

DFT modeling of the carbon dioxide and alkene oxide reaction catalyzed by a Cr^{III} complex

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I. Figures

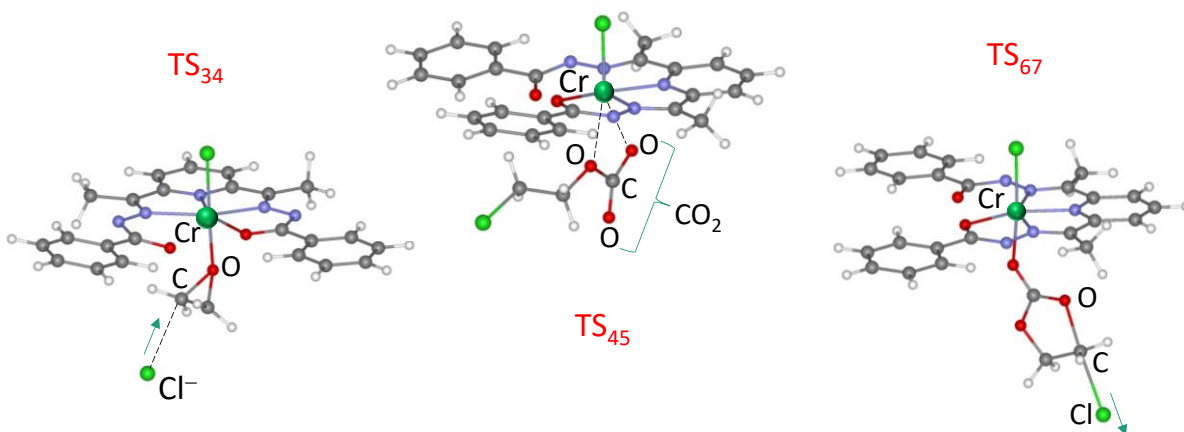


Figure S1. Optimized structures of the key transition states on the reaction path.

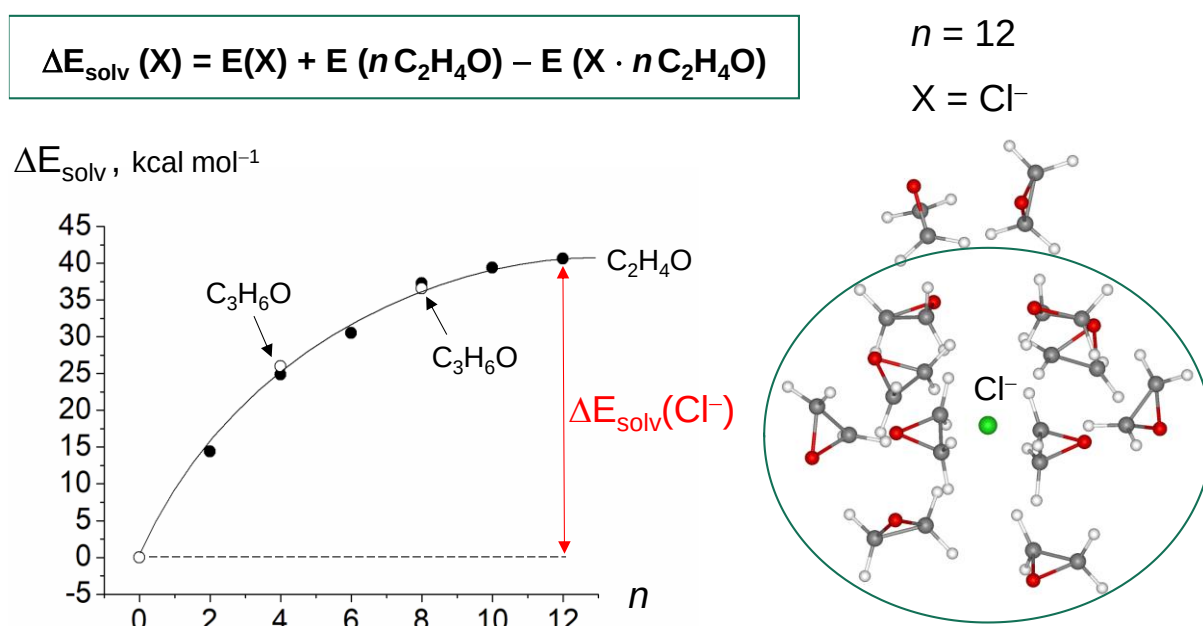


Figure S2. Formular for ΔE_{solv} energy calculation, ΔE_{solv} dependence on the number of epoxide molecules for $X = \text{Cl}^-$, optimized structure of the system $\{\text{Cl}^- + 12\text{C}_2\text{H}_4\text{O}\}$.

II. Atomic coordinates, total energies without (E) and with ZPE (E_0) corrections (a.u.).

Stable structures

1

E = -3276.149365 a.u., E_0 = -3275.765949 a.u.

Atomic Coordinates:

24	0.82407147	-0.09520378	0.24186170
6	-4.36984873	0.74480146	2.26565313
6	-4.96722221	-0.58917218	0.32573935
1	-4.67568207	-1.27413392	-0.46845272
6	-3.99863625	-0.14662734	1.24323106
6	-6.65133095	0.73349535	1.45585096
6	-5.68841791	1.18096173	2.36790538
6	-6.28663635	-0.15024209	0.43632078
8	-2.33544135	-1.28527415	0.00724286
1	-7.03321266	-0.49882066	-0.27787447
6	-2.59715223	-0.60579419	1.12154627
7	-1.77480948	-0.33521903	2.10599685
6	0.22069521	-0.93453979	3.02053142
6	4.37054157	-1.17556548	2.18882203
1	5.42311239	-1.21430397	1.91509652
6	3.41225839	-0.74525893	1.25604963
6	1.66917086	-1.05786288	2.84520173
6	2.58972049	-1.50075543	3.80881858
6	3.94292212	-1.55317760	3.46300840
7	2.10364914	-0.70425469	1.61937356
1	4.67284393	-1.89364207	4.19746017
6	3.66194940	-0.32582539	-0.11559953
7	2.55098176	0.01342127	-0.75259084
7	-0.44406086	-0.56628537	1.94023085
6	1.24961841	0.67421538	-2.38344979
6	1.78651726	1.74433303	-5.97733307
6	-0.57776076	1.86420941	-5.46126032
1	-1.60154927	2.08386493	-5.76588869
6	0.47335708	2.02548409	-6.37032032
6	0.99734640	1.13974988	-3.76478982
6	2.05108356	1.30355990	-4.68193150
6	-0.31980950	1.42368388	-4.16444969
8	0.25125229	0.52960944	-1.58268690
1	-1.12506735	1.29318643	-3.44263911
7	2.53392196	0.42049509	-2.03132558
1	2.25629497	-1.80167520	4.79906178
1	3.06774592	1.08131611	-4.36210775
1	2.60662150	1.87007916	-6.68512249
1	-5.96776915	1.87708914	3.15932751
1	-3.60929680	1.09286940	2.96290016
1	-7.68322945	1.07660091	1.53868937
1	0.26960820	2.37062883	-7.38480186
6	5.02031708	-0.29002827	-0.73395413
1	4.94302702	0.06653382	-1.76586711

1	5.68921328	0.38120371	-0.17406431
1	5.47895050	-1.29072261	-0.73688263
6	-0.45398360	-1.20275652	4.32588625
1	0.23700817	-1.08759511	5.16825247
1	-1.30033028	-0.51390475	4.44243574
1	-0.86593246	-2.22369528	4.35355616
17	0.44298157	-2.33399701	-0.43490624
17	0.92595863	2.06493878	0.98526996
1	-1.39555812	-1.65999734	-0.04302195

2

E = -2815.471275 a.u., E₀ = -2815.100312 a.u.

Atomic Coordinates:

24	0.69470945	0.19040899	0.59532755
6	-4.31642776	0.38558093	2.19827141
6	-3.98325295	-0.23502569	-0.12705905
1	-3.30073844	-0.49485653	-0.93520977
6	-3.45114385	0.03838581	1.14467168
6	-6.21608889	0.18234479	0.71022925
6	-5.69029568	0.45806694	1.97786301
6	-5.35947468	-0.16351151	-0.33982560
8	-1.22510498	-0.35268599	0.34771900
1	-5.76640533	-0.37534272	-1.32921228
6	-1.99040180	-0.03440177	1.35403103
7	-1.49600233	0.19071000	2.57921402
6	0.57480064	-0.40539576	3.48429820
6	4.03071950	-2.12154084	1.76917436
1	4.88437686	-2.57208671	1.26754513
6	3.01583367	-1.50164669	1.02022761
6	1.84272135	-0.94453069	3.01830710
6	2.85207096	-1.51845124	3.80349058
6	3.94002583	-2.11796718	3.16245758
7	1.94000485	-0.96576752	1.66019092
1	4.73059248	-2.57789507	3.75542121
6	2.99672454	-1.29530103	-0.41438086
7	1.98711897	-0.52220474	-0.79814105
7	-0.15405364	0.03829224	2.47772399
6	0.89219375	0.79422526	-2.14830230
6	0.94759444	1.54492630	-5.86085194
6	-0.72336687	2.94080134	-4.79810413
1	-1.49471072	3.70879191	-4.86495245
6	-0.04450548	2.52782689	-5.94944735
6	0.58050323	1.38652006	-3.46856241
6	1.26210940	0.97567039	-4.62809229
6	-0.41469426	2.37419740	-3.56241839
8	0.22293783	1.17605554	-1.11845491
1	-0.93094718	2.68448558	-2.65476166
7	1.88286318	-0.12168891	-2.08006749
1	2.77965079	-1.49921931	4.88920507
1	2.03404753	0.21234955	-4.54320827

1	1.47848577	1.22324647	-6.75757481
1	-6.35648902	0.73100336	2.79709354
1	-3.89405735	0.59776297	3.17944669
1	-7.29221299	0.23889488	0.54160675
1	-0.28684130	2.97284923	-6.91537664
6	4.03112103	-1.78763199	-1.37107500
1	3.54802309	-2.15932143	-2.28423273
1	4.69536831	-0.96516412	-1.67973907
1	4.64033700	-2.58629867	-0.93317082
6	0.07922638	-0.53526323	4.88727112
1	0.81503805	-0.12636501	5.59490421
1	-0.86623885	0.00526973	4.99725706
1	-0.08976661	-1.58990289	5.15594549
17	1.96402208	1.99080067	1.19332771

3

$E = -2969.145638$ a.u., $E_0 = -2968.717477$ a.u.

Atomic Coordinates:

24	0.62923980	0.28059247	0.43375444
6	-4.88313913	0.52045041	1.61851466
6	-4.53357840	0.09384112	-0.74341422
1	-3.84280610	-0.12976430	-1.55626655
6	-4.01395178	0.21995600	0.55529964
6	-6.75879574	0.56029421	0.08629082
6	-6.24763870	0.68809628	1.38232291
6	-5.89769745	0.26440650	-0.97608310
8	-1.79575670	-0.29233527	-0.18873861
1	-6.29297209	0.17056449	-1.98849106
6	-2.54694986	0.03564743	0.76465744
7	-2.11240315	0.22086295	2.05408454
6	-0.23427130	0.18960406	3.33237195
6	3.98475814	0.14665778	3.01109719
1	5.06240034	0.14640348	2.86268306
6	3.11893320	0.16787127	1.90884435
6	1.21225488	0.17352311	3.32806134
6	2.04732943	0.16048235	4.46623468
6	3.42797422	0.14288083	4.29414701
7	1.77176690	0.16716006	2.09085369
1	4.08094692	0.13416670	5.16729164
6	3.53752136	0.22048149	0.51553982
7	2.52220821	0.27517694	-0.32717133
7	-0.78212726	0.18633400	2.12123847
6	1.50172317	0.37356427	-2.25677991
6	2.58507943	0.53197193	-5.88828468
6	0.16770183	0.64609295	-5.77703857
1	-0.79847884	0.72929603	-6.27608967
6	1.34589839	0.62968028	-6.53108644
6	1.46717787	0.46181831	-3.73642516
6	2.64917350	0.44956419	-4.49820089
6	0.22530924	0.56230366	-4.38650513

8	0.39108402	0.30964848	-1.61244833
1	-0.67952859	0.58235341	-3.77969527
7	2.71249795	0.35084283	-1.65856707
1	1.61355650	0.16801094	5.46320820
1	3.60650182	0.37768668	-3.98429060
1	3.50450420	0.52290142	-6.47494173
1	-6.91701174	0.92203808	2.21135306
1	-4.47009659	0.62097609	2.62096834
1	-7.82603884	0.69412172	-0.09589939
1	1.29927921	0.69690168	-7.61882734
6	4.97086239	0.24459539	0.09456041
1	5.03219175	0.25440428	-0.99786562
1	5.47601223	1.14121795	0.48559061
1	5.51105690	-0.63319814	0.48001745
6	-1.07530606	0.22088023	4.56817627
1	-1.74375749	-0.65215456	4.60363913
1	-0.47259325	0.24579336	5.48211241
1	-1.73147595	1.10355854	4.54628706
17	0.54573452	2.54142499	0.54717469
6	-0.25317815	-2.83731437	0.73037606
6	0.05274217	-2.65259457	-0.69582391
8	0.76809698	-1.87004793	0.32037467
1	0.16997737	-3.68323278	1.27388644
1	-1.15785849	-2.38231826	1.13090754
1	-0.62784237	-2.05067992	-1.29688239
1	0.70376080	-3.36346173	-1.20610261

4

$E = -3429.321513$ a.u., $E_0 = -3428.893846$ a.u.

Atomic Coordinates:

6	1.64900279	1.79104841	0.49119729
6	2.74303102	2.00566745	-0.55243766
8	1.60211086	0.41521323	0.75895774
1	0.69368792	2.18638062	0.10708133
1	1.90880430	2.35849690	1.40898669
1	3.69948554	1.59479427	-0.21225470
1	2.46564245	1.57293057	-1.51840377
24	0.06818977	-0.69886804	0.51326108
6	0.18972294	-0.12543190	-5.19953060
6	-1.05857301	1.70242846	-4.21912956
1	-1.41356933	2.20476007	-3.31887698
6	-0.28131559	0.54490721	-4.05833864
6	-0.88752002	1.51077008	-6.62761021
6	-0.11232686	0.35571575	-6.47484207
6	-1.35964358	2.18209219	-5.49443483
8	-0.41998407	0.69583809	-1.67737150
1	-1.96524882	3.08339143	-5.60721779
6	0.01474251	0.06460439	-2.66243243
7	0.79236841	-1.06784630	-2.61306548
6	1.75738871	-2.54274321	-1.19635701

6	1.94183433	-3.66406846	2.88059402
1	1.93987429	-3.90628910	3.94153953
6	1.18028748	-2.58499908	2.39921403
6	1.89081061	-2.99517965	0.17005302
6	2.67344618	-4.08798361	0.60982245
6	2.68990111	-4.40880156	1.96459305
7	1.17807400	-2.28036165	1.07560539
1	3.29058766	-5.25078249	2.31290603
6	0.34036946	-1.72538161	3.21160340
7	-0.27641872	-0.78787738	2.51230907
7	0.95974833	-1.49341321	-1.36011350
6	-1.57599354	0.93484229	2.15779233
6	-3.80262613	3.11938930	4.33843184
6	-3.94635582	3.87954354	2.04523063
1	-4.35043812	4.56574965	1.29895377
6	-4.32343102	4.00368977	3.38672090
6	-2.52821970	1.99062645	2.60702181
6	-2.91081238	2.11802197	3.95315552
6	-3.05435681	2.87983537	1.65591788
8	-1.25415587	0.88356143	0.92518526
1	-2.74629045	2.76062942	0.61715496
7	-1.10592270	0.09332698	3.10664368
1	3.25296760	-4.66878843	-0.10405333
1	-2.49716496	1.42045450	4.68019485
1	-4.09478998	3.21180487	5.38617277
1	0.25781941	-0.17236723	-7.35600710
1	0.79079390	-1.02315259	-5.06052542
1	-1.12259507	1.88574111	-7.62561369
1	-5.02131605	4.78623676	3.69013286
6	0.18261907	-1.90142059	4.68900490
1	-0.49609229	-1.13298762	5.07320976
1	-0.23028642	-2.89432883	4.92760468
1	1.15227187	-1.81413913	5.20441771
6	2.43768430	-3.19322157	-2.36174464
1	3.04866481	-4.05151939	-2.05956984
1	1.68870592	-3.52549148	-3.09625006
1	3.07506084	-2.46575499	-2.88685727
17	-1.77035129	-2.13450146	0.10399599
17	3.05009937	3.79520750	-0.86162907

5

$E = -3617.804270$ a.u., $E_0 = -3617.361819$ a.u.

Atomic Coordinates:

6	0.61447909	-3.44565353	-3.02391303
6	1.71810038	-3.22423504	-1.99864390
24	0.43198107	0.47286826	0.74190104
6	-5.06946617	0.74529548	2.30457524
6	-4.87533053	0.92111798	-0.10251423
1	-4.23170939	0.92526938	-0.98261902
6	-4.26733981	0.75477000	1.15147364

6	-7.05290826	1.06549922	0.94804083
6	-6.45326852	0.89965312	2.20142138
6	-6.25828455	1.07578507	-0.20371500
8	-2.09846363	0.59159025	0.16392253
1	-6.72069971	1.20502546	-1.18416024
6	-2.77258426	0.59438951	1.21125820
7	-2.27293155	0.45081501	2.48776453
6	-0.35573459	0.15917158	3.65339538
6	3.84704286	-0.02860715	3.19361103
1	4.91901235	-0.06113623	3.01007736
6	2.95212988	0.17025154	2.12949002
6	1.08414041	0.07419010	3.59477225
6	1.94873030	-0.13157572	4.69536217
6	3.32223294	-0.18104661	4.48053633
7	1.61405382	0.21456644	2.35338718
1	3.99530695	-0.33974707	5.32465923
6	3.33467191	0.36067053	0.74161633
7	2.30280502	0.52283190	-0.06737460
7	-0.94802728	0.35712911	2.48035331
6	1.24783107	0.83645382	-1.95287125
6	2.30654454	1.39430771	-5.56420703
6	-0.11040123	1.40238131	-5.43528546
1	-1.08372871	1.48856161	-5.92124348
6	1.06121281	1.50623188	-6.19273359
6	1.20757982	1.07272003	-3.42360894
6	2.38186628	1.17886617	-4.18783536
6	-0.03975493	1.18765797	-4.05855208
8	0.14867468	0.71979002	-1.32085476
1	-0.93693691	1.10301128	-3.44524347
7	2.47197795	0.75543764	-1.38033521
1	1.53992825	-0.24957651	5.69615466
1	3.34262787	1.08797488	-3.68294340
1	3.22295606	1.47331994	-6.15178830
1	-7.06914462	0.89047809	3.10296994
1	-4.58465200	0.61495310	3.27118423
1	-8.13507729	1.18590318	0.86932341
1	1.00460841	1.67243635	-7.26995417
6	4.75881504	0.39739163	0.28623411
1	4.78616657	0.50371248	-0.80301335
1	5.29719822	1.24462216	0.73987501
1	5.28866018	-0.52410327	0.57293715
6	-1.15248664	0.04078580	4.91563523
1	-1.85786132	-0.80057268	4.84130430
1	-0.51604865	-0.10288747	5.79619231
1	-1.76719887	0.94209902	5.05876134
17	0.49944316	2.78449300	1.04737625
1	0.40337730	-2.53642154	-3.59545560
1	-0.29344328	-3.82687311	-2.54824441
1	2.64432847	-2.90645481	-2.49652228
1	1.88969621	-4.14521229	-1.42535418
8	1.35219071	-2.14809234	-1.12581538
17	1.13768092	-4.70884347	-4.23877477

8	0.14865053	-3.67562535	0.09135188
6	0.50211001	-2.50641667	-0.05706387
8	0.19467067	-1.50139813	0.68372257

6

E = -3617.807237 a.u., E₀ = -3617.364807 a.u.

Atomic Coordinates:

6	0.87395275	-5.10191965	1.15966022
6	0.93303597	-4.56033707	-0.26253498
24	0.43590343	0.77955866	0.28937480
6	-5.07211304	0.73217964	1.86071873
6	-4.88523436	1.14042675	-0.51846975
1	-4.24098253	1.26771259	-1.38890457
6	-4.27000523	0.90045476	0.71993303
6	-7.06994247	1.04228938	0.52293938
6	-6.46304321	0.80292398	1.76087666
6	-6.27533484	1.21083665	-0.61649311
8	-2.09342003	0.99083823	-0.25961268
1	-6.74336338	1.39784908	-1.58491385
6	-2.76742744	0.83288378	0.77529997
7	-2.26166654	0.58944941	2.03361368
6	-0.33018157	0.31593421	3.18135548
6	3.87028742	0.25430337	2.69491386
1	4.94074965	0.24068294	2.50181508
6	2.96514273	0.44747630	1.64068568
6	1.11219072	0.27468961	3.11464858
6	1.98722196	0.07208886	4.20585823
6	3.36033797	0.06482653	3.98191023
7	1.62849724	0.45545316	1.87308931
1	4.04349518	-0.09230015	4.81811428
6	3.33398342	0.64360946	0.25015110
7	2.29627085	0.80682069	-0.54677486
7	-0.93217266	0.54203147	2.01841426
6	1.22632897	1.13740158	-2.42618775
6	2.26098228	1.59164310	-6.06093550
6	-0.14858532	1.75016284	-5.89507103
1	-1.12238479	1.89310920	-6.36668396
6	1.01508009	1.77561486	-6.67134619
6	1.17828369	1.35773861	-3.90081692
6	2.34458303	1.38413894	-4.68368578
6	-0.06948142	1.54206133	-4.51773214
8	0.13293757	1.10149562	-1.77614725
1	-0.95979029	1.51714778	-3.88933086
7	2.45284152	0.98574710	-1.87311041
1	1.58777583	-0.07393182	5.20679951
1	3.30561113	1.23850906	-4.19222546
1	3.17134261	1.61018312	-6.66296196
1	-7.07878399	0.67094415	2.65289617
1	-4.58168030	0.54714209	2.81554842
1	-8.15759850	1.09723544	0.44672137

1	0.95192611	1.93792212	-7.74891853
6	4.75047064	0.62782228	-0.22529331
1	4.78181839	0.91481382	-1.28121650
1	5.37251663	1.32128251	0.36037377
1	5.17949820	-0.38127959	-0.11943121
6	-1.11815262	0.13364971	4.44144917
1	-1.82961512	-0.69769883	4.32549095
1	-0.47628450	-0.06195814	5.30794573
1	-1.72763038	1.02836394	4.63975525
17	0.52747041	3.07019567	0.69204271
8	0.14434445	-1.15825069	-0.06973583
1	-0.15936048	-5.23246765	1.49695146
1	1.43224967	-4.46056557	1.84726524
1	0.44120601	-5.25595999	-0.95634943
1	1.97778404	-4.40191078	-0.56142145
6	0.90493923	-2.18400812	0.06206988
8	2.06960797	-2.28384447	0.45667303
8	0.19070761	-3.33826399	-0.33961910
17	1.65285349	-6.75494242	1.24057221

7

$E = -3617.791155$ a.u., $E_0 = -3617.347717$ a.u.

Atomic Coordinates:

6	2.18268132	-3.90392494	0.49349004
6	0.91842151	-4.61117744	0.01058109
24	0.32395998	0.74053454	0.33477938
6	-5.17971802	0.96605551	1.81063306
6	-4.91197824	1.34486687	-0.56739628
1	-4.24305296	1.42381716	-1.42460525
6	-4.34350729	1.07330775	0.68695253
6	-7.12029028	1.39838278	0.42476311
6	-6.55985928	1.12780297	1.67786634
6	-6.29137039	1.50659537	-0.69737977
8	-2.14250040	0.99548709	-0.23875710
1	-6.72416401	1.71756124	-1.67686689
6	-2.85487080	0.90675032	0.78067207
7	-2.38713980	0.65471697	2.05306864
6	-0.48587731	0.28014758	3.22713113
6	3.71336651	0.04383862	2.77697420
1	4.78438711	-0.01127764	2.59540105
6	2.82802558	0.28141475	1.71603084
6	0.95333463	0.17574237	3.17075920
6	1.80923760	-0.07003652	4.26817608
6	3.18240333	-0.13411975	4.05784988
7	1.48839092	0.33896536	1.93319452
1	3.84969831	-0.32777226	4.89855242
6	3.22133994	0.46665752	0.32943586
7	2.19756651	0.66023654	-0.48074269
7	-1.06394565	0.54020029	2.05865955
6	1.16039336	1.02443850	-2.37145519

6	2.23108697	1.40809035	-5.99838829
6	-0.17039859	1.67789781	-5.84650183
1	-1.13375187	1.86174095	-6.32468271
6	0.99768478	1.64458501	-6.61569309
6	1.12734151	1.23832595	-3.84409285
6	2.29856753	1.20624065	-4.61989117
6	-0.10834304	1.47555447	-4.46786308
8	0.06157556	1.02906883	-1.72316015
1	-1.00331366	1.49615550	-3.84627652
7	2.37440968	0.83097517	-1.80486608
1	1.39423037	-0.20668732	5.26385307
1	3.25029325	1.01981723	-4.12442064
1	3.14376116	1.37980044	-6.59582090
1	-7.20325470	1.04209697	2.55547857
1	-4.72621584	0.75518930	2.77812123
1	-8.19972706	1.52400720	0.32301968
1	0.94747490	1.80145311	-7.69448996
6	4.64372206	0.42158720	-0.12611328
1	4.69288015	0.66908926	-1.19099414
1	5.25959873	1.13518393	0.44160789
1	5.07177353	-0.58176738	0.02541330
6	-1.29403865	0.12766488	4.47745132
1	-2.04310966	-0.66764778	4.34898424
1	-0.67236269	-0.10431714	5.34918594
1	-1.86120224	1.04978991	4.67510366
17	0.51726747	2.99052930	0.72892237
8	-0.07419019	-1.25938320	-0.02406349
1	2.47042775	-4.16054153	1.51338530
1	3.03511643	-4.01214314	-0.17797798
1	0.47714576	-5.27747917	0.75284207
1	1.04117334	-5.13441133	-0.93852431
6	0.53339648	-2.33664989	0.07949672
8	1.79198635	-2.44849133	0.48847935
8	-0.05301231	-3.48808908	-0.21943589
17	2.87707448	-6.71644640	0.53414422

8

$E = -3157.643075$ a.u., $E_0 = -3157.198606$ a.u.

Atomic Coordinates:

6	-1.05854249	-3.03385568	-1.73935521
6	-1.30743754	-3.88532829	-0.49184519
24	0.80288315	0.62737662	0.59908587
6	-4.78676748	0.26474008	1.65790212
6	-4.38936234	-0.02420004	-0.71448278
1	-3.67712021	-0.13419491	-1.53257549
6	-3.88713908	0.09287567	0.59180701
6	-6.65325499	0.19082178	0.11417836
6	-6.16054726	0.30940723	1.41817963
6	-5.76280546	0.02775171	-0.95243514
8	-1.63891912	-0.28817192	-0.14007831

1	-6.14233208	-0.05197677	-1.97224414
6	-2.40565729	0.03247649	0.80457169
7	-2.00222683	0.32027644	2.07927299
6	-0.18269964	0.45021254	3.42536378
6	4.04075670	0.72081244	3.30434895
1	5.12203741	0.79084969	3.20713234
6	3.22706652	0.68937856	2.16377020
6	1.25970292	0.55057478	3.49466729
6	2.04067993	0.58710527	4.67034864
6	3.42555261	0.66989142	4.56015301
7	1.87766612	0.59997129	2.28940797
1	4.03710032	0.69920355	5.46241283
6	3.69624996	0.75933862	0.78568512
7	2.71094370	0.74048030	-0.09332217
7	-0.67613810	0.40473297	2.19106221
6	1.73552406	0.76982051	-2.04704905
6	2.90054035	0.91955507	-5.65464115
6	0.47904021	0.94464749	-5.60243893
1	-0.47720432	0.98682845	-6.12550306
6	1.67484093	0.96265841	-6.32835340
6	1.73447812	0.83642966	-3.52857423
6	2.93378544	0.85840708	-4.26215792
6	0.50636590	0.88080311	-4.20980644
8	0.61145431	0.67961687	-1.43220973
1	-0.41221413	0.87446922	-3.62364292
7	2.93275762	0.80434918	-1.42003095
1	1.56429362	0.55041373	5.64699602
1	3.88016105	0.82893133	-3.72434855
1	3.83383608	0.93726313	-6.21885777
1	-6.85215473	0.44103575	2.25159240
1	-4.38884878	0.36164466	2.66686249
1	-7.72760630	0.23101158	-0.07076008
1	1.65221775	1.01481545	-7.41773748
6	5.14004898	0.86370724	0.41667920
1	5.23772573	0.90189904	-0.67263895
1	5.58707857	1.77332330	0.84615612
1	5.71029091	0.00352899	0.79928672
6	-1.07640076	0.39309728	4.62263107
1	-1.63026202	-0.55716544	4.64829063
1	-0.52149755	0.50637245	5.55995369
1	-1.83484447	1.18649626	4.55415010
17	0.54894274	2.87634873	0.71975750
8	0.95071238	-1.52012193	0.60343307
1	-0.82935882	-3.61317515	-2.63903856
1	-1.85774183	-2.30530047	-1.92354727
1	-0.85355031	-4.88435698	-0.54529655
1	-2.36339617	-3.96010971	-0.21347086
6	0.19103199	-2.23947930	-0.03643081
8	0.13054694	-2.28074527	-1.37388909
8	-0.62027889	-3.13756919	0.55162323

$E = -3157.647108$ a.u., $E_0 = -3157.203046$ a.u.

Atomic Coordinates:

6	0.61965877	-3.33102345	-0.04592742
6	-0.91069406	-3.31657076	0.02241408
24	0.51238775	1.10082984	0.55824345
6	-4.67836523	0.22837067	1.05094206
6	-3.68252611	-0.35840181	-1.08435369
1	-2.79263020	-0.45248023	-1.70613050
6	-3.53605413	0.07397372	0.24488576
6	-6.08219099	-0.48321018	-0.79042941
6	-5.94170046	-0.04994535	0.53306901
6	-4.95014906	-0.63397050	-1.59729075
8	-1.14407170	0.05423061	0.04759551
1	-5.05690527	-0.96153575	-2.63212919
6	-2.18721032	0.37132338	0.77331418
7	-2.07051992	0.92506152	1.98120439
6	-0.22532405	0.94537437	3.41203690
6	3.81601143	-0.14820988	2.86928892
1	4.83598423	-0.46579814	2.66332054
6	2.92334270	0.09141900	1.81268239
6	1.20354378	0.66370964	3.35257268
6	2.06853747	0.46515289	4.43583965
6	3.37725568	0.04893041	4.18004084
7	1.64564288	0.46659920	2.08326149
1	4.06255293	-0.12142602	5.01016855
6	3.22395110	0.03763661	0.39351943
7	2.21388149	0.46398297	-0.35317510
7	-0.73739201	1.07275963	2.20562673
6	1.25211418	1.22838151	-2.15808105
6	2.06095147	1.28658843	-5.86118746
6	-0.04741831	2.42193580	-5.49573088
1	-0.90887696	2.96482062	-5.88625479
6	0.95337582	1.97705710	-6.36593103
6	1.16435075	1.48233652	-3.61546803
6	2.16981864	1.04002726	-4.49351978
6	0.05509961	2.17680645	-4.12700796
8	0.29429874	1.62886620	-1.39804363
1	-0.71182048	2.51974177	-3.43345547
7	2.34642029	0.59107488	-1.69159794
1	1.71608222	0.61776608	5.45376778
1	3.02925038	0.50971788	-4.08612967
1	2.84411192	0.94268906	-6.53789568
1	-6.82327080	0.07029048	1.16375995
1	-4.55514097	0.56471020	2.07934046
1	-7.07281590	-0.69966799	-1.19216263
1	0.87262714	2.17123985	-7.43623638
6	4.54788303	-0.35184178	-0.17591736
1	4.41187143	-0.77603638	-1.17747867
1	5.19906950	0.53058916	-0.28503355
1	5.06066751	-1.07883382	0.46578714

6	-1.03295541	0.85651815	4.66307974
1	-1.09430718	-0.18987951	5.00132036
1	-0.56928182	1.44550455	5.46692705
1	-2.04761267	1.22375500	4.47987509
17	1.25088620	3.21784329	0.98019069
8	-0.00049185	-2.52680278	3.25500488
1	1.03966248	-4.34447527	-0.12143153
1	1.02205670	-2.69339490	-0.84136111
1	-1.37830567	-4.22375870	-0.37523144
1	-1.33754206	-2.41799378	-0.44188726
6	-0.05436624	-2.82293773	2.09013677
8	1.01219285	-2.77018476	1.23002839
8	-1.17560422	-3.25923991	1.44723415

Transition states

TS₂₃

E = -2969.141212 a.u., E₀ = -2968.713792 a.u., v_i = 35i cm⁻¹

Atomic Coordinates:

24	0.49543988	0.51410095	0.54931448
6	-4.81319778	0.47290393	1.39366400
6	-4.10775778	-0.23855931	-0.81780889
1	-3.29862428	-0.48001962	-1.50639823
6	-3.78236705	0.14193480	0.49533992
6	-6.46194434	0.03968533	-0.32699252
6	-6.14361892	0.42082087	0.98153214
6	-5.44056739	-0.28770694	-1.22487949
8	-1.44275598	-0.18612580	0.08606257
1	-5.68531807	-0.57886604	-2.24713050
6	-2.36163364	0.19114658	0.90892198
7	-2.06935493	0.60629733	2.15282025
6	-0.17595336	0.63983329	3.47148810
6	3.94278492	-0.11035957	2.99265528
1	4.99606732	-0.30492134	2.80380121
6	3.03586663	-0.04879443	1.92322721
6	1.25226593	0.42535091	3.41459064
6	2.13056846	0.39977294	4.50908782
6	3.47822262	0.11406076	4.28944333
7	1.70894535	0.17252977	2.15411605
1	4.17241464	0.08333677	5.12910791
6	3.37862532	-0.12052939	0.52212535
7	2.34242348	0.12631956	-0.26514809
7	-0.72926434	0.61799898	2.27194406
6	1.35880762	0.56369364	-2.15188302
6	2.29521596	0.58902877	-5.82113655
6	-0.01316667	1.28733444	-5.59257457
1	-0.94841282	1.62209789	-6.04274195
6	1.09371641	1.01089015	-6.40186057
6	1.28058675	0.71593387	-3.62157514
6	2.39226367	0.44243797	-4.43852472
6	0.07687864	1.14139588	-4.20877951

8	0.29717863	0.76448568	-1.44590651
1	-0.77221057	1.35881975	-3.56161784
7	2.52993145	0.21332143	-1.59971306
1	1.75850493	0.59617821	5.51221210
1	3.32192569	0.11980954	-3.97188650
1	3.16016695	0.37649800	-6.45062577
1	-6.93817053	0.68027945	1.68227171
1	-4.55142215	0.77048094	2.40811272
1	-7.50412623	0.00088433	-0.64647233
1	1.02202099	1.12750751	-7.48400785
6	4.75080729	-0.34628483	-0.02168218
1	4.70916887	-1.05635583	-0.85808316
1	5.16359968	0.59054427	-0.42701191
1	5.43296898	-0.73027353	0.74453823
6	-0.98348291	0.76179328	4.72221401
1	-1.51957826	-0.17635438	4.93553810
1	-0.35674279	1.00844824	5.58641757
1	-1.74812726	1.53897617	4.59461886
17	0.85805768	2.75200822	0.73869942
6	-0.36242619	-3.08209206	0.68232470
6	0.11074314	-2.80981497	-0.68344696
8	0.73015725	-2.15415774	0.45600184
1	-0.06223462	-4.00387313	1.18564363
1	-1.28706787	-2.61253809	1.02115081
1	-0.47495242	-2.13966322	-1.31531657
1	0.75815400	-3.53165016	-1.18578162

TS₃₄

E = -3429.277317 a.u., E₀ = -3428.850647 a.u., v_i = 36i cm⁻¹

Atomic Coordinates:

6	1.74344227	1.96508416	0.35709307
6	2.79163654	0.99220900	0.06482146
8	1.56048458	0.59676851	0.87814926
1	1.02354188	2.22504082	-0.41905992
1	1.90792782	2.69377554	1.15192549
1	3.70768939	0.98839944	0.64934629
1	2.82572572	0.53075078	-0.91873915
24	-0.01244058	-0.68883946	0.44633277
6	0.02985160	-0.01886546	-5.19534365
6	-1.26341509	1.73415927	-4.13431417
1	-1.59972950	2.21221432	-3.21417768
6	-0.41941682	0.61769773	-4.02625761
6	-1.20317709	1.56846180	-6.54899381
6	-0.36027003	0.45624867	-6.44812610
6	-1.65398333	2.20536854	-5.38765523
8	-0.38823903	0.77034032	-1.63945009
1	-2.31096624	3.07368049	-5.46161533
6	-0.02788817	0.14089683	-2.66058783
7	0.74258266	-0.99582792	-2.64723767
6	1.78776418	-2.43909720	-1.24449455

6	2.04180139	-3.50991844	2.84066000
1	2.06203324	-3.73745815	3.90443377
6	1.22540779	-2.47652763	2.35507787
6	1.94453452	-2.87602167	0.12414535
6	2.78048714	-3.92245511	0.57036469
6	2.82118170	-4.22671650	1.92840415
7	1.20093201	-2.18499962	1.02664948
1	3.46803283	-5.03044706	2.28243637
6	0.35480055	-1.64685559	3.16767069
7	-0.31121537	-0.74727600	2.46436802
7	0.95079490	-1.41850366	-1.40144044
6	-1.65409167	0.93712740	2.09873919
6	-3.92320587	3.09655846	4.25119110
6	-4.09496163	3.81766244	1.94649223
1	-4.51879440	4.48234062	1.19212711
6	-4.46917794	3.95234780	3.28767104
6	-2.62856415	1.97440436	2.53198772
6	-3.00816608	2.11230370	3.87827649
6	-3.18009121	2.83490149	1.56852155
8	-1.32154938	0.88088930	0.86471229
1	-2.87457985	2.70894629	0.52997851
7	-1.16406007	0.11423662	3.05239186
1	3.38933149	-4.47558608	-0.14059133
1	-2.57402316	1.43864763	4.61572773
1	-4.21274097	3.19888969	5.29839278
1	-0.00332831	-0.04077704	-7.35193087
1	0.68717527	-0.88169875	-5.09852465
1	-1.50554064	1.93931633	-7.52997054
1	-5.18432445	4.72228091	3.58211093
6	0.22959550	-1.80196895	4.64974704
1	-0.50913285	-1.08801029	5.02747669
1	-0.08884675	-2.82237118	4.91292682
1	1.19338507	-1.61619352	5.14903964
6	2.48883075	-3.05773113	-2.41206427
1	3.10539475	-3.91469595	-2.11968216
1	1.75089760	-3.38100023	-3.16097720
1	3.12657542	-2.31291006	-2.91122263
17	-1.75289401	-2.14082115	0.05762622
17	5.27697605	2.47162453	-0.63455876

TS₄₅

E = -3617.777330 a.u., E₀ = -3617.335840 a.u., v_i = 133i cm⁻¹

Atomic Coordinates:

6	-0.98440623	-2.33200309	-2.10234099
6	0.48003119	-2.42706311	-1.70073084
24	0.56842437	0.30820514	0.69296208
6	-4.91139361	0.33294281	1.93620788
6	-4.55343660	0.13181908	-0.45061826
1	-3.85328361	0.03382777	-1.28030973
6	-4.02978683	0.20525123	0.84961646

6	-6.80476459	0.31301735	0.42309956
6	-6.28943217	0.38626255	1.72221697
6	-5.93151544	0.18585236	-0.66245926
8	-1.78672862	-0.00663332	0.04622069
1	-6.32748458	0.12732585	-1.67780170
6	-2.54326299	0.14510469	1.03660322
7	-2.11957197	0.25120766	2.33253968
6	-0.21915998	0.23140470	3.58253029
6	3.98314931	0.06697456	3.17583654
1	5.05647989	0.02421194	3.00257642
6	3.09663372	0.15593695	2.09118418
6	1.22284222	0.18796373	3.54739368
6	2.07792419	0.11106314	4.66761259
6	3.45326539	0.04429133	4.46894504
7	1.75768689	0.20182610	2.30092582
1	4.12189762	-0.02503357	5.32820525
6	3.48932986	0.25692242	0.69635496
7	2.46564673	0.39406356	-0.12662418
7	-0.78810884	0.25205525	2.38623273
6	1.45548956	0.80091875	-2.03279317
6	2.66419448	1.47054918	-5.57952318
6	0.24903309	1.61630071	-5.52518646
1	-0.70103398	1.78184057	-6.03551860
6	1.44941020	1.68792296	-6.23944500
6	1.47677970	1.10931508	-3.49306853
6	2.68040539	1.18320237	-4.21454558
6	0.26123629	1.32909134	-4.16017613
8	0.33816238	0.72163813	-1.43272674
1	-0.66121602	1.26849744	-3.58315438
7	2.66092506	0.62181786	-1.43754168
1	1.65950876	0.08806781	5.67117245
1	3.61682652	1.01061326	-3.68592627
1	3.60304748	1.52354368	-6.13369963
1	-6.96711570	0.48438370	2.57249913
1	-4.49222079	0.38631916	2.94005318
1	-7.88300837	0.35353220	0.25790010
1	1.43888208	1.91019922	-7.30795696
6	4.91806441	0.27601963	0.25358205
1	4.95898907	0.23432377	-0.83958006
1	5.42491574	1.19585439	0.58731308
1	5.46952388	-0.57848965	0.67320985
6	-1.03312607	0.20298430	4.83725016
1	-1.56295899	-0.75795130	4.92834908
1	-0.41726334	0.35312080	5.73148757
1	-1.80698108	0.98209915	4.79443730
17	0.53291175	2.60050124	0.94570439
1	-1.33942001	-1.29849024	-2.08541273
1	-1.61009604	-2.96711260	-1.46788713
1	1.11203762	-1.85360692	-2.39202667
1	0.80566182	-3.47608714	-1.67478070
8	0.64290668	-1.87474500	-0.38954486
17	-1.20263463	-2.94899288	-3.81444309

8	0.48600080	-4.02497820	0.49329849
6	0.55685331	-2.82368472	0.74980207
8	0.58433363	-2.14531515	1.80249959

TS₅₆

E = -3617.801919 a.u., E₀ = -3617.359799 a.u., $v_i = 36i \text{ cm}^{-1}$

Atomic Coordinates:

6	1.10989814	-4.60340758	-2.13761074
6	1.84638881	-3.27586285	-2.02489584
24	0.34228509	0.57542901	0.67352933
6	-5.13387176	0.85419244	2.29361401
6	-4.94496650	1.25973054	-0.08598950
1	-4.30392313	1.33843687	-0.96450236
6	-4.33566508	0.96184199	1.14276588
6	-7.11625548	1.33806659	0.98470787
6	-6.51519263	1.04124280	2.21305115
6	-6.32547966	1.44681127	-0.16460339
8	-2.17370669	0.86245275	0.13152046
1	-6.78891573	1.67882401	-1.12546460
6	-2.84367864	0.76889351	1.17779825
7	-2.34191621	0.48533996	2.42819966
6	-0.42309867	0.04604730	3.54542698
6	3.76046034	-0.28232065	3.01604313
1	4.82626445	-0.35991235	2.81194695
6	2.86418800	0.03503483	1.98344473
6	1.01265100	-0.08605518	3.46439950
6	1.87814266	-0.41013583	4.53397145
6	3.24550711	-0.50356287	4.29625366
7	1.53381022	0.13051407	2.23123702
1	3.92040671	-0.75611803	5.11554859
6	3.23761950	0.28623436	0.60190997
7	2.20641712	0.55763452	-0.17820818
7	-1.01803375	0.35399089	2.39799758
6	1.14325707	1.04256156	-2.02743236
6	2.19168950	1.68315078	-5.62975224
6	-0.21357670	1.88866033	-5.45331958
1	-1.18332817	2.08162788	-5.91534096
6	0.95101541	1.93164644	-6.22754672
6	1.10205828	1.34934469	-3.48626596
6	2.26919524	1.39357090	-4.26695563
6	-0.14040409	1.59934642	-4.09052810
8	0.05279201	1.00553780	-1.37724574
1	-1.03144742	1.55888503	-3.46398500
7	2.36791928	0.82130729	-1.48689024
1	1.47501114	-0.58819292	5.52816180
1	3.22633219	1.19699171	-3.78576892
1	3.10260005	1.71461280	-6.23035162
1	-7.12799774	0.95559464	3.11269874
1	-4.64798275	0.62297607	3.24067274
1	-8.19640875	1.48417279	0.92366046

1	0.89248501	2.15743668	-7.29387582
6	4.65323961	0.24305437	0.12181996
1	4.67993251	0.48378214	-0.94574761
1	5.27736727	0.96617143	0.66962459
1	5.08916304	-0.75642884	0.27561915
6	-1.21303723	-0.14182518	4.80315902
1	-1.94780511	-0.95056315	4.67234091
1	-0.57484022	-0.37420180	5.66318961
1	-1.79547345	0.76593169	5.02097120
17	0.53435120	2.84197275	1.15559764
1	0.19761843	-4.50696892	-2.73496022
1	0.88970037	-5.01544341	-1.14883962
1	2.12567367	-2.90565950	-3.02044193
1	2.74112269	-3.39453505	-1.39916013
8	0.96600327	-2.28978373	-1.46892344
17	2.15549522	-5.83563433	-2.99440206
8	1.50786184	-3.11688376	0.60221141
6	0.88269467	-2.28608599	-0.05780737
8	0.07838746	-1.36947201	0.35372249

TS₆₇

E = -3617.782766 a.u., E₀ = -3617.340755 a.u., $v_i = 359i \text{ cm}^{-1}$

Atomic Coordinates:

6	2.18157053	-4.26125956	0.46894148
6	0.80725783	-4.61734390	-0.06043041
24	0.33781675	0.74046636	0.34000698
6	-5.17571878	0.93539971	1.82361865
6	-4.92301273	1.32190478	-0.55403203
1	-4.25773716	1.41244102	-1.41304696
6	-4.34509182	1.05758488	0.69742268
6	-7.12871599	1.33874905	0.44589794
6	-6.55894566	1.07532084	1.69639206
6	-6.30546665	1.46168125	-0.67891407
8	-2.14741731	1.02398694	-0.23807874
1	-6.74507761	1.66704988	-1.65670037
6	-2.85162592	0.91454250	0.78389972
7	-2.37865186	0.66116315	2.05374837
6	-0.47552279	0.30728054	3.22914100
6	3.72556138	0.09126382	2.78958869
1	4.79720736	0.04105065	2.60994768
6	2.84039116	0.31445542	1.72480607
6	0.96444172	0.21031472	3.17729211
6	1.81946957	-0.02174643	4.27847433
6	3.19363046	-0.07862365	4.07082891
7	1.50117910	0.36812970	1.94045234
1	3.86077666	-0.25956434	4.91477823
6	3.23354959	0.49150044	0.33773172
7	2.21066642	0.67815918	-0.47425833
7	-1.05381298	0.55635911	2.05858040
6	1.17464685	1.02885973	-2.36864829

6	2.25853872	1.40586030	-5.99499798
6	-0.14513007	1.65759468	-5.85413551
1	-1.10809767	1.83219779	-6.33682299
6	1.02611816	1.63046587	-6.61878347
6	1.14739943	1.23603022	-3.84399009
6	2.32159829	1.20990467	-4.61520767
6	-0.08706591	1.46118128	-4.47427034
8	0.07430147	1.03496671	-1.72661150
1	-0.98419034	1.47699070	-3.85551167
7	2.38876152	0.84108192	-1.79924154
1	1.40349293	-0.15190580	5.27472019
1	3.27226591	1.03295171	-4.11414862
1	3.17417359	1.38282490	-6.58841944
1	-7.19756174	0.97832531	2.57650685
1	-4.71452427	0.73044193	2.78879714
1	-8.21048355	1.44747615	0.34837869
1	0.97921067	1.78312528	-7.69844580
6	4.65586805	0.44136617	-0.11761282
1	4.70696259	0.70408082	-1.17891467
1	5.27914429	1.13956368	0.46099052
1	5.07207870	-0.56950247	0.01761856
6	-1.28480852	0.15796502	4.47949171
1	-2.03008151	-0.64149100	4.35383272
1	-0.66266680	-0.06673130	5.35303688
1	-1.85671878	1.07826495	4.67226696
17	0.51937062	3.00958610	0.72333831
8	-0.04507010	-1.22276688	-0.00808795
1	2.38965917	-4.29648829	1.52905619
1	3.01596522	-4.13150644	-0.20566562
1	0.28347927	-5.28536987	0.63012707
1	0.87856269	-5.09713650	-1.04167044
6	0.61910695	-2.28863668	0.11256600
8	1.82618105	-2.41141820	0.51409400
8	-0.03381445	-3.42653704	-0.22351864
17	2.76660681	-6.54188299	0.46379483

TS₈₉

E = -3157.638750 a.u., E₀ = -3157.195205 a.u., v_i = 79i cm⁻¹

Atomic Coordinates:

6	-0.70434745	-3.31816954	-1.87551549
6	-1.58590116	-3.62948650	-0.65935315
24	0.65216048	0.75661757	0.70405134
6	-4.72987566	0.17174450	1.53853832
6	-4.02477125	-0.15646312	-0.75898857
1	-3.21342080	-0.21542357	-1.48488137
6	-3.69804897	0.06578604	0.58949883
6	-6.38069524	-0.17305064	-0.20132843
6	-6.06156341	0.05041754	1.14270407
6	-5.35845129	-0.27271004	-1.15117050
8	-1.35209938	-0.07733675	0.12852566

1	-5.60457257	-0.43419687	-2.20172648
6	-2.26835643	0.18496077	0.97997656
7	-2.00267128	0.55653490	2.24950351
6	-0.15939954	0.74614462	3.60455016
6	4.04238680	0.55520307	3.28120170
1	5.11853776	0.50253119	3.13266161
6	3.17565436	0.52516238	2.17783923
6	1.28761498	0.72303276	3.60002646
6	2.11965299	0.77646963	4.73173097
6	3.49992112	0.68163616	4.56138926
7	1.82669526	0.58075160	2.35926321
1	4.15850339	0.71783143	5.42926984
6	3.58133656	0.50390715	0.78762549
7	2.55862791	0.61999823	-0.04286644
7	-0.67480002	0.68692321	2.38944066
6	1.58155601	0.87721946	-1.96692591
6	2.63629025	0.91185171	-5.60652918
6	0.25193247	1.31697368	-5.47267703
1	-0.70153579	1.51874787	-5.96250553
6	1.41220894	1.15960980	-6.23813088
6	1.53847899	0.97415603	-3.44416480
6	2.70294509	0.82040679	-4.21710295
6	0.31207954	1.22478595	-4.08248795
8	0.47871736	0.95543573	-1.30662110
1	-0.57801186	1.35370698	-3.46733422
7	2.77453880	0.71038475	-1.37100022
1	1.68692307	0.88349211	5.72381181
1	3.64889088	0.63289456	-3.71109136
1	3.54267663	0.79291601	-6.20152722
1	-6.85676210	0.13275455	1.88483907
1	-4.46752657	0.34918220	2.58054484
1	-7.42349226	-0.26421320	-0.50800024
1	1.36418445	1.23487321	-7.32531416
6	4.99582732	0.44225541	0.31199608
1	5.05246890	-0.15879609	-0.60385251
1	5.36366540	1.44833692	0.05479800
1	5.65896272	0.01322461	1.07190058
6	-1.01031740	0.74268762	4.83290657
1	-1.42787006	-0.25963136	5.01698531
1	-0.44603131	1.05255177	5.71955882
1	-1.86437378	1.41763625	4.69082787
17	0.68041611	3.01602178	0.89195170
8	0.92646709	-1.71632002	0.71359340
1	-0.15561009	-4.19350725	-2.24960971
1	-1.24723434	-2.83529701	-2.69500711
1	-1.80948264	-4.69462904	-0.53709787
1	-2.51229001	-3.04030213	-0.64271465
6	0.19546296	-2.37019149	-0.00211660
8	0.25982405	-2.37145974	-1.35392649
8	-0.76609597	-3.20657412	0.46005719

Intermediates

I₂₃

E = -2969.143402 a.u., E₀ = -2968.716054 a.u.

Atomic Coordinates:

24	0.43226508	1.00431638	0.67584099
6	-4.79932906	0.70396124	1.21631423
6	-3.87357839	-0.44605555	-0.71260964
1	-2.99910636	-0.77779629	-1.27091391
6	-3.68116875	0.25357465	0.49094654
6	-6.27232104	-0.24451247	-0.45582694
6	-6.08563585	0.45578306	0.74171629
6	-5.16376885	-0.69296797	-1.18084634
8	-1.30117524	0.04997476	0.28104763
1	-5.30606574	-1.23363066	-2.11723272
6	-2.30791085	0.51262183	0.97238307
7	-2.13705964	1.18068170	2.12016751
6	-0.27254565	1.21845135	3.53133784
6	3.60612354	-0.39014287	3.07605233
1	4.57289079	-0.85531152	2.89492871
6	2.73169965	-0.14254217	2.00524819
6	1.11412815	0.77399167	3.49307021
6	1.97280512	0.58610780	4.58493166
6	3.21676323	-0.01281999	4.36305997
7	1.50843708	0.39626285	2.24715049
1	3.89192301	-0.18136348	5.20205622
6	3.00668076	-0.35816525	0.59570856
7	2.04308256	0.11449354	-0.18245522
7	-0.79656464	1.24716394	2.32109757
6	1.12294651	0.80669846	-2.03890317
6	1.84359896	0.43665816	-5.74210145
6	-0.12442332	1.81929822	-5.45469112
1	-0.93408429	2.41178114	-5.88214862
6	0.80296468	1.19241672	-6.29350030
6	1.02706717	0.93260513	-3.51210791
6	1.95881743	0.30630584	-4.35904739
6	-0.01542429	1.69126265	-4.07066026
8	0.23462288	1.38392150	-1.30709577
1	-0.72649096	2.17456784	-3.40176651
7	2.14658046	0.09111170	-1.53022594
1	1.66628029	0.89213136	5.58338684
1	2.76674569	-0.27452779	-3.91661828
1	2.56926210	-0.05028747	-6.39464780
1	-6.94876559	0.80961404	1.30674797
1	-4.64018734	1.24789382	2.14632574
1	-7.28074544	-0.43764554	-0.82383015
1	0.71691491	1.29460325	-7.37605508
6	4.25904198	-0.98951245	0.08777662
1	4.29054534	-0.92111657	-1.00387194
1	5.14722721	-0.49165022	0.50399095
1	4.29347809	-2.04992677	0.38068092

6	-1.05453295	1.39275802	4.79167416
1	-1.15757490	0.43945711	5.33340918
1	-0.54774475	2.10154024	5.46283062
1	-2.05541678	1.76934932	4.55821838
17	1.38100852	3.06606524	0.91348574
6	0.33438847	-3.34917365	0.07688033
6	1.34721853	-3.57018749	-0.96786764
8	1.73889347	-3.40955219	0.41473392
1	-0.25480389	-4.19688140	0.43733002
1	-0.12903216	-2.36349780	0.17670033
2	1.62741872	-2.74111168	-1.62351124
1	1.49363636	-4.57704530	-1.36869437

I₃₄

E = -3429.286829 a.u., E₀ = -3428.859201 a.u.

Atomic Coordinates:

6	2.01779056	1.88938200	0.17868714
6	2.87710953	0.72731847	0.48504221
8	1.45747602	0.72626263	0.84825093
1	1.62709916	2.03003907	-0.83005393
1	2.04778790	2.76325583	0.83201885
1	3.51896048	0.68639225	1.37578416
1	3.11146951	0.04539585	-0.33563510
24	-0.06138085	-0.67338389	0.37164822
6	-0.26422304	-0.03722407	-5.27594042
6	-1.20934331	1.91694999	-4.20340586
1	-1.39646661	2.47039723	-3.28281021
6	-0.51301724	0.70187265	-4.10705137
6	-1.39629912	1.64633310	-6.60305834
6	-0.70322174	0.43356150	-6.51436234
6	-1.64872026	2.38544130	-5.44235706
8	-0.26848722	0.94762343	-1.73830700
1	-2.19294024	3.32970548	-5.50463486
6	-0.06084048	0.23587827	-2.75187707
7	0.58880424	-0.96618450	-2.75342512
6	1.68034112	-2.40865421	-1.37572539
6	2.41166377	-3.16267323	2.72159100
1	2.62621641	-3.22429895	3.78394914
6	1.45318341	-2.25334477	2.25169587
6	1.95329964	-2.79619741	-0.00429183
6	2.87811422	-3.76719308	0.42155141
6	3.10192180	-3.93586922	1.78793538
7	1.25529587	-2.09088945	0.92122823
1	3.85093951	-4.65089607	2.12878704
6	0.60130310	-1.41636527	3.09406757
7	-0.23791981	-0.68011725	2.39563084
7	0.86304420	-1.37244570	-1.50553620
6	-1.69592023	0.90118206	2.02041078
6	-3.98837972	3.04615450	4.16121387
6	-4.33707190	3.60004520	1.83095515

1	-4.84840298	4.18256426	1.06268692
6	-4.64627981	3.79798388	3.18063736
6	-2.71424890	1.90102613	2.44174886
6	-3.02788115	2.10284948	3.79687715
6	-3.37637925	2.65785146	1.46137691
8	-1.42637169	0.79739344	0.76458240
1	-3.11983871	2.48401690	0.41649517
7	-1.10818577	0.17529801	2.98480439
1	3.43650842	-4.34987593	-0.30804247
1	-2.50550389	1.51021707	4.54667807
1	-4.22563076	3.19793010	5.21562338
1	-0.50619364	-0.14833356	-7.41684818
1	0.27333382	-0.98051268	-5.18819094
1	-1.73986709	2.01207113	-7.57241869
1	-5.39748859	4.53555298	3.46860290
6	0.74630618	-1.37202787	4.57464743
1	0.01992621	-0.67504275	5.00272560
1	0.60552365	-2.37032080	5.01694250
1	1.77925408	-1.03483725	4.78861856
6	2.27576256	-3.08887982	-2.56831312
1	2.84925628	-3.97998214	-2.28985977
1	1.47332132	-3.37470317	-3.26388979
1	2.93000460	-2.40095162	-3.12549162
17	-1.72874236	-2.20717263	0.03999377
17	4.03422832	-0.41956824	3.58803701

I_{45}

$E = -3617.801332$ a.u., $E_0 = -3617.361465$ a.u.

Atomic Coordinates:

6	-0.81850627	-2.35544137	-1.59235057
6	0.58289495	-2.25162684	-0.99358359
24	0.59279228	0.36078194	0.44003175
6	-4.98867595	0.26275968	1.81747788
6	-4.74803663	0.54527179	-0.57451595
1	-4.08530349	0.63094357	-1.43611610
6	-4.16011814	0.37416794	0.68842425
6	-6.95618194	0.49143982	0.41936831
6	-6.37705663	0.32071857	1.68186817
6	-6.13580826	0.60389621	-0.70849388
8	-1.96314298	0.38997309	-0.25070125
1	-6.58141225	0.73779493	-1.69608125
6	-2.65806278	0.31472960	0.78231307
7	-2.18624972	0.16676130	2.06513535
6	-0.30396110	-0.02005171	3.30228039
6	3.91973276	-0.01090140	3.02167376
1	4.99878946	0.00416952	2.88227627
6	3.06209841	0.14898405	1.92004003
6	1.14057210	-0.03331143	3.30725959
6	1.96638842	-0.19752860	4.44278844
6	3.35044839	-0.18663564	4.28539120

7	1.71397319	0.12861017	2.08655595
1	3.99404662	-0.31387365	5.15735500
6	3.48994503	0.36850491	0.55198619
7	2.48154299	0.51003832	-0.29209347
7	-0.85503273	0.14588571	2.10438111
6	1.49995973	0.87260216	-2.21518904
6	2.70466084	1.64501797	-5.74051424
6	0.28459261	1.62222937	-5.71692949
1	-0.66817866	1.72810238	-6.23830246
6	1.48608814	1.78184676	-6.41519140
6	1.51869891	1.18744375	-3.67212564
6	2.72330326	1.35016317	-4.37717711
6	0.29896712	1.32710484	-4.35347781
8	0.37604247	0.71054990	-1.63419589
1	-0.62353502	1.20098322	-3.78702723
7	2.69977667	0.76995228	-1.59853480
1	1.52198264	-0.33060263	5.42647999
1	3.66248326	1.24146140	-3.83643254
1	3.64449391	1.76898843	-6.28162142
1	-7.01282028	0.23248110	2.56523280
1	-4.51946176	0.13059643	2.79153445
1	-8.04198481	0.53661006	0.31525391
1	1.47372951	2.01214522	-7.48207403
6	4.92859884	0.46346614	0.15309798
1	4.99455902	0.60203801	-0.93086502
1	5.42174359	1.31346301	0.65085170
1	5.47692945	-0.44891438	0.43465327
6	-1.14502931	-0.17674395	4.53112090
1	-1.78852902	-1.06476693	4.43992789
1	-0.53868787	-0.26655265	5.43971603
1	-1.82327992	0.68337469	4.63353666
17	0.52877652	2.69059920	0.82301194
1	-1.20483254	-1.37364132	-1.87821583
1	-1.50861541	-2.84935583	-0.90084836
1	1.26060481	-1.78650661	-1.73388748
1	0.97316140	-3.27230092	-0.80679652
8	0.51845499	-1.54911355	0.21758568
17	-0.80510914	-3.38911739	-3.11714106
8	-0.03698483	-3.46116582	2.68123825
6	1.06331379	-3.47805286	2.27571190
8	2.18045135	-3.56044511	1.92492335