4.23453210
6	5.42958876	-1.47775191	2.88921704
6	4.51056700	-1.72043233	1.86035902
6	-2.99195577	1.78021069	-4.07471288
1	-3.96527820	4.15466295	-3.35262940
6	-3.24735187	6.19540030	-1.67869905
1	-0.96373775	5.26253591	-0.49184089
6	0.54745384	3.06451387	-0.61375445
6	1.30504329	-2.08630565	3.93509242
1	3.37979031	-1.62953850	5.57788806
6	6.06115046	-1.12722673	5.32003502
1	6.48373242	-1.35906142	2.62445213
6	5.02438324	-1.89639131	0.45214529
1	-3.71783592	2.30625457	-4.70920498
1	-3.53521009	0.95202853	-3.58981367
1	-2.22538635	1.33285055	-4.72411058
1	0.53937146	2.02490852	-0.25626854
1	0.59406944	3.73480453	0.25477201
1	1.48394471	3.20565340	-1.17624242
1	-2.94282045	6.94073448	-2.43079615
1	-3.00916373	6.61319151	-0.69097494
1	-4.33854760	6.08858323	-1.75206706
1	1.19122937	-2.01019385	5.02385503
1	0.93567078	-3.07967498	3.63304785
1	0.63762989	-1.34680305	3.46848531
1	4.82871621	-1.02698245	-0.19511158
1	4.55032951	-2.76698854	-0.02514593
1	6.11068420	-2.05459225	0.46139200
1	7.07194272	-1.43988151	5.02342670
1	5.80509138	-1.64231240	6.25637226
1	6.10594270	-0.04909368	5.54381295
1	1.27610238	-2.40134661	1.56098600

Energy = -7584.952263 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 11

Atomic N.	X	Y	Z
8	-3.13383108	0.06790528	2.40440953
6	-3.34134064	0.82470691	1.47457571
8	-3.65805802	2.12765996	1.77898430
6	-3.94153934	3.06529307	0.72086373
1	-4.88452693	2.81448099	0.21282506
1	-3.12024109	3.11899666	-0.00512808
1	-4.04876961	4.03641340	1.21637586
8	-0.45792171	0.28946873	-1.48802794

6	-3.24415569	0.43710467	0.01512805
1	-2.28179830	0.83004238	-0.36792102
1	-4.03826448	0.93258797	-0.56449546
6	-3.30827661	-1.07760133	-0.19640236
1	-2.49563665	-1.56184946	0.36042028
1	-4.24451322	-1.44930872	0.24945681
6	-3.25620014	-1.50689101	-1.67220883
1	-3.91459219	-0.85270301	-2.27250385
1	-3.69931595	-2.51382245	-1.74206583
6	-1.87282124	-1.57800898	-2.34237749
1	-1.20875267	-2.22990139	-1.75111985
1	-2.00898953	-2.07720268	-3.31848849
6	-1.13127221	-0.26065324	-2.61826060
1	-1.84933223	0.49217157	-3.00098872
1	-0.41834721	-0.44840069	-3.45144152
50	1.62669951	0.23650758	-1.58449818
7	3.91797082	-0.12789128	-0.03758997
6	5.02954057	0.28464371	-0.90340193
1	5.99335192	0.30587336	-0.35732975
1	4.84094640	1.28522087	-1.31104187
1	5.11323963	-0.41207679	-1.74817099
7	1.77037778	1.86905315	-0.21806292
6	3.66679194	0.85460447	1.02993351
1	4.60745495	1.10539424	1.56422794
1	2.97463470	0.40153702	1.75240015
6	3.02058789	2.13077204	0.49569229
1	2.83432629	2.78301565	1.36455969
1	3.74873452	2.68789244	-0.13107855
6	0.85125428	2.96003743	-0.15821361
6	0.61300568	3.78325940	-1.28974247
6	-0.23668907	4.88969383	-1.17579793
6	-0.87126720	5.22161249	0.02703953
6	-0.64482100	4.39244535	1.12862180
6	0.19207738	3.27031832	1.05911137
7	1.87393983	-2.33475030	0.03304713
6	4.15936582	-1.48545901	0.47901035
1	4.95595928	-1.47954058	1.25222379
1	4.54443808	-2.08733209	-0.36062772
6	2.93074784	-2.18353905	1.05501673
1	3.25912996	-3.16604464	1.44308270
1	2.52661328	-1.62895324	1.91059496
6	0.80578924	-3.23565603	0.35328005
6	-0.10294477	-2.93736430	1.39218845
6	-1.14108088	-3.83965489	1.65818778
6	-1.32298669	-5.01283653	0.91862646
6	-0.43251351	-5.26636688	-0.13068793
6	0.62953110	-4.40412072	-0.42433424
6	1.26462064	3.50562943	-2.62249218
1	-0.39513126	5.52073061	-2.05459797
6	-1.78872589	6.41774248	0.11723669
1	-1.14782080	4.60930952	2.07472204
6	0.35543935	2.40371366	2.28218265
6	-0.02864472	-1.64970687	2.17210427
1	-1.85062349	-3.58911617	2.45006144
6	-2.44101049	-5.97325034	1.24458823
1	-0.56407026	-6.16306780	-0.74112164
6	1.55572644	-4.72464573	-1.57561552
1	1.20981452	4.38976546	-3.27176291

1	0.76028729	2.68204256	-3.15448521
1	2.32032634	3.21975744	-2.51204346
1	0.53027906	1.35946260	1.99453783
1	-0.54055366	2.44962685	2.91450486
1	1.20982128	2.72018153	2.90354140
1	-1.34457952	7.30165384	-0.36306996
1	-2.01072372	6.67334177	1.16183623
1	-2.74830755	6.22764283	-0.39023298
1	-1.01630345	-1.37552088	2.56403556
1	0.31766209	-0.82812149	1.52961013
1	0.65912217	-1.72139959	3.03037724
1	2.60757193	-4.80820217	-1.25650255
1	1.51164228	-3.96148420	-2.37056675
1	1.27873073	-5.68190894	-2.03395504
1	-2.74161447	-6.55344104	0.36174672
1	-3.32408412	-5.44247869	1.62547524
1	-2.13324030	-6.69201348	2.02052880
1	2.31868074	-2.65702684	-0.82851905

Energy = -7584.959448 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 12

Atomic N.	X	Y	Z
8	-0.17548158	-2.71363380	-1.54134184
6	-0.26244486	-3.91954145	-1.71505093
8	-0.92438572	-4.46225866	-2.77219498
6	-1.56031433	-3.50161570	-3.65066442
1	-0.81556553	-2.81210451	-4.06739352
1	-2.31769536	-2.92864833	-3.10075231
1	-2.02327162	-4.09880002	-4.44210611
8	1.90413130	-1.56173411	1.45824044
6	0.30305391	-5.00220015	-0.81848115
1	0.78120990	-5.76131975	-1.45828793
1	-0.56650636	-5.50322892	-0.36136101
6	1.25214367	-4.47673994	0.25815472
1	0.77948059	-3.64002751	0.78681847
1	1.40862153	-5.27232255	1.00458292
6	2.61722170	-4.02221011	-0.27724152
1	2.47223897	-3.32805669	-1.12247014
1	3.14998448	-4.89871564	-0.68393751
6	3.49074968	-3.33346210	0.78604044
1	3.37173305	-3.84356537	1.75713277
1	4.55506958	-3.42935134	0.50970912
6	3.21319931	-1.83575170	0.97100824
1	3.40379933	-1.32773286	0.00055756
1	3.95969196	-1.43036031	1.68411513
50	0.61550020	-0.37949139	0.31946095
7	0.67666200	1.17697893	2.27620724
6	2.05303305	1.49580135	2.70179576
1	2.06159637	2.07085374	3.64536260
1	2.55990673	2.06871867	1.91647398
1	2.58732349	0.54961900	2.84917079
7	1.03621572	3.21212779	0.02511591
6	-0.16041733	2.38977582	2.06504642
1	-0.50171136	2.76903875	3.04766427
1	-1.05748046	2.07091673	1.51232604
6	0.50067136	3.56584573	1.34595393

1	-0.27309209	4.35539346	1.27699484
1	1.30256276	3.97671135	1.97585727
6	1.26822205	4.25264079	-0.91298698
6	2.23399566	5.25496960	-0.66321850
6	2.44571087	6.25236989	-1.62443406
6	1.75536696	6.28080207	-2.83953386
6	0.83547364	5.25434243	-3.08589879
6	0.57517242	4.24912275	-2.14971554
7	-1.14124888	-0.85129561	1.45993061
6	0.04051626	0.28137128	3.28439043
1	-0.10163121	0.83025706	4.23498363
1	0.74816679	-0.54415711	3.44639736
6	-1.28538314	-0.28986465	2.79718977
1	-1.59248765	-1.04460536	3.54374797
1	-2.07572582	0.49115563	2.82796602
6	-2.16871916	-1.73077627	1.03187160
6	-3.02075126	-1.37520304	-0.04769580
6	-4.01674115	-2.26227228	-0.47327903
6	-4.21083549	-3.50996414	0.13062701
6	-3.36912423	-3.85124749	1.19356926
6	-2.35793687	-2.99597850	1.65231673
6	3.09391950	5.23350249	0.57658255
1	3.20002119	7.01690638	-1.42095795
6	1.98563988	7.38135169	-3.84697163
1	0.29423762	5.23689409	-4.03529583
6	-0.43040922	3.16825789	-2.47002592
6	-2.87247953	-0.04761812	-0.74925540
1	-4.67111735	-1.96114299	-1.29648730
6	-5.27063091	-4.46286506	-0.36896169
1	-3.49106771	-4.82401854	1.67869838
6	-1.46402727	-3.46179831	2.77602362
1	4.00538161	5.82460542	0.41915759
1	3.38884904	4.20423127	0.82898716
1	2.58181201	5.65442893	1.45639423
1	0.03044271	2.16734230	-2.50732497
1	-0.89230514	3.35195641	-3.44805317
1	-1.23972444	3.12169449	-1.72366901
1	1.23220201	8.17892358	-3.74634037
1	1.92158039	7.00363161	-4.87691979
1	2.97231939	7.84520172	-3.71343784
1	-3.76996760	0.18092754	-1.34003094
1	-2.01228803	-0.04839144	-1.43787595
1	-2.70285840	0.76752248	-0.03200555
1	-1.86323785	-3.17967714	3.76422924
1	-0.45994949	-3.02439043	2.68770073
1	-1.37541046	-4.55685702	2.77031959
1	-4.90470932	-5.05627121	-1.22241219
1	-6.16605005	-3.92416315	-0.70988162
1	-5.57466214	-5.17047661	0.41417143
1	0.47501567	2.46971629	-0.39509165

Energy = -7584.976379 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 13

Atomic N.	X	Y	Z
8	3.56442163	-1.42434056	-0.17023376
6	4.29544323	-1.36753245	-1.14419919

8	5.54539340	-1.92079271	-1.16154194
6	5.94073639	-2.55708700	0.07588198
1	5.24242151	-3.36295502	0.33479687
1	5.96133207	-1.82680482	0.89517710
1	6.94249710	-2.95641003	-0.11077122
8	-0.20924725	-0.25712092	-0.93519109
6	3.99441489	-0.67552452	-2.45821282
1	4.44071291	-1.26712673	-3.27276329
1	4.55081969	0.27705364	-2.43378809
6	2.50500340	-0.41263536	-2.68359800
1	2.08904637	0.11424784	-1.81661062
1	2.39766580	0.26937730	-3.54213960
6	1.69363052	-1.68770582	-2.94989087
1	1.88063850	-2.42019238	-2.14576366
1	2.05904728	-2.15188843	-3.88247633
6	0.17771939	-1.45208280	-3.05695259
1	-0.02060121	-0.52444474	-3.62032454
1	-0.28018902	-2.27365904	-3.63500512
6	-0.56940772	-1.38797503	-1.71845216
1	-0.38369453	-2.34067992	-1.17375741
1	-1.65562241	-1.35456549	-1.92812301
50	0.36975142	-0.53383978	1.03428871
7	-0.72479224	0.40614886	3.44485248
6	0.19996836	-0.07964515	4.47743305
1	-0.02444829	0.35451854	5.47198366
1	1.23250720	0.17779647	4.21211652
1	0.13409613	-1.17391130	4.54116357
7	0.80503563	1.56643503	1.21403639
6	-0.58203415	1.85778028	3.23067431
1	-0.64469198	2.40171555	4.19724981
1	-1.41449754	2.18869958	2.59464434
6	0.72323684	2.21200228	2.51962931
1	0.72950764	3.30948724	2.39100731
1	1.57914369	1.99283073	3.19290096
6	1.66020335	2.23238628	0.28078062
6	3.07021521	2.24088109	0.43698845
6	3.86805063	2.90868555	-0.50388781
6	3.31914471	3.57620564	-1.60221856
6	1.92548450	3.57540646	-1.73428745
6	1.09049223	2.92391560	-0.81919214
7	-2.65676445	-0.99553280	1.60494932
6	-2.10796010	0.02550850	3.78421539
1	-2.51768271	0.69239760	4.57095406
1	-2.07261022	-0.98591297	4.22110695
6	-3.07412989	0.00818465	2.60277455
1	-4.08405380	-0.20856299	2.99923768
1	-3.12472421	0.99732887	2.13010452
6	-3.62017337	-1.42760491	0.64510198
6	-4.16582021	-0.52934385	-0.29881240
6	-5.09063548	-1.01270016	-1.23389911
6	-5.47553710	-2.35554043	-1.28747801
6	-4.88911547	-3.23490267	-0.36975852
6	-3.97598875	-2.79770739	0.59442636
6	3.74223581	1.53891635	1.59154573
1	4.95377799	2.89967576	-0.37158463
6	4.19746699	4.25687895	-2.62508037
1	1.46854176	4.10490652	-2.57471709
6	-0.40253917	2.96626060	-1.01268233

6	-3.72274108	0.91018555	-0.37443574
1	-5.49924780	-0.31141090	-1.96573783
6	-6.49136495	-2.84041607	-2.29333853
1	-5.15123391	-4.29540980	-0.40004709
6	-3.36896103	-3.79505236	1.55448593
1	4.79619760	1.33548003	1.36014195
1	3.25145975	0.58245506	1.81987369
1	3.72095539	2.14984656	2.50829016
1	-0.77416007	1.96339706	-1.26912738
1	-0.66903970	3.66581034	-1.81642332
1	-0.91722737	3.27474030	-0.09122518
1	3.74522377	5.19258433	-2.98310163
1	4.35251614	3.61526831	-3.50744880
1	5.18756431	4.49126394	-2.21108910
1	-3.94175442	1.32276459	-1.36757947
1	-2.64037505	0.99339140	-0.20287661
1	-4.23694773	1.54845914	0.36181574
1	-3.57136314	-3.53758446	2.60723980
1	-2.27493159	-3.87151780	1.43842875
1	-3.78247159	-4.79577806	1.37900298
1	-6.24979853	-3.84990504	-2.65400614
1	-6.54427454	-2.17010247	-3.16169343
1	-7.49958107	-2.88566380	-1.85156876
1	-2.30128629	-1.81170945	2.10379179

Energy = -7584.971009 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 14

Atomic N.	X	Y	Z
8	-0.59545159	-2.18564145	-2.76437189
6	0.57700425	-1.86220025	-2.76575791
8	0.86743043	-0.53994401	-2.99364269
6	2.22625259	-0.06568869	-2.88478300
1	2.89026760	-0.57159207	-3.59953039
1	2.59761738	-0.19422393	-1.85876264
1	2.18000464	1.00161128	-3.12675065
8	0.91802365	-1.46189085	0.09767862
6	1.74378177	-2.81962958	-2.60818935
1	2.46383104	-2.38686920	-1.90007207
1	2.25506124	-2.84576547	-3.58668489
6	1.34133809	-4.23915164	-2.17843505
1	0.29374678	-4.41129555	-2.46664856
1	1.94773957	-4.95587658	-2.75347996
6	1.52860401	-4.57324369	-0.68724025
1	2.57363562	-4.36341280	-0.39509706
1	1.41222291	-5.66563249	-0.59876740
6	0.57826207	-3.91810025	0.33825141
1	-0.42677492	-3.79150987	-0.09520799
1	0.45947224	-4.62072773	1.18103971
6	1.02584084	-2.58902250	0.96271716
1	2.08670286	-2.68198104	1.27258398
1	0.43248385	-2.42758308	1.88103705
50	-0.61238340	-0.07792526	0.13903949
7	0.14549250	1.34302344	2.16292203
6	1.59252617	1.23551662	2.42495198
1	1.89444725	1.81661911	3.31582737
1	2.15023324	1.58701349	1.54910395

1	1.84171049	0.18012139	2.58458452
7	0.86779841	3.05591672	-0.27930908
6	-0.28849076	2.74880758	1.92734744
1	-0.37124669	3.26835960	2.90147333
1	-1.30225881	2.71225370	1.49707045
6	0.61475318	3.62095953	1.05120143
1	0.11635040	4.60867437	0.99170917
1	1.56770996	3.79119375	1.57145790
6	1.36835651	3.90468897	-1.30233073
6	2.63887609	4.51618704	-1.18979872
6	3.10234176	5.32391992	-2.23730966
6	2.36720877	5.52828532	-3.40820565
6	1.13271438	4.87658800	-3.51898732
6	0.61785888	4.07703048	-2.49394527
7	-1.75018872	-0.87030235	1.79350026
6	-0.64445262	0.74730507	3.27946837
1	-0.80327305	1.50375707	4.07105950
1	-0.04616094	-0.07098189	3.70028250
6	-1.97546339	0.16221176	2.80307130
1	-2.49951121	-0.24705498	3.67957489
1	-2.62955569	0.98022930	2.42984978
6	-2.54427821	-2.04193547	1.85536732
6	-3.38949337	-2.41730307	0.77348049
6	-4.14660051	-3.59236260	0.85335512
6	-4.11789461	-4.42956714	1.97284808
6	-3.28390130	-4.05665867	3.02996631
6	-2.49607250	-2.89913388	2.99289642
6	3.54137278	4.26363867	-0.00669831
1	4.08796819	5.78613067	-2.13831601
6	2.87892683	6.42355379	-4.51079129
1	0.54293876	4.99845274	-4.43096798
6	-0.71906968	3.39746550	-2.67500962
6	-3.51068167	-1.57254414	-0.47104307
1	-4.79273567	-3.85228695	0.01063291
6	-4.92594904	-5.70408763	2.01854067
1	-3.22087232	-4.70034022	3.91183637
6	-1.56610092	-2.63530851	4.15244015
1	4.58348623	4.48941984	-0.26754000
1	3.48642801	3.21197986	0.31134630
1	3.28399290	4.88551735	0.86538129
1	-0.63462047	2.29852144	-2.67632852
1	-1.17161185	3.69067008	-3.63033427
1	-1.42978920	3.66229003	-1.87555902
1	2.43041267	7.42791017	-4.44946641
1	2.63336484	6.02016451	-5.50312564
1	3.96865790	6.54739965	-4.45155836
1	-4.40513067	-1.85737140	-1.04145515
1	-2.65521070	-1.70105787	-1.15728115
1	-3.58429478	-0.50147940	-0.23133417
1	-0.60107044	-2.24493328	3.79780456
1	-1.38019017	-3.56216225	4.71087968
1	-1.96702210	-1.90219393	4.87094241
1	-4.39498705	-6.53135994	1.52080647
1	-5.89108130	-5.58545637	1.50614396
1	-5.12355783	-6.01679936	3.05286970
1	0.04217762	2.54820143	-0.60422468

Energy = -7584.954615 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 15

Atomic N.	X	Y	Z
8	3.15922360	-3.31579165	2.11475356
6	2.89898726	-3.62606465	0.96895513
8	1.58232715	-3.90337649	0.67620165
6	1.20847609	-4.31741491	-0.65422513
1	1.74695307	-5.22543756	-0.95883506
1	1.37531720	-3.51185593	-1.38270920
1	0.13668560	-4.53704905	-0.59917099
8	2.79252209	-0.82320794	-0.20708423
6	3.90920758	-3.78386236	-0.14992932
1	3.54391274	-3.22490778	-1.02409619
1	3.90111694	-4.85003098	-0.43619530
6	5.33833684	-3.34862378	0.20795946
1	5.50521819	-3.51536929	1.28264014
1	6.03374245	-4.01491568	-0.32596432
6	5.71334509	-1.89999150	-0.15580816
1	5.49250232	-1.72820465	-1.22363221
1	6.80857546	-1.82781375	-0.06324363
6	5.07528143	-0.76958676	0.68571511
1	4.72236978	-1.17122262	1.64791374
1	5.85065406	-0.02070792	0.92183998
6	3.93314111	-0.00742609	0.00531120
1	4.29887398	0.38813569	-0.96432770
1	3.68975335	0.87943057	0.62442388
50	0.78918692	-0.30804316	-0.37996358
7	0.45466677	-0.04755514	2.07925137
6	1.75703840	-0.27036787	2.75642974
1	1.66136792	-0.05407801	3.83512074
1	2.52219923	0.38366575	2.32893304
1	2.07540243	-1.31063550	2.61997817
7	0.81321328	1.82176562	-0.07425355
6	0.03121797	1.37231449	2.19898780
1	0.08445212	1.69614035	3.25664512
1	-1.00733115	1.43888720	1.85352276
6	0.88310402	2.28154960	1.30941587
1	0.46679694	3.30009663	1.39442775
1	1.91211261	2.33984919	1.71799188
6	0.76032878	2.79480552	-1.10234267
6	1.73771632	3.82460722	-1.20880006
6	1.63752388	4.78150201	-2.22682755
6	0.61325700	4.76070978	-3.17717893
6	-0.33757654	3.74134497	-3.07089950
6	-0.29286771	2.77206493	-2.06135447
7	-2.31039036	-0.87220682	0.95166988
6	-0.51535716	-1.01184792	2.68564135
1	-0.40764198	-0.96761841	3.78557265
1	-0.18639971	-2.01646083	2.37684214
6	-2.00149423	-0.82736012	2.38625322
1	-2.52054316	-1.62989574	2.94763958
1	-2.35820933	0.12009141	2.81193036
6	-3.67082906	-1.01766436	0.56032939
6	-4.61727376	0.00009052	0.82012579
6	-5.94055872	-0.17689234	0.39504129
6	-6.35919453	-1.31366505	-0.30269492
6	-5.39674585	-2.28954317	-0.58781452

6	-4.06895971	-2.16640722	-0.16763517
6	2.92894107	3.88451211	-0.28397256
1	2.40598619	5.55723474	-2.28745725
6	0.55217650	5.77715988	-4.29192592
1	-1.16378261	3.70733481	-3.78651428
6	-1.39785351	1.74542231	-2.00834266
6	-4.22637229	1.29880863	1.48122828
1	-6.66040542	0.62053407	0.59647855
6	-7.79770003	-1.48814829	-0.72574503
1	-5.68773071	-3.18024471	-1.15031652
6	-3.07242096	-3.25056605	-0.50755083
1	3.71025966	4.52713045	-0.71035902
1	3.35341358	2.88320465	-0.12442980
1	2.67908908	4.28862615	0.70946370
1	-1.10783994	0.79558407	-2.48824827
1	-2.28783817	2.11217060	-2.53724308
1	-1.67601785	1.49890445	-0.97429155
1	-0.48650557	6.00551280	-4.56961729
1	1.05624329	5.40683856	-5.19917852
1	1.04434895	6.71668382	-4.00572494
1	-4.95537200	2.08353634	1.24185624
1	-3.23719285	1.63209297	1.13510426
1	-4.18501454	1.21946283	2.57933401
1	-2.59171271	-3.66804288	0.39205777
1	-2.26860969	-2.88136833	-1.16616228
1	-3.56875670	-4.07703500	-1.03115845
1	-7.87321165	-2.02244677	-1.68282009
1	-8.30289410	-0.51885211	-0.83371751
1	-8.36375238	-2.07125011	0.01812962
1	-1.74420968	-1.59674842	0.50864604

Energy = -7584.958782 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 16

Atomic N.	X	Y	Z
8	3.16149861	-2.65793759	4.06237865
6	3.16562228	-3.82146028	3.70530736
8	2.23069069	-4.73185751	4.10271306
6	1.22568098	-4.20086715	5.00293329
1	0.68644085	-3.37367773	4.52507741
1	1.69364758	-3.84198362	5.92849855
1	0.55148601	-5.03823591	5.20818351
8	1.57456993	-2.05464434	-1.25463693
6	4.20836988	-4.45326396	2.80039235
1	3.83625776	-5.41606403	2.42351847
1	5.07808442	-4.67180351	3.44240952
6	4.62394071	-3.51704434	1.65740862
1	4.84170702	-2.52613348	2.08504986
1	5.56224664	-3.88828519	1.21473579
6	3.55547946	-3.39005000	0.56570803
1	2.58676206	-3.12117313	1.01445491
1	3.40995652	-4.37109504	0.07962398
6	3.91105946	-2.34443687	-0.49392359
1	3.97092778	-1.34976622	-0.01859376
1	4.91239021	-2.55609090	-0.91157228
6	2.91783920	-2.28272452	-1.66071356
1	2.94451077	-3.24987531	-2.20057675

1	3.27160020	-1.51288151	-2.37929058
50	0.83949328	-0.13697492	-0.92143308
7	-0.47312413	-0.28629769	-3.07199891
6	0.06127523	-1.45356725	-3.81454898
1	-0.59278486	-1.69504706	-4.67063831
1	0.15609828	-2.31424770	-3.14530601
1	1.06490473	-1.21356239	-4.18903620
7	-1.05627380	-0.90409362	-0.31748866
6	-1.85245010	-0.56512905	-2.58349231
1	-2.46596720	-0.97576490	-3.40848006
1	-2.28543071	0.38464562	-2.24944936
6	-1.83377656	-1.51743297	-1.38756985
1	-2.87930025	-1.66077023	-1.06209200
1	-1.47307654	-2.51275770	-1.71274552
6	-1.35112427	-1.24709237	1.02513998
6	-1.46890164	-2.59218684	1.46585862
6	-1.82932629	-2.85323182	2.79615318
6	-2.04012430	-1.83590583	3.73025409
6	-1.87073555	-0.51540038	3.29579352
6	-1.53719026	-0.20290796	1.97473518
7	-0.54179279	2.69112958	-2.26631875
6	-0.40404672	0.89054026	-3.98830604
1	-0.86253121	0.61297415	-4.95689507
1	0.66582066	1.06830932	-4.18324432
6	-1.06480409	2.19328201	-3.54277658
1	-0.89855866	2.91281983	-4.36977642
1	-2.15242525	2.06035867	-3.47262958
6	-0.84314369	4.03094586	-1.89188296
6	-2.17037547	4.43299630	-1.62200421
6	-2.41380665	5.75962866	-1.23934198
6	-1.38889645	6.69613701	-1.08382527
6	-0.07685332	6.26664738	-1.32085598
6	0.21424089	4.96038745	-1.72260670
6	-1.13033738	-3.75443369	0.56285884
1	-1.92011988	-3.89604707	3.11365563
6	-2.40032293	-2.14363561	5.16428835
1	-2.02056208	0.30397281	4.00416636
6	-1.39110764	1.24247362	1.57073539
6	-3.32433030	3.46214348	-1.67598344
1	-3.44458279	6.05768256	-1.03157488
6	-1.67562478	8.11002700	-0.63877180
1	0.74867912	6.97197258	-1.19599093
6	1.64937399	4.55276505	-1.96329844
1	-0.91608919	-4.64836112	1.16362173
1	-0.24613734	-3.52467366	-0.05071767
1	-1.95132788	-4.01467495	-0.12437034
1	-0.33242700	1.53794359	1.47505276
1	-1.84523820	1.90432192	2.31985260
1	-1.85002152	1.43012673	0.59078285
1	-3.26610249	-1.55287607	5.49850708
1	-1.56905135	-1.90556773	5.84701882
1	-2.64637792	-3.20609075	5.29443592
1	-4.15828440	3.82664884	-1.06251471
1	-3.02442804	2.47544066	-1.29437028
1	-3.71224291	3.32151695	-2.69774845
1	1.80984133	4.17909674	-2.98773370
1	1.97818798	3.75902877	-1.27218452
1	2.32042836	5.40798529	-1.81651860

1	-1.37624784	8.26686219	0.40941171
1	-2.74574031	8.34289380	-0.71544913
1	-1.12320012	8.84212394	-1.24553675
1	0.46761212	2.54425486	-2.23390175

Energy = -7584.973553 Hartree
Number of imaginary frequencies = 0.

Compound I5b isomer 17

Atomic N.	X	Y	Z
8	2.43218750	-1.38623188	-1.17942197
6	3.65360857	-1.28864970	-1.07097532
8	4.50500723	-1.80893546	-1.98869167
6	3.87861912	-2.46041050	-3.12122209
1	3.24577437	-1.74993809	-3.66745132
1	3.26954479	-3.30914245	-2.78597669
1	4.70622592	-2.80304271	-3.74913861
8	2.25985368	1.57490004	0.36117297
6	4.36158013	-0.56557121	0.03803273
1	4.03597556	0.48432700	-0.07383770
1	5.44794444	-0.63034001	-0.09851913
6	3.93468305	-1.04634893	1.43958201
1	2.88199773	-1.36704980	1.40879008
1	4.52492142	-1.93876457	1.69959085
6	4.10259628	0.02326846	2.53569437
1	5.02514573	0.60216497	2.35393645
1	4.25914604	-0.49474983	3.49547837
6	2.91640139	0.98735726	2.72299150
1	1.99481782	0.39749110	2.87339483
1	3.07782224	1.54151583	3.66470010
6	2.66307906	2.04912491	1.63922388
1	3.59479228	2.63096650	1.49553468
1	1.91626275	2.76252537	2.04047870
50	0.52942473	0.45310321	0.02958800
7	-0.95686660	-1.30782891	-1.72508790
6	-0.57070178	-2.71858912	-1.83648525
1	-1.14211120	-3.25079166	-2.62466713
1	-0.72558118	-3.22331355	-0.87515028
1	0.49742582	-2.76873490	-2.07791648
7	-2.26082260	-2.03103696	0.92900275
6	-2.38646802	-1.12592417	-1.40547362
1	-3.00093852	-1.25665923	-2.32216785
1	-2.52826024	-0.08305400	-1.07573447
6	-2.97511799	-2.06801636	-0.35486920
1	-4.03481991	-1.77270926	-0.23372418
1	-2.98607415	-3.09352882	-0.75324825
6	-2.96132307	-2.39684900	2.10485621
6	-3.46533067	-3.70959331	2.26601024
6	-4.14307373	-4.04261103	3.44614224
6	-4.32016180	-3.13128451	4.49121184
6	-3.77724120	-1.85079684	4.33105318
6	-3.11081808	-1.46525041	3.16365547
7	0.21230227	1.46457949	-1.79955463
6	-0.60143515	-0.57909940	-2.95451783
1	-1.24573020	-0.90287364	-3.80119502
1	0.43874374	-0.84356544	-3.19408990
6	-0.69003229	0.93987483	-2.82396916
1	-0.40819951	1.35580846	-3.80845850

1	-1.74526203	1.24440584	-2.66803211
6	0.56791927	2.83808045	-1.98898711
6	-0.32950569	3.87970031	-1.65028289
6	0.04609802	5.21307922	-1.86993849
6	1.28404189	5.55350564	-2.42114962
6	2.15623767	4.51195014	-2.76007385
6	1.82427245	3.16903680	-2.55222077
6	-3.22317220	-4.77917728	1.22931551
1	-4.52021881	-5.06267028	3.55749430
6	-5.07859531	-3.50791558	5.74121361
1	-3.88367101	-1.11975049	5.13670397
6	-2.55751164	-0.06541319	3.04758107
6	-1.68844450	3.59334051	-1.05857995
1	-0.65345172	6.00749837	-1.59612328
6	1.68290189	6.99643652	-2.61871934
1	3.12896092	4.75099997	-3.19827357
6	2.81009466	2.08985711	-2.91813848
1	-3.33018877	-5.77597303	1.67674273
1	-2.20983920	-4.69278931	0.80999086
1	-3.93138276	-4.72182027	0.38756995
1	-1.45868755	-0.05708088	2.95967135
1	-2.82119355	0.52745142	3.93239384
1	-2.94885983	0.46096254	2.16222626
1	-6.13154731	-3.18894742	5.68084766
1	-4.64688452	-3.03207042	6.63277872
1	-5.07528578	-4.59513911	5.89829807
1	-2.05680619	4.45913333	-0.49279006
1	-1.66006527	2.72353070	-0.38641084
1	-2.43348309	3.37190342	-1.83956318
1	2.33883368	1.28959121	-3.50577448
1	3.20827382	1.62784263	-2.00341249
1	3.64672633	2.50727227	-3.49395034
1	2.32706753	7.34605818	-1.79630898
1	0.80412903	7.65442546	-2.65072468
1	2.24820237	7.13240762	-3.55156460
1	-1.76447858	-1.14544419	1.03961392

Energy = -7584.961395 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 18

Atomic N.	X	Y	Z
8	3.66040372	-3.40555225	-2.60732740
6	4.19226997	-2.31981419	-2.48460611
8	4.33978743	-1.55318938	-3.61902548
6	4.96705706	-0.25806334	-3.53861245
1	6.03674508	-0.34747447	-3.29977228
1	4.47441776	0.38888573	-2.80011150
1	4.85727560	0.17954020	-4.53664082
8	2.36830303	-0.24484190	0.40110374
6	4.64963647	-1.72771499	-1.16847697
1	3.94567808	-0.90967006	-0.91779724
1	5.64195926	-1.26404092	-1.28341560
6	4.66791256	-2.74739191	-0.02757910
1	3.71873722	-3.30235476	-0.01845567
1	5.44508080	-3.49747877	-0.24189363
6	4.92870827	-2.13024376	1.35741892
1	5.74835101	-1.39261427	1.28729460

1	5.30924271	-2.93105085	2.01211719
6	3.73315019	-1.48255245	2.08234166
1	2.89322250	-2.19711271	2.12878559
1	4.04370918	-1.30830615	3.12778531
6	3.19681850	-0.14087078	1.55665360
1	4.05389897	0.52604854	1.33109280
1	2.64762381	0.34477545	2.39112646
50	0.35709144	0.40216624	0.63901255
7	-0.11539924	-1.37994871	-0.99243990
6	0.50725507	-2.66846782	-0.61088555
1	0.46849746	-3.38681479	-1.44701176
1	-0.00324015	-3.09417160	0.25988976
1	1.55157497	-2.47806640	-0.34363353
7	-2.65478437	-0.95901234	0.78264448
6	-1.54760654	-1.56014399	-1.35405795
1	-1.61004298	-2.29935807	-2.17493426
1	-1.90482412	-0.59979891	-1.75302846
6	-2.48159831	-2.00900372	-0.23257663
1	-3.44258738	-2.29041213	-0.70810868
1	-2.10696895	-2.91797940	0.25449172
6	-3.51989466	-1.26645921	1.87805587
6	-3.08851951	-2.14204082	2.89907589
6	-3.94850264	-2.41029675	3.97182073
6	-5.21356284	-1.82449526	4.08052627
6	-5.60669055	-0.93263932	3.07566261
6	-4.78962769	-0.64862411	1.97635727
7	0.12203445	1.38883260	-1.24286444
6	0.62563106	-0.81765947	-2.16574454
1	0.48125206	-1.46886721	-3.04657206
1	1.68528817	-0.84048337	-1.88443417
6	0.22047428	0.62181627	-2.47551978
1	0.98408745	1.01735491	-3.17146776
1	-0.73284706	0.64607387	-3.04709122
6	0.11035437	2.80549202	-1.35918178
6	-1.06700732	3.53430869	-1.05197799
6	-1.07050870	4.93077066	-1.15133714
6	0.06257602	5.64788895	-1.55108165
6	1.22108431	4.92163198	-1.84543758
6	1.27043113	3.52501088	-1.75141070
6	-1.70687940	-2.74672733	2.88666396
1	-3.60198303	-3.08224939	4.76099940
6	-6.12964324	-2.14995886	5.23532497
1	-6.58287432	-0.44602331	3.14330898
6	-5.26525204	0.32491050	0.92250254
6	-2.32453103	2.81970303	-0.61932811
1	-1.99010598	5.47371167	-0.91675234
6	0.04625549	7.15604300	-1.62270210
1	2.12615208	5.45899376	-2.14236250
6	2.57082166	2.81202034	-2.03061210
1	-1.38925865	-2.99914848	3.90655348
1	-0.97780824	-2.04266198	2.46033820
1	-1.66068023	-3.67742044	2.29744029
1	-4.67053834	1.25326592	0.91561266
1	-6.30695293	0.61320451	1.10991094
1	-5.21728196	-0.10104761	-0.09181950
1	-6.84347136	-2.94386190	4.96391054
1	-6.71889586	-1.27423225	5.54029932
1	-5.56329309	-2.50326708	6.10736880

1	-3.18164255	3.50631133	-0.62334260
1	-2.22568395	2.41320432	0.40029306
1	-2.54945054	1.97252557	-1.28338851
1	2.64227745	2.48686258	-3.08182659
1	2.66708925	1.91643044	-1.39935072
1	3.42370401	3.47763586	-1.84098185
1	0.34511766	7.60294832	-0.66100596
1	-0.95750652	7.53487073	-1.85945877
1	0.74294260	7.52923676	-2.38571070
1	-2.98403530	-0.11079574	0.31936998

Energy = -7584.964512 Hartree
Number of imaginary frequencies = 0.

Compound I5b isomer 19

Atomic N.	X	Y	Z
8	2.13267804	-2.20539062	0.70096368
6	2.85301585	-3.18597720	0.58463845
8	2.57226293	-4.38906985	1.14559130
6	1.31441498	-4.43749005	1.87454028
1	0.47968678	-4.22014088	1.19859766
1	1.31516001	-3.70267312	2.68795897
1	1.25009725	-5.45753391	2.26472887
8	-0.38787707	-2.43121182	-1.97575241
6	4.13739488	-3.22524634	-0.21598050
1	4.51277811	-2.19427456	-0.25871163
1	4.87446092	-3.85028021	0.30726731
6	3.93249402	-3.76050262	-1.65347479
1	3.71264145	-4.83833791	-1.60755809
1	4.90023915	-3.66576528	-2.16825598
6	2.82303234	-3.03290216	-2.44674937
1	2.59522523	-2.07276598	-1.95420838
1	3.19225924	-2.77405737	-3.45154815
6	1.53089139	-3.85105133	-2.60205500
1	1.25766412	-4.33289017	-1.64943524
1	1.71224352	-4.66666063	-3.32343577
6	0.31234327	-3.02962446	-3.05654986
1	0.64427304	-2.28018818	-3.80801499
1	-0.39601379	-3.70002614	-3.57897993
50	0.07127367	-0.59379966	-1.11224515
7	-1.96594936	0.44554244	-2.26634172
6	-2.38187143	-0.51453267	-3.31402688
1	-3.36685583	-0.23355651	-3.72815329
1	-2.41193429	-1.52924370	-2.90449913
1	-1.64069318	-0.50663343	-4.12417844
7	-1.52779467	-0.83581827	0.29834183
6	-2.96046121	0.48666754	-1.16310107
1	-3.98232639	0.59817424	-1.57665700
1	-2.72861410	1.35524231	-0.53578789
6	-2.86314000	-0.76236749	-0.28684788
1	-3.61833673	-0.66324403	0.51206187
1	-3.15554498	-1.65045188	-0.87979236
6	-1.39690097	-1.40454985	1.58420842
6	-2.01124243	-2.63722815	1.94002284
6	-1.91476178	-3.10532776	3.25886365
6	-1.19660944	-2.42479146	4.24563682
6	-0.54101582	-1.24662403	3.86584272
6	-0.62397473	-0.72799946	2.57019244

7	-0.36845567	2.84442351	-1.15860611
6	-1.76352483	1.76604453	-2.92770743
1	-2.64861687	1.99179487	-3.55418815
1	-0.91134871	1.64125696	-3.61545349
6	-1.52886601	2.98906665	-2.04353735
1	-1.41358765	3.84432169	-2.73928279
1	-2.42890849	3.20189539	-1.45044722
6	0.18437639	4.01500247	-0.57239884
6	-0.55719208	4.78537410	0.35230984
6	0.03393852	5.92330336	0.91787877
6	1.34381446	6.31232577	0.62409826
6	2.07671396	5.50909155	-0.25837271
6	1.52402970	4.37633158	-0.86293333
6	-2.68080963	-3.51426370	0.90736775
1	-2.39903659	-4.05349769	3.51065534
6	-1.13235546	-2.93329624	5.66623194
1	0.04537003	-0.69860406	4.60855823
6	0.10325462	0.54888615	2.23736208
6	-1.93895498	4.37457678	0.79823684
1	-0.54750357	6.50719373	1.63571354
6	1.94661253	7.55708207	1.22926245
1	3.11092848	5.77441381	-0.49114991
6	2.36209577	3.54497841	-1.80604518
1	-2.73914733	-4.54868969	1.27259463
1	-2.11339217	-3.50532645	-0.03571753
1	-3.70909961	-3.19700611	0.67221039
1	1.02962397	0.34868126	1.67306875
1	0.39019100	1.08471019	3.15192435
1	-0.51110424	1.20803268	1.60833065
1	-1.80290672	-2.36263041	6.32864262
1	-0.11831674	-2.84434806	6.08258499
1	-1.43402456	-3.98808945	5.72585676
1	-2.17891891	4.83215876	1.76660866
1	-2.00540187	3.28228803	0.90798528
1	-2.72323632	4.68605090	0.08979733
1	1.90315002	3.46145175	-2.80460432
1	2.51399652	2.51850699	-1.43326401
1	3.35422941	3.99497768	-1.93531406
1	3.00259395	7.40542166	1.49357392
1	1.40748134	7.86112147	2.13645922
1	1.90762761	8.40275332	0.52421236
1	0.36006871	2.30683642	-1.62961874

Energy = -7584.968175 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 20

Atomic N.	X	Y	Z
8	0.59947913	-1.16807995	-2.22164847
6	1.71975143	-1.69083768	-2.15395968
8	2.65313549	-1.53950896	-3.10333891
6	2.36910380	-0.52929933	-4.10620503
1	2.29358015	0.44632550	-3.61109217
1	1.43695253	-0.76380880	-4.63363933
1	3.22221729	-0.56001428	-4.79039595
8	2.27919081	0.54019357	-0.85686565
6	2.12151407	-2.68276542	-1.08644881
1	1.48772964	-2.48164289	-0.21027161

1	1.78589457	-3.65983638	-1.47950506
6	3.60432814	-2.78574754	-0.69383618
1	4.22823125	-2.75832948	-1.59964996
1	3.74387274	-3.78862042	-0.25969247
6	4.13001396	-1.76460234	0.33414910
1	3.42296040	-1.70748456	1.18065909
1	5.05295837	-2.19890217	0.75031104
6	4.45979105	-0.33492173	-0.15097872
1	4.75406601	-0.34921679	-1.21319603
1	5.34037392	0.02696359	0.40747430
6	3.35936282	0.71497761	0.03834168
1	3.03018333	0.68081612	1.10302620
1	3.80414611	1.71875390	-0.11685499
50	0.30680101	0.42740566	-0.15017256
7	-2.36822870	-0.16443136	-0.89372603
6	-2.64102185	-1.49727154	-1.44570191
1	-3.68997370	-1.60506298	-1.78800067
1	-2.42697131	-2.26204472	-0.68924538
1	-1.97111320	-1.66533879	-2.29685969
7	-2.22522106	-1.51092136	1.85413987
6	-3.21839508	0.16442715	0.27084002
1	-4.22131961	0.49016144	-0.07711930
1	-2.76598403	1.02915754	0.78469424
6	-3.46055438	-0.95351484	1.28581605
1	-4.10591225	-0.51853180	2.07317929
1	-4.05156079	-1.75099241	0.81170885
6	-2.29517952	-2.15344159	3.11625403
6	-3.05606694	-3.33466711	3.28483966
6	-3.09187512	-3.95200418	4.54220083
6	-2.37990774	-3.45894460	5.63950932
6	-1.59998702	-2.31305680	5.44207694
6	-1.54856379	-1.65023716	4.21185684
7	-0.37327637	2.02502002	-1.36192600
6	-2.50247617	0.86906464	-1.93806710
1	-3.57446815	1.06228517	-2.15713383
1	-2.03532719	0.46950255	-2.84835414
6	-1.81063826	2.18768209	-1.58552206
1	-1.98854440	2.88130220	-2.42254689
1	-2.31139552	2.65372280	-0.71237951
6	0.46844264	3.03545365	-1.90302758
6	1.18688353	3.91045823	-1.04941874
6	2.01464471	4.89637268	-1.60179430
6	2.16336643	5.05638550	-2.98279989
6	1.44661594	4.19107171	-3.81610708
6	0.61025682	3.18973796	-3.30834286
6	-3.76922604	-3.98547978	2.12502931
1	-3.67882682	-4.86748626	4.65405475
6	-2.45739949	-4.12826584	6.99062108
1	-1.01831694	-1.91148610	6.27588280
6	-0.69715142	-0.41183065	4.06594531
6	1.06557648	3.81792713	0.45256756
1	2.55308786	5.56742676	-0.92724800
6	3.08693902	6.10486233	-3.55524924
1	1.54973115	4.28666384	-4.90072772
6	-0.09715595	2.26777971	-4.27052846
1	-3.95924058	-5.04527248	2.33940316
1	-3.16480881	-3.91872494	1.20838594
1	-4.74275794	-3.51732308	1.90949955

1	0.12197131	-0.55028786	3.34163750
1	-0.24408382	-0.14119714	5.02794463
1	-1.28315362	0.45320153	3.71613244
1	-3.20285379	-3.63772520	7.63692717
1	-1.49387575	-4.08471589	7.51732143
1	-2.74927250	-5.18319967	6.89786542
1	1.39513346	4.75316013	0.92498610
1	1.69386501	3.01203849	0.86626691
1	0.03197258	3.61208728	0.76312402
1	-0.12066605	1.24176556	-3.87815491
1	0.40702967	2.26662442	-5.24641448
1	-1.14187974	2.56981723	-4.44952624
1	4.06840045	5.67424097	-3.81052747
1	3.26291359	6.91755253	-2.83754730
1	2.67659464	6.54329214	-4.47571174
1	-1.47443188	-0.81860647	1.82278768

Energy = -7584.961006 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 21

Atomic N.	X	Y	Z
8	5.08347673	-4.06500407	0.24373110
6	4.02176614	-4.01107323	0.83230541
8	3.83668943	-2.98793267	1.72763143
6	2.62819356	-2.90732070	2.51514111
1	2.56332720	-3.74463097	3.22440533
1	1.72742743	-2.87439998	1.88983958
1	2.71040309	-1.96932866	3.07331885
8	0.26223830	-2.15918971	-2.02269714
6	2.88422264	-4.98916578	0.58678559
1	3.35698683	-5.92834468	0.26854943
1	2.32054690	-5.18704334	1.50891917
6	1.91238418	-4.50397256	-0.51546849
1	1.44304888	-3.55349263	-0.22771814
1	1.09277216	-5.23816363	-0.58084802
6	2.56780305	-4.36002886	-1.89416168
1	3.38905050	-3.62674407	-1.84568760
1	3.04340282	-5.32041939	-2.15512000
6	1.60317930	-3.96429924	-3.02378908
1	0.69546515	-4.59098404	-2.98897514
1	2.09311011	-4.17834204	-3.98952576
6	1.17608672	-2.49295331	-3.06321413
1	2.08739204	-1.85764852	-3.02741402
1	0.70323799	-2.30437723	-4.05034210
50	0.32071111	-0.27708054	-1.13070242
7	-1.71416766	0.40977200	-2.43943768
6	-1.90862015	-0.62612222	-3.48367183
1	-2.89683965	-0.50871116	-3.96137260
1	-1.80600518	-1.62500959	-3.04744116
1	-1.12848972	-0.51627032	-4.24785734
7	-1.31189500	-0.75513858	0.16076437
6	-2.79605002	0.33211725	-1.41836401
1	-3.78202077	0.29735218	-1.92028704
1	-2.73679190	1.23638243	-0.80188949
6	-2.60602788	-0.87542004	-0.50011714
1	-3.41901164	-0.85353133	0.24713356
1	-2.74656902	-1.80747242	-1.08137583

6	-1.12736076	-1.36280495	1.42602045
6	-1.45659147	-2.72292521	1.68162636
6	-1.28922586	-3.24433975	2.97230832
6	-0.77960367	-2.48358560	4.02907802
6	-0.41581693	-1.15998616	3.75392693
6	-0.57888327	-0.58852136	2.48700131
7	-0.50080316	3.02204528	-1.34050775
6	-1.66129985	1.73240405	-3.13114243
1	-2.53790429	1.81650607	-3.80165551
1	-0.76900377	1.70805406	-3.77712096
6	-1.63386767	2.99436350	-2.27192436
1	-1.60875571	3.84367716	-2.98407600
1	-2.57490342	3.09497059	-1.71552338
6	-0.18548445	4.25644072	-0.70338422
6	-1.08074811	4.85659142	0.21062692
6	-0.71424503	6.05932312	0.82975298
6	0.51774751	6.67748058	0.59855628
6	1.40701570	6.04295417	-0.27732653
6	1.07947098	4.85280172	-0.93320182
6	-1.90522433	-3.64763987	0.57523909
1	-1.54649421	-4.29305610	3.14650636
6	-0.64433040	-3.06025202	5.41805543
1	-0.00733016	-0.54027869	4.55695746
6	-0.18093198	0.84949475	2.26897000
6	-2.39037238	4.20783954	0.58640200
1	-1.41263148	6.51056067	1.53911165
6	0.87634522	7.98507775	1.26198727
1	2.38737270	6.48914448	-0.46179485
6	2.08151055	4.21085205	-1.86478803
1	-1.75368398	-4.69422960	0.87151735
1	-1.33704202	-3.45796369	-0.34758222
1	-2.97383767	-3.53155844	0.33392185
1	0.78109797	0.93641381	1.73611493
1	-0.06885363	1.37237578	3.22784528
1	-0.92010078	1.37577301	1.65060168
1	-1.51910472	-2.81203637	6.04028758
1	0.24161517	-2.66546855	5.93509367
1	-0.56531298	-4.15577813	5.39049644
1	-2.73049690	4.57347603	1.56375607
1	-2.28398375	3.11508036	0.64754898
1	-3.19301813	4.42539200	-0.13660190
1	1.68086067	4.08534359	-2.88393473
1	2.39871990	3.21481183	-1.51403155
1	2.98444867	4.82878002	-1.94146169
1	1.94045482	8.01943660	1.53380745
1	0.28468512	8.14634903	2.17301055
1	0.68532336	8.83755454	0.59086027
1	0.33014488	2.66304785	-1.81197809

Energy = -7584.961791 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 22

Atomic N.	X	Y	Z
8	1.06133078	-4.09880739	-3.97350558
6	1.53211328	-3.10663387	-4.49209297
8	0.65021896	-2.15366161	-4.95473664
6	1.13208144	-0.96378158	-5.61124103

1	1.60359218	-1.20405597	-6.57492078
1	1.83326280	-0.40194240	-4.97938449
1	0.24098471	-0.35275866	-5.79310536
8	2.03986024	-1.11949278	-0.61538668
6	3.01983455	-2.83280145	-4.59905949
1	3.51247846	-3.80701787	-4.72227252
1	3.25316677	-2.22410082	-5.48214241
6	3.54988426	-2.14062326	-3.31560849
1	2.86630857	-1.34046738	-2.99544365
1	4.51000070	-1.65670735	-3.55631857
6	3.75711830	-3.11462646	-2.14845962
1	2.85060463	-3.72548297	-2.00962620
1	4.55860570	-3.81896398	-2.42745017
6	4.11106825	-2.41939462	-0.82080131
1	4.71016847	-1.51307504	-1.01217629
1	4.74124683	-3.09001270	-0.21214068
6	2.89834178	-2.04879893	0.03756017
1	2.35157029	-2.98892761	0.27036191
1	3.26330670	-1.65356891	1.00866053
50	0.76880035	0.02949107	0.61474696
7	-1.01665256	-1.09662039	-0.68879185
6	-0.82647840	-2.56486392	-0.73018514
1	-1.51586842	-3.02989731	-1.45565466
1	-0.99599577	-3.00075897	0.26055646
1	0.20553121	-2.76942652	-1.03505323
7	-2.19851018	-0.36349088	2.11308808
6	-2.41471771	-0.74253130	-0.32993049
1	-3.09584923	-1.20987457	-1.06682056
1	-2.51376900	0.34711577	-0.44279430
6	-2.88143875	-1.14138712	1.06868379
1	-3.98027271	-0.99634534	1.09403346
1	-2.71221831	-2.21019006	1.24957198
6	-2.57152603	-0.63318950	3.46482111
6	-2.14359672	-1.82199480	4.09718228
6	-2.50387235	-2.04917488	5.43153526
6	-3.25533432	-1.12988105	6.17043336
6	-3.63807291	0.05749609	5.53560539
6	-3.31764877	0.31951254	4.19936844
7	0.18417331	1.43182403	-0.88272583
6	-0.68861891	-0.53923146	-2.03755551
1	-1.43540689	-0.88359803	-2.77611040
1	0.28690786	-0.96607552	-2.30131780
6	-0.58499705	0.98398490	-2.03324924
1	-0.11961954	1.26720347	-2.99721643
1	-1.59582874	1.44741289	-2.05303029
6	0.65390773	2.77316734	-0.90243720
6	0.09310703	3.73970144	-0.02942046
6	0.57151882	5.05561384	-0.04454440
6	1.59814571	5.46070083	-0.90453422
6	2.14900709	4.49923039	-1.75833328
6	1.70568352	3.17076625	-1.77019548
6	-1.26216034	-2.81809019	3.38620204
1	-2.16034530	-2.96777386	5.91386499
6	-3.65049019	-1.41204970	7.59978186
1	-4.21042287	0.80278475	6.09357099
6	-3.75492576	1.62046674	3.56620222
6	-1.02081842	3.36737133	0.91924366
1	0.12192004	5.78785629	0.63161253

6	2.12147342	6.87694403	-0.88254622
1	2.96532084	4.78531585	-2.42758208
6	2.38128152	2.17263129	-2.67796551
1	-0.69407423	-3.41493772	4.11121311
1	-0.55019862	-2.30362787	2.72463315
1	-1.84144731	-3.52611137	2.77101562
1	-2.90005821	2.27404903	3.32580839
1	-4.40382041	2.18055671	4.25077995
1	-4.31714094	1.46179053	2.63265566
1	-4.65604279	-1.85885958	7.65281721
1	-3.67176756	-0.49213913	8.20010140
1	-2.95457846	-2.11617548	8.07531492
1	-1.46802295	4.26633766	1.36421163
1	-0.65366247	2.73287595	1.74217619
1	-1.80979782	2.80045563	0.40405751
1	2.40644836	1.17669757	-2.21257563
1	3.40851336	2.48890070	-2.90365050
1	1.85434205	2.07574336	-3.64209156
1	2.97488720	6.97417534	-0.19256266
1	1.34991981	7.58391087	-0.54811354
1	2.46917396	7.19239236	-1.87586822
1	-2.33114391	0.62952329	1.91725740

Energy = -7584.963343 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 23

Atomic N.	X	Y	Z
8	4.96034720	-2.86277662	-1.19418113
6	5.47892525	-1.79238845	-1.45540366
8	5.82475267	-1.41813981	-2.72479009
6	5.51013491	-2.38788413	-3.75008147
1	4.42641495	-2.54970576	-3.80379362
1	6.00586765	-3.34423708	-3.54044025
1	5.88137930	-1.95373345	-4.68364908
8	0.42574663	0.47999974	0.24594035
6	5.83119854	-0.70020876	-0.46765728
1	5.78780697	-1.14057691	0.53721293
1	6.86641827	-0.38579147	-0.66740888
6	4.90166681	0.53001875	-0.55803211
1	4.85722702	0.87112688	-1.60444278
1	5.37122186	1.34763781	0.01313062
6	3.48707329	0.29458442	-0.01704891
1	3.00429674	-0.53755575	-0.55034573
1	3.55678817	-0.01059249	1.04259746
6	2.60801137	1.54526726	-0.12598349
1	2.35103612	1.72872863	-1.18256560
1	3.17807017	2.42764535	0.21971493
6	1.31658006	1.49152206	0.69611406
1	1.59367040	1.35206981	1.76554946
1	0.82434213	2.48154791	0.63218317
50	-0.42952918	-0.77794013	1.67264531
7	-2.95414672	-1.63713188	2.28944397
6	-3.20032536	-1.74293863	3.72964992
1	-4.12846738	-2.30740302	3.94898425
1	-3.28322971	-0.74710207	4.18128674
1	-2.35368889	-2.25543710	4.20578785
7	-2.42347011	1.11884866	1.38410164

6	-3.96005494	-0.81322459	1.60705497
1	-4.98911922	-1.08923312	1.91751116
1	-3.88520673	-1.01394396	0.52949036
6	-3.76053098	0.68428428	1.84427368
1	-4.56556580	1.23129146	1.31980100
1	-3.85784577	0.92761019	2.90894481
6	-2.11810219	2.51181699	1.57510801
6	-1.89880472	3.03075575	2.86883639
6	-1.59603196	4.39219195	3.00630147
6	-1.48517746	5.24902541	1.90738808
6	-1.66461560	4.69960747	0.63261305
6	-1.97876694	3.34995872	0.44445964
7	-1.18696427	-1.98845501	0.06947577
6	-2.78796276	-2.97302749	1.69188797
1	-3.72945752	-3.55952996	1.73849446
1	-2.04125933	-3.49672605	2.30985700
6	-2.29258258	-2.92080294	0.24721594
1	-1.99538523	-3.95410330	-0.01934169
1	-3.14559601	-2.68838527	-0.42652780
6	-0.52956312	-2.13084039	-1.18915356
6	-1.13248451	-1.67298179	-2.38659914
6	-0.48081543	-1.86279393	-3.61221446
6	0.76137388	-2.49628442	-3.70037632
6	1.34962222	-2.94481294	-2.51168603
6	0.73129303	-2.77561995	-1.26707835
6	-1.92725339	2.16028526	4.10200849
1	-1.41841986	4.78529612	4.01041755
6	-1.18586900	6.71725851	2.08852315
1	-1.55094844	5.33768719	-0.24692898
6	-2.11618491	2.79708231	-0.95461469
6	-2.46592021	-0.96893855	-2.37413889
1	-0.96001102	-1.49519348	-4.52408311
6	1.45817271	-2.66428550	-5.02999190
1	2.31965586	-3.44735818	-2.54456422
6	1.41926715	-3.29757128	-0.02980453
1	-1.30036935	2.59805452	4.88957105
1	-1.54880226	1.14984761	3.88892135
1	-2.94278307	2.06026882	4.51906081
1	-1.35273051	2.02680676	-1.15487432
1	-1.98627072	3.59534060	-1.69550661
1	-3.10536491	2.34447878	-1.13144396
1	-2.11477809	7.30482083	2.16180377
1	-0.61365673	7.11730728	1.24055566
1	-0.61175905	6.89854310	3.00717114
1	-2.54419520	-0.26222666	-3.21118275
1	-2.59884465	-0.41726140	-1.43362860
1	-3.30831533	-1.67443522	-2.46169968
1	0.73641683	-3.88708804	0.59862632
1	1.80002200	-2.47606317	0.59928746
1	2.28546357	-3.91499860	-0.29804723
1	2.13303789	-1.81761685	-5.23667682
1	0.73726688	-2.71344408	-5.85760604
1	2.06579768	-3.57993008	-5.05093742
1	-2.33913910	0.91010251	0.38552802

Energy = -7584.974200 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 24

Atomic N.	X	Y	Z
8	4.19747395	-3.39275358	-1.12137222
6	4.89327893	-2.48742503	-1.54439459
8	5.15578404	-2.29997298	-2.87276935
6	4.50898365	-3.24557718	-3.75596834
1	3.41841098	-3.15614319	-3.67480264
1	4.80686604	-4.27155183	-3.50519331
1	4.84468266	-2.97779406	-4.76270800
8	0.44009397	0.62484240	-0.03663981
6	5.56686889	-1.41642889	-0.71274921
1	5.58401040	-1.77250732	0.32581119
1	6.60285991	-1.30339907	-1.06429224
6	4.84759021	-0.05286640	-0.80020923
1	4.79286521	0.25823290	-1.85534060
1	5.47892508	0.69227086	-0.28877543
6	3.44855501	-0.04158224	-0.17591359
1	2.80301348	-0.77818049	-0.67886533
1	3.52165462	-0.36250248	0.87868911
6	2.78548920	1.33697368	-0.23997844
1	2.60289280	1.61619022	-1.29097633
1	3.47119939	2.09630775	0.17877984
6	1.46321343	1.43043029	0.53014695
1	1.65855948	1.16611250	1.59318381
1	1.13376347	2.48751844	0.53061758
50	-0.29978107	-0.99067030	1.05885800
7	-2.83554977	-1.68421062	1.76270204
6	-2.95028483	-2.20075334	3.13042602
1	-3.93805075	-2.66982249	3.30969087
1	-2.80573576	-1.39816785	3.86201649
1	-2.16707698	-2.95158740	3.29929127
7	-2.05512463	1.18672850	1.82758898
6	-3.76877476	-0.57878241	1.50126406
1	-4.80607735	-0.85677867	1.78283408
1	-3.76673561	-0.39159818	0.41805573
6	-3.39761455	0.71624707	2.22476738
1	-4.17797703	1.46848470	2.00222784
1	-3.40657708	0.57485760	3.31262285
6	-1.58825436	2.36292492	2.51069711
6	-1.13879367	2.28118667	3.84650740
6	-0.67740899	3.44384460	4.47803942
6	-0.63138058	4.68036543	3.82758926
6	-1.05623270	4.73095658	2.49516267
6	-1.53763609	3.60021451	1.82697760
7	-1.34836117	-1.63938346	-0.68893801
6	-2.97312698	-2.78700845	0.79273487
1	-4.00199799	-3.20359251	0.80375478
1	-2.28865793	-3.58166087	1.12900158
6	-2.59770023	-2.38430538	-0.63066476
1	-2.54203855	-3.32348622	-1.21534658
1	-3.43343155	-1.81485387	-1.09622984
6	-0.82930509	-1.55307881	-2.01970889
6	-1.14977237	-0.45444150	-2.85092038
6	-0.67078517	-0.41701669	-4.16612404
6	0.11794955	-1.44438558	-4.69577165
6	0.42510211	-2.52588272	-3.86359067
6	-0.02352517	-2.59608499	-2.53723917
6	-1.10166734	0.97439850	4.59938262

1	-0.32125702	3.36882440	5.50847653
6	-0.15220784	5.92159965	4.54040064
1	-1.01427455	5.67982536	1.95498994
6	-1.96613306	3.71389075	0.38297329
6	-1.97246291	0.69147851	-2.32162658
1	-0.92512000	0.44033973	-4.79520186
6	0.64338669	-1.37335495	-6.10982888
1	1.02718335	-3.34897572	-4.25840507
6	0.38357302	-3.76862404	-1.67804197
1	-0.35191993	1.01580621	5.39993040
1	-0.84762282	0.13711667	3.93328286
1	-2.06829299	0.74371455	5.07691548
1	-1.29004287	3.15703862	-0.28526655
1	-1.95385630	4.76264906	0.06175070
1	-2.98436672	3.32932582	0.21579199
1	-0.99639890	6.47797694	4.97772445
1	0.36575744	6.60427090	3.85306284
1	0.53482372	5.67214822	5.36007938
1	-2.18185396	1.42182663	-3.11436377
1	-1.41219261	1.18966329	-1.51659980
1	-2.93358845	0.35220671	-1.90671292
1	-0.46845790	-4.21012278	-1.14285933
1	1.11916687	-3.47011487	-0.91542075
1	0.85103795	-4.55151239	-2.28908307
1	1.59080906	-0.81246667	-6.15359877
1	-0.06561168	-0.86333928	-6.77668844
1	0.83686225	-2.37540807	-6.51669858
1	-2.05159019	1.37136562	0.82107908

Energy = -7584.974313 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 25

Atomic N.	X	Y	Z
8	0.38523842	-0.86942986	0.20326958
6	1.05847011	-1.47870431	1.04347656
8	2.16006552	-2.17318642	0.73002361
6	2.65122586	-1.99372671	-0.62547130
1	2.89007721	-0.93457890	-0.77893030
1	1.89922017	-2.32595222	-1.35088254
1	3.54928434	-2.61559051	-0.68503647
8	2.38367820	0.85990771	1.14310568
6	0.65087501	-1.63493823	2.48981885
1	-0.00279280	-0.78337985	2.72909859
1	-0.00514252	-2.52426361	2.49944119
6	1.74940865	-1.81235638	3.54915681
1	2.48004297	-2.55848922	3.20240649
1	1.26042021	-2.25351024	4.43235718
6	2.48331538	-0.53866160	4.01284011
1	1.74041410	0.25400234	4.21158688
1	2.92665863	-0.77838146	4.99218416
6	3.60521427	0.02647793	3.11017167
1	4.02051222	-0.76890084	2.47074946
1	4.43408978	0.36773775	3.75394279
6	3.22217637	1.21823798	2.22486451
1	2.75674402	1.99514610	2.87578397
1	4.15430332	1.66793667	1.82663373
50	0.52472737	1.80612163	0.91720982

7	-2.05361909	2.44893412	-0.33069259
6	-2.09671005	3.83268698	0.15253155
1	-2.81742357	4.45204302	-0.41998087
1	-1.10632956	4.30197077	0.08296812
1	-2.39363970	3.83612395	1.20974256
7	0.82582459	2.26349885	-1.13270870
6	-1.62066875	2.37296157	-1.73091831
1	-2.31335792	2.93331920	-2.39840781
1	-1.64365275	1.31720770	-2.03428671
6	-0.20361460	2.90540924	-1.95754701
1	0.02217669	2.74636533	-3.02465539
1	-0.19604434	4.00651524	-1.82613627
6	2.09031326	2.13350437	-1.78313027
6	3.17528240	2.97668394	-1.43878771
6	4.40223308	2.82759263	-2.09723332
6	4.60072115	1.86515540	-3.09298092
6	3.51821723	1.04671121	-3.43106160
6	2.27255732	1.16178557	-2.80018057
7	-2.76994737	-0.57105277	0.31253685
6	-3.37912278	1.84254868	-0.09612818
1	-4.15494658	2.42695163	-0.64162523
1	-3.58765061	1.94452419	0.97942761
6	-3.57039405	0.37448650	-0.47760004
1	-4.63132002	0.15321308	-0.29391068
1	-3.42945756	0.23389677	-1.56704477
6	-3.35200052	-1.85628342	0.52634463
6	-2.95241076	-2.98872861	-0.22166978
6	-3.51879694	-4.23682366	0.06919236
6	-4.49132741	-4.39874221	1.06193648
6	-4.88097981	-3.26506706	1.78475606
6	-4.32693054	-2.00275245	1.54242875
6	3.03522528	4.04785647	-0.38442600
1	5.22737533	3.49138597	-1.82581354
6	5.94546410	1.69950871	-3.75953734
1	3.64455051	0.28734909	-4.20774145
6	1.15179286	0.23390485	-3.19983170
6	-1.94375399	-2.86921027	-1.34032397
1	-3.20061962	-5.10544595	-0.51328425
6	-5.12005270	-5.74556336	1.32852477
1	-5.62395467	-3.36709300	2.58016035
6	-4.73786758	-0.82506459	2.39017608
1	3.82806438	4.80028066	-0.49120787
1	3.11971053	3.62776352	0.63026931
1	2.06221976	4.55409769	-0.44464528
1	0.60034711	-0.11478833	-2.31593384
1	1.54420455	-0.63625434	-3.74325191
1	0.42410724	0.72671364	-3.86498129
1	6.46684309	2.66206861	-3.85552295
1	5.84531386	1.26184425	-4.76205722
1	6.59949777	1.03332397	-3.17437162
1	-1.86990744	-3.81532395	-1.89154609
1	-0.93862747	-2.61317122	-0.97403971
1	-2.22535116	-2.08314517	-2.05723001
1	-5.45132364	-0.16567048	1.86974778
1	-3.86297704	-0.20904037	2.64207076
1	-5.22327246	-1.16215972	3.31534533
1	-5.31686896	-5.89177420	2.39992830
1	-4.47441759	-6.56439173	0.98394610

1 -6.08470405 -5.84496340 0.80580348
 1 -1.81622526 -0.64919484 -0.04320550
 Energy = -7584.958777 Hartree
 Number of imaginary frequencies = 0.

Compound I5b isomer 26

Atomic N.	X	Y	Z
8	0.35278915	0.82032627	-0.91021116
6	1.55148110	0.86383143	-1.20554318
8	2.22383563	2.01602672	-1.35299013
6	1.50426360	3.21333059	-0.95768440
1	1.22452101	3.13448750	0.09956001
1	0.60912732	3.34166901	-1.57798672
1	2.20937822	4.03421062	-1.11921048
8	1.75675254	0.70006512	1.49209450
6	2.37676159	-0.34843787	-1.56867630
1	1.89098298	-1.21571702	-1.09943105
1	2.21894217	-0.47604171	-2.65470246
6	3.88537817	-0.32785781	-1.27623623
1	4.30375574	0.65069872	-1.55529084
1	4.34648952	-1.06075648	-1.95732402
6	4.32212547	-0.69364251	0.15587950
1	3.79494439	-1.61225460	0.46945642
1	5.38585624	-0.97262782	0.09006644
6	4.18283666	0.37551462	1.26422974
1	4.22724541	1.38745575	0.82989716
1	5.05272009	0.29166199	1.93848669
6	2.93467603	0.27914139	2.15037440
1	2.85662536	-0.76843318	2.52444207
1	3.09896200	0.91435361	3.04487512
50	0.09187432	-0.56302586	1.35803141
7	-2.81191010	-1.65769877	1.20850372
6	-3.05146586	-2.33941250	2.48144697
1	-4.13264388	-2.43028141	2.72011399
1	-2.56278172	-1.79865640	3.30163653
1	-2.61779008	-3.34760903	2.44147997
7	-1.28363489	0.88787867	2.06224915
6	-3.35309866	-0.29160946	1.20826866
1	-4.45191083	-0.30901168	1.39368969
1	-3.18918956	0.13662320	0.20893315
6	-2.72077340	0.64842778	2.23315552
1	-3.26609373	1.60274058	2.14142643
1	-2.94852120	0.29133461	3.25829729
6	-0.87496689	2.17714651	2.52456896
6	-0.18908561	2.31902103	3.75569627
6	0.19208506	3.59413110	4.19096954
6	-0.08052659	4.74664487	3.44584242
6	-0.77051402	4.59346230	2.23919520
6	-1.17458863	3.33748828	1.76669565
7	-1.38437679	-2.24839403	-1.35240440
6	-3.36588385	-2.45300176	0.10089228
1	-4.47674705	-2.39021244	0.08235379
1	-3.11338221	-3.50782750	0.29596671
6	-2.84088983	-2.08175431	-1.28564817
1	-3.35387917	-2.73519138	-2.01531509
1	-3.12629651	-1.04928799	-1.53595950
6	-0.73532705	-2.56997620	-2.56029798

6	-0.88235112	-1.76265095	-3.71517403
6	-0.18759442	-2.11074301	-4.88059873
6	0.67485026	-3.21025628	-4.94542431
6	0.84326526	-3.96650628	-3.77949769
6	0.15559704	-3.67410773	-2.59771746
6	0.12726521	1.12240055	4.61956317
1	0.71433605	3.68848787	5.14678477
6	0.37740274	6.10571110	3.91857272
1	-1.00097431	5.47853844	1.63958142
6	-1.90771739	3.24244844	0.45101382
6	-1.69572589	-0.49100018	-3.69267541
1	-0.30736182	-1.47509540	-5.76202017
6	1.38621775	-3.57482122	-6.22629937
1	1.52413764	-4.82160678	-3.78943917
6	0.37112550	-4.53166330	-1.37296901
1	0.33746603	1.43519214	5.65117855
1	1.01536200	0.58620625	4.25090095
1	-0.70083371	0.40098739	4.63375203
1	-1.55794139	2.37971333	-0.13172394
1	-1.76137697	4.15679371	-0.13982448
1	-2.99424814	3.12360724	0.59335999
1	0.32118385	6.19001431	5.01293485
1	-0.23107101	6.90858985	3.48077414
1	1.42479741	6.29346409	3.63283870
1	-1.44018524	0.13717652	-4.55601390
1	-1.49375965	0.08186949	-2.77545709
1	-2.77991586	-0.67820816	-3.73557308
1	-0.56869373	-4.98254251	-1.01394105
1	0.79709016	-3.96088097	-0.53050419
1	1.06610705	-5.35108961	-1.59469603
1	2.35516931	-4.05270019	-6.02608385
1	1.56470456	-2.68890978	-6.85135991
1	0.79251685	-4.28244355	-6.82711619
1	-1.05697569	-2.82492738	-0.58100929

Energy = -7584.958338 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 27

Atomic N.	X	Y	Z
8	3.81564413	-3.63138104	-1.21693571
6	4.35461913	-2.89303677	-2.01654656
8	4.15500271	-3.14134154	-3.35200440
6	4.78019301	-2.31826511	-4.35538668
1	5.87265706	-2.44444756	-4.35043262
1	4.52302059	-1.25755957	-4.23483925
1	4.38356127	-2.67604881	-5.31163045
8	0.36510938	0.29443248	0.39076172
6	5.21355673	-1.70916443	-1.60287243
1	5.65377495	-1.98667343	-0.63574646
1	6.03667007	-1.54497970	-2.31235147
6	4.41180865	-0.39677014	-1.43055697
1	3.98307594	-0.08056852	-2.39529654
1	5.13407822	0.38610079	-1.14551108
6	3.29781043	-0.46559314	-0.38067186
1	2.50633579	-1.14656679	-0.73013220
1	3.69717344	-0.90576411	0.54894738
6	2.69646956	0.90851315	-0.07307102

1	2.32107180	1.37477825	-0.99933550
1	3.48452640	1.57291006	0.32460618
6	1.54768045	0.87148672	0.94172409
1	1.88535119	0.32976458	1.85052360
1	1.32598131	1.90610839	1.26306615
50	-0.20111389	-1.61518377	1.02343158
7	-2.65717877	-1.47753257	1.64527678
6	-2.88765697	-1.82635767	3.05735763
1	-3.96564598	-1.93139908	3.27826002
1	-2.45458305	-1.05617325	3.70461014
1	-2.38763771	-2.77903747	3.27444884
7	-1.73574018	1.32833660	2.34797787
6	-3.34742277	-0.22296910	1.25013660
1	-4.43658923	-0.41639817	1.18226840
1	-2.99107889	0.02985022	0.24153912
6	-3.14899753	0.97618308	2.17405190
1	-3.73957153	1.80293843	1.72825581
1	-3.60085426	0.78259114	3.15948250
6	-1.50227190	2.59571869	2.96923379
6	-1.53385637	2.70089177	4.37715378
6	-1.29016014	3.94360595	4.97607149
6	-0.99866975	5.08601356	4.22329048
6	-0.95571164	4.95776042	2.82977631
6	-1.21361222	3.74045226	2.18842822
7	-1.30402042	-1.92839988	-0.77016006
6	-3.09169471	-2.59379481	0.76458131
1	-4.18731016	-2.73298148	0.83929747
1	-2.60695173	-3.50509788	1.14924466
6	-2.68138066	-2.38269511	-0.69365573
1	-2.83584301	-3.35154462	-1.21062570
1	-3.38459205	-1.67475770	-1.18389490
6	-0.73955630	-1.89453283	-2.07981761
6	-0.92278595	-0.75840962	-2.91083432
6	-0.36633336	-0.74302474	-4.19366033
6	0.37950551	-1.82061435	-4.69026464
6	0.55949739	-2.92943314	-3.86058655
6	0.01390463	-2.98857466	-2.56863528
6	-1.77448227	1.48678167	5.23843245
1	-1.30673664	4.01178425	6.06681941
6	-0.75837188	6.41964865	4.88938580
1	-0.72602071	5.83451053	2.21877563
6	-1.19115963	3.66712891	0.67910620
6	-1.67777762	0.44677092	-2.40921409
1	-0.51377301	0.14123267	-4.82018445
6	0.96216726	-1.78060898	-6.08364949
1	1.14908335	-3.77684455	-4.21836135
6	0.26595707	-4.21386086	-1.72296792
1	-1.49977616	1.68943433	6.28166088
1	-1.18172056	0.63543884	4.87393248
1	-2.83133948	1.17442347	5.23442967
1	-0.41288958	2.98660259	0.30091646
1	-1.00360673	4.65971829	0.25060756
1	-2.14867776	3.30357807	0.27577864
1	-1.68344144	7.01669555	4.92812758
1	-0.01205232	7.01269061	4.34302716
1	-0.40733497	6.29347516	5.92247161
1	-1.62243563	1.26858772	-3.13541825
1	-1.25138905	0.78570833	-1.45404373

1	-2.74388597	0.22504647	-2.24195131
1	-0.58762289	-4.44464997	-1.07299510
1	1.14706419	-4.07837375	-1.07572972
1	0.47444003	-5.08441540	-2.35880874
1	1.61942516	-0.90805576	-6.22091596
1	0.17230099	-1.70644804	-6.84685858
1	1.54719781	-2.68550120	-6.29562191
1	-1.23240017	1.25813747	1.45490158

Energy = -7584.963174 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 28

Atomic N.	X	Y	Z
8	0.32875440	-0.91982607	0.07036937
6	0.88980837	-1.68437528	0.86440841
8	1.99127133	-2.37981270	0.55191802
6	2.62319060	-2.02364121	-0.70683623
1	2.92085980	-0.96895377	-0.66827871
1	1.93442243	-2.19700227	-1.54204513
1	3.49553389	-2.67970666	-0.78023900
8	2.28979731	0.54305766	1.45229086
6	0.33246729	-2.03708373	2.22363679
1	-0.31008550	-1.19890115	2.53060125
1	-0.35350787	-2.88219858	2.03235655
6	1.31115106	-2.43068133	3.34068364
1	2.04427260	-3.15328114	2.95188278
1	0.71927421	-2.97384884	4.09461298
6	2.04237642	-1.28225694	4.06342842
1	1.31412236	-0.48982450	4.31106379
1	2.37438326	-1.68970283	5.03133936
6	3.27122854	-0.64884333	3.36915438
1	3.71611251	-1.35876330	2.65360042
1	4.04443094	-0.45673917	4.13280831
6	3.02764851	0.68391389	2.65127765
1	2.52973076	1.37610664	3.37028925
1	4.01243764	1.13757001	2.41887238
50	0.50220996	1.61396076	1.20858320
7	-1.90699455	2.58314864	-0.14954551
6	-1.93374217	3.88375494	0.52706412
1	-2.56880469	4.61941327	-0.00796338
1	-0.92119680	4.29984999	0.61383479
1	-2.32876397	3.75315445	1.54332975
7	1.02229118	2.35440678	-0.71098089
6	-1.34764742	2.68258779	-1.50257254
1	-1.94943294	3.36987764	-2.13880891
1	-1.38708944	1.68351520	-1.95823264
6	0.10584270	3.16149017	-1.52385341
1	0.42602920	3.14035003	-2.57832948
1	0.14785513	4.23133975	-1.23489861
6	2.34014334	2.25686825	-1.25205720
6	3.41557940	2.98104576	-0.68113417
6	4.69622925	2.86870424	-1.23634533
6	4.95816647	2.05771796	-2.34584663
6	3.88563237	1.35688440	-2.90644330
6	2.58775763	1.44056116	-2.38525154
7	-2.80296834	-0.45113200	-0.02435786
6	-3.27354945	2.02549610	-0.12164033

1	-3.96914154	2.72377260	-0.64082069
1	-3.57695405	1.98550547	0.93528147
6	-3.49098003	0.63933854	-0.72904563
1	-4.57230688	0.45146304	-0.66709093
1	-3.26002488	0.64870526	-1.81209104
6	-3.45780771	-1.71892629	-0.04104797
6	-3.04966799	-2.75650345	-0.91313977
6	-3.69224495	-3.99912275	-0.84748595
6	-4.74834296	-4.24419159	0.03800489
6	-5.14454620	-3.20313304	0.88466992
6	-4.51729820	-1.95125530	0.86766214
6	3.20964304	3.88779454	0.50806219
1	5.51382552	3.44055494	-0.78949830
6	6.35623061	1.92414128	-2.90049627
1	4.06141067	0.71696606	-3.77561450
6	1.47980919	0.64224096	-3.02713354
6	-1.95076719	-2.53647996	-1.92665314
1	-3.36667102	-4.79396092	-1.52377311
6	-5.45472349	-5.57869671	0.05910061
1	-5.95343470	-3.37413269	1.59979810
6	-4.94421670	-0.88245416	1.84219510
1	4.03824849	4.60316238	0.59608627
1	3.17165109	3.31597463	1.44872179
1	2.26861943	4.44957649	0.43334426
1	0.82648017	0.19786145	-2.26382039
1	1.89349789	-0.15840026	-3.65498530
1	0.84499372	1.26523770	-3.67805975
1	6.34168253	1.64296198	-3.96224622
1	6.92420468	1.14796514	-2.36299758
1	6.91847152	2.86313962	-2.80155998
1	-1.86755413	-3.40304747	-2.59489536
1	-0.96950752	-2.37824375	-1.45545132
1	-2.14636373	-1.64975609	-2.54857023
1	-5.58776986	-0.12198351	1.37077017
1	-4.06706556	-0.35278732	2.24021584
1	-5.51331402	-1.31855384	2.67354972
1	-5.88964430	-5.78506146	1.04657378
1	-4.77005102	-6.40011148	-0.19291485
1	-6.27814743	-5.60464003	-0.67239177
1	-1.82745020	-0.53312065	-0.31399829

Energy = -7584.958759 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 29

Atomic N.	X	Y	Z
8	0.40342582	0.79469165	-0.88221000
6	1.61324845	0.80929188	-1.13250847
8	2.31479324	1.94514165	-1.26813709
6	1.60676426	3.16200720	-0.91322836
1	1.28317454	3.10009305	0.13250265
1	0.74031727	3.30347300	-1.57033034
1	2.33587622	3.96553261	-1.05406039
8	1.71233683	0.67667882	1.56808740
6	2.42479047	-0.42441126	-1.45146180
1	1.90173444	-1.27619980	-0.99418026
1	2.30711710	-0.55897466	-2.54175255
6	3.92083904	-0.43400068	-1.09999031

1	4.37195025	0.53165427	-1.37294794
1	4.39130935	-1.18491138	-1.75452021
6	4.29257348	-0.79285693	0.35207175
1	3.73099938	-1.69442761	0.65522840
1	5.35077259	-1.09852397	0.33109184
6	4.13709167	0.29311394	1.44167052
1	4.22404541	1.29807973	0.99764338
1	4.97743417	0.19630796	2.15075999
6	2.85319699	0.23878976	2.27884632
1	2.73558055	-0.80081274	2.66440870
1	2.99741916	0.88354522	3.16996380
50	0.02427783	-0.54947748	1.38724250
7	-2.90056522	-1.58181658	1.10833634
6	-3.20617049	-2.26501571	2.36622972
1	-4.29791536	-2.33577579	2.55926421
1	-2.74211223	-1.73756758	3.20914511
1	-2.79057815	-3.28121512	2.33920019
7	-1.34874558	0.93945442	2.01204738
6	-3.41285959	-0.20455382	1.09482150
1	-4.51711663	-0.20010736	1.24552409
1	-3.20930145	0.22175149	0.10203178
6	-2.79396979	0.72136757	2.14109031
1	-3.32029389	1.68500753	2.03830992
1	-3.05677097	0.36405899	3.15766971
6	-0.93729787	2.23534868	2.45270049
6	-0.28958957	2.40255960	3.70114834
6	0.09568376	3.68456182	4.11228863
6	-0.13663540	4.81919008	3.32741127
6	-0.79034370	4.64143509	2.10394545
6	-1.19629356	3.37796152	1.65371474
7	-1.36787842	-2.22845723	-1.37945894
6	-3.42561283	-2.35732150	-0.02746821
1	-4.53124984	-2.25639550	-0.10114604
1	-3.21919805	-3.42042185	0.17612928
6	-2.81754564	-2.00085521	-1.38361749
1	-3.31901708	-2.62862523	-2.14292314
1	-3.04752311	-0.95588543	-1.63954748
6	-0.67372026	-2.58933220	-2.54984310
6	-0.73919842	-1.79634779	-3.72219595
6	-0.00060485	-2.18454302	-4.84727119
6	0.82839208	-3.31135499	-4.85448315
6	0.91595968	-4.05401462	-3.67111126
6	0.18207156	-3.72148584	-2.52838429
6	-0.01885305	1.22709105	4.60827761
1	0.58872257	3.79908475	5.08137011
6	0.32570169	6.18465567	3.77684533
1	-0.98954502	5.51227509	1.47311229
6	-1.88821348	3.25553309	0.31822010
6	-1.51108675	-0.49921284	-3.75814052
1	-0.05739440	-1.55955849	-5.74250904
6	1.58861763	-3.71764715	-6.09408127
1	1.56862930	-4.93021539	-3.63602179
6	0.31128664	-4.56533231	-1.28219382
1	0.16000922	1.56677738	5.63724026
1	0.87423272	0.67064728	4.28485811
1	-0.85636327	0.51648679	4.61361168
1	-1.52424619	2.37803435	-0.23293071
1	-1.71874124	4.15517844	-0.28870808

1	-2.97925254	3.14420059	0.42881502
1	-0.26242754	6.98301805	3.30430709
1	1.38179187	6.35347741	3.51199494
1	0.24417631	6.29722995	4.86703359
1	-1.19521179	0.10519963	-4.61847746
1	-1.33369187	0.08322478	-2.84188573
1	-2.59764649	-0.65222789	-3.84895232
1	-0.65926403	-4.97767384	-0.96046126
1	0.71766759	-3.99533661	-0.42955540
1	0.98665620	-5.41161302	-1.45909989
1	2.52860100	-4.22692952	-5.84035730
1	1.82975385	-2.84686033	-6.71939256
1	1.00019485	-4.41143391	-6.71588597
1	-1.09917147	-2.80348164	-0.58478079

Energy = -7584.958317 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 30

Atomic N.	X	Y	Z
8	0.67367474	-2.26282908	-1.92858053
6	1.00992586	-3.40703707	-2.19604623
8	2.07468088	-3.68973616	-2.99965086
6	2.79274768	-2.53174262	-3.48873608
1	3.18165272	-1.93973975	-2.65063271
1	2.13172591	-1.90026792	-4.09543740
1	3.61060090	-2.93349176	-4.09455877
8	0.69236565	-2.18327839	2.00646272
6	0.33813806	-4.67499034	-1.71907536
1	-0.64215387	-4.38986960	-1.31566372
1	0.17804388	-5.31153101	-2.60223513
6	1.13295568	-5.48451107	-0.66547040
1	2.14249874	-5.69948162	-1.05063062
1	0.62551674	-6.45744875	-0.57340069
6	1.20635243	-4.83072459	0.72387451
1	0.21850272	-4.41504503	0.97637117
1	1.41500586	-5.61157157	1.47389034
6	2.25080100	-3.71625199	0.87524670
1	2.27483622	-3.08143556	-0.02465908
1	3.26088836	-4.15020857	0.97710395
6	1.97084831	-2.80056539	2.07619499
1	2.00590272	-3.39809446	3.00799379
1	2.79000749	-2.05436924	2.14752383
50	0.36916487	-0.56995218	0.70763575
7	-0.44326456	0.59632866	2.75364104
6	0.53433652	0.45775067	3.85359210
1	0.09913087	0.79443578	4.81171591
1	1.43272601	1.05037341	3.64584320
1	0.81953951	-0.59872925	3.92473169
7	0.56538557	3.01531516	0.83770185
6	-0.90089187	2.00781832	2.60436363
1	-1.37244595	2.30830891	3.56083399
1	-1.67519452	2.02464221	1.82638839
6	0.15391759	3.05621595	2.24824037
1	-0.31674730	4.03045553	2.43422650
1	1.01528929	3.00454088	2.94242078
6	1.30808589	4.13300208	0.35884749
6	2.67459433	3.99752525	0.01476815

6	3.36700220	5.10142450	-0.49528842
6	2.75356852	6.34748034	-0.66852166
6	1.39668473	6.45439989	-0.34568745
6	0.65875908	5.37318049	0.15170454
7	-1.74028011	-0.84360990	0.65584687
6	-1.61895010	-0.28255125	3.03899834
1	-2.19007190	0.12613207	3.89422201
1	-1.20462719	-1.26163632	3.31763439
6	-2.52199512	-0.46021978	1.82388984
1	-3.26546652	-1.22960558	2.10194251
1	-3.11290305	0.46224064	1.63609960
6	-2.46658841	-1.37802666	-0.44072031
6	-2.55795658	-0.66638206	-1.66590239
6	-3.28018980	-1.21230681	-2.73317684
6	-3.92188836	-2.45290903	-2.64199827
6	-3.81635270	-3.15051730	-1.43519651
6	-3.10205667	-2.64437392	-0.34060316
6	3.38669923	2.67498443	0.17557602
1	4.42119386	4.98258733	-0.75829136
6	3.53185599	7.53803207	-1.17486412
1	0.88175338	7.40453530	-0.51037795
6	-0.82234827	5.53264512	0.39280280
6	-1.88533360	0.67272430	-1.84034317
1	-3.34875516	-0.64374619	-3.66477109
6	-4.67445907	-3.02806075	-3.81851768
1	-4.29278562	-4.13072016	-1.34203271
6	-2.98177568	-3.48274670	0.90903685
1	4.45390070	2.78199010	-0.05642516
1	2.97957478	1.89884791	-0.49248916
1	3.30475328	2.28201654	1.20118548
1	-1.35631777	4.60078167	0.15895745
1	-1.22777058	6.33894961	-0.23234532
1	-1.05471050	5.79110663	1.43893032
1	3.97386987	8.10758523	-0.34170982
1	2.88705277	8.22929437	-1.73479205
1	4.35613151	7.22922505	-1.83204655
1	-2.31981622	1.21695103	-2.68969154
1	-0.80804652	0.55708695	-2.04098598
1	-1.97128484	1.29307092	-0.93810090
1	-2.02615071	-3.28935431	1.41720320
1	-3.04700147	-4.55180255	0.66359100
1	-3.78808135	-3.27287606	1.63117470
1	-3.98537530	-3.45339634	-4.56558959
1	-5.26762667	-2.25706891	-4.33103470
1	-5.35569496	-3.83011852	-3.50410535
1	1.06071593	2.14094677	0.64197805

Energy = -7584.972661 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 31

Atomic N.	X	Y	Z
8	4.15089286	-2.23449238	1.19709874
6	4.47220926	-2.20837312	0.02192413
8	4.62118908	-3.34015702	-0.73157265
6	4.33256522	-4.57029256	-0.03033907
1	3.29421109	-4.57408654	0.32569623
1	5.00356191	-4.69102847	0.82974602

1	4.49378664	-5.36740691	-0.76299187
8	0.06154877	-0.07090590	-0.70829449
6	4.80637184	-0.96441708	-0.77617919
1	4.55092493	-0.10396636	-0.14299184
1	5.90296782	-0.96956381	-0.89763830
6	4.15509248	-0.83197199	-2.16795778
1	4.32193627	-1.75704387	-2.74129938
1	4.69721820	-0.03487255	-2.70130505
6	2.66204718	-0.46941937	-2.15052610
1	2.50690813	0.40736999	-1.50277648
1	2.36953614	-0.15682446	-3.16797526
6	1.71442756	-1.58647323	-1.70194378
1	1.99372412	-1.95268974	-0.69971363
1	1.78981223	-2.44672772	-2.39112588
6	0.24988378	-1.13171247	-1.63467691
1	-0.07160370	-0.77885025	-2.63359637
1	-0.38210825	-2.01236048	-1.39231082
50	-0.44438235	-0.53807334	1.24487107
7	-2.35944965	0.52662649	2.96230711
6	-2.14262540	-0.14645818	4.25039882
1	-2.76758339	0.28927403	5.05451320
1	-1.08996147	-0.06264591	4.54634598
1	-2.37911817	-1.21408542	4.15057407
7	0.17607140	1.42582421	1.82825026
6	-1.91692828	1.93348278	3.00912419
1	-2.34286546	2.44517614	3.89742799
1	-2.29477695	2.43567157	2.10777364
6	-0.39390653	2.05713508	3.01011703
1	-0.15896194	3.13726768	3.00805939
1	0.01269851	1.67236156	3.97086558
6	1.48267945	1.89980054	1.48392463
6	2.63205627	1.51976567	2.22043851
6	3.88808973	2.02701249	1.85205543
6	4.04831889	2.90576506	0.77835449
6	2.90294238	3.27603093	0.06184392
6	1.63276698	2.79057583	0.39031932
7	-3.27070222	-0.50817979	0.30836296
6	-3.76792427	0.39742594	2.54527957
1	-4.40800645	1.12688806	3.08214391
1	-4.11214675	-0.60394066	2.85138717
6	-3.99385973	0.54998596	1.04312415
1	-5.08265633	0.50213668	0.85582571
1	-3.65274350	1.53392007	0.69770897
6	-3.64942796	-0.77461957	-1.04480563
6	-3.51000443	0.20249012	-2.05462930
6	-3.87696883	-0.12808440	-3.36607033
6	-4.35198238	-1.39430406	-3.71941756
6	-4.44354901	-2.35788277	-2.70843277
6	-4.10593261	-2.07221396	-1.38220831
6	2.55624764	0.57670158	3.39713364
1	4.76660344	1.71234903	2.42174930
6	5.41299871	3.41465499	0.37884664
1	2.99964855	3.96396255	-0.78252222
6	0.44009695	3.20326002	-0.43193843
6	-2.92062385	1.56178243	-1.77525633
1	-3.75769697	0.63226946	-4.14184825
6	-4.75991532	-1.71073566	-5.13786346
1	-4.79080117	-3.36409377	-2.95558280

6	-4.21779501	-3.15682786	-0.33485609
1	3.46936618	-0.02829507	3.46674642
1	1.70251181	-0.11004684	3.31228578
1	2.44448865	1.12525177	4.34655551
1	0.06516031	2.33738503	-0.99710002
1	0.71128737	4.00088495	-1.13657178
1	-0.38629301	3.55734298	0.20068675
1	5.37372281	4.46872032	0.06941597
1	5.81728052	2.84369139	-0.47261080
1	6.13139644	3.32553805	1.20472162
1	-2.55648977	2.01467397	-2.70624364
1	-2.07020089	1.48064826	-1.08438408
1	-3.65700304	2.25798884	-1.34294233
1	-4.89640503	-2.87589818	0.48756606
1	-3.24109840	-3.40515350	0.11301115
1	-4.61218050	-4.07855309	-0.77978536
1	-4.50614183	-2.74523958	-5.40767778
1	-4.26765950	-1.03918132	-5.85390532
1	-5.84712145	-1.59655637	-5.27423671
1	-3.35964678	-1.37438691	0.84152311

Energy = -7584.969505 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 32

Atomic N.	X	Y	Z
8	0.54528285	-2.46052724	-2.43872471
6	1.74575988	-2.62456370	-2.36038333
8	2.55246517	-1.52500359	-2.54345276
6	3.98725090	-1.64769733	-2.50112913
1	4.36150387	-2.25656300	-3.33658874
1	4.33554427	-2.06538907	-1.54645881
1	4.36740045	-0.62567614	-2.60610047
8	0.11979195	-2.38806125	2.25101105
6	2.38925597	-3.95487848	-2.00989052
1	1.74289611	-4.73650836	-2.43117220
1	3.38205140	-4.05543141	-2.46754957
6	2.49238758	-4.14324816	-0.47440961
1	2.92820518	-3.23769528	-0.02144115
1	3.20622659	-4.95917077	-0.27637709
6	1.15190901	-4.47363022	0.19451366
1	0.38397346	-3.74736397	-0.11523843
1	0.80524016	-5.44868146	-0.18464894
6	1.22331769	-4.51605501	1.72735126
1	2.08892889	-5.12427776	2.04690543
1	0.32269185	-5.01379025	2.11957810
6	1.31508099	-3.13866839	2.40239905
1	1.50162965	-3.29467889	3.48259811
1	2.20074894	-2.58956298	2.01448146
50	0.00334426	-0.81152380	0.88386943
7	-0.63678294	0.57687438	2.82246133
6	0.31045436	0.37401793	3.94017747
1	-0.08642512	0.81418831	4.87226174
1	1.27649696	0.83925903	3.71272316
1	0.46005792	-0.70424040	4.07222161
7	0.51082580	2.72765464	0.61335223
6	-0.88108000	2.02914632	2.58080756
1	-1.22634606	2.46881558	3.53669855

8	1.12958711	-4.22856787	2.96929806
6	1.47580096	-4.56611518	1.85282250
8	0.54934952	-4.44087937	0.84365784
6	0.86720059	-4.84833127	-0.50393394
1	1.04866866	-5.93087070	-0.55870502
1	1.72822159	-4.29611302	-0.90153317
1	-0.02103411	-4.60437553	-1.09674766
8	2.58119487	-1.05072556	0.75246577
6	2.86901746	-5.05887471	1.51448411
1	3.26787950	-5.52431651	2.42589191
1	2.83503833	-5.82677273	0.72957354
6	3.78387329	-3.89070970	1.06774791
1	3.27343239	-3.28179334	0.30913942
1	4.67824193	-4.31997309	0.58820061
6	4.21722513	-2.96016062	2.21222485
1	3.36568032	-2.77801031	2.88614277
1	4.98491317	-3.47041650	2.81631157
6	4.75040631	-1.60948320	1.69761610
1	5.26457874	-1.75382998	0.73251950
1	5.50036016	-1.20197845	2.39587356
6	3.64964458	-0.55113252	1.53495275
1	3.30148533	-0.26747855	2.55167557
1	4.08667631	0.36080607	1.08500962
50	0.89032882	-0.22444637	-0.11246476
7	-0.46729666	-0.28972694	1.98461187
6	0.39785341	-0.80995735	3.07246175
1	-0.12537321	-0.73155881	4.04176974
1	1.32885731	-0.23843670	3.12061951
1	0.64178258	-1.86165825	2.88356658
7	0.93102036	1.80945444	0.59938846
6	-0.78714349	1.14545026	2.20309989
1	-1.17648809	1.29382044	3.22921609
1	-1.56208888	1.42674628	1.47996464
6	0.43505724	2.03091790	1.95396004
1	0.10719668	3.07828893	2.07292050
1	1.18542865	1.85644466	2.75057180
6	1.46330989	2.91331293	-0.10817176
6	2.47753763	3.74536222	0.44650668
6	2.95608731	4.84238781	-0.28079971
6	2.48962844	5.15524355	-1.56072198
6	1.51096545	4.31966725	-2.10717934
6	0.98643502	3.22191368	-1.41418185
7	-2.48993231	-0.56228608	-0.33992792
6	-1.67991959	-1.16421059	1.94459098
1	-2.06847855	-1.26715505	2.97519497
1	-1.33197157	-2.16341781	1.63924699
6	-2.85457134	-0.72623227	1.07290762
1	-3.63589863	-1.49992097	1.21108149
1	-3.28339527	0.20975985	1.45536568
6	-3.53852527	-0.46909125	-1.29734572
6	-4.41357391	0.64105278	-1.31284902
6	-5.41727666	0.70229207	-2.28871291
6	-5.57222718	-0.28271732	-3.26850006
6	-4.66846259	-1.35201424	-3.26129176
6	-3.66306414	-1.46609031	-2.29659540
6	3.11471127	3.43719965	1.78015770
1	3.74303707	5.45742457	0.16491214
6	3.00412968	6.35989259	-2.31148436

1	1.12117558	4.53760983	-3.10531200
6	-0.09643117	2.40596466	-2.07640028
6	-4.25317314	1.79053476	-0.34895752
1	-6.08299315	1.56915480	-2.29386251
6	-6.67865053	-0.20302346	-4.29234837
1	-4.75024794	-2.12775384	-4.02679579
6	-2.71427993	-2.64193489	-2.33860829
1	4.07806402	3.95624907	1.86986904
1	3.29149415	2.35829022	1.89365284
1	2.49372591	3.75233991	2.63329021
1	0.30094684	1.49398017	-2.55322062
1	-0.59052195	2.98950220	-2.86480689
1	-0.85335004	2.07367897	-1.35234913
1	2.39959478	7.25556276	-2.09512025
1	2.97118468	6.20027159	-3.39808666
1	4.04090312	6.59306069	-2.03142481
1	-4.72382709	2.69626387	-0.75231980
1	-3.18961505	2.00564061	-0.17032059
1	-4.72048739	1.59062920	0.62859102
1	-2.72569820	-3.21579371	-1.39773707
1	-1.67252924	-2.32724019	-2.51736730
1	-2.99081989	-3.32842080	-3.14849518
1	-6.35641978	-0.60118451	-5.26444114
1	-7.01249598	0.83284924	-4.44017296
1	-7.55688987	-0.78828169	-3.97619538
1	-1.84378036	-1.30555841	-0.60763735

Energy = -7584.958593 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 34

Atomic N.	X	Y	Z
8	0.81828423	-3.01550386	-0.24753107
6	1.24300899	-4.12282311	0.04805480
8	2.45445093	-4.58757760	-0.34849968
6	3.23731803	-3.64422698	-1.13156019
1	3.43944547	-2.74239710	-0.54266307
1	2.69623237	-3.36131885	-2.04195255
1	4.16403430	-4.17355913	-1.37216170
8	2.05872465	-0.66353957	2.30688727
6	0.51199476	-5.12634749	0.91459310
1	-0.55833440	-4.89809079	0.82509500
1	0.69219394	-6.13977407	0.52954942
6	0.93195470	-5.05650059	2.40229945
1	1.95986130	-5.43757045	2.50436400
1	0.28701075	-5.76227687	2.94680967
6	0.83269356	-3.64398767	3.02192293
1	0.18628062	-3.01455031	2.38758160
1	0.32936714	-3.70117596	3.99986345
6	2.19212607	-2.95385971	3.21786247
1	2.82713091	-3.08208801	2.32644265
1	2.72202573	-3.44613121	4.05178942
6	2.10173058	-1.44310060	3.49283054
1	1.22893069	-1.24977888	4.15407514
1	2.99747616	-1.12957242	4.06152733
50	0.34915960	-0.22416488	1.20395223
7	0.41084385	2.18042730	2.08349934
6	1.32771877	2.17082183	3.24604679

1	1.55822739	3.20276766	3.56638960
1	2.24682177	1.63127837	2.99618785
1	0.84795711	1.63941860	4.07866250
7	1.53346800	0.84381573	-0.23153250
6	1.01428067	2.91483856	0.94131584
1	1.41208587	3.89039482	1.28433366
1	0.22536284	3.08763380	0.20012683
6	2.11111878	2.08642220	0.27161543
1	2.50766532	2.68329152	-0.56800118
1	2.95229355	1.95057371	0.97858818
6	2.08161177	0.28429757	-1.40660150
6	3.48291881	0.12676829	-1.59609468
6	3.96730776	-0.35655362	-2.82025368
6	3.11990792	-0.73444693	-3.86561061
6	1.74086192	-0.63799246	-3.64172910
6	1.20908328	-0.14282986	-2.44690331
7	-2.33180981	1.91155625	0.69340282
6	-0.88340116	2.76108719	2.54184778
1	-0.67988458	3.70496642	3.08451610
1	-1.29692671	2.05383683	3.27913164
6	-1.94511686	3.07958619	1.49105300
1	-2.80437045	3.50063453	2.05070377
1	-1.59090212	3.88397752	0.83192529
6	-3.54474404	1.96453883	-0.04468293
6	-3.71170393	2.88162848	-1.10765502
6	-4.91840881	2.88431746	-1.82026344
6	-5.95752726	1.99266722	-1.53976210
6	-5.75334644	1.06211124	-0.51348661
6	-4.57553960	1.03351848	0.23877002
6	4.46426728	0.36811505	-0.47246903
1	5.04877945	-0.46557374	-2.94489563
6	3.66757218	-1.21850915	-5.18713804
1	1.04910312	-0.94388040	-4.43142778
6	-0.28622049	-0.06284737	-2.28046950
6	-2.59972920	3.80536881	-1.54030126
1	-5.03221416	3.59399420	-2.64375520
6	-7.25552728	2.03287435	-2.30963085
1	-6.53782722	0.33636849	-0.28440244
6	-4.40903819	0.00431960	1.33234462
1	5.40670061	-0.15844415	-0.67594060
1	4.05657608	0.00455254	0.48310382
1	4.71253459	1.43274033	-0.33729376
1	-0.66483931	-0.88386464	-1.64859924
1	-0.79220970	-0.14148628	-3.25188693
1	-0.58543958	0.87385167	-1.78998523
1	3.70195115	-0.40569534	-5.93050867
1	3.04540065	-2.01850397	-5.61331109
1	4.69140473	-1.60281818	-5.07873391
1	-2.75918618	4.13561468	-2.57478598
1	-1.62634723	3.29599081	-1.48816959
1	-2.53457140	4.71170863	-0.91720842
1	-4.21613130	0.46856952	2.31317786
1	-3.57265755	-0.68542232	1.13120197
1	-5.31714519	-0.60374460	1.42798471
1	-7.64633048	1.02209244	-2.49246643
1	-7.12855790	2.53107366	-3.28013391
1	-8.03138896	2.58507892	-1.75564421
1	-2.30788322	1.07303889	1.27467274

Energy = -7584.968179 Hartree
 Number of imaginary frequencies = 0.

Compound I5b isomer 35

Atomic N.	X	Y	Z
8	0.84106147	-0.86450754	2.47090495
6	0.72327218	-2.07247026	2.71174240
8	0.44503193	-2.52569860	3.94524742
6	0.22957860	-1.50950112	4.95817991
1	-0.55900782	-0.81936827	4.63940555
1	1.15863462	-0.95353216	5.13612156
1	-0.06771300	-2.06076124	5.85493746
8	-1.57618960	-1.62219611	1.35514040
6	1.04111911	-3.18292944	1.73998451
1	0.98605392	-2.75600773	0.72952437
1	2.11203858	-3.38868199	1.92337866
6	0.25102357	-4.50422990	1.84372376
1	-0.10298916	-4.64389618	2.87543031
1	0.96360544	-5.32255676	1.65740063
6	-0.92009283	-4.69167500	0.85943248
1	-0.57968610	-4.44076769	-0.16091517
1	-1.13230483	-5.77317699	0.84188082
6	-2.24837920	-3.96212007	1.14233520
1	-2.45479796	-3.95617859	2.22604767
1	-3.06277166	-4.54431157	0.67647453
6	-2.36972399	-2.52967726	0.61485661
1	-2.10140519	-2.53149622	-0.46712093
1	-3.43441592	-2.22560970	0.66760910
50	-0.45778479	-0.14051022	0.36173351
7	1.34619039	1.91423930	0.89569144
6	2.63758152	1.58572110	1.51432351
1	3.23730672	2.49218160	1.73106590
1	3.20726313	0.92246109	0.85239680
1	2.45007223	1.05309875	2.45311213
7	2.51813082	0.81171381	-1.70887402
6	1.49791797	2.67083810	-0.36842408
1	1.69051466	3.74016339	-0.14221139
1	0.53493735	2.62805019	-0.90347151
6	2.61669320	2.22238581	-1.30974591
1	2.56571731	2.89525745	-2.18759740
1	3.59021544	2.41267030	-0.83441933
6	3.15428192	0.40502854	-2.90930856
6	4.56207277	0.46748276	-3.03829235
6	5.15938581	0.04214089	-4.23227436
6	4.41682179	-0.46974855	-5.30020588
6	3.02913877	-0.56150154	-5.13817405
6	2.38560517	-0.13096459	-3.97367361
7	-1.55309710	1.45096327	1.26247405
6	0.50046080	2.66527503	1.84722866
1	0.91395518	3.68251857	2.01244536
1	0.53108471	2.11992156	2.80132461
6	-0.95638868	2.77357624	1.40531157
1	-1.48733905	3.34000082	2.19316218
1	-1.02699165	3.40208329	0.49273138
6	-2.98236764	1.42809732	1.25284359
6	-3.72995459	1.91201905	0.14871491
6	-5.13148064	1.87969646	0.19236541

6	-5.82837230	1.38194782	1.29629324
6	-5.07915944	0.91087647	2.38124923
6	-3.68015143	0.92329140	2.37964291
6	5.43961498	0.91197338	-1.89397846
1	6.24853445	0.09017581	-4.31362386
6	5.08304040	-0.89735686	-6.58584909
1	2.42163718	-0.97221944	-5.94877147
6	0.88399405	-0.24503597	-3.86348252
6	-3.05675243	2.45903194	-1.08692406
1	-5.69174623	2.24980754	-0.67069442
6	-7.33718425	1.32343693	1.30917504
1	-5.59953900	0.52269455	3.26101528
6	-2.92546222	0.39366231	3.57076463
1	6.46183516	0.53438093	-2.02720565
1	5.05152032	0.53559910	-0.93598284
1	5.50592164	2.00848937	-1.81187625
1	0.57384241	-0.92693147	-3.05503786
1	0.45780263	-0.62778449	-4.79930113
1	0.41105808	0.72760675	-3.65301503
1	5.04892036	-0.09460281	-7.33981109
1	4.58629847	-1.77415440	-7.02424332
1	6.14009421	-1.14846813	-6.42382745
1	-3.71766333	2.37262018	-1.95945156
1	-2.12198404	1.92182602	-1.30546328
1	-2.79996370	3.52463968	-0.97518072
1	-2.14855202	1.09987262	3.89740125
1	-2.41846663	-0.54277684	3.29232776
1	-3.60830226	0.20085608	4.40926778
1	-7.69852429	0.32608747	1.01181391
1	-7.77305552	2.05199386	0.61232597
1	-7.73689290	1.52586161	2.31280009
1	1.54577196	0.49908921	-1.67233178

Energy = -7584.959691 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 36

Atomic N.	X	Y	Z
8	0.67177146	-6.49377090	0.32449306
6	1.27094200	-5.60223123	-0.24354868
8	0.63812280	-4.96360995	-1.28004752
6	1.32256463	-3.94956744	-2.04833800
1	2.15429744	-4.38364829	-2.62114799
1	1.68855892	-3.12913461	-1.41879329
1	0.57239341	-3.55984296	-2.74364677
8	1.34362520	-1.23670866	2.35133500
6	2.65778739	-5.13714863	0.17074801
1	3.14644476	-6.01118065	0.62247646
1	3.25209675	-4.82666673	-0.69971733
6	2.61474820	-3.98316938	1.20082678
1	2.11706197	-3.10144284	0.77503278
1	3.65519796	-3.67687842	1.39761287
6	1.94513591	-4.36459877	2.52634099
1	0.90114685	-4.66882783	2.34704278
1	2.44990617	-5.26015405	2.92607022
6	1.97380858	-3.26294121	3.59816506
1	2.98813756	-2.83609907	3.68088272
1	1.74859315	-3.72371876	4.57565546

6	0.97748646	-2.11306117	3.41298613
1	-0.03596182	-2.54255336	3.25870885
1	0.93387703	-1.54614636	4.36706114
50	-0.11744314	-0.34058237	1.16687594
7	0.22603413	1.83355689	2.38315225
6	1.03306769	1.51578787	3.58682923
1	1.39972627	2.44374840	4.05906252
1	1.86909803	0.86201542	3.31810036
1	0.40629033	0.97365477	4.30649132
7	1.35181881	0.67972094	-0.00070768
6	1.02889123	2.62531405	1.40969999
1	1.52037219	3.46982810	1.92980954
1	0.34037793	3.01910073	0.65339637
6	2.05799293	1.74809394	0.69631386
1	2.59190759	2.38812900	-0.02830331
1	2.81886633	1.40493207	1.42399528
6	1.93802376	0.10698909	-1.15490313
6	3.28063481	-0.36302157	-1.18375075
6	3.80818088	-0.87681818	-2.37667804
6	3.05413344	-0.97549666	-3.55023190
6	1.72051726	-0.55347820	-3.49668577
6	1.15239502	-0.01800091	-2.33516938
7	-2.42645493	2.14045580	0.84385280
6	-0.99886795	2.55148035	2.84668435
1	-0.69260370	3.38214534	3.51099348
1	-1.55876765	1.83641166	3.47061515
6	-1.92940576	3.14432539	1.79096077
1	-2.75204001	3.63090639	2.35285481
1	-1.41982815	3.94907527	1.24520551
6	-3.51537286	2.49767370	-0.00234678
6	-3.37698687	3.50245663	-0.98652790
6	-4.47037966	3.80058780	-1.81092020
6	-5.68910427	3.12298951	-1.71566408
6	-5.79028278	2.10224747	-0.76264087
6	-4.73410654	1.78098392	0.09491880
6	4.13070730	-0.40151898	0.06383287
1	4.84175360	-1.23470736	-2.37600573
6	3.65966238	-1.49864707	-4.83074481
1	1.10123996	-0.62454349	-4.39511902
6	-0.28697935	0.43079136	-2.35729386
6	-2.06868968	4.21815351	-1.21746231
1	-4.34889421	4.57516733	-2.57237228
6	-6.85747033	3.48206520	-2.60141274
1	-6.72271504	1.53868207	-0.67802226
6	-4.89977170	0.66625953	1.10190518
1	4.95997494	-1.10992742	-0.06489564
1	3.53435954	-0.71356479	0.93408295
1	4.57594561	0.57722334	0.30342866
1	-0.95475580	-0.29665656	-1.86536074
1	-0.64212735	0.55022557	-3.38929905
1	-0.41552245	1.37708471	-1.81538313
1	4.50228018	-2.17426754	-4.62847362
1	4.04456409	-0.67653876	-5.45527418
1	2.92017893	-2.04385023	-5.43388316
1	-2.03166572	4.62587008	-2.23578500
1	-1.21826343	3.53246581	-1.09207081
1	-1.92121425	5.06344113	-0.52602115
1	-4.20190348	-0.16771628	0.91968479

1	-5.91506775	0.25406608	1.05400104
1	-4.73301190	1.01123223	2.13538973
1	-6.52359805	3.98481069	-3.51894123
1	-7.55177890	4.16509966	-2.08663262
1	-7.43294667	2.59123167	-2.88867141
1	-2.65871762	1.28595718	1.35131829

Energy = -7584.961803 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 37

Atomic N.	X	Y	Z
8	3.60803881	-2.43238171	0.96172255
6	3.66050653	-2.81184647	2.11682747
8	4.26446181	-1.97993377	3.02653422
6	4.43275947	-2.38583521	4.40104018
1	5.11781750	-3.24161118	4.47982560
1	3.47313160	-2.62556139	4.87787481
1	4.87967315	-1.52146059	4.90326564
8	-0.62261055	-0.90450486	2.59265383
6	3.04451942	-4.10972659	2.60203771
1	3.07956301	-4.80761929	1.75491485
1	3.62784022	-4.54576508	3.42418818
6	1.57230035	-3.91373317	3.04693992
1	1.51476440	-3.11240902	3.80008877
1	1.24976970	-4.83775834	3.55391204
6	0.61848505	-3.60812433	1.88779486
1	0.97182915	-2.72008414	1.34255258
1	0.65593503	-4.44248940	1.16796722
6	-0.83539812	-3.37989305	2.32093660
1	-1.20011331	-4.24813650	2.89884080
1	-1.46389328	-3.32471330	1.41616135
6	-1.07425295	-2.11409564	3.16626758
1	-2.15831770	-2.06711913	3.39845145
1	-0.56525899	-2.23154477	4.14406208
50	-1.01062178	-0.27073417	0.61074384
7	0.84977949	1.21985261	1.19721502
6	1.98171893	0.54357813	1.87284554
1	2.70103704	1.28726196	2.25874327
1	2.50554890	-0.13213072	1.18849683
1	1.57123855	-0.04942975	2.69741328
7	1.48026571	0.26348684	-1.69677319
6	1.31208603	2.06027701	0.05745590
1	1.89949111	2.90625230	0.46526910
1	0.41661163	2.47055570	-0.42770661
6	2.17068715	1.36028416	-0.99823364
1	2.43987240	2.12744357	-1.73492590
1	3.12468121	1.01858205	-0.55972818
6	1.76890632	0.07067485	-3.07791112
6	2.39850595	-1.12045064	-3.51417346
6	2.63939294	-1.30506382	-4.87957616
6	2.28486068	-0.34467747	-5.83470505
6	1.63335367	0.80807600	-5.38501007
6	1.35283745	1.02944426	-4.03065487
7	-1.95402614	1.60362105	1.05412518
6	0.14108042	2.07104947	2.20598833
1	0.81858108	2.87818770	2.54163657
1	-0.08029625	1.40681754	3.05210924

6	-1.16029364	2.65781155	1.66871433
1	-1.68765902	3.10683240	2.53301046
1	-0.93727147	3.50128534	0.98427667
6	-3.29888220	1.89697684	0.71761145
6	-3.64027183	2.89592280	-0.23496491
6	-4.98650775	3.15543972	-0.52133059
6	-6.02900377	2.44889528	0.08568774
6	-5.68410693	1.45364460	1.00609758
6	-4.35322332	1.16694098	1.33197902
6	2.79132075	-2.19444396	-2.52762153
1	3.12688325	-2.22811366	-5.20355700
6	2.60037965	-0.54507608	-7.29743600
1	1.30182430	1.55272732	-6.11332506
6	0.54613546	2.23870069	-3.62580082
6	-2.57920317	3.64735470	-0.99867148
1	-5.22365551	3.92453171	-1.26188968
6	-7.47153260	2.72117990	-0.26775018
1	-6.47788561	0.88829131	1.50223299
6	-4.06482921	0.09088635	2.35106019
1	3.33267193	-3.00181854	-3.03642662
1	1.91205446	-2.65041932	-2.04301732
1	3.43825751	-1.81726171	-1.72179494
1	-0.16862198	1.97314886	-2.83354972
1	-0.01353667	2.63013120	-4.48506028
1	1.16784224	3.06407038	-3.24314939
1	3.62555162	-0.21699036	-7.53275022
1	1.91807615	0.03208733	-7.93620515
1	2.52500275	-1.60328277	-7.58377607
1	-2.98469316	4.03463624	-1.94274959
1	-1.73065634	2.98639291	-1.22822362
1	-2.18217190	4.50750241	-0.43617182
1	-3.21165954	0.35568282	2.98921044
1	-3.81022581	-0.86955378	1.87002211
1	-4.94799527	-0.09432853	2.97741942
1	-7.81509117	2.05983902	-1.07942733
1	-7.61307676	3.75609643	-0.60796187
1	-8.13388600	2.54927979	0.59224665
1	1.62279780	-0.61161182	-1.19446204

Energy = -7584.962777 Hartree

Number of imaginary frequencies = 0.

Compound I5b isomer 38

Atomic N.	X	Y	Z
8	3.94709718	-2.41126858	1.75922192
6	3.60340467	-2.84358828	2.84151256
8	3.76571097	-2.02192175	3.93285697
6	3.47369896	-2.49653218	5.26295269
1	4.15836737	-3.30566627	5.55435073
1	2.43249363	-2.83145705	5.36094264
1	3.63834096	-1.63524930	5.91909988
8	-0.84260345	-1.30225715	2.11979534
6	2.95861287	-4.20352574	3.03736292
1	3.33177364	-4.84121708	2.22503272
1	3.26547096	-4.65585097	3.99054462
6	1.41227189	-4.13294057	2.96578280
1	1.03596928	-3.42042837	3.71621800
1	1.02041564	-5.12176901	3.25568639

6	0.87614626	-3.75800053	1.58060918
1	1.27812594	-2.77964029	1.28005023
1	1.25579935	-4.48427162	0.84318166
6	-0.65519798	-3.71142869	1.49861885
1	-1.08112314	-4.68436591	1.80423751
1	-0.94307610	-3.56426671	0.44425310
6	-1.32221288	-2.61391403	2.34957847
1	-2.41782369	-2.68337188	2.18733649
1	-1.16668814	-2.84150953	3.42264022
50	-1.00986324	-0.33744933	0.24063505
7	0.67418746	1.08876115	1.34355974
6	1.75332425	0.31610031	2.00315738
1	2.37650240	0.98041643	2.62726566
1	2.39173762	-0.17758270	1.26403808
1	1.28365727	-0.45358448	2.62446268
7	1.23350694	1.03789233	-1.71274003
6	1.24113713	2.16767344	0.49094444
1	1.87673050	2.81609682	1.12352216
1	0.40078409	2.78259700	0.13797437
6	2.06792347	1.71813152	-0.71204634
1	2.55390253	2.62541598	-1.12375618
1	2.87967605	1.04829785	-0.40370692
6	1.86834892	0.61046053	-2.91683262
6	2.77128357	-0.47656420	-2.90495098
6	3.35990213	-0.87893063	-4.11106522
6	3.06685247	-0.26237507	-5.33149420
6	2.13495956	0.78237697	-5.32579762
6	1.53641913	1.23246510	-4.14476395
7	-2.07179385	1.42704476	0.86463710
6	-0.19640585	1.68941937	2.40228935
1	0.38437791	2.43212616	2.98087196
1	-0.47728305	0.85735948	3.06139466
6	-1.45808886	2.32971273	1.82642391
1	-2.13111059	2.53225444	2.68300905
1	-1.21767785	3.32598699	1.39948224
6	-3.35830012	1.77297017	0.37886822
6	-3.56753550	2.91132231	-0.44664338
6	-4.85638184	3.21881129	-0.90012874
6	-5.96601682	2.43033229	-0.58043222
6	-5.74952642	1.30304998	0.21898654
6	-4.47990792	0.96159539	0.70080319
6	3.06291620	-1.24792439	-1.64299676
1	4.05230868	-1.72439917	-4.09301624
6	3.73671793	-0.70190264	-6.61101184
1	1.86782580	1.26815691	-6.26768706
6	0.53044943	2.35968233	-4.19614008
6	-2.41439536	3.77275132	-0.89581125
1	-4.99116008	4.09616268	-1.53919857
6	-7.34107102	2.76023200	-1.10995092
1	-6.59994613	0.67156488	0.49068987
6	-4.33085486	-0.26429358	1.56969968
1	3.40608550	-2.26243317	-1.88142956
1	2.16269827	-1.32706183	-1.01760760
1	3.85122644	-0.78554210	-1.02866181
1	-0.47827483	2.03053862	-3.89535139
1	0.44796708	2.75392643	-5.21655790
1	0.81068109	3.19923158	-3.54011847
1	4.61198989	-0.07265164	-6.83839062

1	3.05335702	-0.62890902	-7.46841092
1	4.08954584	-1.73964144	-6.54099920
1	-2.66462801	4.30563008	-1.82266676
1	-1.52355712	3.15225283	-1.07487620
1	-2.13604384	4.53126579	-0.14670298
1	-3.57412825	-0.11846064	2.35122196
1	-4.01013614	-1.14111968	0.98158645
1	-5.29080325	-0.52749364	2.03432147
1	-7.54147217	2.23104160	-2.05541500
1	-7.44772402	3.83541338	-1.30839978
1	-8.12547458	2.46291914	-0.40000057
1	0.44560474	1.64332044	-1.94595118

Energy = -7584.962774 Hartree

Number of imaginary frequencies = 0.

Transition state 4 (TS4)

Atomic N.	X	Y	Z
50	0.46286991	-0.15286328	-0.41808099
7	0.83436179	-0.77661002	2.59058261
6	2.05380750	-0.88564825	3.39693713
1	1.82966948	-0.95348656	4.48221254
1	2.70373464	-0.01657934	3.23272967
1	2.60972500	-1.79770899	3.12633109
7	0.48095605	1.58017170	0.84626085
6	0.07380040	0.42825508	2.97671437
1	0.08575796	0.56188530	4.07839489
1	-0.97087795	0.28786096	2.67072797
6	0.59009165	1.68777013	2.29403591
1	-0.01909990	2.53397131	2.66650915
1	1.62736571	1.89707839	2.62568855
6	0.75264543	2.78347683	0.12489545
6	-0.31048915	3.44444418	-0.54436523
6	-0.05693801	4.61939812	-1.26251090
6	1.22428215	5.17413187	-1.34829140
6	2.26487398	4.51355934	-0.68781352
6	2.05877113	3.33452392	0.04007894
7	-0.78724599	-1.72492743	0.38994420
6	0.03217628	-2.00368500	2.70636296
1	-0.32302034	-2.15900993	3.74903297
1	0.69218028	-2.84795117	2.45085740
6	-1.17131197	-2.01583552	1.76323283
1	-1.61499393	-3.02566123	1.82625318
1	-1.95029175	-1.33108521	2.15719843
6	-1.60303807	-2.33218741	-0.61471158
6	-2.96058631	-1.95834517	-0.79927164
6	-3.72231460	-2.57761598	-1.79828751
6	-3.18917108	-3.56032562	-2.63829708
6	-1.84726501	-3.91123176	-2.45752835
6	-1.05096722	-3.32407880	-1.46644330
6	-1.72105491	2.90757513	-0.48420963
1	-0.88953716	5.11858225	-1.76523376
6	1.48097754	6.42157173	-2.15919948
1	3.27869034	4.91868401	-0.75061655
6	3.24374270	2.66105962	0.68778419
6	-3.59283876	-0.87680715	0.04085185
1	-4.76217985	-2.26715255	-1.93248129

6	-4.03826427	-4.23457623	-3.68902469
1	-1.40393889	-4.67408037	-3.10305858
6	0.38579687	-3.76285481	-1.32271230
1	-2.43876004	3.67680335	-0.79922360
1	-1.97920847	2.56840038	0.52776146
1	-1.85556877	2.04065609	-1.15092647
1	3.36452031	2.96922088	1.73903275
1	4.17117119	2.92976499	0.16452409
1	3.13874555	1.56739891	0.67357117
1	1.70390391	6.17223692	-3.20901561
1	2.33877683	6.98560143	-1.76832497
1	0.60515052	7.08502054	-2.16197419
1	-4.45489597	-0.43672401	-0.47732091
1	-2.87085915	-0.07847799	0.26556757
1	-3.95401263	-1.26517236	1.00640118
1	0.66016090	-3.89028621	-0.26650444
1	1.07678497	-3.01381397	-1.74167264
1	0.55579054	-4.70783663	-1.85581815
1	-3.43727851	-4.53705263	-4.55750465
1	-4.84073687	-3.57177424	-4.04072571
1	-4.51680088	-5.14349270	-3.29050326
1	2.78642297	-1.37771499	1.15078461
8	3.09503627	-0.99963391	0.30778569
6	3.86513519	-1.98867321	-0.39911181
1	4.08502007	-1.56535363	-1.38561308
1	3.30618119	-2.92766261	-0.53230876
1	4.81446934	-2.19512534	0.11964095

Energy = -7200.136201 Hartree

Number of imaginary frequencies = 1.

Transition state 5 (TS5)

Atomic N.	X	Y	Z
8	0.70718300	-0.45696205	1.52609086
8	1.62673771	1.82974935	1.41658342
6	2.34951282	2.84666514	2.07738280
1	2.19177938	3.82094741	1.57957745
1	3.43604064	2.64700484	2.03584766
1	2.06384254	2.95904732	3.14221978
8	1.45542359	0.25758255	3.47449875
6	1.70515025	0.04530491	2.12637043
6	3.11961985	-0.32163495	1.70871878
1	3.84608436	0.44831374	2.00695157
1	3.10303426	-0.34312239	0.61486804
6	3.55183673	-1.69552016	2.26179051
1	2.70557213	-2.39735818	2.19300270
1	4.33893299	-2.09697008	1.60550082
6	4.09368706	-1.63989103	3.69525599
1	4.99314213	-0.99921429	3.70571327
1	4.42970085	-2.64416385	3.99787235
6	3.10234928	-1.10778010	4.73662090
1	2.25161028	-1.79813874	4.85451698
1	3.60372734	-1.05687988	5.71754408
6	2.54392314	0.28108022	4.42976999
1	3.33949471	0.96887290	4.10167599
1	2.08227468	0.70926970	5.32989120
50	-0.09317036	-0.76399958	-0.68621302

7	-0.87118447	2.36853290	1.24684501
6	-0.85911250	3.63186026	2.03325438
1	-1.87241542	4.05438757	2.08904529
1	-0.18799964	4.35283756	1.55191696
1	-0.49424928	3.42137432	3.04589152
7	0.19131362	1.19211161	-1.58628607
6	-1.27234006	2.65370250	-0.18043607
1	-1.70454776	3.66410446	-0.21308845
1	-2.04914212	1.94459045	-0.48195365
6	-0.11708792	2.55413008	-1.17214441
1	-0.41735089	3.15452433	-2.04980421
1	0.77364779	3.06917763	-0.75011766
6	0.79443610	1.13177109	-2.88408089
6	0.00010073	1.32182121	-4.05064058
6	0.59048444	1.24197197	-5.31668758
6	1.95514607	0.98170167	-5.48671818
6	2.72958064	0.81162453	-4.33680010
6	2.18043852	0.88661945	-3.04882884
7	-2.01413727	-0.56495512	0.29429486
6	-1.72364271	1.34666002	1.98775971
1	-2.39167094	1.91382420	2.65469599
1	-1.02665937	0.75768006	2.59631133
6	-2.62680793	0.42106348	1.17145967
1	-3.22138500	-0.09354722	1.94823468
1	-3.37890911	1.04560971	0.63552105
6	-2.74226117	-1.79601407	0.23150073
6	-3.42329359	-2.16647434	-0.95637888
6	-4.11241674	-3.38531613	-1.01671100
6	-4.16189957	-4.26394892	0.06896301
6	-3.49229050	-3.88883924	1.23907721
6	-2.78551793	-2.68482280	1.34231102
6	-1.47987819	1.59699392	-3.95343590
1	-0.04167162	1.37553334	-6.19903994
6	2.55979991	0.85935503	-6.86480141
1	3.80180073	0.62249601	-4.43904829
6	3.08778119	0.70914233	-1.85793149
6	-3.43110776	-1.25971031	-2.16275692
1	-4.63379669	-3.64896536	-1.94086099
6	-4.88065863	-5.58836603	-0.02790839
1	-3.50214648	-4.56474590	2.09894514
6	-2.05244255	-2.37516642	2.62505245
1	-2.00174975	1.24803364	-4.85439157
1	-1.69045639	2.67494416	-3.85553026
1	-1.91170132	1.10183656	-3.07455921
1	2.70674706	1.24825978	-0.98086870
1	4.10400438	1.05817640	-2.08914471
1	3.16535830	-0.35594496	-1.58261776
1	2.41036177	-0.15235515	-7.27462769
1	3.64177251	1.04795694	-6.84490824
1	2.10042834	1.56566346	-7.57045698
1	-4.25203085	-1.52650273	-2.84207940
1	-2.49305034	-1.33518934	-2.73624110
1	-3.53709030	-0.20724005	-1.86850643
1	-2.65826201	-1.75383186	3.30595255
1	-1.12107635	-1.82662594	2.42977905
1	-1.81697536	-3.30241251	3.16452694
1	-4.18331909	-6.39982557	-0.29115450
1	-5.66079092	-5.56437016	-0.80094439

1 -5.35114098 -5.86205769 0.92682326
 1 0.30497614 2.04495311 1.30227709
 Energy = -7584.900031 Hartree
 Number of imaginary frequencies = 1.

Transition state 6 (TS6)

Atomic N.	X	Y	Z
8	0.77720958	-1.79072309	0.06783146
8	-1.42207539	-2.51366544	-1.01366246
6	0.08685140	-2.83956337	0.20854874
6	0.63632321	-4.16536999	-0.30375692
1	-0.15069561	-4.93059969	-0.34028077
1	1.33244801	-4.47672415	0.49529964
6	1.38606966	-4.10453463	-1.64097869
1	1.85579765	-3.11645842	-1.73883438
1	2.20945287	-4.83456278	-1.60399866
6	0.53238714	-4.43380690	-2.87368298
1	0.13509570	-5.45885181	-2.76036215
1	1.19484377	-4.46586132	-3.75425339
6	-0.64352834	-3.49632621	-3.17880201
1	-0.27733091	-2.48076200	-3.40046167
1	-1.13492882	-3.86069965	-4.09824228
6	-1.71379161	-3.39838529	-2.07747889
1	-1.91335940	-4.41951036	-1.68763566
1	-2.66503263	-3.08272767	-2.55119538
50	1.09910774	0.25759774	1.13555253
7	-2.17338610	-0.05931803	-1.38460636
6	-3.26373720	-0.40678403	-2.34606385
1	-3.90977883	0.46640471	-2.50677538
1	-3.85025549	-1.23451066	-1.93339562
1	-2.82007718	-0.71371692	-3.30028415
7	-0.97096795	0.78355026	1.64898086
6	-2.80963588	0.42968419	-0.09484942
1	-3.81668973	-0.01117591	-0.08427133
1	-2.91928887	1.52145338	-0.15978293
6	-2.13062406	0.00313293	1.21956253
1	-2.92926121	0.11125309	1.97400069
1	-1.92823827	-1.07884157	1.14679539
6	-1.07044804	1.33425617	2.96813512
6	-1.02132523	2.74363089	3.13942885
6	-1.10050631	3.30007458	4.42220020
6	-1.23822081	2.51142597	5.56845665
6	-1.29175901	1.12597191	5.39423132
6	-1.20180452	0.52532715	4.13113928
7	0.92631155	1.15036201	-0.81327975
6	-1.28639483	0.95849591	-2.08311105
1	-1.98305321	1.66541588	-2.56610656
1	-0.75549293	0.40764719	-2.86998701
6	-0.30711311	1.78712344	-1.23397994
1	-0.08671583	2.67190337	-1.86023772
1	-0.86006296	2.15812325	-0.35427022
6	2.10701394	1.50642645	-1.54028189
6	2.82159829	2.69535136	-1.21941209
6	3.98444200	3.02723551	-1.92323422
6	4.49072981	2.21777511	-2.94706774
6	3.78376889	1.05589259	-3.25949836

6	2.60881495	0.69086570	-2.58474350
6	-0.93063223	3.66960788	1.95284295
1	-1.06472778	4.38809776	4.52406168
6	-1.28584480	3.13152695	6.94407845
1	-1.38497531	0.48127329	6.27260351
6	-1.20622981	-0.97980690	4.04816389
6	2.35322738	3.61524534	-0.12037596
1	4.51651096	3.94400907	-1.65505254
6	5.77200222	2.57528043	-3.66105843
1	4.15272188	0.40455589	-4.05691767
6	1.89364004	-0.56405050	-3.01489258
1	-0.87620234	4.71567535	2.28284621
1	-1.80876231	3.56471467	1.29712641
1	-0.05083134	3.45977187	1.33226407
1	-2.16784120	-1.37271428	3.68186569
1	-1.02470005	-1.41823828	5.03816414
1	-0.43661031	-1.34650326	3.35512471
1	-0.27316049	3.24418092	7.36335230
1	-1.86145306	2.51129603	7.64476824
1	-1.73956621	4.13196087	6.91749239
1	3.04913378	4.45524693	0.00263583
1	2.28368902	3.08798194	0.84353966
1	1.35624897	4.03021240	-0.32908973
1	1.25122142	-0.37170109	-3.89119220
1	1.26639521	-0.95287985	-2.20529866
1	2.61338735	-1.33811176	-3.31683898
1	6.65179014	2.30513716	-3.05570507
1	5.83507538	3.65497065	-3.85780978
1	5.85653734	2.04595900	-4.61962652
1	-1.67326558	-1.08916223	-1.20584834
8	-0.61967522	-2.90413570	1.39444184
6	-1.51498652	-4.00545454	1.60865188
1	-2.05819249	-3.76730084	2.53047705
1	-0.97230804	-4.95144892	1.75003254
1	-2.22430158	-4.08809805	0.77387500

Energy = -7584.902985 Hartree

Number of imaginary frequencies = 1.

Transition state 7 (TS7)

Atomic N.	X	Y	Z
8	2.47709417	1.22070158	1.45128405
6	3.38565373	2.33117986	1.41246581
1	3.05346251	3.05506587	0.65581155
1	4.41979694	2.01520801	1.20019948
1	3.35619426	2.81220508	2.40040803
1	3.02312088	0.13763013	1.68964779
8	1.11345756	-0.15862933	-0.00985993
8	3.37188172	-0.74934781	0.95494246
6	2.25553274	0.24555236	0.03713335
6	3.12575269	0.63344890	-1.12684631
1	4.11618519	0.94776142	-0.77708113
1	2.64672828	1.47745764	-1.64703810
6	3.25535679	-0.57019353	-2.08593369
1	2.25876975	-0.80088568	-2.49352336
1	3.87312150	-0.23838606	-2.93502617
6	3.86725593	-1.86445868	-1.50723636

1	4.84313536	-1.64453173	-1.04487526
1	4.07443333	-2.52573729	-2.36333299
6	2.96794772	-2.64195299	-0.52073091
1	1.92798650	-2.59944105	-0.87378204
1	3.25317669	-3.70518231	-0.52578706
6	3.03402972	-2.14656544	0.93601656
1	3.83684182	-2.65610194	1.49111521
1	2.07932973	-2.32685971	1.45157480
50	-1.17370951	0.43770766	1.57270801
7	-3.63763380	0.77350414	1.73032820
6	-4.03024912	1.22275782	3.07998776
1	-5.12896252	1.29788494	3.16991138
1	-3.59061575	2.20648003	3.28643942
1	-3.65294909	0.51265764	3.82692027
7	-1.64808583	2.03789639	0.11171695
6	-3.98039365	1.80278504	0.70762688
1	-4.91699409	2.31491041	0.99454242
1	-4.14021444	1.29068351	-0.24932308
6	-2.82936788	2.78491902	0.53851914
1	-3.11685371	3.52284098	-0.23213263
1	-2.71277618	3.36581182	1.48098576
6	-0.63657421	2.81631017	-0.50907755
6	-0.23704316	2.48138928	-1.83318329
6	0.70984632	3.26557732	-2.50159574
6	1.30197287	4.38854027	-1.90894222
6	0.93074131	4.69273424	-0.59661865
6	-0.01113814	3.93193436	0.11350077
7	-2.05329895	-1.35963595	0.70944285
6	-4.23756599	-0.54561257	1.40480995
1	-5.30123234	-0.41939566	1.12461257
1	-4.18662930	-1.16510797	2.31125140
6	-3.44512725	-1.23752236	0.29393968
1	-3.89345527	-2.23293948	0.13737677
1	-3.58413506	-0.68251252	-0.65553266
6	-1.40334821	-2.58925867	0.46720946
6	-1.37116635	-3.17855549	-0.82926786
6	-0.74256033	-4.41498899	-1.02252674
6	-0.11640648	-5.10787773	0.01779797
6	-0.14735323	-4.52157545	1.28725910
6	-0.77474028	-3.29372931	1.53388357
6	-0.83791167	1.28973103	-2.52949142
1	0.98058277	2.99769139	-3.52702761
6	2.28866220	5.24439621	-2.66701388
1	1.39631569	5.54694176	-0.09581015
6	-0.29307362	4.30093288	1.55010080
6	-1.95352721	-2.46843863	-2.02683973
1	-0.72562635	-4.83730459	-2.03138304
6	0.59252739	-6.41870832	-0.22504427
1	0.31283742	-5.04879951	2.12791491
6	-0.80200207	-2.77210593	2.94898963
1	-0.59315062	1.29703128	-3.60035801
1	-1.92888212	1.26855850	-2.40456343
1	-0.45421714	0.35493219	-2.09453344
1	-1.20125127	4.91605616	1.65468872
1	0.54090995	4.88133669	1.96762836
1	-0.43261933	3.40312576	2.17024779
1	2.99913597	4.63148975	-3.24072623
1	2.86406612	5.88748693	-1.98711944

1	1.77786207	5.90255833	-3.38781786
1	-1.50421977	-2.84833455	-2.95412207
1	-1.77057540	-1.38788271	-1.96536994
1	-3.04306006	-2.60565758	-2.11274171
1	-1.78625357	-2.34871149	3.19692993
1	-0.07217075	-1.96281731	3.11290407
1	-0.56984460	-3.57616353	3.66068077
1	1.63996458	-6.25900984	-0.52985674
1	0.10787327	-6.99618053	-1.02454138
1	0.60942185	-7.03870487	0.68215901

Energy = -7584.888346 Hartree
Number of imaginary frequencies = 1.

Transition state 8 (TS8)

Atomic N.	X	Y	Z
8	2.37836218	1.73317015	0.63084698
8	4.13576937	2.45984435	-0.49862760
6	3.34858251	1.38969100	-0.10276914
6	4.04336643	0.04719738	0.12019593
1	4.44683886	-0.34924224	-0.81993288
1	3.25202394	-0.64288831	0.44155389
6	5.15407467	0.12471003	1.18638563
1	4.84069777	0.79271144	2.00510693
1	5.28167725	-0.87342227	1.63394165
6	6.50488043	0.57246757	0.61056477
1	6.81063414	-0.15815425	-0.15879907
1	7.27429771	0.52935803	1.39818954
6	6.50860929	1.97360981	-0.01384407
1	6.38000202	2.74255919	0.76533616
1	7.49208927	2.15843844	-0.47800767
6	5.43522215	2.20774651	-1.07731080
1	5.38317537	1.37638831	-1.79796302
1	5.65939236	3.12441778	-1.64077914
1	1.02354836	0.74852788	-1.43138456
8	2.49316573	0.85947526	-1.79590833
6	2.66359067	1.71885419	-2.89542818
1	1.72104216	1.82907355	-3.47015238
1	3.42664409	1.34150267	-3.60669208
1	2.97443366	2.73688698	-2.58501577
50	0.31312689	0.13408791	1.23225009
7	-0.58738923	2.38731480	1.46428132
6	0.38107616	3.36684179	2.01974678
1	-0.11510813	4.34072304	2.17095637
1	1.23702753	3.46229982	1.34510970
1	0.75238615	2.99808955	2.98397708
7	-0.04611607	0.87679511	-1.13767982
6	-1.05936098	2.82050323	0.11465210
1	-1.14002895	3.92223787	0.09838598
1	-2.06521749	2.41398525	-0.02256603
6	-0.14060064	2.35241079	-1.00959802
1	-0.42866477	2.82594490	-1.95680046
1	0.88504130	2.68081284	-0.78720397
6	-0.88722724	0.13190699	-2.05591106
6	-2.10732985	0.56900436	-2.64495134
6	-2.75738978	-0.27843684	-3.56382418
6	-2.29148793	-1.54030514	-3.91582632

6	-1.11950827	-1.97212839	-3.29036880
6	-0.41824588	-1.17879641	-2.38106871
7	-1.70431256	-0.12210787	1.97859395
6	-1.74853039	2.25258994	2.39400506
1	-2.35395408	3.17715740	2.36217189
1	-1.33333504	2.14259768	3.40556669
6	-2.59155440	1.02174997	2.07115197
1	-3.32377911	0.89679247	2.88973737
1	-3.19745350	1.20338058	1.15713847
6	-2.23755717	-1.40757859	2.27798295
6	-3.24073434	-2.00658250	1.47180605
6	-3.72606993	-3.27914214	1.79843724
6	-3.24883294	-3.99850535	2.89826226
6	-2.26276541	-3.39741516	3.68753815
6	-1.75233805	-2.12423539	3.40435982
6	-2.88330984	1.83926690	-2.34032965
1	-3.68624878	0.08140280	-4.01261711
6	-3.01185155	-2.40352488	-4.92136621
1	-0.72470868	-2.96551228	-3.51609516
6	0.82514191	-1.77142811	-1.76458848
6	-3.77201295	-1.30963171	0.24541096
1	-4.49317217	-3.72514534	1.15951562
6	-3.75707078	-5.38644934	3.20622349
1	-1.88389611	-3.93003035	4.56391716
6	-0.71189666	-1.53528821	4.32766390
1	-3.68409014	1.95175695	-3.08160996
1	-2.29930449	2.76344085	-2.36241937
1	-3.37945533	1.77693272	-1.35840094
1	1.71844149	-1.15457666	-1.94765568
1	0.99538189	-2.77806711	-2.16653514
1	0.72784477	-1.87450409	-0.66979706
1	-3.18502235	-3.41614199	-4.52849150
1	-2.42380929	-2.51366782	-5.84559536
1	-3.98438358	-1.97273052	-5.19334555
1	-4.24419689	-2.02856660	-0.43632385
1	-2.96622014	-0.79602540	-0.29694834
1	-4.53160477	-0.55244869	0.49888843
1	-0.91412002	-0.47621465	4.53906393
1	0.29869336	-1.58039963	3.89203644
1	-0.68541503	-2.08733249	5.27664423
1	-3.14910054	-6.15344143	2.70022607
1	-4.79428864	-5.51830053	2.86909986
1	-3.71621108	-5.59828806	4.28361034

Energy = -7584.922994 Hartree

Number of imaginary frequencies = 1.