DFT modeling of the first step of plastoquinol oxidation by the iron–sulfur protein of the cytochrome b_6f complex

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I.   Tables

Table S1 The energy characteristics of the models M1-M6 and their products obtained after the H-transfer from $TMBQH_2$ to His155.

Model	number of fixed geometry parameters	E^M, a.u. (ΔE^M, kcal mol^{-1})	$\Delta E_{opt} = E(P^{opt}) - E(M)$, kcal mol^{-1}	$\Delta E_{nop} = E(P^{nop}) - E(M)$, kcal mol^{-1}	$\Delta E_{rel} = \Delta E_{nop} - \Delta E_{opt}$, kcal mol^{-1}
M1	0	-7957.766824 (0)	- [a]	-	-
M2	14	-7957.722766 (27.6)	3.6	17.4 [b] <u>16.6</u> [b]	13.8 [b] <u>13.0</u> [b]
M3	16	-7957.716974 (31.3)	0.2	19.9 <u>18.8</u>	19.7 <u>18.6</u>
M4	18	-7957.716079 (31.8)	0.5	<u>9.9</u> 10.7	<u>9.4</u> 10.2
M5	20	-7957.713359 (33.5)	-0.2	<u>7.8</u> 8.2 7.7 [c]	<u>8.0</u> 8.4 *8.0* [c]
M6	14	-7957.722865 (27.6)	0.1	<u>8.9</u> 9.2	<u>8.8</u> 9.1

[a] The product was not found because the non-optimized form obtained after the H-transfer gradually transformed to M1.
[b] The structures of the non-optimized products (P^{nop}) were obtained using two different approaches as described in the text. The data for the best approximation of two are underlined.
[c] The refined values were obtained by detailed scanning of $E(P^{nop})$ versus the H atom position with regard to His155.[14]

Table S2 The geometry parameters of the models M1-M6 and their products obtained after the H-transfer from TMBQH$_2$ to His155.

Model	number of fixed geometry parameters	bond lengths/ val. angles/ torsions	RMSD, Å	l_{H-N_ε} (M), Å	l_{H-N_ε} (P^{opt},P^{nop}), Å	Δl ,[b] Å
M1	0	0	– [a]	1.643	-	-
M2	14	4/8/2	– [a]	2.068	1.056	1.117 [c] <u>1.095</u> [c]
M3	16	4/8/4	0.99	2.139	1.049	1.463 <u>1.403</u>
M4	18	6/8/4	0.44	2.062	1.051	<u>1.048</u> 1.056
M5	20	8/8/4	0.47	2.046	1.051 *1.062* [d]	<u>1.034</u> 1.036 *1.023* [d]
M6	14	7/5/2	0.70	2.070	1.050	<u>1.057</u> 1.055

[a] Not determined due to critical changes in geometry of M1 and M2 with respect to the initial structure M0.

[b] The distance between the H atom positions before and after the H-transfer in structures M and P^{nop}, respectively.

[c] The structures of the non-optimized products (P^{nop}) were obtained using two different approaches as described in the text. The data for the best approximation of two are underlined.

[d] The refined values were obtained by detailed scanning of E(P^{nop}) versus the H atom position with regard to His155.[14]

II. Calculation details

The contraction schemes for orbital basis sets used in this work are (5s1p)/[3s1p] for H; (11s6p2d)/[6s3p2d] for C, N, and O; (15s11p2d)/[10s6p2d] for S, and (17s13p8d)/[12s9p4d] for Fe. The auxiliary basis sets were applied for the electron density expansion and represented the following uncontracted sets of Gaussian functions: (5s2p) for H, (10s3p3d1f) for C, N, and O, (14s3p3d1f1g) for S, (18s6p6d5f5g) for Fe.

In this work, we did not consider the effects of protein surroundings beyond the domain of the model system. This approximation can be approved because we virtually consider the translocation of the neutral particle (the concerted transfer of electron and proton). In this case, electrostatic interactions with the dielectric surroundings should be comparatively low [9].

III. Cartesian coordinates and total energies (a.u.) calculated for the models M1-M6 and corresponding products P^{opt} and P^{nop} obtained after the H-transfer from quinol to the iron-sulfur protein of the cytochrome b_6f complex. List of the fixed internal coordinates for the models M2-M6 and products P2^{opt}–P6^{opt}.

1. Model M0, Z = −1, m=1

Atomic Coordinates

N	M0 Atom number	X	Y	Z
1	6	-1.70109367	3.12616754	-4.60085344
2	6	-2.30609322	4.05817461	-3.55485559
3	8	-1.58909416	4.67116594	-2.76485467
4	6	-1.00409317	1.94817376	-3.90885186
5	16	-2.05209351	0.89916253	-2.87985253
6	1	-2.42669296	2.77936578	-5.19525194
7	1	-0.59939384	1.37247491	-4.61935472
8	1	-0.27999309	2.32006097	-3.32805657
9	1	-1.03379440	3.63106561	-5.14845324
10	7	-3.63009453	4.15517473	-3.54585290
11	6	-4.31609344	5.03417253	-2.60785699
12	6	-4.19509315	4.59816790	-1.14785802
13	8	-4.77909470	5.22417498	-0.25985751
14	1	-4.16629410	3.61516595	-4.19455767
15	1	-3.92829323	5.95177507	-2.69535089
16	1	-5.28609467	5.05716753	-2.85005212
17	7	-3.44809341	3.53017449	-0.89185363
18	6	-3.28609467	3.05316949	0.47714201
19	6	-2.17109299	3.79816461	1.20014918
20	8	-2.42909431	4.73116350	1.95914423
21	6	-2.97509384	1.55516839	0.49814573
22	6	-2.60409355	1.04317498	1.85514796
23	7	-1.77809334	-0.04483768	2.04214454
24	6	-2.94109344	1.47817254	3.09314704
25	6	-1.62309456	-0.25482914	3.33714271
26	7	-2.31709290	0.65416741	3.99714637
27	1	-2.99389458	3.05007195	-1.64235723
28	1	-4.15079308	3.22426629	0.94944733
29	1	-3.78419304	1.05927300	0.18284574
30	1	-2.21289444	1.38117242	-0.12535128
31	1	-3.53359413	2.25437188	3.30844855
32	1	-1.07229424	-0.98082709	3.74874854
33	1	-2.37829399	0.73006463	4.99234724
34	7	-0.93309402	3.37216973	0.96214265
35	6	0.22690579	3.98416924	1.59514582
36	6	1.26190567	4.55216265	0.61914796
37	8	2.32590675	5.00716448	1.04814875
38	1	-0.79529381	2.60956597	0.33014646
39	1	-0.09389308	4.73046160	2.17834449
40	1	0.67690659	3.29067254	2.15784431
41	7	0.96690559	4.50417376	-0.68485290
42	6	1.86990547	5.09716082	-1.66185796
43	6	2.59190559	4.29616594	-2.73185754
44	8	3.11690712	4.88216448	-3.68185449
45	1	0.12430570	4.06006670	-0.98955566
46	1	1.33070564	5.78266191	-2.15115380
47	1	2.58560562	5.55167437	-1.13155401
48	7	2.63190651	2.97716546	-2.60285211
49	6	3.33190536	2.14916253	-3.57685113

50	6	3.31690598	0.70417047	-3.10785699
51	16	4.11290550	0.56316400	-1.48785436
52	1	2.17510605	2.54407525	-1.82585180
53	1	2.87480545	2.21746087	-4.46365404
54	1	2.37030602	0.38936642	-3.03895593
55	1	3.80990601	0.13767269	-3.76825738
56	1	4.27750587	2.46256280	-3.66375756
57	6	-0.86409378	-2.50283027	-4.10685778
58	16	0.32190701	-1.52083564	-3.14685082
59	1	-0.36929324	-3.14513373	-4.69205523
60	1	-1.41869354	-1.89463019	-4.67475176
61	1	-1.45879364	-3.01062751	-3.48355126
62	6	2.93690681	-3.57382941	-0.42985567
63	6	2.02690697	-4.18683577	0.63414735
64	8	2.51890564	-4.79183149	1.58814204
65	6	2.96690559	-2.04982734	-0.33185610
66	16	4.42190552	-1.42583442	-1.23185766
67	1	3.86470604	-3.92552924	-0.30525240
68	1	2.13460541	-1.67153144	-0.73705322
69	1	3.02450562	-1.77683234	0.62844819
70	1	2.59990692	-3.83443427	-1.33455694
71	7	0.71190643	-4.04582930	0.48314634
72	6	-0.20709422	-4.62883711	1.45514643
73	6	-1.34909439	-5.38883162	0.79214448
74	8	-2.34909439	-5.72182417	1.43014491
75	6	-0.75509453	-3.55083442	2.38014960
76	6	0.30390546	-2.67783332	2.97014594
77	7	0.82290649	-1.58882880	2.30214667
78	6	0.95990562	-2.74582648	4.15114546
79	6	1.75290680	-1.02283454	3.05014777
80	7	1.85590553	-1.70482612	4.17714643
81	1	0.35230634	-3.53823066	-0.29975161
82	1	0.31490704	-5.29132795	1.99244654
83	1	-1.38469315	-2.97573066	1.85784876
84	1	-1.25039291	-3.99582648	3.12624335
85	1	0.81910706	-3.42623115	4.87034559
86	1	2.28850555	-0.21472904	2.80494666
87	7	-1.19209290	-5.65782881	-0.49785647
88	6	-2.19309425	-6.41483259	-1.21785772
89	6	-3.45109367	-5.69083357	-1.64285314
90	8	-4.54509354	-6.22583723	-1.48485601
91	1	-0.37549403	-5.33473921	-0.97615081
92	1	-1.75969315	-6.77133894	-2.04555535
93	1	-2.47029305	-7.17623091	-0.63185149
94	7	-3.31009293	-4.48082685	-2.17485070
95	6	-4.46709442	-3.72983527	-2.65385461
96	6	-4.16909409	-2.22383857	-2.67285180
97	8	-4.11309433	-1.68183112	-1.36185491
98	1	-2.39749336	-4.07863569	-2.24815392
99	1	-4.69279289	-4.03102827	-3.58035302
100	1	-3.28889465	-2.07363105	-3.12315392
101	1	-4.89009285	-1.75763679	-3.18535638
102	1	-3.91779327	-0.70253730	-1.41355169
103	1	-5.24379349	-3.90273261	-2.04815698
104	26	-0.20809367	-0.58083320	0.89714783
105	26	-0.69109344	-0.29582950	-1.74685705
106	16	-1.32809448	-1.97882819	-0.42185244
107	16	0.44690701	1.10117364	-0.38285097
108	6	5.04430580	-0.26932499	7.65414381
109	6	6.08150673	0.46346310	8.23514557
110	6	7.29360771	0.54296136	7.53294325
111	6	7.47190666	-0.08733341	6.28854322

112	6	6.41460609	-0.82433295	5.71364546
113	6	5.20130539	-0.90323615	6.41784620
114	8	4.16650581	-1.62873054	5.84754896
115	8	8.30680656	1.27477288	8.12844849
116	6	6.55810738	-1.51813483	4.37964582
117	1	7.36050606	-2.27133918	4.39794874
118	1	5.62780571	-2.02783942	4.10964918
119	1	6.79670525	-0.80623603	3.57484412
120	6	8.81060600	0.05097225	5.60204268
121	1	8.83740807	-0.48133060	4.64604902
122	1	9.05280495	1.10627007	5.38724470
123	1	9.63010597	-0.35823795	6.21824598
124	6	5.92820549	1.15096307	9.56554413
125	1	6.66640663	0.78096795	10.29224396
126	1	6.09780693	2.23426080	9.47544861
127	1	4.92360687	0.98976922	9.97714233
128	1	4.09000587	-0.34513065	8.18384552
129	1	3.40810585	-1.58412910	6.45374250
130	1	9.08230782	1.24646783	7.54174757

2. Model M1, Z = –1, m=1

E(M1) = -7957.76682372 a.u.

Atomic Coordinates

N	M1 Atom number	X	Y	Z
1	6	-2.09095094	3.29319803	-3.64538618
2	6	-2.06373809	4.42902480	-2.63219091
3	8	-1.04843370	5.10275681	-2.41717164
4	6	-1.39244712	2.04123356	-3.09548920
5	16	-2.29304692	1.35375455	-1.63255926
6	1	-3.12085282	3.04545523	-3.94205882
7	1	-1.34354333	1.26094208	-3.86632434
8	1	-0.36654247	2.28822789	-2.79415299
9	1	-1.54756446	3.64279690	-4.53619410
10	7	-3.23549834	4.64242555	-1.95523526
11	6	-3.34842453	5.62884389	-0.89504786
12	6	-2.80680900	5.26557103	0.50190629
13	8	-2.93740272	6.07831652	1.41746578
14	1	-3.96370929	3.94113357	-2.05340821
15	1	-2.78893085	6.52490966	-1.19644861
16	1	-4.40109830	5.91506373	-0.77409103
17	7	-2.18910683	4.05700930	0.62095277
18	6	-1.45589605	3.68438346	1.82382931
19	6	0.03246702	4.12614964	1.76698973
20	8	0.48268427	4.92803390	2.58420826
21	6	-1.61945477	2.16886756	2.06975296
22	6	-0.75191402	1.63102143	3.16349650
23	7	0.08554499	0.53107552	2.98607798
24	6	-0.60447364	2.07919571	4.45679182
25	6	0.71042831	0.32641242	4.15084113
26	7	0.31493949	1.24673225	5.05799718
27	1	-2.16271429	3.41238990	-0.17834316
28	1	-1.87835124	4.26946656	2.65113693
29	1	-2.68085318	1.96813301	2.28318272
30	1	-1.39456084	1.62036644	1.14337692
31	1	-1.04718560	2.92098578	4.97382462
32	1	1.43582192	-0.45253842	4.36167606
33	1	0.66988480	1.31899904	6.01871457

34	7	0.77781973	3.58082274	0.75041262
35	6	2.21189867	3.81254620	0.67099532
36	6	2.76048909	4.33748486	-0.66127629
37	8	3.97373807	4.50432116	-0.78916251
38	1	0.42717635	2.74231434	0.28083044
39	1	2.46747290	4.54606169	1.44720363
40	1	2.76969866	2.88828908	0.88716400
41	7	1.85429812	4.55893917	-1.66337180
42	6	2.25929838	5.14472894	-2.93070063
43	6	2.36274806	4.18375727	-4.12527088
44	8	2.47166850	4.62489341	-5.27209319
45	1	0.85528264	4.56208485	-1.45278549
46	1	1.54467559	5.92479368	-3.22010069
47	1	3.25225344	5.59862215	-2.79882546
48	7	2.35246842	2.85343794	-3.83444600
49	6	2.41128543	1.84553481	-4.88694303
50	6	2.69423804	0.45472361	-4.33742051
51	16	4.38562808	0.35721108	-3.56727551
52	1	2.19544858	2.57292812	-2.86942975
53	1	1.45151002	1.81435139	-5.43470752
54	1	1.94298468	0.15921548	-3.59144557
55	1	2.68462441	-0.27475406	-5.15563963
56	1	3.18067661	2.14942170	-5.61033313
57	6	-2.55646094	-2.01658399	-3.35937357
58	16	-0.78881588	-1.76942620	-2.89475850
59	1	-2.57501616	-2.50402716	-4.34197872
60	1	-3.05821444	-1.04316121	-3.41490016
61	1	-3.07368670	-2.65444681	-2.63406917
62	6	2.92927534	-2.81801966	-2.56102620
63	6	2.55921536	-4.02412793	-1.69413740
64	8	3.13953914	-5.10730852	-1.79640615
65	6	4.44175461	-2.63389169	-2.63695810
66	16	5.02128266	-1.56719373	-4.02244190
67	1	2.53217516	-3.02733920	-3.56685475
68	1	4.85374090	-2.23601906	-1.70118527
69	1	4.92704147	-3.60052469	-2.84431245
70	1	2.44375502	-1.90068545	-2.19971048
71	7	1.50785006	-3.82105976	-0.83713341
72	6	1.02076495	-4.86551815	0.04683436
73	6	-0.18265348	-5.64816362	-0.50542514
74	8	-0.57590429	-6.67623874	0.07524849
75	6	0.64022830	-4.32575169	1.45690262
76	6	1.69269978	-3.45534443	2.05964556
77	7	1.71501452	-2.07300896	1.88501439
78	6	2.84361425	-3.79246340	2.74800931
79	6	2.88745070	-1.66146067	2.45654422
80	7	3.58932478	-2.65804650	2.99771147
81	1	1.12765609	-2.88055665	-0.75417565
82	1	1.83456249	-5.59913920	0.14139528
83	1	-0.30217069	-3.76218503	1.38283898
84	1	0.44263811	-5.19989499	2.08997502
85	1	3.18156708	-4.77690992	3.05805510
86	1	3.20666417	-0.62240573	2.46783760
87	7	-0.79499550	-5.14304357	-1.60248832
88	6	-1.93650758	-5.80722773	-2.22077903
89	6	-3.29356434	-5.51874135	-1.54201673
90	8	-4.24164809	-5.03129480	-2.16935373
91	1	-0.49840384	-4.23496704	-1.97407156
92	1	-2.01965125	-5.47190792	-3.25974580
93	1	-1.75383819	-6.89264621	-2.20097423
94	7	-3.34198386	-5.86678648	-0.22961242
95	6	-4.51114757	-5.59958829	0.59521883

96	6	-4.54793854	-4.18160315	1.17173988
97	8	-3.49774095	-3.97340371	2.12306423
98	1	-2.48924301	-6.26512551	0.17903312
99	1	-5.41212721	-5.75392076	-0.01831359
100	1	-4.49280502	-3.45172141	0.34932619
101	1	-5.51786339	-4.04324458	1.68276622
102	1	-2.89611004	-3.29338649	1.76115892
103	1	-4.51757637	-6.32463125	1.42164097
104	26	0.33304560	-0.72740851	1.31795366
105	26	-0.91929452	-0.41759209	-1.05322525
106	16	-1.65957005	-1.46587338	0.74210779
107	16	1.08631517	0.31531815	-0.48051305
108	6	3.37808550	-1.52322704	6.14370406
109	6	2.47396951	-0.79732119	6.92455734
110	6	2.72608993	0.56973874	7.09355003
111	6	3.87282984	1.19290982	6.57582088
112	6	4.77974894	0.44452737	5.79727653
113	6	4.49956276	-0.92028222	5.54665165
114	8	5.31794151	-1.63006031	4.72385977
115	8	1.72579450	1.31976857	7.74049170
116	6	6.00525682	1.07298094	5.18059176
117	1	6.72033202	1.41176105	5.94699067
118	1	6.51062923	0.33836593	4.54489264
119	1	5.75159330	1.94700175	4.56218376
120	6	4.07475606	2.67018870	6.82911392
121	1	5.08439023	2.98943695	6.55128952
122	1	3.37021968	3.29146318	6.25047574
123	1	3.94948224	2.92966194	7.89577726
124	6	1.26421401	-1.44805010	7.54862476
125	1	1.20125376	-1.22819463	8.62406023
126	1	0.32158418	-1.09194185	7.10306364
127	1	1.30312442	-2.53615569	7.41461703
128	1	3.20590082	-2.58680673	5.97286515
129	1	4.72596885	-2.19110262	4.08761278
130	1	2.10058753	2.20001216	7.92640580

3. Model M2, Z = −1, m=1

E(M2) = -7957.72276619 a.u.
E(P2^{opt}) = -7957.71705914 a.u.
E(P2^{nop}) = -7957.69501616 a.u. (approximation 1)
E(P2^{nop}) = -7957.69630583 a.u. (approximation 2)

Atomic Coordinates

N	M2				P2^{opt}			
	Atom				Atom			
	number	X	Y	Z	number	X	Y	Z
1	6	-2.17614722	2.95177424	-4.77777395	6	-2.86392691	3.13692266	-5.18115979
2	6	-2.69358353	3.98730289	-3.78944681	6	-3.18379742	4.16320409	-4.10398052
3	8	-1.94983730	4.80787992	-3.23800285	8	-2.32648954	4.91784144	-3.62838128
4	6	-1.37606011	1.85637906	-4.06464405	6	-2.08471628	1.95035847	-4.60345680
5	16	-2.45185478	0.84045972	-2.94859269	16	-3.10482233	0.96704669	-3.40943132
6	1	-2.99553052	2.50411718	-5.35952470	1	-3.77668640	2.78124054	-5.68186353
7	1	-0.91056594	1.17490348	-4.78756227	1	-1.75933199	1.26906239	-5.39967556
8	1	-0.57818691	2.30723228	-3.46051017	1	-1.19007844	2.31036136	-4.07882537
9	1	-1.50627412	3.47932423	-5.47418926	1	-2.23365593	3.64209394	-5.92912936
10	7	-4.03954384	3.93687590	-3.53750618	7	-4.48899764	4.18108248	-3.68524213
11	6	-4.69503087	4.82023824	-2.58957555	6	-4.96356476	5.05939349	-2.63183154
12	6	-4.65349614	4.44960005	-1.09433786	6	-4.76846738	4.62197866	-1.16772183
13	8	-5.32120853	5.10934579	-0.29894745	8	-5.28453562	5.29306692	-0.27412288

14	1	-4.55346861	3.14097743	-3.90197361	1	-5.08596435	3.42044939	-3.99509196
15	1	-4.21647544	5.80755093	-2.65598121	1	-4.42928127	6.01589529	-2.72040361
16	1	-5.75036243	4.93825450	-2.86629167	1	-6.03389945	5.25779606	-2.77181759
17	7	-3.83443198	3.41624632	-0.74592855	7	-3.99204154	3.52115972	-0.95566371
18	6	-3.49052948	3.14551767	0.64568368	6	-3.50784618	3.17891637	0.37718919
19	6	-2.32375261	4.04372449	1.14808386	6	-2.23796664	3.98829748	0.76851733
20	8	-2.49701963	4.84492762	2.06583531	8	-2.25212704	4.75313839	1.73341638
21	6	-3.19871255	1.63810277	0.80164287	6	-3.28934754	1.65348167	0.45801472
22	6	-2.58658818	1.25420338	2.11158036	6	-2.56272944	1.20306433	1.68587724
23	7	-1.49937925	0.38783123	2.19997634	7	-1.53639021	0.26026009	1.64542399
24	6	-2.94024377	1.64422393	3.38313752	6	-2.74345965	1.60553176	2.99003694
25	6	-1.21195906	0.25297155	3.49534712	6	-1.12081632	0.09621803	2.90046110
26	7	-2.06543373	1.00035436	4.23534332	7	-1.82860460	0.89347388	3.73788011
27	1	-3.32146627	2.91250333	-1.47567478	1	-3.61183356	3.00629429	-1.75658779
28	1	-4.34884135	3.45326195	1.25709536	1	-4.26990843	3.51351345	1.09328849
29	1	-4.14157285	1.08913597	0.64460186	1	-4.27252641	1.15974579	0.39272366
30	1	-2.51390731	1.31678811	0.00206477	1	-2.71218009	1.31839091	-0.41726209
31	1	-3.69367154	2.33601818	3.73745793	1	-3.39672777	2.34999732	3.42688948
32	1	-0.42212788	-0.36324053	3.91368642	1	-0.34206637	-0.58074912	3.23136794
33	1	-2.03965948	1.09021803	5.24452105	1	-1.68157591	0.97647509	4.73724780
34	7	-1.13551572	3.88917639	0.48298890	7	-1.14877284	3.79736321	-0.03958621
35	6	0.06614833	4.57491750	0.93421507	6	0.13787795	4.38658052	0.29841555
36	6	1.01508151	5.07533497	-0.15948167	6	1.00632709	4.84426582	-0.87709617
37	8	2.09322049	5.57684571	0.16166178	8	2.14984227	5.24617087	-0.65863762
38	1	-0.97938581	3.01803008	-0.03834849	1	-1.10679506	2.93978897	-0.60675993
39	1	-0.25047437	5.43858186	1.53369733	1	-0.05258177	5.25561582	0.94195479
40	1	0.67319594	3.93176999	1.59176333	1	0.76102241	3.68725076	0.87923293
41	7	0.62107033	4.90429673	-1.45969763	7	0.46507577	4.75456963	-2.13202930
42	6	1.38931400	5.48247564	-2.55120343	6	1.17156828	5.29761147	-3.28137500
43	6	2.37404377	4.57042421	-3.29972564	6	1.96266783	4.32058649	-4.16570474
44	8	2.91911142	4.99078950	-4.32593985	8	2.47847180	4.73819821	-5.20806413
45	1	-0.35054155	4.66493754	-1.66085667	1	-0.53969921	4.60664439	-2.23358176
46	1	0.69536492	5.87395727	-3.30546045	1	0.44976812	5.79584489	-3.94117675
47	1	1.98872355	6.31622043	-2.15751337	1	1.89722066	6.04377198	-2.92735651
48	7	2.61524774	3.33304546	-2.78950532	7	2.07580483	3.02850355	-3.75531056
49	6	3.56595204	2.44716503	-3.45943521	6	2.73425620	2.05941401	-4.63149116
50	6	3.44669435	0.98238781	-3.04743456	6	2.67633426	0.62616354	-4.11663551
51	16	4.37766204	0.62596653	-1.47633145	16	3.93822242	0.28320508	-2.79493338
52	1	2.14383522	3.03585418	-1.93814641	1	1.53447267	2.70297910	-2.95501781
53	1	3.37775465	2.52870689	-4.54081367	1	2.24316643	2.08728047	-5.61909768
54	1	2.39982328	0.67870075	-2.92620319	1	1.68189417	0.37707814	-3.72682836
55	1	3.90962003	0.35257204	-3.81549477	1	2.91353381	-0.05956894	-4.93753167
56	1	4.59596685	2.80933246	-3.30231945	1	3.77434455	2.37690180	-4.80188798
57	6	-0.56085659	-2.50237764	-4.24681093	6	-1.63113129	-2.45126027	-5.04079218
58	16	0.49859626	-1.24464597	-3.42510235	16	-0.39696399	-1.28219196	-4.34093887
59	1	0.02953790	-2.97335125	-5.04275795	1	-1.17958014	-2.94201152	-5.91224796
60	1	-1.44817319	-2.02557768	-4.68178244	1	-2.53282691	-1.90936752	-5.35325443
61	1	-0.87722688	-3.26831314	-3.52780195	1	-1.90538661	-3.21099081	-4.29775736
62	6	3.03660368	-3.60532540	-0.90465860	6	2.16892328	-3.66940750	-2.05670566
63	6	2.28771177	-4.44311300	0.14356001	6	1.59685836	-4.48463744	-0.89013713
64	8	2.81867616	-5.39597531	0.71335399	8	2.28310589	-5.29155226	-0.26118333
65	6	3.23670350	-2.13563805	-0.50529894	6	2.91857969	-2.42497544	-1.55324406
66	16	4.61144830	-1.43629805	-1.54360383	16	4.08820599	-1.78619075	-2.85514180
67	1	4.00526560	-4.10805571	-1.02670852	1	2.86732817	-4.34415626	-2.57165644
68	1	2.34291860	-1.53098723	-0.69826764	1	2.22943618	-1.60383720	-1.32716234
69	1	3.53094416	-2.03966829	0.54624935	1	3.51958237	-2.66112639	-0.66650124
70	1	2.50474604	-3.65022863	-1.86786308	1	1.38653764	-3.36384927	-2.76705854
71	7	0.97591884	-4.07972266	0.36804272	7	0.26326792	-4.25746316	-0.61530866
72	6	0.19500980	-4.65633557	1.45630573	6	-0.38238249	-4.81930306	0.56254216
73	6	-0.98013706	-5.54585706	0.98935444	6	-1.67093819	-5.61610917	0.25361330
74	8	-1.64833471	-6.18184222	1.80565151	8	-2.28463608	-6.18187432	1.16047907
75	6	-0.39368791	-3.60052905	2.45193489	6	-0.74824675	-3.76756921	1.66461662

N		X	Y	Z		X	Y	Z
76	6	0.55206346	-2.52338793	2.87629763	6	0.36034689	-2.82430842	1.99517370
77	7	0.89846341	-1.45368751	2.05201298	7	0.68374156	-1.74853636	1.16799896
78	6	1.29871479	-2.39210370	4.03414756	6	1.29629111	-2.88645472	3.00665355
79	6	1.83379506	-0.74295300	2.77027893	6	1.78545544	-1.18646593	1.69366831
80	7	2.09781654	-1.26641471	3.96526934	7	2.17871931	-1.85138361	2.79927215
81	1	0.63667111	-3.20134670	-0.02952222	1	-0.18359887	-3.42868161	-1.02912237
82	1	0.88396897	-5.31990937	1.99877220	1	0.33897240	-5.53568316	0.98333963
83	1	-1.28774835	-3.15194577	1.99370276	1	-1.62396756	-3.19534553	1.32544664
84	1	-0.73652491	-4.16375934	3.32900729	1	-1.05087074	-4.33419494	2.55371540
85	1	1.32241209	-3.05468360	4.89512562	1	1.42028172	-3.59125094	3.81956360
86	1	2.30280924	0.15613756	2.37783454	1	2.29649786	-0.31363353	1.30185394
87	7	-1.24463231	-5.52687127	-0.35651346	7	-2.08197766	-5.60723059	-1.05197803
88	6	-2.23719777	-6.39130608	-0.96763675	6	-3.22255583	-6.37439333	-1.51823731
89	6	-3.35996877	-5.73079311	-1.78841668	6	-4.36312517	-5.61719504	-2.22406596
90	8	-4.04609184	-6.43490873	-2.53624937	8	-5.21305100	-6.26943234	-2.83963926
91	1	-0.54643206	-5.06828688	-0.93738261	1	-1.43651628	-5.20052028	-1.72467996
92	1	-1.76628291	-7.12547205	-1.63810157	1	-2.90911590	-7.16439969	-2.21684939
93	1	-2.71556599	-6.95001347	-0.14911365	1	-3.65444368	-6.86721994	-0.63485237
94	7	-3.54531451	-4.39167143	-1.63603724	7	-4.38042870	-4.26192293	-2.12822269
95	6	-4.66584687	-3.70543462	-2.27264238	6	-5.49908771	-3.48813287	-2.66277214
96	6	-4.40499999	-2.21767312	-2.45858530	6	-5.15023556	-2.01619120	-2.82820506
97	8	-4.27691935	-1.64166775	-1.15498122	8	-4.86402070	-1.50001911	-1.52675180
98	1	-3.00815899	-3.88590379	-0.93172849	1	-3.71561225	-3.78162630	-1.51948198
99	1	-4.83971566	-4.18210248	-3.24714586	1	-5.78017678	-3.91896782	-3.63386707
100	1	-3.48944349	-2.05186591	-3.05058470	1	-4.28157809	-1.89238991	-3.49650535
101	1	-5.25703446	-1.77975625	-3.00935575	1	-6.01435697	-1.50329434	-3.28788411
102	1	-4.12212466	-0.68419450	-1.19304602	1	-4.66095497	-0.55216454	-1.54750618
103	1	-5.58373854	-3.83762220	-1.67394431	1	-6.37512231	-3.58109255	-1.99818164
104	26	-0.22549381	-0.51039037	0.70278517	26	-0.57670299	-0.65159512	-0.08523669
105	26	-0.87415853	-0.32366104	-1.83571195	26	-1.48285457	-0.34991926	-2.53883131
106	16	-1.44307562	-1.94334424	-0.44728211	16	-1.99518051	-1.98292947	-1.14070829
107	16	0.31940770	1.12079863	-0.66428185	16	-0.08467985	0.99442249	-1.45853819
108	6	5.07218527	-0.09993114	7.22370310	6	4.03874095	-0.46090388	6.65043890
109	6	5.92442570	0.29266281	8.25878456	6	4.51207391	-0.01077568	7.87303016
110	6	7.26421842	-0.11259574	8.19063130	6	5.89305395	0.25527336	7.98840282
111	6	7.74662571	-0.88684381	7.12098591	6	6.78354418	0.07530147	6.90615079
112	6	6.87725218	-1.27578823	6.08062386	6	6.30286968	-0.37793549	5.67313025
113	6	5.52641404	-0.87251573	6.14438532	6	4.88645086	-0.66003084	5.50904081
114	8	4.69823891	-1.26119697	5.13688578	8	4.41770811	-1.06883941	4.38339967
115	8	8.09556040	0.28686037	9.23230720	8	6.33898884	0.70316858	9.21915791
116	6	7.35197538	-2.10442960	4.91031103	6	7.19964430	-0.58746126	4.48248414
117	1	7.74188145	-3.08243517	5.23309649	1	7.98869357	-1.32987089	4.68212909
118	1	6.52452600	-2.28495396	4.21690400	1	6.59010194	-0.94758757	3.64549654
119	1	8.15638098	-1.60014185	4.35282958	1	7.69954856	0.34318659	4.17039631
120	6	9.20630758	-1.28043627	7.12361621	6	8.24634281	0.38881321	7.13110522
121	1	9.46616951	-1.88006028	6.24543732	1	8.83670144	0.21578637	6.22577764
122	1	9.87018955	-0.39768318	7.11527963	1	8.40276676	1.44421604	7.41689990
123	1	9.46801282	-1.88229055	8.01190660	1	8.68602972	-0.23973135	7.92578750
124	6	5.44068825	1.12461743	9.41797100	6	3.60737079	0.19847492	9.06019742
125	1	5.59108349	0.60329147	10.37558715	1	3.91800138	-0.42087430	9.91520877
126	1	5.99669806	2.07159336	9.48978721	1	3.63582479	1.24270099	9.40638358
127	1	4.37291454	1.35606821	9.31187290	1	2.57094090	-0.05600182	8.80434004
128	1	4.02297455	0.20389934	7.25245280	1	2.97544822	-0.67610327	6.52422016
129	1	3.75902384	-0.95781496	5.15840395	1	2.98498052	-1.58455065	3.42610342
130	1	8.98715543	-0.04928954	9.03751829	1	7.29817068	0.85391392	9.14568907

N	P2^{nop} – approximation 1			P2^{nop} – approximation 2		
	Atom			Atom		
	number	X	Y	Z	number	X	Y	Z
1	6	-2.24340248	4.17481041	-7.68184948	6	-2.75577164	2.98418212	-5.40032816
2	6	-2.76083875	5.21033955	-6.69352150	6	-3.27320814	4.01971054	-4.41200113
3	8	-2.01709223	6.03091621	-6.14207745	8	-2.52946186	4.84028769	-3.86055684
4	6	-1.44331515	3.07941389	-6.96871853	6	-1.95568466	1.88878691	-4.68719816

5	16	-2.51910996	2.06349492	-5.85266733	16	-3.03147936	0.87286758	-3.57114673
6	1	-3.06278586	3.72715259	-8.26360035	1	-3.57515526	2.53652501	-5.98207903
7	1	-0.97782129	2.39793849	-7.69163799	1	-1.49019051	1.20731139	-5.41011667
8	1	-0.64544213	3.53026795	-6.36458492	1	-1.15781140	2.33964014	-4.08306456
9	1	-1.57352936	4.70236111	-8.37826443	1	-2.08589864	3.51173210	-6.09674358
10	7	-4.10679913	5.15991211	-6.44158077	7	-4.61916828	3.96928358	-4.16006041
11	6	-4.76228619	6.04327488	-5.49365044	6	-5.27465534	4.85264587	-3.21212959
12	6	-4.72075176	5.67263699	-3.99841237	6	-5.23312092	4.48200798	-1.71689200
13	8	-5.38846397	6.33238220	-3.20302129	8	-5.90083313	5.14175367	-0.92150158
14	1	-4.62072468	4.36401367	-6.80604839	1	-5.13309336	3.17338514	-4.52452803
15	1	-4.28373098	7.03058720	-5.56005621	1	-4.79610014	5.83995867	-3.27853537
16	1	-5.81761789	6.16129112	-5.77036667	1	-6.32998705	4.97066212	-3.48884583
17	7	-3.90168691	4.63928318	-3.65000224	7	-4.41405630	3.44865417	-1.36848259
18	6	-3.55778480	4.36855316	-2.25839019	6	-4.07015419	3.17792535	0.02312958
19	6	-2.39100790	5.26676083	-1.75599015	6	-2.90337706	4.07613230	0.52552968
20	8	-2.56427455	6.06796455	-0.83823895	8	-3.07664394	4.87733555	1.44328117
21	6	-3.26596761	2.86113787	-2.10243082	6	-3.77833700	1.67051065	0.17908877
22	6	-2.65384316	2.47723842	-0.79249370	6	-3.16621256	1.28661132	1.48902631
23	7	-1.56663454	1.61086619	-0.70409763	7	-2.07900381	0.42023909	1.57742238
24	6	-3.00749898	2.86725903	0.47906309	6	-3.51986837	1.67663181	2.76058340
25	6	-1.27921426	1.47600663	0.59127265	6	-1.79158354	0.28537941	2.87279296
26	7	-2.13268876	2.22338963	1.33126891	7	-2.64505816	1.03276229	3.61278939
27	1	-3.38872123	4.13553905	-4.37974977	1	-3.90109062	2.94491100	-2.09822893
28	1	-4.41609621	4.67629814	-1.64697874	1	-4.92846584	3.48566961	0.63454121
29	1	-4.20882845	2.31217122	-2.25947189	1	-4.72119761	1.12154388	0.02204776
30	1	-2.58116221	2.53982306	-2.90200901	1	-3.09353161	1.34919596	-0.62048936
31	1	-3.76092625	3.55905366	0.83338362	1	-4.27329588	2.36842585	3.11490393
32	1	-0.48938310	0.85979474	1.00961208	1	-1.00175238	-0.33083269	3.29113245
33	1	-2.10691476	2.31325316	2.34044647	1	-2.61928415	1.12262595	4.62196684
34	7	-1.20277083	5.11221313	-2.42108488	7	-1.71514022	3.92158413	-0.13956523
35	6	-0.00110694	5.79795361	-1.96985865	6	-0.51347619	4.60732508	0.31166095
36	6	0.94782639	6.29837132	-3.06355548	6	0.43545699	5.10774279	-0.78203583
37	8	2.02596545	6.79988194	-2.74241209	8	1.51359594	5.60925341	-0.46089235
38	1	-1.04664099	4.24106598	-2.94242239	1	-1.55901027	3.05043793	-0.66090262
39	1	-0.31772962	6.66161823	-1.37037694	1	-0.83009887	5.47098970	0.91114324
40	1	0.60594076	5.15480614	-1.31231093	1	0.09357142	3.96417785	0.96920925
41	7	0.55381501	6.12733364	-4.36377287	7	0.04144579	4.93670464	-2.08225179
42	6	1.32205892	6.70551205	-5.45527840	6	0.80968952	5.51488352	-3.17375755
43	6	2.30678868	5.79346085	-6.20380020	6	1.79441917	4.60283184	-3.92227960
44	8	2.85185647	6.21382618	-7.23001432	8	2.33948708	5.02319717	-4.94849396
45	1	-0.41779688	5.88797379	-4.56493187	1	-0.93016613	4.69734526	-2.28341079
46	1	0.62810963	7.09699345	-6.20953512	1	0.11574036	5.90636492	-3.92801452
47	1	1.92146838	7.53925514	-5.06158829	1	1.40909898	6.34862804	-2.78006744
48	7	2.54799247	4.55608177	-5.69358015	7	2.03562307	3.36545324	-3.41205931
49	6	3.49869680	3.67020059	-6.36350965	6	2.98632765	2.47957277	-4.08198929
50	6	3.37943912	2.20542288	-5.95150900	6	2.86706972	1.01479566	-3.66998863
51	16	4.31040668	1.84900200	-4.38040638	16	3.79803753	0.65837443	-2.09888554
52	1	2.07658029	4.25889015	-4.84222126	1	1.56421077	3.06826186	-2.56070042
53	1	3.31049943	3.75174189	-7.44488811	1	2.79813004	2.56111455	-5.16336775
54	1	2.33256817	1.90173626	-5.83027792	1	1.82019866	0.71110862	-3.54875731
55	1	3.84236503	1.57560694	-6.71956921	1	3.32999563	0.38497990	-4.43804884
56	1	4.52871132	4.03236866	-6.20639420	1	4.01634216	2.84174013	-3.92487359
57	6	-0.62811184	-1.27934277	-7.15088558	6	-1.14048111	-2.46996999	-4.86936522
58	16	0.43134090	-0.02161081	-6.32917690	16	-0.08102828	-1.21223807	-4.04765654
59	1	-0.03771736	-1.75031650	-7.94683361	1	-0.55008662	-2.94094348	-5.66531229
60	1	-1.51542842	-0.80254245	-7.58585739	1	-2.02779770	-1.99316990	-5.30433655
61	1	-0.94448227	-2.04527855	-6.43187666	1	-1.45685148	-3.23590541	-4.15035629
62	6	2.96934867	-2.38229060	-3.80873275	6	2.45697927	-3.57291770	-1.52721274
63	6	2.22045684	-3.22007847	-2.76051378	6	1.70808733	-4.41070509	-0.47899413
64	8	2.75142121	-4.17293930	-2.19071984	8	2.23905182	-5.36356735	0.09079987
65	6	3.16944814	-0.91260278	-3.40937281	6	2.65707874	-2.10323024	-1.12785304
66	16	4.54419279	-0.21326278	-4.44767904	16	4.03182364	-1.40389013	-2.16615796

67	1	3.93801069	-2.88502073	-3.93078303	1	3.42564106	-4.07564783	-1.64926267
68	1	2.27566361	-0.30795196	-3.60234141	1	1.76329410	-1.49857938	-1.32082176
69	1	3.46368909	-0.81663311	-2.35782456	1	2.95131969	-2.00726056	-0.07630479
70	1	2.43749094	-2.42719388	-4.77193832	1	1.92512143	-3.61782098	-2.49041724
71	7	0.90866369	-2.85668802	-2.53603125	7	0.39629430	-4.04731512	-0.25451142
72	6	0.12775460	-3.43330097	-1.44776845	6	-0.38461474	-4.62392759	0.83375162
73	6	-1.04739225	-4.32282162	-1.91471934	6	-1.55976152	-5.51344919	0.36680031
74	8	-1.71559000	-4.95880604	-1.09842277	8	-2.22795916	-6.14943457	1.18309736
75	6	-0.46094316	-2.37749410	-0.45213932	6	-0.97331244	-3.56812119	1.82938075
76	6	0.48480815	-1.30035293	-0.02777643	6	-0.02756107	-2.49098015	2.25374365
77	7	0.83120817	-0.23065226	-0.85206127	7	0.31883889	-1.42127967	1.42945886
78	6	1.23145938	-1.16906857	1.13007307	6	0.71909022	-2.35969591	3.41159368
79	6	1.76654005	0.48008239	-0.13379526	6	1.25417054	-0.71054512	2.14772487
80	7	2.03056145	-0.04337956	1.06119490	7	1.51819193	-1.23400688	3.34271526
81	1	0.56941599	-1.97831190	-2.93359613	1	0.05704659	-3.16893888	-0.65207636
82	1	0.81671375	-4.09687424	-0.90530205	1	0.30434442	-5.28750181	1.37621808
83	1	-1.35500360	-1.92891109	-0.91037154	1	-1.86737287	-3.11953807	1.37114859
84	1	-0.80378026	-2.94072437	0.42493302	1	-1.31614947	-4.13135147	2.70645332
85	1	1.25515676	-1.83164871	1.99105072	1	0.74278760	-3.02227592	4.27257109
86	1	2.23555422	1.37917268	-0.52623963	1	1.72318470	0.18854541	1.75528049
87	7	-1.31188762	-4.30383587	-3.26058722	7	-1.82425690	-5.49446344	-0.97906756
88	6	-2.30445337	-5.16826916	-3.87171125	6	-2.81682253	-6.35889816	-1.59019089
89	6	-3.42722392	-4.50775719	-4.69249153	6	-3.93959332	-5.69838524	-2.41097069
90	8	-4.11334753	-5.21187210	-5.44032431	8	-4.62571669	-6.40250111	-3.15880346
91	1	-0.61368740	-3.84525156	-3.84145689	1	-1.12605667	-5.03587914	-1.55993676
92	1	-1.83353829	-5.90243530	-4.54217672	1	-2.34590745	-7.09306431	-2.26065564
93	1	-2.78282094	-5.72697735	-3.05318737	1	-3.29519033	-6.91760588	-0.77166778
94	7	-3.61256957	-3.16863728	-4.54011250	7	-4.12493896	-4.35926390	-2.25859141
95	6	-4.73310232	-2.48239970	-5.17671728	6	-5.24547148	-3.67302680	-2.89519644
96	6	-4.47225571	-0.99463785	-5.36266041	6	-4.98462486	-2.18526530	-3.08113933
97	8	-4.34417439	-0.41863242	-4.05905628	8	-4.85654402	-1.60925984	-1.77753544
98	1	-3.07541394	-2.66286898	-3.83580303	1	-3.58778334	-3.85349607	-1.55428267
99	1	-4.90697098	-2.95906782	-6.15122032	1	-5.41934013	-4.14969492	-3.86969995
100	1	-3.55669856	-0.82883060	-5.95465946	1	-4.06906796	-2.01945806	-3.67313886
101	1	-5.32428980	-0.55672103	-5.91343021	1	-5.83665895	-1.74734843	-3.63190985
102	1	-4.18938017	0.53884101	-4.09712076	1	-4.70174932	-0.65178663	-1.81560016
103	1	-5.65099382	-2.61458731	-4.57801962	1	-6.16336298	-3.80521441	-2.29649854
104	26	-0.29274908	0.71264505	-2.20128870	26	-0.80511832	-0.47798249	0.08023107
105	26	-0.94141382	0.89937443	-4.73978710	26	-1.45378304	-0.29125318	-2.45826602
106	16	-1.51033103	-0.72030896	-3.35135603	16	-2.02270031	-1.91093636	-1.06983626
107	16	0.25215250	2.34383368	-3.56835580	16	-0.26021683	1.15320647	-1.28683591
108	6	5.00492954	1.12310421	4.31962872	6	4.49256039	-0.06752329	6.60114861
109	6	5.85717010	1.51569784	5.35470963	6	5.34480095	0.32507065	7.63622999
110	6	7.19696283	1.11043966	5.28655624	6	6.68459368	-0.08018788	7.56807661
111	6	7.67936945	0.33619145	4.21691179	6	7.16700125	-0.85443592	6.49843168
112	6	6.80999660	-0.05275296	3.17654991	6	6.29762745	-1.24338031	5.45806932
113	6	5.45915842	0.35051951	3.24031162	6	4.94678926	-0.84010786	5.52183104
114	8	4.63098335	-0.03816177	2.23281097	8	4.11861420	-1.22878909	4.51433134
115	8	8.02830410	1.50989544	6.32823229	8	7.51593542	0.31926823	8.60975361
116	6	7.28471994	-0.88139427	2.00623655	6	6.77235079	-2.07202172	4.28775692
117	1	7.67462492	-1.85940015	2.32902193	1	7.16225672	-3.05002737	4.61054230
118	1	6.45727062	-1.06191897	1.31282961	1	5.94490147	-2.25254631	3.59435010
119	1	8.08912468	-0.37710661	1.44875491	1	7.57675600	-1.56773400	3.73027539
120	6	9.13905239	-0.05740105	4.21954203	6	8.62668324	-1.24802840	6.50106192
121	1	9.39891434	-0.65702504	3.34136343	1	8.88654518	-1.84765244	5.62288284
122	1	9.80293465	0.82535207	4.21120548	1	9.29056549	-0.36527532	6.49272537
123	1	9.40075779	-0.65925533	5.10783195	1	8.88838863	-1.84988272	7.38935232
124	6	5.37343264	2.34765267	6.51389503	6	4.86106348	1.15702534	8.79541683
125	1	5.52382803	1.82632697	7.47151136	1	5.01145887	0.63569933	9.75303364
126	1	5.92944241	3.29462814	6.58571148	1	5.41707325	2.10400105	8.86723328
127	1	4.30565882	2.57910323	6.40779734	1	3.79328966	1.38847613	8.68931866
128	1	3.95571947	1.42693460	4.34837866	1	3.44334984	0.23630720	6.62989855

| 129 | 1 | 2.67831159 | 0.35702854 | 1.79316378 | 1 | 2.18785214 | -0.87079895 | 4.07399559 |
| 130 | 1 | 8.91989994 | 1.17374575 | 6.13344336 | 1 | 8.40753078 | -0.01688168 | 8.41496468 |

4. Model M3, Z = −1, m=1

E(M3) = -7957.71697411 a.u.
E(P3^{opt}) = -7957.71672176 a.u.
E(P3^{nop}) = -7957.68522889 a.u. (approximation 1)
E(P3^{nop}) = -7957.68700445 a.u. (approximation 2)

Atomic Coordinates

| N | M3 | | | | P3^{opt} | | | |
| | Atom | | | | Atom | | | |
	number	X	Y	Z	number	X	Y	Z
1	6	-1.56642025	2.93703489	-4.80350827	6	-2.57529328	3.29434013	-4.96295963
2	6	-2.34344351	3.92877661	-3.94928915	6	-2.77246769	4.29486272	-3.83346138
3	8	-1.78557978	4.79994550	-3.27071402	8	-1.83095154	4.90930703	-3.31732428
4	6	-0.84221647	1.90411848	-3.93354877	6	-1.90989109	2.01102837	-4.45616918
5	16	-2.03653703	0.80623573	-3.03751717	16	-3.00826186	1.07060501	-3.29687660
6	1	-2.22007339	2.42973548	-5.52850674	1	-3.52660989	3.05630575	-5.46169104
7	1	-0.19337832	1.26218572	-4.54233355	1	-1.65675019	1.34294884	-5.28869417
8	1	-0.21536264	2.41358893	-3.19034559	1	-0.98047489	2.25858567	-3.92727681
9	1	-0.81443128	3.51524748	-5.36236618	1	-1.90886327	3.76940222	-5.69962760
10	7	-3.70540384	3.77936015	-3.97010492	7	-4.06916933	4.45677336	-3.41879200
11	6	-4.60021209	4.61186750	-3.18618365	6	-4.44306611	5.34033930	-2.33009863
12	6	-4.83890520	4.24197542	-1.70946387	6	-4.33683516	4.81124607	-0.88760980
13	8	-5.70356891	4.84680370	-1.07674522	8	-4.79319779	5.49267881	0.03037613
14	1	-4.07732919	2.94938453	-4.42084066	1	-4.75669094	3.80030671	-3.77471212
15	1	-4.18775602	5.63059448	-3.16584103	1	-3.78375483	6.21931071	-2.36489252
16	1	-5.58261266	4.65596265	-3.67318762	1	-5.47444755	5.68707894	-2.47352745
17	7	-4.03257745	3.27442238	-1.18612151	7	-3.69736586	3.61888345	-0.71879475
18	6	-3.95914491	3.03274017	0.25077840	6	-3.28174862	3.16183789	0.60315119
19	6	-2.99470035	4.02305345	0.96468485	6	-1.95676832	3.83265280	1.06872221
20	8	-3.41404322	4.80525008	1.81719901	8	-1.92488805	4.52430964	2.08695254
21	6	-3.58579565	1.55413145	0.48904483	6	-3.20098989	1.62098942	0.59621659
22	6	-3.21218847	1.22630502	1.90030811	6	-2.56046050	1.03148022	1.81308535
23	7	-2.09805389	0.45127752	2.21338719	7	-1.64188966	-0.01574794	1.74366115
24	6	-3.83263984	1.59461128	3.07234316	6	-2.73650182	1.37985933	3.13341778
25	6	-2.05398260	0.34923510	3.54240207	6	-1.28790442	-0.29369479	2.99779884
26	7	-3.08949061	1.02963934	4.08961726	7	-1.92978052	0.53029132	3.86173257
27	1	-3.34299827	2.81485319	-1.78813156	1	-3.35075709	3.10995267	-1.53788358
28	1	-4.94575578	3.26977140	0.66982187	1	-4.03040804	3.52154081	1.32124948
29	1	-4.43281149	0.92948599	0.16159646	1	-4.22124237	1.22329812	0.47087990
30	1	-2.73412110	1.28714197	-0.15516075	1	-2.62658847	1.28827182	-0.28172317
31	1	-4.69122236	2.22619190	3.26138646	1	-3.31609331	2.16874956	3.59552293
32	1	-1.31302702	-0.19960429	4.11536244	1	-0.59983934	-1.07016144	3.31077751
33	1	-3.26451781	1.12799710	5.08304061	1	-1.80215719	0.54375188	4.86718848
34	7	-1.68810091	3.96752968	0.55542396	7	-0.87367885	3.61225484	0.26020073
35	6	-0.66171432	4.74513616	1.23339367	6	0.45003777	4.06664080	0.65950416
36	6	0.45482994	5.31382471	0.35217688	6	1.41908579	4.41193533	-0.47494906
37	8	1.39938011	5.90065967	0.88165993	8	2.59187570	4.67213915	-0.20286750
38	1	-1.36058696	3.11237803	0.08955727	1	-0.88998263	2.78562992	-0.35323598
39	1	-1.15977274	5.58380173	1.73744802	1	0.32373397	4.95918144	1.28653442
40	1	-0.15906582	4.15274384	2.01512275	1	0.96728153	3.31523004	1.27833005
41	7	0.35789520	5.10670462	-0.99810456	7	0.93064160	4.38813024	-1.75452697
42	6	1.29312847	5.74083294	-1.91427746	6	1.75741829	4.83014438	-2.86695159
43	6	2.48389221	4.90996669	-2.41788227	6	2.48281997	3.76061611	-3.70230660
44	8	3.21049743	5.37862504	-3.30077295	8	3.12350868	4.11654485	-4.69663993
45	1	-0.52928218	4.79295072	-1.39340618	1	-0.07871374	4.36715190	-1.90404689
46	1	0.74679400	6.07119594	-2.80665027	1	1.13411318	5.39896809	-3.56897743

47	1	1.72732776	6.62260417	-1.42117720	1	2.54298117	5.49446174	-2.47983384
48	7	2.69768744	3.68913188	-1.85853659	7	2.40007024	2.46295160	-3.29904534
49	6	3.82172384	2.87375715	-2.31672550	6	2.96746969	1.41372246	-4.14711139
50	6	3.73542492	1.40758903	-1.90208961	6	2.87272203	0.01787317	-3.54460780
51	16	4.37564999	1.12956545	-0.17734864	16	4.05544902	-0.25571054	-2.13670223
52	1	2.05830068	3.33627211	-1.14955941	1	1.72911400	2.20651305	-2.57335382
53	1	3.84029476	2.92953046	-3.41619167	1	2.43216758	1.39588698	-5.11329224
54	1	2.70983739	1.02548876	-1.97300997	1	1.85667307	-0.20220666	-3.19557695
55	1	4.37951292	0.80965967	-2.55654949	1	3.14835458	-0.71780736	-4.30878970
56	1	4.77186784	3.31718223	-1.97517402	1	4.00995154	1.67755560	-4.37397046
57	6	0.35846874	-2.38116397	-3.85040480	6	-1.62842861	-2.37159197	-5.08780644
58	16	1.11520191	-1.02161187	-2.87128871	16	-0.39428668	-1.25743183	-4.30373362
59	1	1.13596617	-2.80355009	-4.49924697	1	-1.15386005	-2.85069895	-5.95341237
60	1	-0.46241040	-1.99366109	-4.46672252	1	-2.50109752	-1.79674170	-5.42299916
61	1	-0.02600336	-3.16530294	-3.18629304	1	-1.95570606	-3.14265314	-4.37901645
62	6	3.23877603	-3.18275725	0.17181802	6	2.12342296	-3.70982035	-1.86945137
63	6	2.36829652	-4.06475069	1.08059766	6	1.41304782	-4.68977659	-0.92639796
64	8	2.85400310	-4.94612002	1.78913016	8	2.00907763	-5.62965038	-0.39593106
65	6	3.27091817	-1.70625615	0.59496247	6	3.41513910	-3.20807819	-1.21490007
66	16	4.76844335	-0.90997305	-0.16639637	16	4.56902303	-2.26313610	-2.30837148
67	1	4.24323464	-3.62308249	0.22827679	1	2.37207820	-4.26518019	-2.78685554
68	1	2.39322462	-1.15688217	0.23557029	1	3.21414732	-2.57017579	-0.34594143
69	1	3.35426084	-1.60097564	1.68281793	1	4.01439505	-4.06497410	-0.87492303
70	1	2.89064823	-3.25370219	-0.87029395	1	1.46902490	-2.87500998	-2.15753194
71	7	1.01142160	-3.82359578	1.01597114	7	0.06875545	-4.44943042	-0.73212213
72	6	0.07552257	-4.43988795	1.94972221	6	-0.67135300	-5.09882309	0.34104499
73	6	-0.92134956	-5.41859621	1.28889040	6	-1.96670103	-5.80965525	-0.11008937
74	8	-1.70059728	-6.08013165	1.97621997	8	-2.64361051	-6.43950807	0.70510455
75	6	-0.76350601	-3.41423626	2.78611687	6	-1.05703022	-4.12743859	1.51001830
76	6	0.01800159	-2.26914751	3.34515122	6	0.06052517	-3.24178940	1.95505201
77	7	0.41124966	-1.17944953	2.57027989	7	0.46353343	-2.13351658	1.20784739
78	6	0.57909263	-2.08963506	4.59806633	6	0.93343737	-3.39008037	3.01330739
79	6	1.19127128	-0.41262194	3.40853845	6	1.54703869	-1.63628630	1.82697595
80	7	1.30600325	-0.91557768	4.63513005	7	1.85926469	-2.37778426	2.91065185
81	1	0.68844167	-2.98598773	0.52630773	1	-0.30799228	-3.55008768	-1.05628939
82	1	0.69074603	-5.04278530	2.63344796	1	-0.00542354	-5.88202835	0.73276688
83	1	-1.58183369	-3.03667949	2.15509340	1	-1.90269301	-3.50569472	1.18152653
84	1	-1.22767979	-3.98721608	3.59863171	1	-1.41032308	-4.75013942	2.34090921
85	1	0.52685109	-2.74996072	5.45926910	1	0.98423614	-4.13645191	3.79612917
86	1	1.65285307	0.51482927	3.07738529	1	2.10167695	-0.75691583	1.51708099
87	7	-0.90554741	-5.45119169	-0.08265769	7	-2.30826720	-5.65756262	-1.42652464
88	6	-1.69432869	-6.39871719	-0.84800838	6	-3.44129542	-6.34179913	-2.02330310
89	6	-2.66195958	-5.83887480	-1.90633398	6	-4.53973085	-5.49075789	-2.68895855
90	8	-3.13512014	-6.60728283	-2.74976710	8	-5.37514646	-6.05983960	-3.39990628
91	1	-0.13320323	-4.96013041	-0.52709610	1	-1.62085246	-5.20195105	-2.02199939
92	1	-1.05042698	-7.11633454	-1.37789712	1	-3.10952599	-7.05608906	-2.79144347
93	1	-2.29564287	-6.96703428	-0.12244277	1	-3.92024021	-6.91968222	-1.21940137
94	7	-2.95568497	-4.51175227	-1.84909955	7	-4.53889178	-4.15317645	-2.45323817
95	6	-3.96443924	-3.92342525	-2.72555615	6	-5.61436348	-3.30060235	-2.95526515
96	6	-3.78234332	-2.42162090	-2.88962719	6	-5.21360079	-1.83296145	-2.99863318
97	8	-3.96894034	-1.82754158	-1.60142617	8	-4.96294352	-1.42133149	-1.65328906
98	1	-2.61353551	-3.95368650	-1.06682391	1	-3.87971095	-3.74864793	-1.78587423
99	1	-3.89163832	-4.42073746	-3.70255998	1	-5.88087577	-3.64733895	-3.96340375
100	1	-2.77897117	-2.18972327	-3.28450228	1	-4.31678274	-1.68994214	-3.62426846
101	1	-4.53212394	-2.05549546	-3.61396096	1	-6.04329191	-1.25935522	-3.45040159
102	1	-3.89248974	-0.86073726	-1.63289740	1	-4.70797533	-0.48699965	-1.59947896
103	1	-4.97568867	-4.12278873	-2.33055261	1	-6.51207286	-3.41206273	-2.32312342
104	26	-0.48885457	-0.34309527	1.00857797	26	-0.69242335	-0.89577042	-0.01345614
105	26	-0.62318708	-0.21968463	-1.60838493	26	-1.49228902	-0.39297096	-2.47569331
106	16	-1.32511446	-1.87760626	-0.33155683	16	-2.13551345	-2.08092775	-1.19853106
107	16	0.17615475	1.33271997	-0.24503450	16	-0.06624860	0.80044077	-1.26681922
108	6	5.51705158	-0.39178226	7.13740280	6	3.75879961	-0.26212958	6.87205811

	6	6.86071271	-0.12484807	7.41405975	6	4.28255069	0.76162742	7.64508958
109	6	6.86071271	-0.12484807	7.41405975	6	4.28255069	0.76162742	7.64508958
110	6	7.82523775	-0.70239439	6.57427248	6	5.37968224	1.48394892	7.12777937
111	6	7.47022564	-1.52116921	5.48907655	6	5.94682973	1.18737123	5.86763199
112	6	6.10966022	-1.77851289	5.22004181	6	5.41819089	0.15068213	5.09138921
113	6	5.13436467	-1.20551711	6.06406461	6	4.27694212	-0.60729583	5.57825839
114	8	3.81373374	-1.52967460	5.84718679	8	3.74601177	-1.55039448	4.88309219
115	8	9.15602799	-0.43203468	6.86340517	8	5.87971077	2.50169287	7.91803296
116	6	5.68397559	-2.64588435	4.06022259	6	5.97997585	-0.21518687	3.74399528
117	1	6.10608479	-3.65974085	4.12899593	1	7.05600590	-0.44292040	3.78969604
118	1	4.59365764	-2.73747392	4.04373443	1	5.45343435	-1.10275791	3.37403257
119	1	6.00978193	-2.22123955	3.09778919	1	5.85073694	0.59257958	3.00585193
120	6	8.57569473	-2.09417973	4.63168720	6	7.11685304	2.02532622	5.40157457
121	1	8.17726846	-2.68678101	3.80236334	1	7.45199380	1.72688159	4.40341239
122	1	9.20049812	-1.30125294	4.18340935	1	6.85548027	3.09651700	5.33893987
123	1	9.24405277	-2.75667232	5.20989760	1	7.98655406	1.93260639	6.07577737
124	6	7.28314490	0.74691914	8.56809204	6	3.72123768	1.11903943	8.99741829
125	1	7.93141905	0.19888881	9.26876983	1	4.48346113	1.02398848	9.78558423
126	1	7.86437394	1.61515277	8.22219879	1	3.37563362	2.16349320	9.02441282
127	1	6.40693255	1.11277880	9.11884082	1	2.87697230	0.46452695	9.24878887
128	1	4.74035673	0.02561458	7.78144610	1	2.91057441	-0.84593189	7.23520980
129	1	3.18990299	-0.79951968	5.64205104	1	2.60214112	-2.12902844	3.60825197
130	1	9.69539901	-0.87487519	6.18551903	1	6.60511615	2.92584880	7.42556209

N	$P3^{nop}$ – approximation 1				$P3^{nop}$ – approximation 2			
	Atom				Atom			
	number	X	Y	Z	number	X	Y	Z
1	1	2.26661038	-1.08686733	1.46895480	6	-2.14604497	2.96944189	-5.42606258
2	6	-2.85738087	4.18820000	-7.14489269	6	-2.92306805	3.96118355	-4.57184362
3	6	-3.18040919	5.16988468	-6.02745819	8	-2.36520457	4.83235264	-3.89326859
4	8	-2.30823541	5.83722305	-5.45773125	6	-1.42184114	1.93652570	-4.55610323
5	6	-2.15090442	2.94211245	-6.60083866	16	-2.61616158	0.83864290	-3.66007137
6	16	-3.26672959	1.94562638	-5.50666857	1	-2.79969811	2.46214247	-6.15106106
7	1	-3.76100254	3.89840913	-7.70143795	1	-0.77300304	1.29459286	-5.16488791
8	1	-1.81800807	2.29016089	-7.41796398	1	-0.79498732	2.44599628	-3.81290007
9	1	-1.26756823	3.23598886	-6.01927090	1	-1.39405608	3.54765463	-5.98492050
10	1	-2.17555189	4.70446110	-7.83840466	7	-4.28502846	3.81176710	-4.59265947
11	7	-4.50432253	5.25147820	-5.68340588	6	-5.17983675	4.64427471	-3.80873823
12	6	-4.98798418	6.10653782	-4.61429787	6	-5.41852999	4.27438259	-2.33201838
13	6	-4.90812302	5.58510303	-3.16637588	8	-6.28319359	4.87921095	-1.69929969
14	8	-5.44646645	6.23318863	-2.26981020	1	-4.65695381	2.98179150	-5.04339504
15	1	-5.13407326	4.56292200	-6.08295536	1	-4.76738071	5.66300154	-3.78839540
16	1	-4.39317703	7.03093433	-4.62179184	1	-6.16223717	4.68836975	-4.29574203
17	1	-6.03411388	6.37751198	-4.80493069	7	-4.61220217	3.30682945	-1.80867589
18	7	-4.19988060	4.43613625	-2.97123456	6	-4.53876972	3.06514740	-0.37177601
19	6	-3.80965996	3.99382567	-1.63680422	6	-3.57432508	4.05546093	0.34213042
20	6	-2.52023911	4.70569181	-1.13553882	8	-3.99366784	4.83765745	1.19464457
21	8	-2.54604387	5.42387390	-0.13660254	6	-4.16542053	1.58653867	-0.13350961
22	6	-3.68421054	2.45555806	-1.63847637	6	-3.79181314	1.25871217	1.27775371
23	6	-3.03321886	1.88301790	-0.41899192	7	-2.67767859	0.48368469	1.59083283
24	7	-2.04978228	0.89973950	-0.49379909	6	-4.41226482	1.62701845	2.44978857
25	6	-3.24849749	2.18689394	0.90602601	6	-2.63360715	0.38164225	2.91984749
26	6	-1.68769264	0.61326134	0.75742710	7	-3.66911530	1.06204653	3.46706295
27	7	-2.39489818	1.37492001	1.62587130	1	-3.92262292	2.84726048	-2.41068602
28	1	-3.79103041	3.95470142	-3.77754807	1	-5.52538061	3.30217838	0.04726744
29	1	-4.59006071	4.33158875	-0.94249475	1	-5.01243591	0.96189314	-0.46095794
30	1	-4.69203186	2.02933621	-1.77102971	1	-3.31374574	1.31954908	-0.77771521
31	1	-3.09506941	2.14120698	-2.51354909	1	-5.27084684	2.25859928	2.63883209
32	1	-3.88946366	2.92004108	1.37850535	1	-1.89265180	-0.16719712	3.49280834
33	1	-0.94678921	-0.12257271	1.05395949	1	-3.84414244	1.16040421	4.46048641
34	1	-2.28699160	1.36570132	2.63361692	7	-2.26772571	3.99993706	-0.06713045
35	7	-1.39892340	4.49111748	-1.89347851	6	-1.24133897	4.77754354	0.61083925
36	6	-0.10163974	4.98981905	-1.46193969	6	-0.12479478	5.34623194	-0.27037755
37	6	0.84090930	5.48016071	-2.56567788	8	0.81975538	5.93306684	0.25910550

38	8	1.98540664	5.82605839	-2.26994944	1	-1.94021177	3.14478540	-0.53299713
39	1	-1.37530649	3.66459107	-2.50315094	1	-1.73939753	5.61620903	1.11489356
40	1	-0.28015617	5.82322788	-0.76994789	1	-0.73869050	4.18515110	1.39256823
41	1	0.45860183	4.22256374	-0.90337574	7	-0.22172952	5.13911200	-1.62065899
42	7	0.36289757	5.47621059	-3.84907985	6	0.71350378	5.77324009	-2.53683186
43	6	1.13763893	6.06512117	-4.93052387	6	1.90426755	4.94237375	-3.04043674
44	6	1.97358334	5.12496424	-5.81303978	8	2.63087273	5.41103220	-3.92332745
45	8	2.52699351	5.58215761	-6.81906605	1	-1.10890687	4.82535791	-2.01596069
46	1	-0.63954788	5.36949635	-4.00888348	1	0.16716927	6.10360336	-3.42920446
47	1	0.45648989	6.59855270	-5.60532284	1	1.14770293	6.65501165	-2.04373169
48	1	1.84731734	6.78828096	-4.50321960	7	2.11806273	3.72153902	-2.48109102
49	7	2.08058357	3.82148004	-5.44118834	6	3.24209929	2.90616417	-2.93928003
50	6	2.86801434	2.90133238	-6.26044750	6	3.15580034	1.43999624	-2.52464390
51	6	2.60590553	1.42724454	-5.96508217	16	3.79602528	1.16197264	-0.79990304
52	16	3.59931064	0.81701821	-4.51502991	1	1.47867608	3.36867905	-1.77211380
53	1	1.58784461	3.48651052	-4.61585712	1	3.26067019	2.96193743	-4.03874588
54	1	2.61496377	3.10126591	-7.31323433	1	2.13021278	1.05789590	-2.59556437
55	1	1.54212868	1.23278677	-5.78194332	1	3.79988813	0.84206682	-3.17910385
56	1	2.93121052	0.82523501	-6.82085133	1	4.19224310	3.34958935	-2.59772849
57	1	3.94165468	3.13159323	-6.15842390	6	-0.22115597	-2.34875679	-4.47295904
58	6	-1.83053505	-1.45360839	-7.21991253	16	0.53557724	-0.98920476	-3.49384308
59	16	-0.59767199	-0.38257292	-6.37574577	1	0.55634147	-2.77114296	-5.12180138
60	1	-1.34318006	-1.90690100	-8.09219360	1	-1.04203510	-1.96125388	-5.08927679
61	1	-2.68973947	-0.85633987	-7.54963684	1	-0.60562807	-3.13289595	-3.80884743
62	1	-2.17773223	-2.24590373	-6.54492950	6	2.65915132	-3.15035009	-0.45073640
63	6	1.76953232	-3.25530958	-4.23514175	6	1.78867197	-4.03234339	0.45804322
64	6	1.00575316	-4.09605026	-3.19988656	8	2.27437854	-4.91371250	1.16657579
65	8	1.47472835	-5.13293028	-2.73141503	6	2.69129348	-1.67384899	-0.02759194
66	6	2.19691563	-1.87535560	-3.71271253	16	4.18881893	-0.87756586	-0.78895080
67	16	3.57531977	-1.24173391	-4.78764343	1	3.66360998	-3.59067535	-0.39427763
68	1	2.64884949	-3.85884905	-4.49662113	1	1.81360006	-1.12447500	-0.38698411
69	1	1.38135338	-1.14528286	-3.76694345	1	2.77463627	-1.56856847	1.06026351
70	1	2.57495642	-1.93320262	-2.68545699	1	2.31102347	-3.22129488	-1.49284840
71	1	1.15924346	-3.12640381	-5.14242601	7	0.43179685	-3.79118872	0.39341676
72	7	-0.24822065	-3.62782383	-2.86577129	6	-0.50410211	-4.40748072	1.32716775
73	6	-1.01560414	-4.20157623	-1.76578987	6	-1.50097430	-5.38618898	0.66633594
74	6	-2.31986523	-4.90392494	-2.20628905	8	-2.28022194	-6.04772425	1.35366559
75	8	-3.01089001	-5.51444006	-1.38938880	6	-1.34313071	-3.38182926	2.16356230
76	6	-1.39526963	-3.17412329	-0.64536417	6	-0.56162310	-2.23674011	2.72259665
77	6	-0.28844026	-2.25994515	-0.22849979	7	-0.16837505	-1.14704239	1.94772542
78	7	0.09842956	-1.15563118	-0.98579693	6	-0.00053209	-2.05722809	3.97551203
79	6	0.59866250	-2.34640718	0.83094156	6	0.61164659	-0.38021478	2.78598404
80	6	1.20141530	-0.64845353	-0.33359778	7	0.72637850	-0.88317055	4.01257563
81	7	1.52580929	-1.32441580	0.76575172	1	0.10881698	-2.95358038	-0.09624672
82	1	-0.51565045	-2.69011116	-3.17349672	1	0.11112130	-5.01037788	2.01089334
83	1	-0.37593567	-4.98443317	-1.33307517	1	-2.16145849	-3.00427246	1.53253901
84	1	-2.25776887	-2.58500576	-0.99072015	1	-1.80730462	-3.95480871	2.97607708
85	1	-1.73864675	-3.76702833	0.21177994	1	-0.05277359	-2.71755362	4.83671474
86	1	0.64065880	-3.09919643	1.61326611	1	1.07322836	0.54723644	2.45483065
87	1	1.73488390	0.22614789	-0.69894445	7	-1.48517203	-5.41878462	-0.70521212
88	7	-2.66248059	-4.75311089	-3.52630782	6	-2.27395344	-6.36631012	-1.47056282
89	6	-3.79041052	-5.44521761	-4.12174988	6	-3.24158430	-5.80646753	-2.52888823
90	6	-4.86804485	-4.59566545	-4.81923103	8	-3.71474481	-6.57487535	-3.37232161
91	8	-5.68215704	-5.15432644	-5.56140232	1	-0.71282792	-4.92772293	-1.14965057
92	1	-1.94911826	-4.34080410	-4.12338018	1	-1.63005161	-7.08392715	-2.00045156
93	1	-3.45677781	-6.18094778	-4.86846161	1	-2.87526751	-6.93462706	-0.74499720
94	1	-4.28497553	-5.99919271	-3.30949879	7	-3.53530955	-4.47934484	-2.47165394
95	7	-4.87205791	-3.25844145	-4.56968594	6	-4.54406404	-3.89101791	-3.34811068
96	6	-5.93648243	-2.39884305	-5.07926798	6	-4.36196804	-2.38921356	-3.51218176
97	6	-5.51255703	-0.93959695	-5.15824318	8	-4.54856491	-1.79513443	-2.22398043
98	8	-5.24322557	-0.50244641	-3.82273841	1	-3.19316006	-3.92127943	-1.68937838
99	1	-4.23874903	-2.87538648	-3.86780310	1	-4.47126293	-4.38832998	-4.32511425

N	Atom number	X	Y	Z	Atom number	X	Y	Z
100	1	-6.21494389	-2.76471734	-6.07713699	1	-3.35859585	-2.15731621	-3.90705681
101	1	-4.61844444	-0.82529026	-5.79394722	1	-5.11174870	-2.02308846	-4.23651552
102	1	-6.33628893	-0.36035553	-5.61285686	1	-4.47211456	-0.82833010	-2.25545168
103	1	-4.98993301	0.43367317	-3.79132128	1	-5.55531311	-4.09038162	-2.95310688
104	1	-6.83166122	-2.48008513	-4.43847847	26	-1.06847930	-0.31068811	0.38602352
105	26	-0.99012321	0.02089917	-2.16014457	26	-1.20281172	-0.18727747	-2.23093939
106	26	-1.76328361	0.51711899	-4.61741114	16	-1.90473914	-1.84519911	-0.95411122
107	16	-2.42491603	-1.15916693	-3.34284711	16	-0.40346998	1.36512709	-0.86758894
108	16	-0.35399920	1.71762121	-3.40074515	6	4.93742704	-0.35937509	6.51484871
109	6	6.25555658	-1.84561384	2.04085255	6	6.28108788	-0.09244090	6.79150534
110	6	7.65062475	-1.84394085	1.95680726	6	7.24561310	-0.66998720	5.95171833
111	6	8.23581696	-2.45388222	0.83674300	6	6.89060116	-1.48876202	4.86652231
112	6	7.46180677	-3.04858661	-0.17383803	6	5.53003550	-1.74610567	4.59748745
113	6	6.05455875	-3.03913021	-0.07700028	6	4.55473995	-1.17310989	5.44151020
114	6	5.45936441	-2.43242788	1.04970801	8	3.23410916	-1.49726748	5.22463226
115	8	4.09021997	-2.50187778	1.17970908	8	8.57640266	-0.39962751	6.24085093
116	8	9.62256527	-2.44842505	0.76849353	6	5.10435104	-2.61347723	3.43766832
117	6	5.18503428	-3.65956688	-1.14361858	1	5.52646017	-3.62733364	3.50644159
118	1	5.40408611	-4.72896576	-1.28126931	1	4.01403284	-2.70506668	3.42118025
119	1	4.13070011	-3.56689215	-0.86562169	1	5.43015718	-2.18883228	2.47523499
120	1	5.33003521	-3.16848779	-2.11867595	6	7.99607038	-2.06177235	4.00913286
121	6	8.17680931	-3.67497897	-1.34935188	1	7.59764338	-2.65437365	3.17980909
122	1	7.47142744	-4.07613087	-2.08365703	1	8.62087345	-1.26884580	3.56085491
123	1	8.80851650	-2.94290924	-1.88346803	1	8.66442776	-2.72426510	4.58734322
124	1	8.82811451	-4.51057339	-1.03743315	6	6.70352030	0.77932632	7.94553804
125	6	8.51644802	-1.21789205	3.01916504	1	7.35179424	0.23129597	8.64621544
126	1	9.20246983	-1.95489204	3.46365547	1	7.28474951	1.64755988	7.59964418
127	1	9.14783764	-0.41889331	2.60154438	1	5.82730770	1.14518595	8.49628639
128	1	7.89947271	-0.79027945	3.82002306	1	4.16073227	0.05802175	7.15889168
129	1	5.76675606	-1.39667928	2.90789270	1	1.25134242	-0.47863612	4.82569647
130	1	9.87305069	-2.87848115	-0.06746639	1	9.11577415	-0.84246802	5.56296492

5. Model M4, Z = −1, m=1

E(M4) = -7957.71607876 a.u.
E(P4^{opt}) = -7957.71520485 a.u.
E(P4^{nop}) = -7957.70032013 a.u. (approximation 1)
E(P4^{nop}) = -7957.69904931 a.u. (approximation 2)

Atomic Coordinates

N	M4 Atom number	X	Y	Z	P4^{opt} Atom number	X	Y	Z
1	6	-1.67277174	3.09574908	-4.56389605	6	-2.30845819	3.17182060	-5.15349786
2	6	-2.24220346	4.09770835	-3.56968361	6	-2.77668019	4.17235033	-4.10676407
3	8	-1.52574945	4.87536777	-2.92702472	8	-1.99538176	4.91601076	-3.50058935
4	6	-0.97365735	1.93654719	-3.84482691	6	-1.63157207	1.96099438	-4.50115387
5	16	-2.17453369	0.91040727	-2.87706887	16	-2.82376003	0.95983340	-3.49691727
6	1	-2.45215866	2.70795238	-5.23648196	1	-3.14024009	2.83963781	-5.79234462
7	1	-0.47239850	1.27366200	-4.56123902	1	-1.19957938	1.29689687	-5.26042206
8	1	-0.21440240	2.32482730	-3.15364873	1	-0.81976776	2.29527768	-3.84200063
9	1	-0.92823375	3.63329543	-5.17093595	1	-1.57154266	3.68980851	-5.78621652
10	7	-3.60379942	4.06738544	-3.41972508	7	-4.12689421	4.17924292	-3.87007830
11	6	-4.30875454	4.91979738	-2.47884036	6	-4.74360417	5.02903687	-2.86807380
12	6	-4.37536081	4.48429399	-1.00186041	6	-4.74457391	4.55517680	-1.40213605
13	8	-5.07344466	5.13168709	-0.22248450	8	-5.37592047	5.20540078	-0.56913645
14	1	-4.10378218	3.29822387	-3.85453231	1	-4.67146041	3.42307674	-4.27365013
15	1	-3.81223151	5.90028892	-2.46772813	1	-4.20802969	5.98882677	-2.86000594
16	1	-5.34067042	5.06926506	-2.82106733	1	-5.78656917	5.22833270	-3.14576882
17	7	-3.61343667	3.40993305	-0.64808388	7	-4.00234079	3.44759124	-1.11605233

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18	6	-3.37005292	3.06833166	0.74930121	6	-3.70225006	3.06786636	0.26008767
19	6	-2.20321254	3.89686012	1.35982999	6	-2.48575942	3.84998433	0.83317429
20	8	-2.40345818	4.67297915	2.29356642	8	-2.62021305	4.60440884	1.79704139
21	6	-3.14822744	1.54504979	0.85756864	6	-3.51419811	1.53818195	0.33297471
22	6	-2.63431516	1.08101120	2.18377771	6	-2.96235614	1.05069207	1.63535036
23	7	-1.60878612	0.14513516	2.29668752	7	-1.94745163	0.09757131	1.70898119
24	6	-3.03259253	1.44900285	3.44879132	6	-3.31400011	1.42344754	2.91317528
25	6	-1.40140162	-0.05173816	3.59929951	6	-1.70633017	-0.10183494	3.00384281
26	7	-2.24671968	0.72239638	4.32110033	7	-2.51386431	0.68303447	3.75882518
27	1	-3.07197938	2.91784075	-1.36562471	1	-3.52280213	2.94823973	-1.87250480
28	1	-4.25300101	3.38701851	1.31858827	1	-4.54827101	3.39806260	0.87709930
29	1	-4.10015541	1.04278173	0.61955006	1	-4.48577804	1.06032027	0.12715385
30	1	-2.42800367	1.22809752	0.08787136	1	-2.83017372	1.21309631	-0.46575705
31	1	-3.76048978	2.17459166	3.78869793	1	-4.01531001	2.16334787	3.27725523
32	1	-0.67491246	-0.73118983	4.03401611	1	-0.98562328	-0.79576267	3.41989709
33	1	-2.27078998	0.77587632	5.33293395	1	-2.50355246	0.73824804	4.77076127
34	7	-0.98102058	3.71455849	0.76727815	7	-1.29884988	3.64965485	0.17969653
35	6	0.21526590	4.33284883	1.31870672	6	-0.06228144	4.21620612	0.69556661
36	6	1.25392301	4.82072850	0.30367406	6	0.94853129	4.70340054	-0.34677670
37	8	2.34229659	5.23693701	0.70461859	8	2.06104984	5.08069549	0.02338416
38	1	-0.82566229	2.85540904	0.22576650	1	-1.19197859	2.80224819	-0.39408822
39	1	-0.10427102	5.19222859	1.92315520	1	-0.32870211	5.06573336	1.33830643
40	1	0.74962410	3.64525000	1.99391291	1	0.47967598	3.49252310	1.32565028
41	7	0.92246911	4.73667263	-1.02124596	7	0.56290084	4.66639527	-1.66008916
42	6	1.77874369	5.31560441	-2.04419030	6	1.41257133	5.23010006	-2.69663716
43	6	2.76529808	4.38662975	-2.76964385	6	2.31140519	4.26495417	-3.48596835
44	8	3.35547069	4.80647469	-3.77056563	8	2.97551910	4.69933574	-4.43310238
45	1	-0.04720624	4.55836992	-1.28586653	1	-0.42281206	4.53376023	-1.88914180
46	1	1.14770577	5.76431191	-2.82111793	1	0.78154498	5.74144567	-3.43477029
47	1	2.39089536	6.10675593	-1.58652807	1	2.08699089	5.96781088	-2.23895414
48	7	2.95570600	3.13752130	-2.26233827	7	2.34778370	2.96211982	-3.09717784
49	6	3.95036312	2.25108764	-2.86230676	6	3.12464567	2.00299307	-3.88133442
50	6	3.68124931	0.76308079	-2.63858633	6	2.99428088	0.56612144	-3.39275625
51	16	4.41543095	0.17834660	-1.03214488	16	3.98728294	0.24116998	-1.85538728
52	1	2.48504780	2.87185089	-1.40060239	1	1.70086173	2.62850688	-2.38339215
53	1	3.93944906	2.46291030	-3.94106498	1	2.78024007	2.03938149	-4.92903154
54	1	2.60850665	0.53715436	-2.65577044	1	1.94835828	0.29882192	-3.19845096
55	1	4.17837726	0.17963345	-3.42191549	1	3.39604568	-0.10962619	-4.15608267
56	1	4.96255686	2.51422094	-2.50847702	1	4.17825059	2.32119539	-3.89626653
57	6	-0.39977177	-2.44948815	-4.24444950	6	-1.21309333	-2.44378190	-5.01040186
58	16	0.67374111	-1.30221218	-3.29040137	16	-0.05874596	-1.33317822	-4.10790007
59	1	0.21213932	-2.90877242	-5.03086707	1	-0.65809035	-2.92238764	-5.82716250
60	1	-1.23095550	-1.89811362	-4.70172948	1	-2.04850207	-1.86597918	-5.42583620
61	1	-0.80129272	-3.23456312	-3.59178811	1	-1.60764187	-3.21649295	-4.33828150
62	6	2.92004013	-4.05234264	-0.70319049	6	2.15859753	-3.72487002	-1.52386472
63	6	2.00157199	-4.87677311	0.21507654	6	1.41607949	-4.58986145	-0.49740116
64	8	2.36998258	-5.95179958	0.68817573	8	2.00304525	-5.41860722	0.20005609
65	6	2.99525570	-2.54988488	-0.40305869	6	2.82135631	-2.51340784	-0.84660712
66	16	4.49761038	-1.88317467	-1.26834733	16	4.19935544	-1.82213005	-1.89063179
67	1	3.90791672	-4.52043770	-0.59609199	1	2.92849322	-4.37848652	-1.95750743
68	1	2.12333077	-2.00649900	-0.78858847	1	2.10812333	-1.69512102	-0.69875195
69	1	3.11846896	-2.35959383	0.66885343	1	3.26406755	-2.79897060	0.11567830
70	1	2.59776817	-4.20565241	-1.74588214	1	1.49474490	-3.37946765	-2.33026234
71	7	0.73868653	-4.36917197	0.42658779	7	0.05363956	-4.37789355	-0.42595527
72	6	-0.16641591	-4.94770677	1.41413731	6	-0.75582621	-4.97070910	0.62973084
73	6	-1.34942709	-5.73865652	0.80961391	6	-1.99654780	-5.73734986	0.11732032
74	8	-2.11224011	-6.37673729	1.53631479	8	-2.73168763	-6.32988931	0.90966183
75	6	-0.76519033	-3.89859631	2.41071885	6	-1.26292771	-3.95119805	1.70639471
76	6	0.21822767	-2.91085454	2.95158089	6	-0.20251203	-3.03805485	2.22528488
77	7	0.67965242	-1.82374346	2.21101135	7	0.27385208	-1.95978461	1.47836056
78	6	0.91642098	-2.90387519	4.14756002	6	0.54270998	-3.12460947	3.38306181
79	6	1.65391082	-1.24682222	2.99575175	6	1.28649739	-1.43134688	2.18412463

N	Atom number	X	Y	Z	Atom number	X	Y	Z
80	7	1.80568906	-1.84918372	4.17442563	7	1.45657825	-2.09620010	3.34543045
81	1	0.52654576	-3.42482317	0.10179725	1	-0.32673189	-3.53011977	-0.86727980
82	1	0.42820894	-5.68284776	1.97552693	1	-0.10738384	-5.71076188	1.12193399
83	1	-1.58901640	-3.37042230	1.90844894	1	-2.07543718	-3.35432657	1.26689001
84	1	-1.21066532	-4.47451575	3.23156569	1	-1.69457109	-4.54244338	2.52321929
85	1	0.84604012	-3.60791876	4.97208931	1	0.51844796	-3.84004253	4.19551156
86	1	2.20613216	-0.36578968	2.67727731	1	1.87857880	-0.57110871	1.89056358
87	7	-1.50409305	-5.63511784	-0.54892049	7	-2.22843644	-5.67128235	-1.23001539
88	6	-2.48259575	-6.41623208	-1.28256098	6	-3.30533407	-6.40030816	-1.87474993
89	6	-3.50850610	-5.65915233	-2.14497267	6	-4.34440923	-5.59670535	-2.67963633
90	8	-4.17258895	-6.28871864	-2.97458059	8	-5.11682773	-6.21020425	-3.42390957
91	1	-0.74250415	-5.17976526	-1.04677630	1	-1.49633944	-5.24626209	-1.79382793
92	1	-1.99247315	-7.13404598	-1.95699045	1	-2.91001592	-7.15818141	-2.56732916
93	1	-3.04723721	-6.99556877	-0.53662403	1	-3.84850394	-6.93103168	-1.07915468
94	7	-3.63662812	-4.32091442	-1.93697353	7	-4.36337427	-4.24717942	-2.52409023
95	6	-4.67234134	-3.54558088	-2.61302018	6	-5.39640834	-3.43335072	-3.16135431
96	6	-4.32140101	-2.06762052	-2.70188381	6	-5.00378226	-1.96543390	-3.24388827
97	8	-4.24516403	-1.56838007	-1.36301378	8	-4.87741453	-1.48235619	-1.90456510
98	1	-3.12811488	-3.87975442	-1.17072455	1	-3.76785114	-3.80203055	-1.82361441
99	1	-4.80035191	-3.96456804	-3.62055873	1	-5.57021324	-3.83273964	-4.17027171
100	1	-3.36233050	-1.92400980	-3.22709871	1	-4.05511887	-1.84469049	-3.79349208
101	1	-5.11203264	-1.55405480	-3.27824042	1	-5.79344419	-1.42524249	-3.79702485
102	1	-4.04431717	-0.61928465	-1.34075235	1	-4.64813310	-0.54031309	-1.87903607
103	1	-5.63610062	-3.65567724	-2.08623416	1	-6.34586553	-3.52359778	-2.60614193
104	26	-0.29316700	-0.75203444	0.83482757	26	-0.78948323	-0.79490555	0.09404087
105	26	-0.73917891	-0.40361004	-1.72453333	26	-1.36337900	-0.41643550	-2.44741334
106	16	-1.49445450	-2.05331269	-0.46857712	16	-2.09980544	-2.06000772	-1.16106589
107	16	0.42566456	0.92493952	-0.38004678	16	-0.07961555	0.86167483	-1.16693095
108	6	4.94747564	-0.02269860	7.48892015	6	4.13770943	-0.14877358	6.91167663
109	6	5.98244500	0.72160693	8.05679344	6	4.99616716	0.74026524	7.52993563
110	6	7.21872690	0.74558835	7.39437845	6	6.22613141	1.03934271	6.90634618
111	6	7.42717488	0.04482600	6.19637043	6	6.59970435	0.45088150	5.68020186
112	6	6.37145020	-0.70128164	5.63560272	6	5.73558435	-0.45522164	5.06237050
113	6	5.12387876	-0.73225803	6.29605005	6	4.45246579	-0.78143338	5.66698019
114	8	4.12541936	-1.53804086	5.80444105	8	3.63326592	-1.61035319	5.12331994
115	8	8.23473219	1.49048101	7.97654405	8	7.05351190	1.93733400	7.55276090
116	6	6.54701865	-1.46895472	4.34696300	6	6.07499480	-1.12433183	3.75641324
117	1	7.34985680	-2.21829840	4.42335612	1	7.02802797	-1.67341088	3.80535559
118	1	5.61746160	-1.99234683	4.10078388	1	5.27845255	-1.83599687	3.50925275
119	1	6.80088780	-0.80393214	3.50717698	1	6.15911441	-0.40250748	2.92825301
120	6	8.78826311	0.12454253	5.54341060	6	7.93322776	0.83491308	5.07906813
121	1	8.82296579	-0.44479224	4.60935448	1	8.09736798	0.33949660	4.11713022
122	1	9.06285727	1.16440610	5.29172312	1	8.00089144	1.92110336	4.89121582
123	1	9.58230292	-0.27923772	6.19633584	1	8.77732931	0.55632848	5.73434684
124	6	5.80266761	1.48523460	9.34419186	6	4.65343428	1.40037090	8.84248187
125	1	6.51203397	1.14620097	10.11447957	1	5.39972816	1.16563423	9.61657164
126	1	5.99002873	2.56039460	9.20196848	1	4.63876119	2.49661372	8.74765981
127	1	4.78324082	1.35848803	9.73097901	1	3.66911147	1.06735509	9.19515146
128	1	3.97951970	-0.07594439	7.99065798	1	3.17957341	-0.39923481	7.37067148
129	1	3.32304464	-1.15141847	5.38303228	1	2.22495649	-1.90442573	4.03605580
130	1	9.01077609	1.42889125	7.39310546	1	7.84153403	2.06291010	6.99436261

N	P4^{nop} – approximation 1			P4^{nop} – approximation 2		
	Atom			Atom		
	number	X	Y	Z	number	X	Y	Z
1	6	-3.11565804	5.17143774	-8.40485764	6	-2.25239635	3.12815666	-5.18645048
2	6	-3.68508983	6.17339611	-7.41064310	6	-2.82182813	4.13011551	-4.19223785
3	8	-2.96863580	6.95105553	-6.76798391	8	-2.10537410	4.90777493	-3.54957891
4	6	-2.41654325	4.01223564	-7.68578672	6	-1.55328202	1.96895456	-4.46738148
5	16	-3.61741996	2.98609543	-6.71802855	16	-2.75415826	0.94281471	-3.49962306
6	1	-3.89504504	4.78364134	-9.07744312	1	-3.03178334	2.74035978	-5.85903645
7	1	-1.91528416	3.34934998	-8.40220070	1	-1.05202305	1.30606937	-5.18379354
8	1	-1.65728760	4.40051556	-6.99460840	1	-0.79402697	2.35723472	-3.77620292

9	1	-2.37111950	5.70898342	-9.01189709	1	-1.50785828	3.66570306	-5.79349041
10	7	-5.04668665	6.14307308	-7.26068449	7	-4.18342400	4.09979296	-4.04227972
11	6	-5.75164175	6.99548531	-6.31979990	6	-4.88837910	4.95220470	-3.10139465
12	6	-5.81824827	6.55998135	-4.84281874	6	-4.95498562	4.51670122	-1.62441468
13	8	-6.51633215	7.20737457	-4.06344366	8	-5.65306950	5.16409445	-0.84503889
14	1	-5.54666948	5.37391233	-7.69549131	1	-4.68340683	3.33063149	-4.47708654
15	1	-5.25511885	7.97597694	-6.30868769	1	-4.39185619	5.93269634	-3.09028244
16	1	-6.78355789	7.14495277	-6.66202688	1	-5.92029524	5.10167217	-3.44362164
17	7	-5.05632401	5.48562098	-4.48904276	7	-4.19306135	3.44234061	-1.27063823
18	6	-4.81294012	5.14402008	-3.09165907	6	-3.94967747	3.10073924	0.12674683
19	6	-3.64609885	5.97254753	-2.48112988	6	-2.78283715	3.92926764	0.73727566
20	8	-3.84634447	6.74866676	-1.54739332	8	-2.98308277	4.70538664	1.67101216
21	6	-4.59111357	3.62073779	-2.98339128	6	-3.72785211	1.57745719	0.23501426
22	6	-4.07720137	3.15669918	-1.65718198	6	-3.21393991	1.11341858	1.56122351
23	7	-3.05167246	2.22082353	-1.54427218	7	-2.18841076	0.17754263	1.67413330
24	6	-4.47547865	3.52469087	-0.39216864	6	-3.61221719	1.48141026	2.82623696
25	6	-2.84428763	2.02395034	-0.24166013	6	-1.98102617	-0.01933070	2.97674513
26	7	-3.68960595	2.79808426	0.48014051	7	-2.82634425	0.75480384	3.69854593
27	1	-4.51486540	4.99352932	-5.20658445	1	-3.65160394	2.95024824	-1.98817897
28	1	-5.69588852	5.46270657	-2.52237177	1	-4.83262587	3.41942596	0.69603390
29	1	-5.54304266	3.11846972	-3.22141027	1	-4.67978001	1.07518911	-0.00300431
30	1	-3.87089014	3.30378556	-3.75308895	1	-3.00762844	1.26050496	-0.53468299
31	1	-5.20337677	4.25027990	-0.05226187	1	-4.34011412	2.20699906	3.16614366
32	1	-2.11779857	1.34449863	0.19305667	1	-1.25453711	-0.69878238	3.41146183
33	1	-3.71367621	2.85156417	1.49197435	1	-2.85041451	0.80828381	4.71037960
34	7	-2.42390633	5.79024696	-3.07368183	7	-1.56064510	3.74696612	0.14472377
35	6	-1.22761941	6.40853691	-2.52225304	6	-0.36435869	4.36525631	0.69615239
36	6	-0.18896219	6.89641571	-3.53728628	6	0.67429847	4.85313559	-0.31888029
37	8	0.89941072	7.31262493	-3.13634157	8	1.76267195	5.26934433	0.08206421
38	1	-2.26854825	4.93109798	-3.61519384	1	-1.40528691	2.88781667	-0.39678788
39	1	-1.54715621	7.26791668	-1.91780472	1	-0.68389559	5.22463608	1.30060077
40	1	-0.69326133	5.72093773	-1.84704685	1	0.16999948	3.67765760	1.37135863
41	7	-0.52041620	6.81235981	-4.86220503	7	0.34284455	4.76907969	-1.64380026
42	6	0.33585808	7.39129162	-5.88514948	6	1.19911909	5.34801149	-2.66674471
43	6	1.32241154	6.46231747	-6.61060286	6	2.18567348	4.41903687	-3.39219809
44	8	1.91258466	6.88216209	-7.61152506	8	2.77584600	4.83888197	-4.39312029
45	1	-1.49009144	6.63405800	-5.12682581	1	-0.62683082	4.59077740	-1.90842080
46	1	-0.29517949	7.84000015	-6.66207743	1	0.56808120	5.79671907	-3.44367218
47	1	0.94800955	8.18244457	-5.42748785	1	1.81127071	6.13916302	-2.20908237
48	7	1.51281977	5.21320963	-6.10329771	7	2.37608123	3.16992879	-2.88489246
49	6	2.50747681	4.32677650	-6.70326662	6	3.37073851	2.28349519	-3.48486114
50	6	2.23836303	2.83876872	-6.47954607	6	3.10162473	0.79548824	-3.26114058
51	16	2.97254467	2.25403500	-4.87310362	16	3.83580637	0.21075407	-1.65469933
52	1	1.04216206	4.94753981	-5.24156141	1	1.90542316	2.90425849	-2.02315664
53	1	2.49656272	4.53859901	-7.78202486	1	3.35982442	2.49531794	-4.56361961
54	1	1.16562080	2.61284232	-6.49673033	1	2.02888203	0.56956184	-3.27832484
55	1	2.73549080	2.25532174	-7.26287508	1	3.59875250	0.21204092	-4.04446983
56	1	3.51966906	4.58991003	-6.34943628	1	4.38293219	2.54662848	-3.13103127
57	6	-1.84265745	-0.37379968	-8.08541012	6	-0.97939634	-2.41708064	-4.86700392
58	16	-0.76914430	0.77347636	-7.13136053	16	0.09411651	-1.26980484	-3.91295576
59	1	-1.23074603	-0.83308399	-8.87182808	1	-0.36748528	-2.87636495	-5.65342140
60	1	-2.67384124	0.17757471	-8.54269028	1	-1.81058002	-1.86570621	-5.32428360
61	1	-2.24417853	-1.15887451	-7.43274736	1	-1.38091731	-3.20215559	-4.21434259
62	6	1.47715402	-1.97665429	-4.54414988	6	2.34041548	-4.01993513	-1.32574487
63	6	0.55868608	-2.80108595	-3.62588358	6	1.42194724	-4.84436560	-0.40747783
64	8	0.92709661	-3.87611222	-3.15278435	8	1.79035783	-5.91939211	0.06562138
65	6	1.55236959	-0.47419637	-4.24401808	6	2.41563106	-2.51747727	-1.02561307
66	16	3.05472422	0.19251366	-5.10930681	16	3.91798592	-1.85076725	-1.89090180
67	1	2.46503043	-2.44474959	-4.43705130	1	3.32829213	-4.48803043	-1.21864629
68	1	0.68044502	0.06918932	-4.62954664	1	1.54370618	-1.97409165	-1.41114283
69	1	1.67558277	-0.28390536	-3.17210674	1	2.53884435	-2.32718635	0.04629904
70	1	1.15488219	-2.12996387	-5.58684206	1	2.01814342	-4.17324495	-2.36843657

71	7	-0.70419890	-2.29348421	-3.41437244	7	0.15906191	-4.33676481	-0.19596657
72	6	-1.60930109	-2.87201929	-2.42682242	6	-0.74604052	-4.91529942	0.79158300
73	6	-2.79231310	-3.66296911	-3.03134632	6	-1.92905164	-5.70624924	0.18705952
74	8	-3.55512643	-4.30104876	-2.30464506	8	-2.69186473	-6.34432983	0.91376048
75	6	-2.20807624	-1.82290781	-1.43024087	6	-1.34481490	-3.86618876	1.78816462
76	6	-1.22465765	-0.83516610	-0.88937867	6	-0.36139691	-2.87844706	2.32902670
77	7	-0.76323301	0.25194484	-1.62994838	7	0.10002780	-1.79133606	1.58845711
78	6	-0.52646434	-0.82818663	0.30660069	6	0.33679640	-2.87146759	3.52500582
79	6	0.21102560	0.82886630	-0.84520781	6	1.07428622	-1.21441483	2.37319756
80	7	0.36280337	0.22650464	0.33346617	7	1.22606444	-1.81677628	3.55187130
81	1	-0.91633958	-1.34913468	-3.73916292	1	-0.05307883	-3.39241576	-0.52075708
82	1	-1.01467645	-3.60716105	-1.86543298	1	-0.15141565	-5.65044069	1.35297251
83	1	-3.03190279	-1.29473376	-1.93251085	1	-2.16864109	-3.33801484	1.28589463
84	1	-2.65355110	-2.39882803	-0.60939425	1	-1.79028988	-4.44210863	2.60901141
85	1	-0.59684527	-1.53223026	1.13112974	1	0.26641554	-3.57551122	4.34953499
86	1	0.76324636	1.70989895	-1.16368222	1	1.62650752	-0.33338222	2.05472302
87	7	-2.94697928	-3.55943060	-4.38987970	7	-2.08371758	-5.60271072	-1.17147493
88	6	-3.92548203	-4.34054422	-5.12352037	6	-3.06222034	-6.38382483	-1.90511537
89	6	-4.95139313	-3.58346510	-5.98593187	6	-4.08813047	-5.62674522	-2.76752687
90	8	-5.61547613	-4.21303082	-6.81553984	8	-4.75221348	-6.25631142	-3.59713483
91	1	-2.18539023	-3.10407805	-4.88773489	1	-1.32212877	-5.14735794	-1.66933060
92	1	-3.43535948	-5.05835819	-5.79795027	1	-2.57209778	-7.10163879	-2.57954478
93	1	-4.49012327	-4.91988087	-4.37758303	1	-3.62686181	-6.96316147	-1.15917838
94	7	-5.07951546	-2.24522638	-5.77793360	7	-4.21625280	-4.28850698	-2.55952787
95	6	-6.11522865	-1.46989226	-6.45397997	6	-5.25196600	-3.51317334	-3.23557448
96	6	-5.76428843	0.00806812	-6.54284334	6	-4.90102577	-2.03521299	-3.32443810
97	8	-5.68805122	0.50730824	-5.20397329	8	-4.82478857	-1.53597271	-1.98556805
98	1	-4.57100105	-1.80406582	-5.01168394	1	-3.70773959	-3.84734678	-1.79327893
99	1	-6.24323940	-1.88887978	-7.46151781	1	-5.37997675	-3.93216062	-4.24311304
100	1	-4.80521774	0.15167853	-7.06805849	1	-3.94195509	-1.89160240	-3.84965301
101	1	-6.55491972	0.52163351	-7.11920023	1	-5.69165707	-1.52164745	-3.90079474
102	1	-5.48720455	1.45640373	-5.18171167	1	-4.62394190	-0.58687717	-1.96330667
103	1	-7.07898808	-1.57998896	-5.92719316	1	-6.21572542	-3.62326980	-2.70878839
104	26	-1.73605239	1.32365406	-3.00613260	26	-0.87279159	-0.71962696	0.21227318
105	26	-2.18206501	1.67207861	-5.56549311	26	-1.31880355	-0.37120259	-2.34708762
106	16	-2.93734074	0.02237573	-4.30953646	16	-2.07407904	-2.02090526	-1.09113145
107	16	-1.01722074	3.00062752	-4.22100639	16	-0.15396002	0.95734698	-1.00260115
108	6	3.50458765	2.05298972	3.64795971	6	4.36785078	0.00970886	6.86636591
109	6	4.53955746	2.79729486	4.21583414	6	5.40282011	0.75401437	7.43423891
110	6	5.77583981	2.82127619	3.55341816	6	6.63910246	0.77799582	6.77182436
111	6	5.98428774	2.12051439	2.35541105	6	6.84755039	0.07723346	5.57381630
112	6	4.92856312	1.37440681	1.79464316	6	5.79182577	-0.66887420	5.01304865
113	6	3.68099141	1.34343052	2.45509052	6	4.54425430	-0.69985056	5.67349577
114	8	2.68253279	0.53764749	1.96348071	8	3.54579449	-1.50563347	5.18188667
115	8	6.79184532	3.56616902	4.13558435	8	7.65510798	1.52288842	7.35398960
116	6	5.10413122	0.60673368	0.50600320	6	5.96739388	-1.43654728	3.72440863
117	1	5.90696955	-0.14260992	0.58239633	1	6.77023220	-2.18589091	3.80080175
118	1	4.17457438	0.08334148	0.25982440	1	5.03783703	-1.95993948	3.47822952
119	1	5.35800028	1.27175641	-0.33378279	1	6.22126293	-0.77152467	2.88462257
120	6	7.34538269	2.20023084	1.70245099	6	8.20863914	0.15694998	4.92085648
121	1	7.38008499	1.63089609	0.76839471	1	8.24334145	-0.41238478	3.98680019
122	1	7.61997652	3.24009418	1.45076346	1	8.48323345	1.19681346	4.66916895
123	1	8.13942242	1.79645085	2.35537624	1	9.00267887	-0.24683025	5.57378149
124	6	4.35978031	3.56092262	5.50323153	6	5.22304296	1.51764202	8.72163677
125	1	5.06914663	3.22188902	6.27352095	1	5.93240929	1.17860842	9.49192524
126	1	4.54714155	4.63608360	5.36100912	1	5.41040421	2.59280205	8.57941341
127	1	3.34035349	3.43417621	5.89002085	1	4.20361614	1.39089549	9.10842419
128	1	2.53663325	1.99974394	4.14969873	1	3.39989495	-0.04353693	7.36810350
129	1	1.07122815	0.44649038	1.07813668	1	1.87902832	-1.54792392	4.33030415
130	1	7.56789589	3.50457931	3.55214500	1	8.43115234	1.46129870	6.77055120

3. Model M5, Z = −1, m=1

E(M5) = -7957.71335871 a.u.
E(P5^{opt}) = -7957.71375241 a.u.
E(P5^{nop}) = -7957.70093802 a.u. (approximation 1)
E(P5^{nop}) = -7957.70026634 a.u. (approximation 2)

Atomic Coordinates

N	M5				P5^{opt}			
	Atom				Atom			
	number	X	Y	Z	number	X	Y	Z
1	6	-1.88238724	3.06420670	-4.55611375	6	-2.45147966	3.12169867	-5.19284471
2	6	-2.35372299	4.09300649	-3.53789987	6	-2.93774017	4.13962783	-4.17140125
3	8	-1.57322731	4.85967089	-2.96018496	8	-2.17282251	4.92935784	-3.60366940
4	6	-1.13907741	1.91001489	-3.87454726	6	-1.72551025	1.95563918	-4.51188608
5	16	-2.26580980	0.93532551	-2.77601575	16	-2.86879442	0.96230548	-3.44762785
6	1	-2.72040176	2.67351428	-5.15213884	1	-3.28110225	2.74101162	-5.80690662
7	1	-0.71756604	1.22035819	-4.61668412	1	-1.29033865	1.27611139	-5.25568645
8	1	-0.31367632	2.30205053	-3.26675595	1	-0.91044533	2.33702256	-3.88338432
9	1	-1.18561953	3.57929897	-5.23522845	1	-1.74154890	3.64230387	-5.85357918
10	7	-3.70120743	4.10142700	-3.29046478	7	-4.28286997	4.10859465	-3.90993619
11	6	-4.31395616	4.98494422	-2.31413630	6	-4.90844317	4.96708392	-2.92052558
12	6	-4.28674927	4.56919946	-0.83010881	6	-4.85313263	4.54510397	-1.43948536
13	8	-4.90561177	5.24851221	-0.01188842	8	-5.47428722	5.21056728	-0.61070803
14	1	-4.25263910	3.34358601	-3.68030632	1	-4.80787565	3.32103137	-4.27785454
15	1	-3.79149484	5.95113305	-2.35220160	1	-4.41342640	5.94757368	-2.95835775
16	1	-5.36319192	5.15902935	-2.58456056	1	-5.96530222	5.11419051	-3.17760064
17	7	-3.53724791	3.47388446	-0.51674302	7	-4.07945384	3.46358726	-1.13848821
18	6	-3.19851185	3.14677049	0.86466288	6	-3.72790301	3.13915884	0.23994233
19	6	-1.97310321	3.95984649	1.37449809	6	-2.50685154	3.96332319	0.74158273
20	8	-2.08157822	4.72998054	2.32819902	8	-2.61947561	4.74150402	1.68935606
21	6	-3.00167161	1.62047472	0.97498488	6	-3.51323146	1.61612333	0.35746464
22	6	-2.43304147	1.14679960	2.27525204	6	-2.93894286	1.17006207	1.66489370
23	7	-1.47225325	0.13939560	2.34204490	7	-1.95252263	0.18787736	1.75259527
24	6	-2.72638910	1.55691586	3.55574699	6	-3.24916256	1.60100148	2.93505577
25	6	-1.20230028	-0.05793370	3.63324948	6	-1.68938410	0.02786910	3.04862033
26	7	-1.94474983	0.78366699	4.39136027	7	-2.45432322	0.86584768	3.79066795
27	1	-3.05566658	2.96226337	-1.26306047	1	-3.60786720	2.95022152	-1.89124851
28	1	-4.03059623	3.49099857	1.49267010	1	-4.55918655	3.47765647	0.87232332
29	1	-3.97518966	1.13787104	0.78806914	1	-4.48021120	1.11822487	0.17803909
30	1	-2.32934010	1.28413741	0.17110029	1	-2.83553532	1.27815787	-0.44123623
31	1	-3.37700614	2.33873150	3.92631965	1	-3.91770714	2.37689232	3.28568464
32	1	-0.49962587	-0.78199278	4.03382599	1	-0.97932814	-0.67136093	3.47390416
33	1	-1.90181471	0.85210720	5.40169530	1	-2.41899082	0.95828731	4.79931486
34	7	-0.81235720	3.77308381	0.67036119	7	-1.34508628	3.77404499	0.04132960
35	6	0.43653965	4.37261806	1.11794512	6	-0.10138120	4.38511383	0.48522325
36	6	1.42557656	4.78176316	0.02135941	6	0.87529235	4.81083003	-0.61569415
37	8	2.54432605	5.18216681	0.34306107	8	1.99887821	5.20578526	-0.30215017
38	1	-0.71502241	2.90572957	0.12923785	1	-1.23898795	2.90282120	-0.49598658
39	1	0.18550850	5.26712612	1.70316941	1	-0.35880820	5.27304226	1.07787032
40	1	0.99126759	3.69687590	1.78882025	1	0.46606391	3.71067922	1.14667770
41	7	1.01438946	4.64968625	-1.28045509	7	0.44602152	4.70247482	-1.91245816
42	6	1.82692799	5.17362977	-2.36846568	6	1.25255467	5.22221642	-3.00559264
43	6	2.59854119	4.16924032	-3.23851347	6	2.04196257	4.21461666	-3.85652459
44	8	3.12576579	4.55957909	-4.28553466	8	2.60888724	4.60730565	-4.88178380
45	1	0.01874033	4.53196911	-1.47614945	1	-0.55029419	4.57618789	-2.09748330
46	1	1.18867668	5.74565196	-3.05380835	1	0.60521942	5.77194945	-3.70075437
47	1	2.57925563	5.85172111	-1.93955552	1	1.99386217	5.91931530	-2.58885647
48	7	2.69454047	2.88358874	-2.80389969	7	2.10291656	2.92426664	-3.42925721
49	6	3.41467387	1.90073985	-3.61435316	6	2.79914077	1.92804420	-4.24327944

50	6	3.44082045	0.50679731	-2.99948991	6	2.84399610	0.54589161	-3.60432160
51	16	4.50262076	0.46442549	-1.48430880	16	3.94217265	0.52102692	-2.11403695
52	1	2.19108142	2.59095505	-1.96830194	1	1.53857288	2.62645860	-2.63409420
53	1	2.93313654	1.82954097	-4.60445604	1	2.29101430	1.83314609	-5.21872946
54	1	2.43251406	0.16849787	-2.73595452	1	1.84373149	0.21060732	-3.30699327
55	1	3.87399804	-0.19709622	-3.71977670	1	3.26032374	-0.17008625	-4.32237387
56	1	4.43573697	2.26999296	-3.79438813	1	3.81236513	2.29878174	-4.45750532
57	6	-0.69918994	-2.47442744	-4.24854794	6	-1.29786528	-2.44246372	-4.94639258
58	16	0.46876423	-1.34535401	-3.38952962	16	-0.12382237	-1.31329730	-4.09492508
59	1	-0.15102665	-2.97470410	-5.05645965	1	-0.75801928	-2.94571828	-5.75834427
60	1	-1.53479946	-1.90307392	-4.67188045	1	-2.13644836	-1.87126319	-5.36461097
61	1	-1.09142688	-3.22717350	-3.55357171	1	-1.68679594	-3.19397624	-4.24768604
62	6	2.84302966	-3.40041605	-0.81686082	6	2.24612695	-3.31924568	-1.41555877
63	6	2.15875701	-4.35329630	0.17753080	6	1.56328643	-4.23255481	-0.38560336
64	8	2.79963370	-5.15642308	0.85349812	8	2.21268368	-4.95498465	0.37200295
65	6	3.64111208	-2.29954723	-0.09964598	6	3.06723612	-2.21498158	-0.73005740
66	16	4.95656614	-1.53726015	-1.17960203	16	4.38877350	-1.48706920	-1.82482319
67	1	3.53542953	-4.03014337	-1.39433926	1	2.92331548	-3.97401891	-1.98415572
68	1	3.00343055	-1.47752539	0.24213141	1	2.43872077	-1.37388502	-0.41711775
69	1	4.18113324	-2.71390030	0.76174788	1	3.59838395	-2.61992094	0.14137144
70	1	2.12452225	-2.95293450	-1.51974679	1	1.52661473	-2.87978318	-2.12220709
71	7	0.77975782	-4.26356421	0.21250206	7	0.18212977	-4.20677764	-0.40466858
72	6	-0.02556285	-4.93273566	1.22874594	6	-0.61510212	-4.86708379	0.62174680
73	6	-1.17857720	-5.77858227	0.64418540	6	-1.78953122	-5.70255981	0.06278422
74	8	-1.88001339	-6.47763847	1.37664863	8	-2.49256864	-6.37023729	0.82392062
75	6	-0.66950267	-3.96771657	2.29025188	6	-1.22581276	-3.89885391	1.69745574
76	6	0.28512364	-2.97828659	2.87333609	6	-0.22429552	-2.95959794	2.28046047
77	7	0.78086527	-1.88604581	2.16050579	7	0.28710165	-1.87796685	1.56027416
78	6	0.99959482	-3.04815127	4.05501394	6	0.48780630	-3.07870653	3.45418687
79	6	1.79909401	-1.38076671	2.94978129	6	1.29700939	-1.38067894	2.29827507
80	7	1.93332819	-2.04057309	4.10152203	7	1.41864632	-2.06964572	3.45443313
81	1	0.36597664	-3.42079976	-0.19733691	1	-0.26317648	-3.39881889	-0.86090944
82	1	0.65399663	-5.62416938	1.74739521	1	0.06433894	-5.56754157	1.12888568
83	1	-1.52606308	-3.45915791	1.82470773	1	-2.04835854	-3.33499875	1.23526634
84	1	-1.07215904	-4.61006430	3.08373391	1	-1.65858438	-4.53242578	2.48144578
85	1	0.91721053	-3.78478770	4.84926732	1	0.43598035	-3.81179739	4.24933593
86	1	2.37771885	-0.50547664	2.66624957	1	1.90721050	-0.52183773	2.04186204
87	7	-1.40065795	-5.63722888	-0.70372028	7	-2.01288063	-5.60439808	-1.28452676
88	6	-2.40338367	-6.40953272	-1.41374936	6	-3.04254187	-6.36952415	-1.96424667
89	6	-3.49218167	-5.63933080	-2.18536359	6	-4.13386017	-5.59932004	-2.73364728
90	8	-4.18609626	-6.24979791	-3.00460273	8	-4.87101146	-6.23104933	-3.49815391
91	1	-0.67027884	-5.15901879	-1.22609211	1	-1.30369397	-5.11903055	-1.82818071
92	1	-1.93962673	-7.08812348	-2.14486787	1	-2.60025712	-7.06745556	-2.69047614
93	1	-2.91371662	-7.03115904	-0.66273837	1	-3.54999786	-6.97004296	-1.19527165
94	7	-3.64047927	-4.31448363	-1.91149331	7	-4.23529351	-4.26053389	-2.52558605
95	6	-4.72973342	-3.53648768	-2.49575619	6	-5.31477940	-3.48359868	-3.13149980
96	6	-4.41382643	-2.04893266	-2.57152828	6	-4.99084119	-1.99781741	-3.20425913
97	8	-4.27990420	-1.57109715	-1.22978069	8	-4.86835993	-1.52204897	-1.86227002
98	1	-3.09697526	-3.89298413	-1.15826693	1	-3.65560475	-3.80477250	-1.81853866
99	1	-4.91755311	-3.93273030	-3.50309538	1	-5.49050741	-3.87943112	-4.14141144
100	1	-3.48782622	-1.87321945	-3.14335756	1	-4.05774437	-1.82739476	-3.76630964
101	1	-5.24529836	-1.54401605	-3.09627487	1	-5.81350926	-1.49028673	-3.74054812
102	1	-4.07600237	-0.62218794	-1.19687967	1	-4.65826221	-0.57533670	-1.82596847
103	1	-5.65461572	-3.67676569	-1.90978411	1	-6.24813800	-3.62158167	-2.55895351
104	26	-0.24325409	-0.78928517	0.82990184	26	-0.80306823	-0.73400739	0.15246988
105	26	-0.78777856	-0.40837580	-1.71191632	26	-1.37619917	-0.38340636	-2.39857675
106	16	-1.49643611	-2.07497125	-0.45244416	16	-2.07561254	-2.03721400	-1.11059312
107	16	0.43531683	0.90341946	-0.38877558	16	-0.12150941	0.93062795	-1.11626251
108	6	4.76714395	-0.20360165	7.67940726	6	4.15735147	-0.30614700	7.07905352
109	6	5.72725070	0.54720498	8.36025761	6	5.06686027	0.50018327	7.74277243
110	6	6.99879595	0.67345327	7.78117241	6	6.32814869	0.71038451	7.14378729
111	6	7.31584166	0.06166091	6.55868612	6	6.67974820	0.11862250	5.91019447

N								
112	6	6.33739618	-0.69920680	5.88889486	6	5.76586840	-0.70856066	5.25120729
113	6	5.05210669	-0.82695901	6.45906306	6	4.45113137	-0.94434450	5.82790913
114	8	4.13882918	-1.66824574	5.87128093	8	3.59736310	-1.72241110	5.26206458
115	8	7.93866785	1.42637982	8.47093766	8	7.21249968	1.52613558	7.82374669
116	6	6.63579000	-1.38373160	4.57605633	6	6.08467497	-1.38022340	3.94231535
117	1	7.47649749	-2.08881920	4.66453954	1	6.98917531	-2.00485617	4.00476487
118	1	5.75645373	-1.94594116	4.24510287	1	5.24101383	-2.02204875	3.66258224
119	1	6.89923060	-0.66038777	3.78892237	1	6.24832131	-0.65344218	3.13054960
120	6	8.70896640	0.24612044	6.00141881	6	8.05332919	0.40979108	5.34746572
121	1	8.82772908	-0.25360031	5.03501775	1	8.20030109	-0.07583846	4.37774072
122	1	8.94807602	1.31213331	5.83869386	1	8.21082218	1.49109866	5.18697109
123	1	9.48042942	-0.16764657	6.67489310	1	8.85792836	0.05071212	6.01332740
124	6	5.43065888	1.21354502	9.67968489	6	4.74875827	1.15489879	9.06281321
125	1	6.11017640	0.85940781	10.46980995	1	5.45778150	0.84464894	9.84529232
126	1	5.56818770	2.30384241	9.61839189	1	4.82179855	2.25078087	8.99419252
127	1	4.39834666	1.01076222	9.99299908	1	3.73410185	0.89224079	9.38783582
128	1	3.77547053	-0.33805861	8.11533752	1	3.17336938	-0.49571178	7.51237962
129	1	3.34958013	-1.32155779	5.39193287	1	2.18075364	-1.91574215	4.16102443
130	1	8.75233495	1.43381507	7.93772539	1	8.02094194	1.59483059	7.28501004

N	P5^{nop} – approximation 1				P5^{nop} – approximation 2			
	Atom				Atom			
	number	X	Y	Z	number	X	Y	Z
1	6	-3.02022719	5.20371771	-8.11701012	6	-2.46201181	3.09661388	-5.17866802
2	6	-3.49156308	6.23251772	-7.09879827	6	-2.93334770	4.12541389	-4.16045427
3	8	-2.71106696	6.99918175	-6.52108431	8	-2.15285182	4.89207840	-3.58273935
4	6	-2.27691770	4.04952669	-7.43544388	6	-1.71870208	1.94242215	-4.49710131
5	16	-3.40364957	3.07483745	-6.33691454	16	-2.84543443	0.96773279	-3.39857006
6	1	-3.85824132	4.81302595	-8.71303463	1	-3.30002642	2.70592165	-5.77469301
7	1	-1.85540509	3.35986996	-8.17757988	1	-1.29719067	1.25276542	-5.23923826
8	1	-1.45151496	4.44156218	-6.82765484	1	-0.89330089	2.33445787	-3.88931036
9	1	-2.32345939	5.71881056	-8.79612446	1	-1.76524401	3.61170626	-5.85778284
10	7	-4.83904600	6.24093771	-6.85136414	7	-4.28083181	4.13383436	-3.91301918
11	6	-5.45179510	7.12445688	-5.87503529	6	-4.89358091	5.01735163	-2.93669033
12	6	-5.42458820	6.70871019	-4.39100790	6	-4.86637402	4.60160685	-1.45266294
13	8	-6.04345083	7.38802385	-3.57278657	8	-5.48523664	5.28091955	-0.63444263
14	1	-5.39047813	5.48309755	-7.24120378	1	-4.83226395	3.37599325	-4.30286074
15	1	-4.92933369	8.09064579	-5.91310072	1	-4.37111950	5.98354053	-2.97475576
16	1	-6.50103092	7.29854155	-6.14545965	1	-5.94281673	5.19143677	-3.20711470
17	7	-4.67508650	5.61339521	-4.07764196	7	-4.11687231	3.50629163	-1.13929725
18	6	-4.33635044	5.28628206	-2.69623446	6	-3.77813649	3.17917776	0.24210870
19	6	-3.11094308	6.09935713	-2.18639922	6	-2.55272770	3.99225378	0.75194395
20	8	-3.21941829	6.86949062	-1.23269868	8	-2.66120291	4.76238775	1.70564473
21	6	-4.13951111	3.75998712	-2.58591247	6	-3.58129621	1.65288198	0.35243070
22	6	-3.57088161	3.28631186	-1.28564525	6	-3.01266623	1.17920685	1.65269792
23	7	-2.61009288	2.27890778	-1.21885276	7	-2.05187774	0.17180285	1.71949065
24	6	-3.86422849	3.69642854	-0.00515080	6	-3.30601382	1.58932316	2.93319273
25	6	-2.34014058	2.08157825	0.07235193	6	-1.78192496	-0.02552645	3.01069546
26	7	-3.08258986	2.92317891	0.83046222	7	-2.52437449	0.81607425	3.76880598
27	1	-4.19350624	5.10177469	-4.82395935	1	-3.63529134	2.99467063	-1.88561463
28	1	-5.16843510	5.63050985	-2.06822705	1	-4.61022091	3.52340579	0.87011588
29	1	-5.11302853	3.27738380	-2.77282786	1	-4.55481434	1.17027831	0.16551495
30	1	-3.46718001	3.42364931	-3.38979769	1	-2.90896463	1.31654465	-0.45145389
31	1	-4.51484489	4.47824335	0.36542177	1	-3.95663071	2.37113881	3.30376530
32	1	-1.63746488	1.35751879	0.47292793	1	-1.07925045	-0.74958551	3.41127157
33	1	-3.03965449	2.99161935	1.84079742	1	-2.48143935	0.88451445	4.77914095
34	7	-1.95019627	5.91259527	-2.89053607	7	-1.39198184	3.80549121	0.04780698
35	6	-0.70129967	6.51212931	-2.44295239	6	-0.14308494	4.40502548	0.49539089
36	6	0.28773707	6.92127323	-3.53953886	6	0.84595197	4.81417036	-0.60119480
37	8	1.40648723	7.32167768	-3.21783710	8	1.96470141	5.21457386	-0.27949312
38	1	-1.85286140	5.04524088	-3.43166018	1	-1.29464698	2.93813682	-0.49331635
39	1	-0.95233089	7.40663767	-1.85772800	1	-0.39411610	5.29953337	1.08061528
40	1	-0.14657184	5.83638716	-1.77207744	1	0.41164297	3.72928309	1.16626608

23

41	7	-0.12344998	6.78919744	-4.84135389	7	0.43476492	4.68209362	-1.90300930
42	6	0.68908864	7.31314039	-5.92936468	6	1.24730349	5.20603704	-2.99101973
43	6	1.46070242	6.30875158	-6.79941273	6	2.01891661	4.20164776	-3.86106777
44	8	1.98792589	6.69908953	-7.84643173	8	2.54614115	4.59198618	-4.90808916
45	1	-1.11909878	6.67147970	-5.03704834	1	-0.56088424	4.56437635	-2.09870362
46	1	0.05083736	7.88516474	-6.61470699	1	0.60905212	5.77805901	-3.67636251
47	1	1.44141674	7.99123478	-5.50045443	1	1.99963093	5.88412857	-2.56210971
48	7	1.55670190	5.02310038	-6.36479902	7	2.11491585	2.91599607	-3.42645407
49	6	2.27683401	4.04025173	-7.17525101	6	2.83504915	1.93314719	-4.23690748
50	6	2.30298090	2.64630938	-6.56038809	6	2.86119580	0.53920460	-3.62204409
51	16	3.36478066	2.60393763	-5.04520798	16	3.92299604	0.49683276	-2.10686302
52	1	1.05324268	4.73046637	-5.52920103	1	1.61145687	2.62336230	-2.59085608
53	1	1.79529715	3.96905279	-8.16535187	1	2.35351181	1.86194825	-5.22701025
54	1	1.29467499	2.30800986	-6.29685354	1	1.85288930	0.20090513	-3.35850859
55	1	2.73615813	1.94241548	-7.28067350	1	3.29437327	-0.16468896	-4.34233093
56	1	3.29789710	4.40950489	-7.35528469	1	3.85611248	2.30240035	-4.41694212
57	6	-1.83702898	-0.33491582	-7.80944395	6	-1.27881455	-2.44202018	-4.87110233
58	16	-0.66907519	0.79415768	-6.95042896	16	-0.11086038	-1.31294668	-4.01208401
59	1	-1.28886557	-0.83519214	-8.61735535	1	-0.73065126	-2.94229674	-5.67901373
60	1	-2.67263913	0.23643769	-8.23277664	1	-2.11442399	-1.87066662	-5.29443455
61	1	-2.22926641	-1.08766174	-7.11447001	1	-1.67105150	-3.19476628	-4.17612600
62	6	1.70519090	-1.26090419	-4.37775993	6	2.26340508	-3.36800885	-1.43941498
63	6	1.02091813	-2.21378446	-3.38336754	6	1.57913232	-4.32088900	-0.44502339
64	8	1.66179490	-3.01691151	-2.70739913	8	2.22000909	-5.12401581	0.23094392
65	6	2.50327229	-0.16003560	-3.66054392	6	3.06148744	-2.26713991	-0.72220016
66	16	3.81872749	0.60225147	-4.74050093	16	4.37694168	-1.50485289	-1.80215621
67	1	2.39758945	-1.89063156	-4.95523834	1	2.95580482	-3.99773598	-2.01689339
68	1	1.86559117	0.66198629	-3.31876636	1	2.42380595	-1.44511807	-0.38042277
69	1	3.04329324	-0.57438838	-2.79914927	1	3.60150862	-2.68149304	0.13919371
70	1	0.98668337	-0.81342250	-5.08064604	1	1.54489756	-2.92052722	-2.14230108
71	7	-0.35808167	-2.12405252	-3.34839630	7	0.20013320	-4.23115683	-0.41005212
72	6	-1.16340184	-2.79322362	-2.33215117	6	-0.60518742	-4.90032816	0.60619175
73	6	-2.31641746	-3.63907075	-2.91671157	6	-1.75820184	-5.74617481	0.02163124
74	8	-3.01785302	-4.33812761	-2.18424869	8	-2.45963788	-6.44523096	0.75409448
75	6	-1.80734181	-1.82820475	-1.27064538	6	-1.24912727	-3.93530917	1.66769779
76	6	-0.85271579	-0.83877450	-0.68756139	6	-0.29450095	-2.94587922	2.25078201
77	7	-0.35697421	0.25346580	-1.40039182	7	0.20124066	-1.85363853	1.53795159
78	6	-0.13824461	-0.90863925	0.49411619	6	0.41997021	-3.01574397	3.43245983
79	6	0.66125447	0.75874490	-0.61111641	6	1.21946931	-1.34835947	2.32722712
80	7	0.79548877	0.09893854	0.54062396	7	1.35370350	-2.00816584	3.47896767
81	1	-0.77186280	-1.28128779	-3.75823498	1	-0.21364796	-3.38839245	-0.81989110
82	1	-0.48384279	-3.48465800	-1.81350219	1	0.07437205	-5.59176207	1.12484097
83	1	-2.66390300	-1.31964600	-1.73618948	1	-2.10568762	-3.42675066	1.20215356
84	1	-2.20999861	-2.47055292	-0.47716403	1	-1.65178370	-4.57765722	2.46117973
85	1	-0.22062889	-1.64527595	1.28836954	1	0.33758593	-3.75238037	4.22671318
86	1	1.23988008	1.63403475	-0.89464790	1	1.79809427	-0.47306940	2.04369545
87	7	-2.53849816	-3.49771762	-4.26461935	7	-1.98028255	-5.60482168	-1.32627439
88	6	-3.54122376	-4.27002192	-4.97464848	6	-2.98300838	-6.37712526	-2.03630352
89	6	-4.63002062	-3.49981952	-5.74626255	6	-4.07180643	-5.60692358	-2.80791759
90	8	-5.32393503	-4.11028671	-6.56550074	8	-4.76572084	-6.21739054	-3.62715673
91	1	-1.80811787	-3.01950741	-4.78699112	1	-1.24990344	-5.12661171	-1.84864628
92	1	-3.07746673	-4.94861269	-5.70576715	1	-2.51925135	-7.05571604	-2.76742220
93	1	-4.05155563	-4.89164734	-4.22363758	1	-3.49334121	-6.99875164	-1.28529263
94	7	-4.77831793	-2.17497206	-5.47239256	7	-4.22010374	-4.28207636	-2.53404760
95	6	-5.86757231	-1.39697576	-6.05665541	6	-5.30935812	-3.50408030	-3.11831045
96	6	-5.55166531	0.09057911	-6.13242722	6	-4.99345112	-2.01652527	-3.19408226
97	8	-5.41774321	0.56841439	-4.79067945	8	-4.85952902	-1.53868985	-1.85233486
98	1	-4.23481464	-1.75347245	-4.71916580	1	-3.67659998	-3.86057687	-1.78082108
99	1	-6.05539179	-1.79321849	-7.06399393	1	-5.49717760	-3.90032291	-4.12564945
100	1	-4.62566471	0.26629212	-6.70425606	1	-4.06745052	-1.84081221	-3.76591158
101	1	-6.38313723	0.59549564	-6.65717411	1	-5.82492304	-1.51160872	-3.71882915
102	1	-5.21384144	1.51732349	-4.75777864	1	-4.65562725	-0.58978069	-1.81943381

N								
103	1	-6.79245472	-1.53725398	-5.47068310	1	-6.23424053	-3.64435840	-2.53233814
104	26	-1.38109303	1.35022652	-2.73099542	26	-0.82287872	-0.75687790	0.20734763
105	26	-1.92561769	1.73113585	-5.27281523	26	-1.36740315	-0.37596855	-2.33447051
106	16	-2.63427615	0.06454046	-4.01334333	16	-2.07606077	-2.04256392	-1.07499838
107	16	-0.70252252	3.04293132	-3.94967437	16	-0.14430776	0.93582666	-1.01132977
108	6	3.62930369	1.93591022	4.11850882	6	4.18751907	-0.17119439	7.05685282
109	6	4.58941174	2.68671703	4.79935884	6	5.14762592	0.57961226	7.73770285
110	6	5.86095715	2.81296539	4.22027397	6	6.41917133	0.70586050	7.15861797
111	6	6.17800283	2.20117307	2.99778819	6	6.73621702	0.09406816	5.93613195
112	6	5.19955730	1.44030476	2.32799697	6	5.75777149	-0.66679955	5.26634073
113	6	3.91426802	1.31255245	2.89816499	6	4.47248220	-0.79455173	5.83650875
114	8	3.00098920	0.47126573	2.31038308	8	3.55920458	-1.63583851	5.24872684
115	8	6.80082893	3.56589198	4.91003895	8	7.35904312	1.45878708	7.84838343
116	6	5.49795103	0.75577992	1.01515830	6	6.05616522	-1.35132432	3.95350218
117	1	6.33865881	0.05069239	1.10364127	1	6.89687300	-2.05641198	4.04198503
118	1	4.61861467	0.19357041	0.68420488	1	5.17682886	-1.91353393	3.62254858
119	1	5.76139164	1.47912383	0.22802445	1	6.31960583	-0.62798047	3.16636801
120	6	7.57112837	2.38563251	2.44052076	6	8.12934208	0.27852768	5.37886429
121	1	7.68989086	1.88591146	1.47412014	1	8.24810505	-0.22119305	4.41246367
122	1	7.81023645	3.45164490	2.27779603	1	8.36845207	1.34454060	5.21613979
123	1	8.34259033	1.97186518	3.11399484	1	8.90080547	-0.13523932	6.05233860
124	6	4.29281950	3.35305691	6.11878586	6	4.85103416	1.24595225	9.05713081
125	1	4.97233772	2.99891973	6.90891171	1	5.53055191	0.89181507	9.84725571
126	1	4.43034887	4.44335413	6.05749321	1	4.98856306	2.33624959	8.99583817
127	1	3.26050639	3.15027404	6.43210077	1	3.81872177	1.04316950	9.37044525
128	1	2.63763070	1.80145299	4.55443907	1	3.19584584	-0.30565137	7.49278307
129	1	1.52888763	0.28114134	1.27039886	1	2.02978969	-1.80143368	4.25663757
130	1	7.61449623	3.57332730	4.37682724	1	8.17271042	1.46622241	7.31517124

3. Model M6, Z = −1, m=1

E(M6) = -7957.72286485 a.u.
E(P6^{opt}) = -7957.72264055 a.u.
E(P6^{nop}) = -7957.70871367 a.u. (approximation 1)
E(P6^{nop}) = -7957.70818593 a.u. (approximation 2)

Atomic Coordinates

N	M6 Atom number	X	Y	Z	P6^{opt} Atom number	X	Y	Z
1	6	-2.14411884	3.17725834	-4.60409649	6	-2.63022258	3.20543080	-5.27626122
2	6	-2.42767194	4.20024400	-3.51326144	6	-2.98843742	4.22219915	-4.20233841
3	8	-1.53267293	4.87515672	-2.98991143	8	-2.14188553	4.94814395	-3.66660911
4	6	-1.35849964	1.98586718	-4.04872921	6	-1.85339573	2.02684409	-4.68121692
5	16	-2.35826656	1.03503796	-2.81221057	16	-2.89053633	1.05164751	-3.49591715
6	1	-3.07119358	2.82977468	-5.08368161	1	-3.52585468	2.84099924	-5.80101819
7	1	-1.06807377	1.29698003	-4.85134586	1	-1.50980864	1.34486595	-5.46884948
8	1	-0.44271764	2.34138096	-3.56002763	1	-0.96885314	2.39813801	-4.14800171
9	1	-1.52925671	3.68048407	-5.36681663	1	-1.98698409	3.72034135	-6.00682988
10	7	-3.74147516	4.31276094	-3.14219485	7	-4.31503579	4.26677953	-3.86086133
11	6	-4.18637151	5.20633546	-2.08790895	6	-4.82786860	5.13658821	-2.81846029
12	6	-4.09091186	4.71698735	-0.63029996	6	-4.73720127	4.65914998	-1.35691690
13	8	-4.59253919	5.40173001	0.26080163	8	-5.28989350	5.32458052	-0.48053356
14	1	-4.39152885	3.62341279	-3.50575720	1	-4.91159777	3.52669985	-4.21728591
15	1	-3.57144160	6.11632725	-2.13048351	1	-4.26061309	6.07740443	-2.85187963
16	1	-5.22981524	5.49578125	-2.26620336	1	-5.88123567	5.37095760	-3.01872260
17	7	-3.41423268	3.55236742	-0.42017403	7	-4.00766654	3.53179233	-1.12486242
18	6	-3.02188177	3.13346906	0.92145051	6	-3.63219521	3.13920814	0.22896002
19	6	-1.73983061	3.86619291	1.41309279	6	-2.38398675	3.91757937	0.73698275
20	8	-1.75388551	4.54761527	2.43708472	8	-2.44983518	4.63756999	1.73343218

21	6	-2.88260443	1.59736407	0.93405714	6	-3.44566373	1.60899112	0.27231125
22	6	-2.34845333	1.02266455	2.20724755	6	-2.91801661	1.08989729	1.57182564
23	7	-1.39501743	0.00569289	2.22769684	7	-1.93477302	0.10288014	1.64533846
24	6	-2.68556170	1.33050530	3.50516728	6	-3.28431481	1.44467531	2.85038163
25	6	-1.17578874	-0.29820174	3.50897559	6	-1.73068200	-0.13508711	2.94099610
26	7	-1.94056530	0.48599126	4.30388446	7	-2.52866521	0.65850252	3.69567767
27	1	-3.01847629	3.04339018	-1.21738712	1	-3.58535178	3.02325804	-1.90987827
28	1	-3.80683091	3.46977148	1.61156505	1	-4.44200237	3.46269829	0.89630952
29	1	-3.87154841	1.16423937	0.71212462	1	-4.41496878	1.13757033	0.04303240
30	1	-2.21724345	1.28759809	0.11404412	1	-2.75302729	1.30023846	-0.52532012
31	1	-3.34834145	2.08229584	3.91387604	1	-3.97152512	2.19652138	3.21658718
32	1	-0.49260367	-1.05703239	3.87724767	1	-1.04008154	-0.85970863	3.35535578
33	1	-1.93539891	0.47207264	5.31733844	1	-2.54069218	0.68916081	4.70860163
34	7	-0.63962295	3.71789143	0.60809666	7	-1.25219030	3.76159032	-0.01995319
35	6	0.65450219	4.24955108	1.01169335	6	0.01256356	4.34002084	0.40835861
36	6	1.61570449	4.61946280	-0.12250111	6	0.98752661	4.72945295	-0.70725195
37	8	2.76043648	4.97585678	0.15508106	8	2.12284782	5.10192886	-0.40946581
38	1	-0.60383335	2.88885472	0.00543799	1	-1.17118481	2.91111585	-0.59174563
39	1	0.47467014	5.14856172	1.61559399	1	-0.21164761	5.23854897	0.99833457
40	1	1.20273015	3.54095658	1.65380785	1	0.56919176	3.65559823	1.06910262
41	7	1.15498563	4.49945769	-1.40982734	7	0.54609723	4.61422642	-2.00000545
42	6	1.95805082	4.98310164	-2.52415052	6	1.35987585	5.10146431	-3.10339160
43	6	2.75904108	3.95810226	-3.34437948	6	2.17257415	4.07764485	-3.91400265
44	8	3.34640201	4.33842238	-4.36242126	8	2.77921968	4.46133699	-4.91959324
45	1	0.14866382	4.43604375	-1.57123862	1	-0.45508411	4.51765098	-2.17468060
46	1	1.30276689	5.50247644	-3.23498389	1	0.71187609	5.61891514	-3.82245032
47	1	2.69616138	5.70142504	-2.13897145	1	2.09042016	5.82194010	-2.70834679
48	7	2.80909509	2.67191396	-2.90285613	7	2.20745486	2.78899851	-3.47705155
49	6	3.54427238	1.67336159	-3.68071847	6	2.91364276	1.78157102	-4.26946305
50	6	3.62698506	0.30777430	-3.00860119	6	3.00817957	0.42008514	-3.59120256
51	16	4.61934707	0.38155400	-1.44754698	16	4.08639755	0.47415316	-2.08768478
52	1	2.23456460	2.38465823	-2.11162960	1	1.59607541	2.49650806	-2.71444534
53	1	3.05504145	1.53907786	-4.66113600	1	2.39382128	1.63836764	-5.23316291
54	1	2.63124546	-0.08601750	-2.77364098	1	2.02006043	0.04893465	-3.29576774
55	1	4.13376744	-0.39203963	-3.68405981	1	3.46226874	-0.29479061	-4.28756213
56	1	4.54933064	2.06966168	-3.88592891	1	3.91227990	2.17373539	-4.50914687
57	6	-0.80307893	-2.22795070	-4.51014041	6	-1.31607078	-2.19252661	-5.16503114
58	16	0.43677913	-1.10705505	-3.74265934	16	-0.07278760	-1.07595350	-4.39630037
59	1	-0.39236529	-2.57837280	-5.46516914	1	-0.89887139	-2.56573611	-6.10872151
60	1	-1.74279695	-1.68991440	-4.68628205	1	-2.24564537	-1.64392160	-5.36275346
61	1	-0.99423542	-3.08740458	-3.85624961	1	-1.53007809	-3.03773302	-4.49918964
62	6	3.02099126	-3.33642484	-1.02016142	6	2.43136941	-3.25341420	-1.51929778
63	6	2.34078906	-4.41102617	-0.15857885	6	1.75407235	-4.25312978	-0.56816633
64	8	2.98850865	-5.29508852	0.40051225	8	2.41113622	-5.02645759	0.13071246
65	6	3.95860348	-2.47482607	-0.16096013	6	3.38974236	-2.33376919	-0.74784773
66	16	5.26686589	-1.55903546	-1.10227851	16	4.68336581	-1.49420590	-1.78340529
67	1	3.61466548	-3.87570744	-1.77252717	1	3.00887200	-3.85822300	-2.23459175
68	1	3.41440873	-1.74024619	0.44283810	1	2.85637559	-1.53817783	-0.21583387
69	1	4.53818130	-3.11911441	0.51611055	1	3.96574639	-2.92397724	-0.02129432
70	1	2.29059394	-2.71023208	-1.55271216	1	1.69888387	-2.66728925	-2.09252528
71	7	0.96481909	-4.31614897	-0.07995927	7	0.37409774	-4.23303031	-0.58157398
72	6	0.20098705	-5.04941614	0.92326573	6	-0.41007842	-4.94560545	0.41886997
73	6	-0.95903777	-5.89675875	0.36343046	6	-1.56347745	-5.80608197	-0.13823807
74	8	-1.50812737	-6.74716709	1.06508008	8	-2.10193650	-6.65072762	0.58021309
75	6	-0.43726754	-4.12012987	2.01192491	6	-1.05835795	-4.00397830	1.49229361
76	6	0.49790818	-3.13164722	2.62538712	6	-0.08497729	-3.06036020	2.11116006
77	7	0.92154467	-1.96311139	1.98887892	7	0.35437717	-1.90348059	1.46552131
78	6	1.17779918	-3.20821565	3.82692513	6	0.64375320	-3.21690975	3.27079453
79	6	1.82920954	-1.39850525	2.86822062	6	1.32406625	-1.38684915	2.24338980
80	7	2.00911011	-2.12137795	3.97157346	7	1.50986431	-2.15464813	3.33847733
81	1	0.55231386	-3.43433216	-0.39736116	1	-0.07278386	-3.40640936	-1.00009777
82	1	0.90454246	-5.74333773	1.40275269	1	0.28342078	-5.63400177	0.92058121

N	Atom				Atom			
83	1	-1.29746875	-3.60054772	1.56247418	1	-1.87473884	-3.43869024	1.01910812
84	1	-0.83464194	-4.78378985	2.79094939	1	-1.50144148	-4.65350830	2.25801404
85	1	1.13251380	-3.99430834	4.57548438	1	0.64076346	-4.00406407	4.01423085
86	1	2.33670126	-0.46109930	2.65406562	1	1.87523689	-0.47407699	2.04606235
87	7	-1.39146975	-5.56595735	-0.89700772	7	-1.98693296	-5.51276116	-1.40650507
88	6	-2.46239138	-6.28474834	-1.56194364	6	-3.05430678	-6.24993799	-2.05760232
89	6	-3.75729636	-5.52058078	-1.89826063	6	-4.36084301	-5.51027372	-2.40376137
90	8	-4.58532862	-6.06845953	-2.63292603	8	-5.20637593	-6.11591808	-3.07085347
91	1	-0.78668524	-4.95444356	-1.43936746	1	-1.42891247	-4.85789362	-1.94812027
92	1	-2.11375592	-6.71951750	-2.50976670	1	-2.70107566	-6.69278379	-3.00026889
93	1	-2.74843105	-7.11497249	-0.89955294	1	-3.32886655	-7.07461825	-1.38494551
94	7	-3.92903903	-4.28752754	-1.34585420	7	-4.52135792	-4.23853261	-1.94754688
95	6	-5.14983319	-3.51795136	-1.56253275	6	-5.74563298	-3.48865051	-2.21431818
96	6	-4.91526043	-2.06355495	-1.95511707	6	-5.51017236	-2.04838449	-2.65451543
97	8	-4.55721296	-1.29726763	-0.79156702	8	-5.17955966	-1.23399908	-1.51708138
98	1	-3.19883769	-3.90081196	-0.75008101	1	-3.77650168	-3.78919833	-1.41450109
99	1	-5.69810019	-4.03657899	-2.36109546	1	-6.27869645	-4.04087743	-3.00061414
100	1	-4.12924677	-2.00099238	-2.72445094	1	-4.71165594	-2.00884314	-3.41218081
101	1	-5.85316034	-1.66801704	-2.38789772	1	-6.44195673	-1.67480441	-3.11848877
102	1	-3.94851884	-0.58780547	-1.07043188	1	-4.49648791	-0.59468708	-1.79097811
103	1	-5.77862042	-3.53732956	-0.65599516	1	-6.38988639	-3.47795904	-1.31847749
104	26	-0.12407879	-0.83723253	0.71260411	26	-0.71234535	-0.74126027	0.06642267
105	26	-0.68741641	-0.32127376	-1.92531158	26	-1.21040606	-0.28786705	-2.57599660
106	16	-1.29559334	-2.05744076	-0.72246047	16	-1.83460800	-2.02806820	-1.36820429
107	16	0.55152428	0.85571747	-0.53419546	16	-0.00721683	0.93832153	-1.18130799
108	6	4.51873261	-0.17576176	7.69710563	6	4.00423288	-0.34596181	7.07064013
109	6	5.37007545	0.64494376	8.44128973	6	4.82026088	0.49940944	7.80589258
110	6	6.66402793	0.86872896	7.94745294	6	6.10278185	0.78680790	7.28721411
111	6	7.10820508	0.28660458	6.74953699	6	6.56442742	0.23689692	6.06853343
112	6	6.23703762	-0.53861009	6.01039834	6	5.74427404	-0.62770450	5.33672984
113	6	4.93181105	-0.76784357	6.49731830	6	4.41192891	-0.94365521	5.82887931
114	8	4.12911850	-1.65364641	5.82135734	8	3.64062283	-1.75035344	5.19086037
115	8	7.49455367	1.69085538	8.69632456	8	6.89527825	1.63757443	8.03273063
116	6	6.67041628	-1.18001949	4.71374160	6	6.18083508	-1.25367724	4.04012480
117	1	7.53062407	-1.85208057	4.85768438	1	7.11085667	-1.83245651	4.15091055
118	1	5.84626271	-1.77025456	4.30060593	1	5.39129106	-1.93097857	3.69425189
119	1	6.96598323	-0.42804286	3.96629637	1	6.35842363	-0.50175508	3.25481790
120	6	8.51809933	0.57864008	6.28879269	6	7.95215813	0.61609718	5.60079609
121	1	8.74883465	0.07298491	5.34603011	1	8.18960560	0.15530836	4.63689774
122	1	8.67976079	1.65791732	6.11846606	1	8.05605262	1.70706116	5.46402470
123	1	9.26914856	0.24301668	7.02577297	1	8.73173557	0.29315037	6.31325293
124	6	4.93479919	1.28255436	9.73576787	6	4.38350515	1.11198490	9.11119796
125	1	5.58514680	0.98007109	10.57059435	1	5.05868765	0.82814924	9.93258997
126	1	4.99151394	2.38032422	9.68075211	1	4.39853550	2.21117861	9.06208363
127	1	3.90254733	0.99987373	9.97977672	1	3.36704170	0.78755906	9.36730925
128	1	3.51277748	-0.38534189	8.06612688	1	3.00635641	-0.59839360	7.43479884
129	1	3.28437513	-1.35637638	5.41188371	1	2.25045565	-1.98908524	4.06447040
130	1	8.33780575	1.76591910	8.21707548	1	7.73100024	1.76127871	7.54793531

N	P6^nop – approximation 1				P6^nop – approximation 2			
	Atom				Atom			
	number	X	Y	Z	number	X	Y	Z
1	6	-3.45434403	4.90182066	-8.09402370	6	-2.72374344	3.20966554	-5.22665071
2	6	-3.73789716	5.92480707	-7.00318861	6	-3.00729656	4.23265123	-4.13581610
3	8	-2.84289765	6.59972000	-6.47983837	8	-2.11229753	4.90756416	-3.61246562
4	6	-2.66872454	3.71042967	-7.53865623	6	-1.93812430	2.01827431	-4.67128372
5	16	-3.66849184	2.75960064	-6.30213737	16	-2.93789124	1.06744528	-3.43476486
6	1	-4.38141918	4.55433750	-8.57360840	1	-3.65081835	2.86218190	-5.70623589
7	1	-2.37829876	3.02154279	-8.34127331	1	-1.64769840	1.32938731	-5.47390032
8	1	-1.75294256	4.06594372	-7.04995441	1	-1.02234232	2.37378836	-4.18258190
9	1	-2.83948159	5.40504694	-8.85674381	1	-2.10888147	3.71289134	-5.98937082
10	7	-5.05170107	6.03732395	-6.63212156	7	-4.32109976	4.34516811	-3.76474905
11	6	-5.49659729	6.93089867	-5.57783604	6	-4.76599598	5.23874283	-2.71046329

12	6	-5.40113783	6.44155025	-4.12022638	6	-4.67053652	4.74939442	-1.25285435
13	8	-5.90276480	7.12629318	-3.22912502	8	-5.17216396	5.43413734	-0.36175272
14	1	-5.70175457	5.34797573	-6.99568415	1	-4.97115374	3.65582013	-4.12831163
15	1	-4.88166714	7.84089041	-5.62041044	1	-4.15106630	6.14873457	-2.75303793
16	1	-6.54004049	7.22034454	-5.75613022	1	-5.80943966	5.52818871	-2.88875771
17	7	-4.72445822	5.27693033	-3.91010094	7	-3.99385738	3.58477473	-1.04272842
18	6	-4.33210707	4.85803175	-2.56847572	6	-3.60150647	3.16587639	0.29889613
19	6	-3.05005550	5.59075546	-2.07683349	6	-2.31945515	3.89860010	0.79053837
20	8	-3.06411052	6.27217817	-1.05284131	8	-2.33351016	4.58002234	1.81453037
21	6	-4.19282961	3.32192683	-2.55586910	6	-3.46222901	1.62977135	0.31150275
22	6	-3.65867853	2.74722719	-1.28267848	6	-2.92807794	1.05507183	1.58469319
23	7	-2.70524216	1.73025584	-1.26222908	7	-1.97464204	0.03810015	1.60514259
24	6	-3.99578691	3.05506802	0.01524143	6	-3.26518631	1.36291254	2.88261294
25	6	-2.48601365	1.42636108	0.01904969	6	-1.75541341	-0.26579449	2.88642120
26	7	-3.25079012	2.21055412	0.81395841	7	-2.52019000	0.51839852	3.68133020
27	1	-4.32870150	4.76795292	-4.70731354	1	-3.59810090	3.07579756	-1.83994150
28	1	-5.11705685	5.19433403	-1.87836087	1	-4.38645554	3.50217867	0.98901063
29	1	-5.18177414	2.88880205	-2.77780151	1	-4.45117283	1.19664669	0.08957028
30	1	-3.52746868	3.01216102	-3.37588263	1	-2.79686809	1.32000542	-0.50851023
31	1	-4.65856695	3.80685854	0.42394996	1	-3.92796612	2.11470318	3.29132175
32	1	-1.80282855	0.66753048	0.38732147	1	-1.07222831	-1.02462506	3.25469327
33	1	-3.24562383	2.19663548	1.82741225	1	-2.51502371	0.50447989	4.69478416
34	7	-1.94984782	5.44245434	-2.88182950	7	-1.21924758	3.75029874	-0.01445770
35	6	-0.65572268	5.97411442	-2.47823286	6	0.07487756	4.28195858	0.38913900
36	6	0.30548000	6.34402609	-3.61242771	6	1.03607988	4.65187025	-0.74505550
37	8	1.45021141	6.70041990	-3.33484554	8	2.18081188	5.00826406	-0.46747330
38	1	-1.91405833	4.61341763	-3.48448849	1	-1.18345809	2.92126203	-0.61711639
39	1	-0.83555472	6.87312508	-1.87433183	1	-0.10495451	5.18096924	0.99303967
40	1	-0.10749446	5.26551914	-1.83611786	1	0.62310553	3.57336378	1.03125358
41	7	-0.15523885	6.22402096	-4.89975405	7	0.57536101	4.53186512	-2.03238177
42	6	0.64782614	6.70766497	-6.01407766	6	1.37842619	5.01550913	-3.14670491
43	6	1.44881594	5.68266535	-6.83430624	6	2.17941642	3.99050951	-3.96693373
44	8	2.03617668	6.06298542	-7.85234785	8	2.76677728	4.37082958	-4.98497534
45	1	-1.16156089	6.16060686	-5.06116581	1	-0.43096083	4.46845102	-2.19379306
46	1	-0.00745758	7.22703934	-6.72491074	1	0.72314227	5.53488350	-3.85753822
47	1	1.38593614	7.42598820	-5.62889862	1	2.11653662	5.73383236	-2.76152587
48	7	1.49887002	4.39647675	-6.39278316	7	2.22947049	2.70432115	-3.52541041
49	6	2.23404717	3.39792442	-7.17064524	6	2.96464777	1.70576882	-4.30327272
50	6	2.31675982	2.03233719	-6.49852800	6	3.04736042	0.34018156	-3.63115549
51	16	3.30912185	2.10611677	-4.93747377	16	4.03972244	0.41396126	-2.07010126
52	1	0.92433971	4.10922098	-5.60155630	1	1.65493989	2.41706562	-2.73418379
53	1	1.74481630	3.26364064	-8.15106297	1	2.47541690	1.57148516	-5.28369045
54	1	1.32102025	1.63854527	-6.26356792	1	2.05162072	-0.05361023	-3.39619517
55	1	2.82354259	1.33252323	-7.17398691	1	3.55414295	-0.35963237	-4.30661440
56	1	3.23910570	3.79422426	-7.37585592	1	3.96970606	2.10206890	-4.50848341
57	6	-2.11330390	-0.50338811	-8.00006676	6	-1.38270354	-2.19554353	-5.13269472
58	16	-0.87344569	0.61750776	-7.23258638	16	-0.14284551	-1.07464778	-4.36521387
59	1	-1.70259011	-0.85381013	-8.95509243	1	-0.97198993	-2.54596543	-6.08772326
60	1	-3.05302191	0.03464844	-8.17620945	1	-2.32242155	-1.65750706	-5.30883646
61	1	-2.30446029	-1.36284161	-7.34617662	1	-1.57386005	-3.05499721	-4.47880411
62	6	1.71076608	-1.61186194	-4.51008749	6	2.44136667	-3.30401754	-1.64271569
63	6	1.03056395	-2.68646312	-3.64850521	6	1.76116443	-4.37861872	-0.78113317
64	8	1.67828357	-3.57052541	-3.08941436	8	2.40888405	-5.26268101	-0.22204211
65	6	2.64837861	-0.75026327	-3.65088654	6	3.37897873	-2.44241881	-0.78351450
66	16	3.95664001	0.16552739	-4.59220457	16	4.68724108	-1.52662814	-1.72483277
67	1	2.30444026	-2.15114474	-5.26245451	1	3.03504086	-3.84330010	-2.39508152
68	1	2.10418344	-0.01568345	-3.04708838	1	2.83478403	-1.70783889	-0.17971626
69	1	3.22795630	-1.39455152	-2.97381592	1	3.95855665	-3.08670712	-0.10644382
70	1	0.98036873	-0.98566943	-5.04263926	1	1.71096921	-2.67782474	-2.17526650
71	7	-0.34540564	-2.59158587	-3.56988573	7	0.38519442	-4.28374147	-0.70251364
72	6	-1.10923779	-3.32485294	-2.56666040	6	-0.37863761	-5.01700878	0.30071139
73	6	-2.26926255	-4.17219543	-3.12649632	6	-1.53866243	-5.86435127	-0.25912389

74	8	-2.81835198	-5.02260399	-2.42484617	8	-2.08775187	-6.71475983	0.44252568
75	6	-1.74749243	-2.39556718	-1.47800076	6	-1.01689219	-4.08772278	1.38937068
76	6	-0.81231666	-1.40708423	-0.86453885	6	-0.08171648	-3.09923983	2.00283289
77	7	-0.38868004	-0.23854865	-1.50104678	7	0.34192002	-1.93070412	1.36632466
78	6	-0.13242529	-1.48365283	0.33699894	6	0.59817457	-3.17580843	3.20437074
79	6	0.51898479	0.32605758	-0.62170529	6	1.24958491	-1.36609793	2.24566627
80	7	0.69888538	-0.39681509	0.48164725	7	1.42948556	-2.08897066	3.34901905
81	1	-0.75791097	-1.70976925	-3.88728809	1	-0.02731079	-3.40192485	-1.01991558
82	1	-0.40568238	-4.01877451	-2.08717370	1	0.32491779	-5.71093035	0.78019828
83	1	-2.60769367	-1.87598515	-1.92745197	1	-1.87709343	-3.56814051	0.93991977
84	1	-2.14486694	-3.05922651	-0.69897652	1	-1.41426659	-4.75138235	2.16839504
85	1	-0.17771088	-2.26974559	1.08555806	1	0.55288911	-3.96190095	3.95292997
86	1	1.02647603	1.26346350	-0.83586031	1	1.75707650	-0.42869204	2.03151131
87	7	-2.70169449	-3.84139490	-4.38693428	7	-1.97109437	-5.53355026	-1.51956201
88	6	-3.77261662	-4.56018543	-5.05187082	6	-3.04201603	-6.25234127	-2.18449807
89	6	-5.06752205	-3.79601789	-5.38818789	6	-4.33692074	-5.48817348	-2.52081490
90	8	-5.89555407	-4.34389639	-6.12285280	8	-5.16495323	-6.03605223	-3.25548029
91	1	-2.09691024	-3.22988033	-4.92929459	1	-1.36630988	-4.92203617	-2.06192183
92	1	-3.42398119	-4.99495459	-5.99969387	1	-2.69338059	-6.68711042	-3.13232112
93	1	-4.05865622	-5.39040947	-4.38947964	1	-3.32805562	-7.08256531	-1.52210736
94	7	-5.23926497	-2.56296468	-4.83578062	7	-4.50866365	-4.25512028	-1.96840858
95	6	-6.46005869	-1.79338872	-5.05245972	6	-5.72945786	-3.48554397	-2.18508720
96	6	-6.22548580	-0.33899227	-5.44504404	6	-5.49488497	-2.03114772	-2.57767153
97	8	-5.86743832	0.42729506	-4.28149319	8	-5.13683748	-1.26486039	-1.41412139
98	1	-4.50906324	-2.17624927	-4.24000740	1	-3.77846241	-3.86840463	-1.37263536
99	1	-7.00832558	-2.31201649	-5.85102224	1	-6.27772474	-4.00417185	-2.98364973
100	1	-5.43947268	-0.27642956	-6.21437788	1	-4.70887136	-1.96858501	-3.34700513
101	1	-7.16338587	0.05654574	-5.87782478	1	-6.43278503	-1.63560975	-3.01045203
102	1	-5.25874472	1.13675749	-4.56035805	1	-4.52814341	-0.55539817	-1.69298625
103	1	-7.08884573	-1.81276715	-4.14592123	1	-6.35824490	-3.50492239	-1.27854943
104	26	-1.43430364	0.88733023	-2.77732205	26	-0.70370346	-0.80482525	0.09004974
105	26	-1.99764144	1.40328908	-5.41523886	26	-1.26704109	-0.28886652	-2.54786587
106	16	-2.60581827	-0.33287808	-4.21238661	16	-1.87521803	-2.02503347	-1.34501481
107	16	-0.75870061	2.58028007	-4.02412224	16	-0.02810037	0.88812476	-1.15674984
108	6	3.20850754	1.54880118	4.20717859	6	3.93910789	-0.14335449	7.07455111
109	6	4.05984974	2.36950636	4.95136309	6	4.79045057	0.67735106	7.81873560
110	6	5.35380268	2.59329152	4.45752621	6	6.08440351	0.90113622	7.32489872
111	6	5.79797935	2.01116753	3.25960994	6	6.52858019	0.31901184	6.12698269
112	6	4.92681217	1.18595278	2.52047205	6	5.65741301	-0.50620282	5.38784409
113	6	3.62158537	0.95671928	3.00739169	6	4.35218620	-0.73543626	5.87476397
114	8	2.81889343	0.07091630	2.33143091	8	3.54949379	-1.62123919	5.19880295
115	8	6.18432808	3.41541815	5.20639706	8	6.91492891	1.72326267	8.07376957
116	6	5.36019087	0.54454321	1.22381556	6	6.09079170	-1.14761221	4.09118748
117	1	6.22039843	-0.12751783	1.36775839	1	6.95099926	-1.81967330	4.23513031
118	1	4.53603745	-0.04569184	0.81067967	1	5.26663828	-1.73784733	3.67805147
119	1	5.65575790	1.29651999	0.47637033	1	6.38635874	-0.39563560	3.34374213
120	6	7.20787334	2.30320263	2.79886627	6	7.93847513	0.61104739	5.66623831
121	1	7.43860960	1.79754782	1.85610402	1	8.16921043	0.10539217	4.72347593
122	1	7.36953497	3.38248014	2.62853956	1	8.10013580	1.69032454	5.49591160
123	1	7.95892382	1.96757972	3.53584599	1	8.68952370	0.27542394	6.40321875
124	6	3.62457371	3.00711727	6.24584103	6	4.35517454	1.31496167	9.11321354
125	1	4.27492142	2.70463371	7.08066893	1	5.00552225	1.01247835	9.94804001
126	1	3.68128824	4.10488701	6.19082451	1	4.41188908	2.41273141	9.05819702
127	1	2.59232259	2.72443652	6.48984909	1	3.32292271	1.03228104	9.35722160
128	1	2.20255232	1.33922100	4.57620001	1	2.93315291	-0.35293463	7.44357252
129	1	1.41120577	-0.19424528	1.22591889	1	2.06763554	-1.87585926	4.15515089
130	1	7.02757835	3.49048185	4.72714853	1	7.75818110	1.79832637	7.59452105

List of the fixed internal coordinates for the models M2-M6 and products P2^{opt}–P6^{opt}

M2	M3	M4	M5	M6
Bond lengths	*Bond lengths*	*Bond lengths*	*Bond lengths*	*Bond lengths*
5 – 102	5 – 102	5 – 102	5 – 102	5 – 102
97 – 105	97 – 105	97 – 105	97 – 105	
102 –106	102 – 106	102 – 106	102 – 106	102 – 106
80 – 114	80 – 114	80 – 114	80 – 114	80 – 114
		66 – 109	66 – 109	66 – 109
		66 – 112	66 – 112	66 – 112
			51 – 109	51 – 109
			51 – 112	51 – 112
Bond angles	*Bond angles*	*Bond angles*	*Bond angles*	*Bond angles*
97–105–104	97–105–104	97–105–104	97–105–104	
102–106–107	102–106–107	102–106–107	102–106–107	102–106–107
102–5–105	102–5–105	102–5–105	102–5–105	
79–80–114	79–80–114	79–80–114	79–80–114	79–80–114
80–114–113	80–114–113	80–114–113	80–114–113	80–114–113
77–104–105	77–104–105	77–104–105	77–104–105	77–104–105
77–104–106	77–104–106	77–104–106	77–104–106	
77–104–107	77–104–107	77–104–107	77–104–107	77–104–107
Torsion angles	*Torsion angles*	*Torsion angles*	*Torsion angles*	*Torsion angles*
76–77–104–106	76–77–104–106	76–77–104–106	76–77–104–106	76–77–104–106
	79–77–104–107	79–77–104–107	79–77–104–107	
	79–80–114–115	79–80–114–115	79–80–114–115	79–80–114–115
79–80–112–109	79–80–112–109	79–80–112–109	79–80–112–109	