

Protonation of Guanine Quartets and Quartet Stacks: Insights From DFT Studies

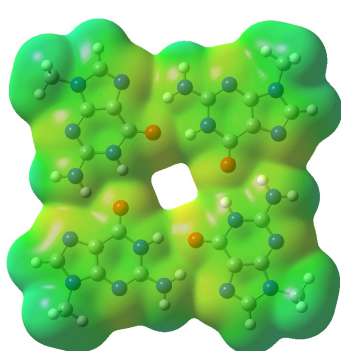
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Canada*

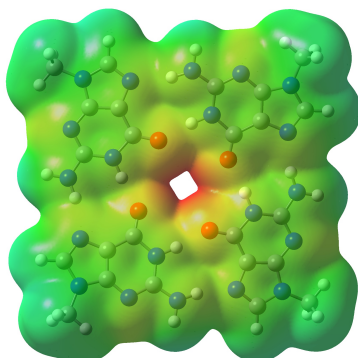
Electronic Supplementary Information

(Table S1-2 and Fig. S1-2, 158 pages)

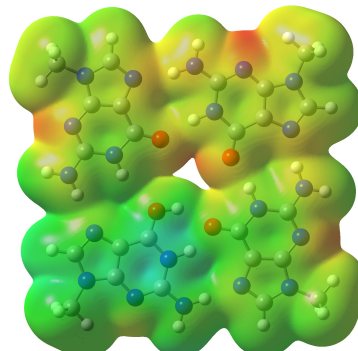
* Email: gauld@uwindsor.ca



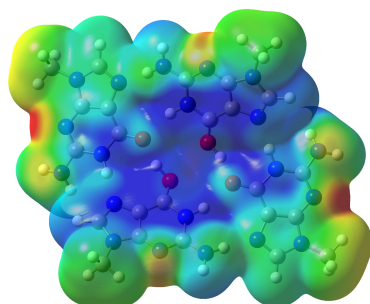
$G4_1$



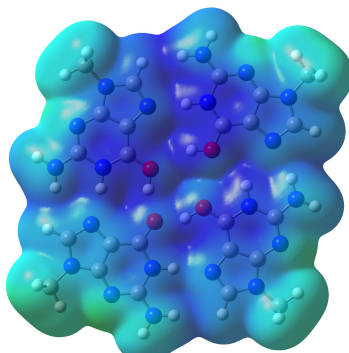
$G4_2$



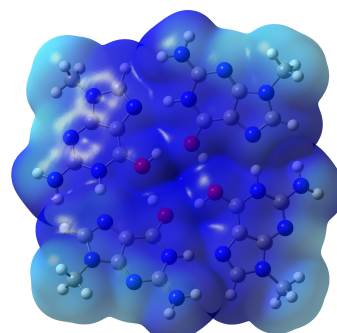
$(G4-H^+)_1$



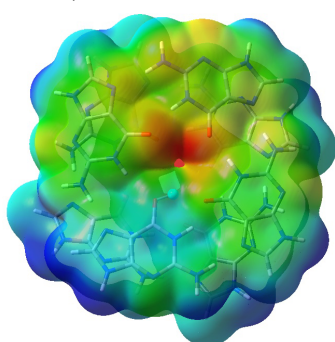
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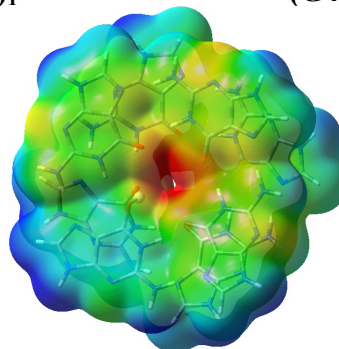
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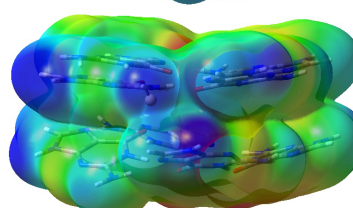
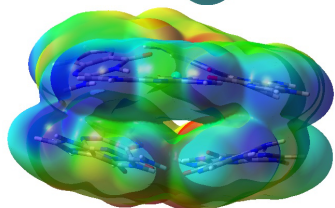
$(G4-4H^+)_1$



$(2G4-H^+)_1$



$(2G4-H^+)_3$



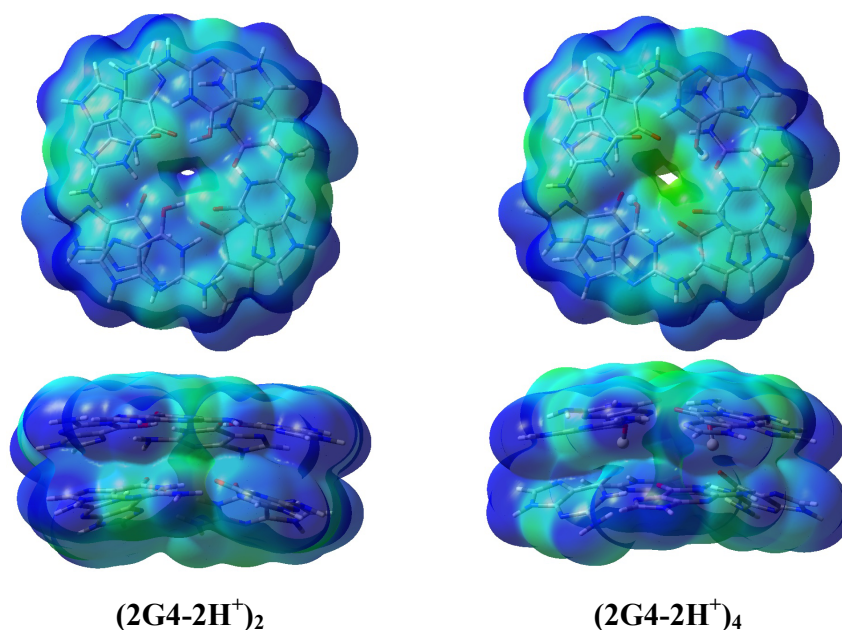
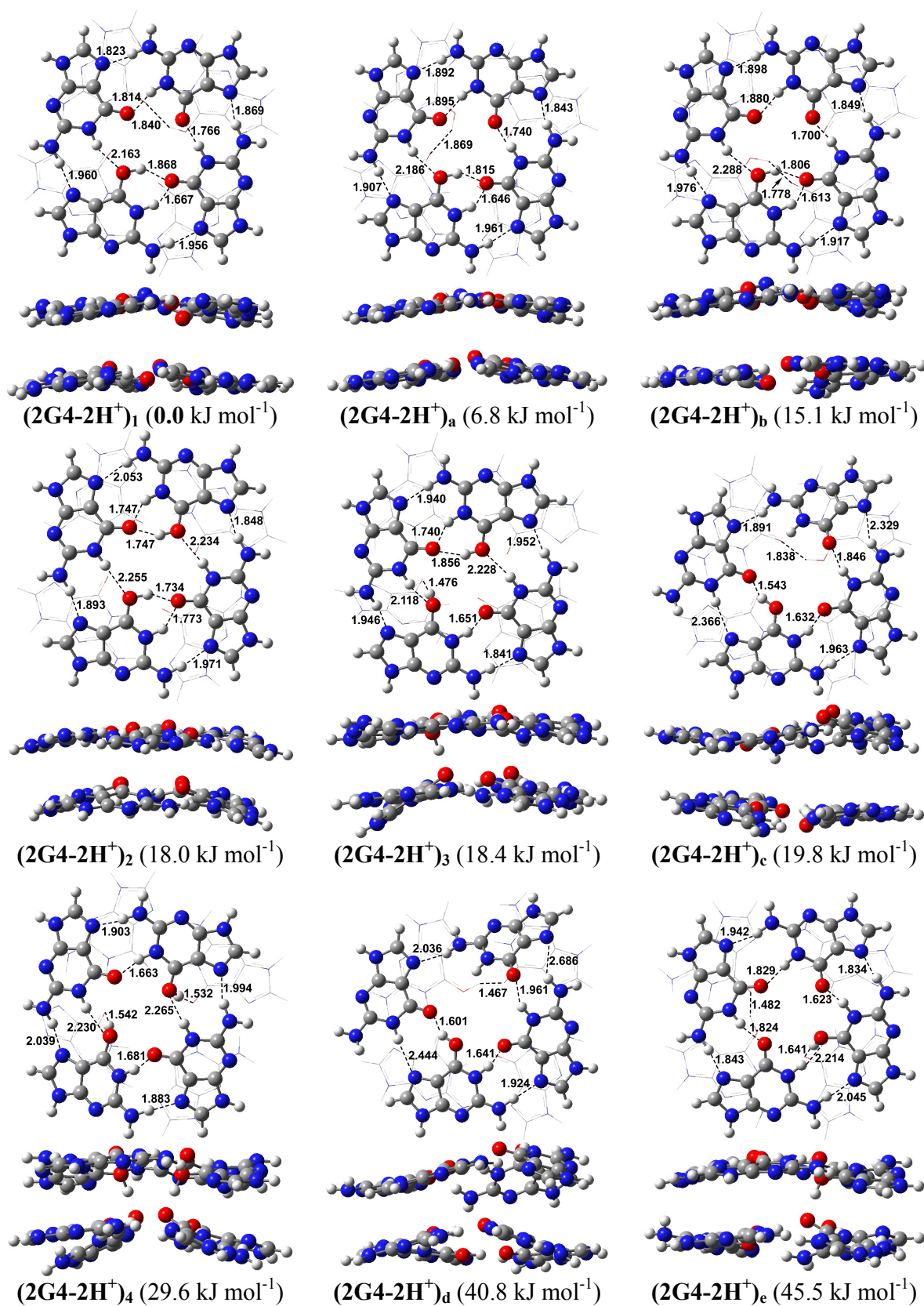
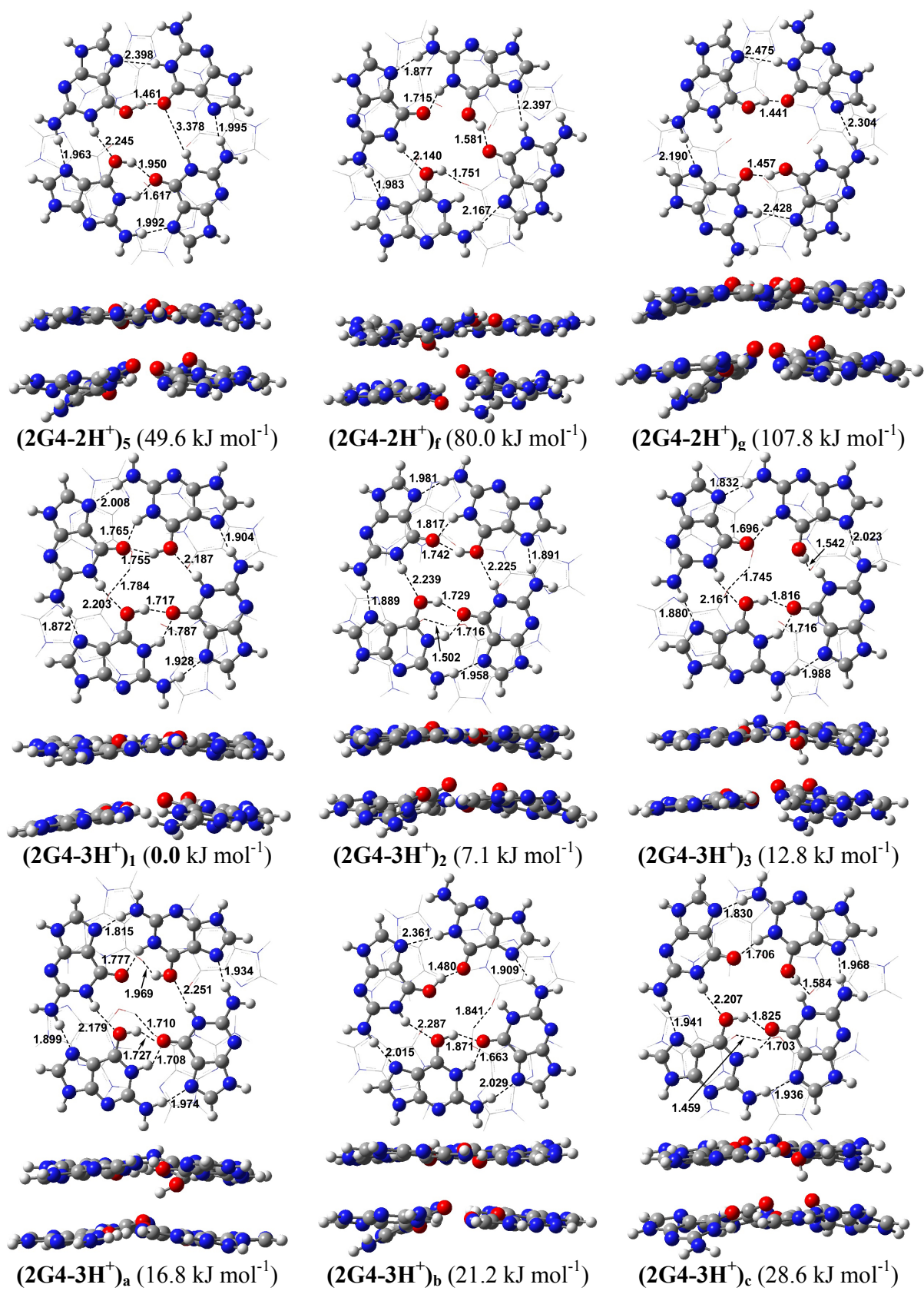
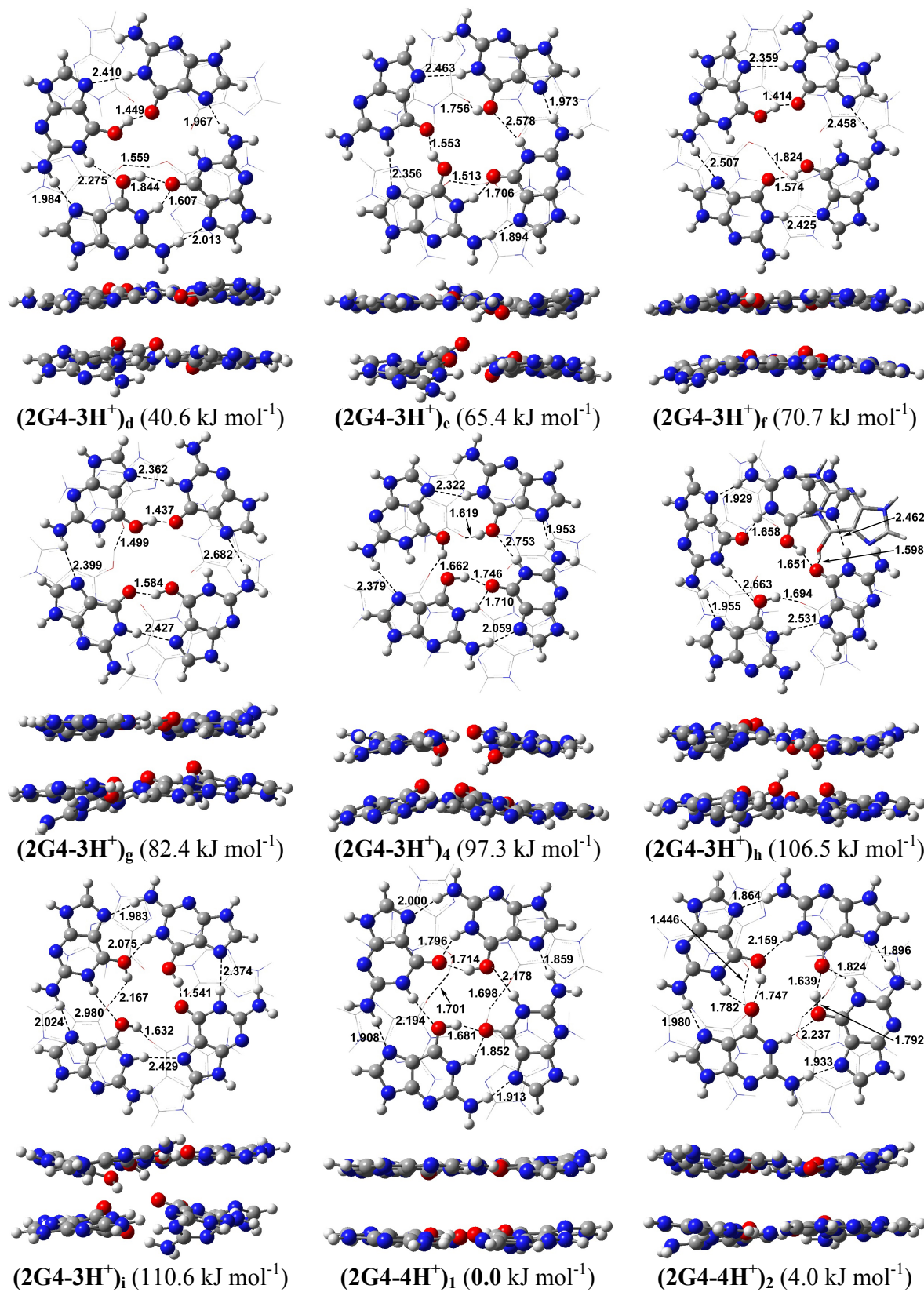
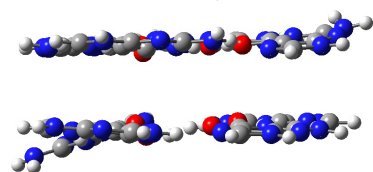
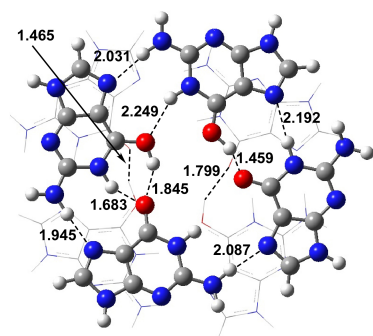


Fig. S1. Electrostatic potential surfaces (EPS's), obtained using GaussView, for the most stable bifurcated and Hoogsteen hydrogen bonded neutral **G4**, the most stable $(G4-nH^+)$ $n=1-4$ complexes, and top- and side-views of $(2G4-H^+)_1$, $(2G4-H^+)_3$, $(2G4-2H^+)_2$ and $(2G4-2H^+)_4$ (see text). The EPS's of the neutral **G4** and protonated **G4** complexes were obtained at the B3LYP/6-31G(d,p) level of theory while those of the protonated **2G4** complexes were obtained at the B3LYP/6-31G(d) level of theory. Blue and red indicate electron-poor and -rich regions respectively.

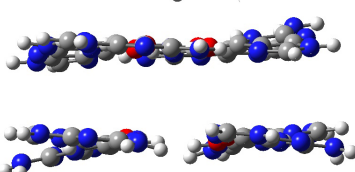
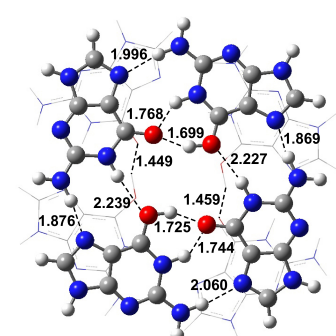




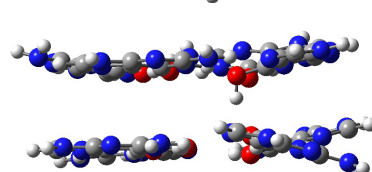
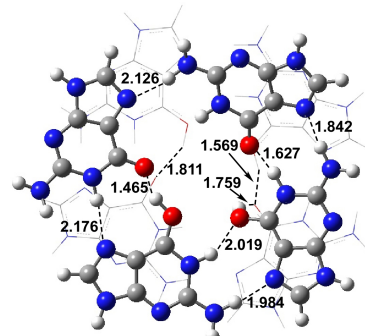




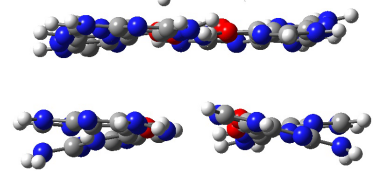
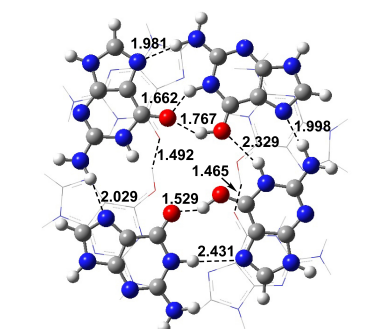
$(2G4-4H^+)_3$ (6.7 kJ mol⁻¹)



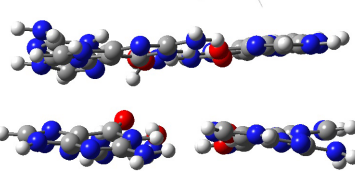
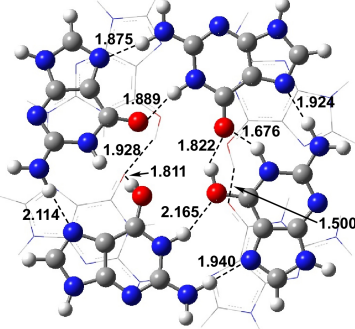
$(2G4-4H^+)_a$ (30.2 kJ mol⁻¹)



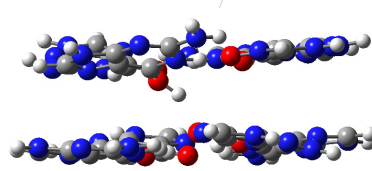
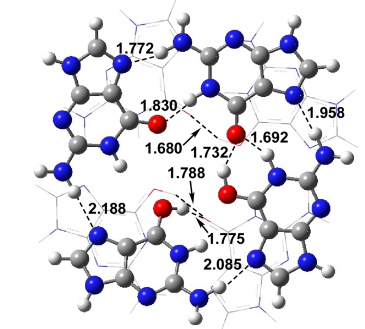
$(2G4-4H^+)_b$ (37.2 kJ mol⁻¹)



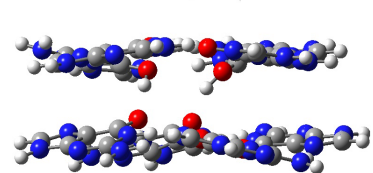
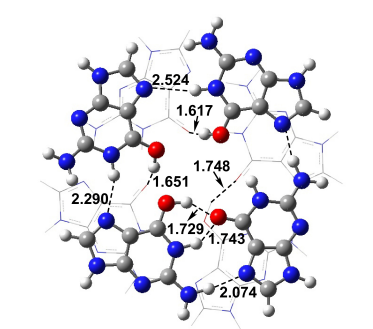
$(2G4-4H^+)_c$ (44.8 kJ mol⁻¹)



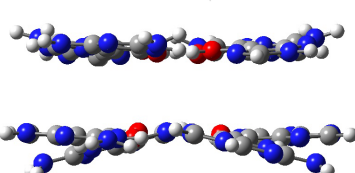
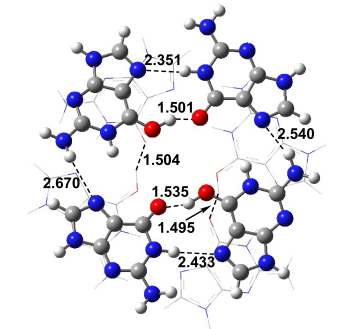
$(2G4-4H^+)_d$ (59.9 kJ mol⁻¹)



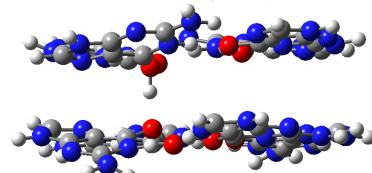
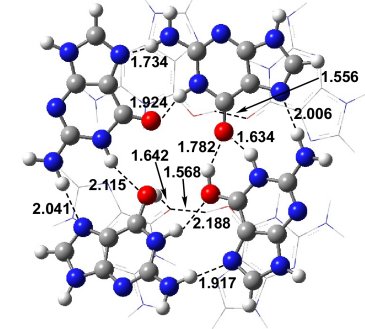
$(2G4-4H^+)_e$ (60.4 kJ mol⁻¹)



$(2G4-4H^+)_f$ (61.0 kJ mol⁻¹)



$(2G4-4H^+)_g$ (66.8 kJ mol⁻¹)



$(2G4-4H^+)_h$ (92.9 kJ mol⁻¹)

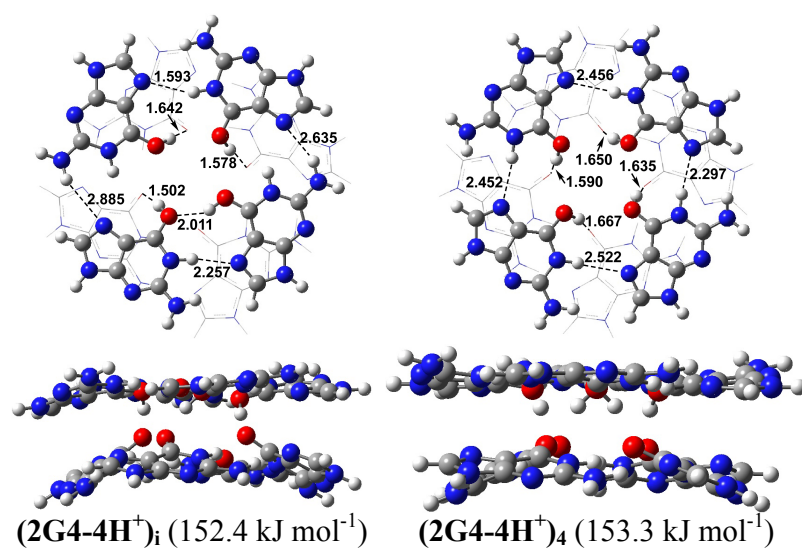


Fig. S2. Optimized structures (top- and side-views) for $(2\text{G4-}n\text{H}^+)$ $n=2-4$. Selected distances are shown in angstroms.

Table S1. Optimized xyz-coordinates and single point energies (h) for all species considered in this present study.

Guanine

C1	2.2553808519	-3.1210147366	-3.8631101686
N2	1.8263065627	-3.1739898867	-5.2498878166
C3	0.5504055166	-3.4095990766	-5.7395014886
C4	2.6260435757	-3.0040896765	-6.3529187303
H5	-0.2819198446	-3.5788006363	-5.0685974422
N6	0.4834473641	-3.4009260327	-7.0458795370
C7	1.7779992744	-3.1477377416	-7.4526337483
N8	3.9596861038	-2.7493567158	-6.3245395142
C9	2.3299444758	-3.0181851987	-8.7739475121
C10	4.4767763631	-2.6282969087	-7.5269073425
O11	1.8177998871	-3.0965330090	-9.8774204105
N12	3.7430375156	-2.7489608787	-8.6798620912
N13	5.8087279565	-2.3674905852	-7.6555088759
H14	4.1853682676	-2.6466993849	-9.5850360845
H15	6.2646129079	-2.2814858421	-8.5464292300
H16	6.3501308433	-2.2873930437	-6.8115086715
H17	3.3065882685	-2.8308168281	-3.8498063451
H18	1.6706842453	-2.3823569957	-3.3071584517
H19	2.1484695833	-4.0986017577	-3.3827440531

Single point energy: -582.0647656

Guanine ‘Hoogsteen protonated’

C1	2.2201930122	-3.1485642502	-3.8403512849
N2	1.8283380519	-3.1795828260	-5.2514394278
C3	0.5510203845	-3.4034664286	-5.7680568022
C4	2.6436070233	-3.0039673517	-6.3259790421
H5	-0.2898553716	-3.5736000351	-5.1079388064
N6	0.4895885611	-3.3836579037	-7.0727645525
C7	1.7920556427	-3.1351351175	-7.4501433206
N8	3.9582368862	-2.7619306737	-6.3364988905
C9	2.3789019256	-2.9948382645	-8.6883417240
C10	4.4842236510	-2.6342630499	-7.5430141125
O11	1.8102945143	-3.0727891999	-9.8741049365
N12	3.7249293249	-2.7452317105	-8.7032083209
N13	5.7968435352	-2.3851481449	-7.6836701465
H14	4.1572014159	-2.6410983004	-9.6160809237
H15	6.2591446118	-2.2957031666	-8.5744316873
H16	6.3505439535	-2.3105082917	-6.8427742093
H17	3.2724323437	-2.8701927831	-3.7887458280
H18	1.6219566601	-2.4089773331	-3.3046251504
H19	2.0823850257	-4.1338127565	-3.3893807181

H2O	0.8577995028	-3.2491822673	-9.7754073896
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Single point energy: -582.4378701

Guanine ‘Watson-Crick protonated’

C1	2.2221002089	-3.1030501867	-3.8507525194
N2	1.8337611462	-3.1611911830	-5.2612527702
C3	0.5599010975	-3.4091545336	-5.7798016087
C4	2.6450476925	-2.9930537957	-6.3353960126
H5	-0.2805312675	-3.5797621272	-5.1189767904
N6	0.5005841009	-3.4109154529	-7.0822738112
C7	1.7997391878	-3.1508485631	-7.4668692284
N8	3.9581855610	-2.7360965650	-6.3324131275
C9	2.3981595602	-3.0238822283	-8.7041362553
C10	4.4974086517	-2.6198619485	-7.5283810423
O11	1.7306120635	-3.1449805573	-9.8336171938
N12	3.7512229813	-2.7589428149	-8.6993446173
N13	5.8099697803	-2.3562639223	-7.6595070896
H14	4.2247927615	-2.6407341246	-9.5878914239
H15	6.2866073108	-2.2793031254	-8.5435001198
H16	6.3503435548	-2.2584532975	-6.8122343226
H17	3.2739328870	-2.8227487818	-3.7999122388
H18	1.6207361970	-2.3548749718	-3.3302017086
H19	2.0831461879	-4.0799536326	-3.3823077531
H20	2.2617152284	-3.0521817590	-10.6387048078

Single point energy: -582.424143

H₂O

O1	0.0000000000	0.0000000000	-0.0665099567
H2	0.0000000000	0.7601633219	0.5277806392
H3	0.0000000000	-0.7601633219	0.5277806392

Single point energy: -76.4602361

H₃O⁺

O1	0.0000000000	0.0000000000	0.0410298196
H2	0.9473163338	0.0000000000	-0.2170576704
H3	-0.4736581669	0.8204000105	-0.2170576704
H4	-0.4736581669	-0.8204000105	-0.2170576704

Single point energy: -76.7325038

NH₃

N1	0.0000000000	0.0000000000	0.0699061873
H2	0.9382587900	0.0000000000	-0.3237670174
H3	-0.4691293950	0.8125559475	-0.3237670174
H4	-0.4691293950	-0.8125559475	-0.3237670174

Single point energy: -56.5841506

NH₄⁺

N1	0.0000000000	0.0000000000	0.0000000000
H2	0.5932436007	-0.5932436007	0.5932436007
H3	-0.5932436007	0.5932436007	0.5932436007
H4	0.5932436007	0.5932436007	-0.5932436007
H5	-0.5932436007	-0.5932436007	-0.5932436007

Single point energy: -56.9207306

G4₁

C1	-1.6767141729	3.3247484730	0.0000000000
C2	-3.5633561219	4.8491597401	0.0000000000
C3	-2.1811129978	4.6589383890	0.0000000000
O4	-0.4898017130	2.9603542978	0.0000000000
N5	-1.5094539594	5.8678129080	0.0000000000
C6	6.9102394634	5.0125701922	0.0000000000
N7	-3.7376519104	6.2142614462	0.0000000000
C8	-2.4638162404	6.7638653176	0.0000000000
N9	-4.9029451660	1.6312807256	0.0000000000
N10	-2.7124869973	2.3810495508	0.0000000000
H11	-4.5497940386	0.6770805339	0.0000000000
H12	-2.4415291188	1.3959318382	0.0000000000
H13	-1.8105831045	-5.8922671829	0.0000000000
N14	-4.5379484735	3.9203042835	0.0000000000
C15	-4.0644023150	2.6796068835	0.0000000000
H16	-1.3959318382	-2.4415291188	0.0000000000
H17	7.8365350992	2.3196577497	0.0000000000
N18	2.3810495508	2.7124869973	0.0000000000
C19	2.6796068835	4.0644023150	0.0000000000
N20	1.6312807256	4.9029451660	0.0000000000
N21	3.9203042835	4.5379484735	0.0000000000
C22	4.8491597401	3.5633561219	0.0000000000
C23	4.6589383890	2.1811129978	0.0000000000
C24	3.3247484730	1.6767141729	0.0000000000
O25	2.9603542978	0.4898017130	0.0000000000
N26	5.8678129080	1.5094539594	0.0000000000
C27	6.7638653176	2.4638162404	0.0000000000
N28	6.2142614462	3.7376519104	0.0000000000
H29	1.3959318382	2.4415291188	0.0000000000
H30	1.8105831045	5.8922671829	0.0000000000
H31	0.6770805339	4.5497940386	0.0000000000
H32	-5.8922671829	1.8105831045	0.0000000000
N33	-3.9203042835	-4.5379484735	0.0000000000
O34	-2.9603542978	-0.4898017130	0.0000000000
H35	2.3196577497	-7.8365350992	0.0000000000
C36	-4.8491597401	-3.5633561219	0.0000000000
C37	5.0125701922	-6.9102394634	0.0000000000

C38	-6.7638653176	-2.4638162404	0.0000000000
N39	-6.2142614462	-3.7376519104	0.0000000000
H40	-2.3196577497	7.8365350992	0.0000000000
C41	-5.0125701922	6.9102394634	0.0000000000
C42	-3.3247484730	-1.6767141729	0.0000000000
N43	-1.6312807256	-4.9029451660	0.0000000000
H44	-0.6770805339	-4.5497940386	0.0000000000
H45	5.8922671829	-1.8105831045	0.0000000000
N46	2.7124869973	-2.3810495508	0.0000000000
C47	4.0644023150	-2.6796068835	0.0000000000
N48	4.9029451660	-1.6312807256	0.0000000000
N49	4.5379484735	-3.9203042835	0.0000000000
C50	3.5633561219	-4.8491597401	0.0000000000
C51	2.1811129978	-4.6589383890	0.0000000000
C52	1.6767141729	-3.3247484730	0.0000000000
O53	0.4898017130	-2.9603542978	0.0000000000
N54	1.5094539594	-5.8678129080	0.0000000000
C55	2.4638162404	-6.7638653176	0.0000000000
N56	3.7376519104	-6.2142614462	0.0000000000
H57	2.4415291188	-1.3959318382	0.0000000000
H58	4.5497940386	-0.6770805339	0.0000000000
N59	-5.8678129080	-1.5094539594	0.0000000000
N60	-2.3810495508	-2.7124869973	0.0000000000
C61	-4.6589383890	-2.1811129978	0.0000000000
H62	-7.8365350992	-2.3196577497	0.0000000000
C63	-2.6796068835	-4.0644023150	0.0000000000
C64	-6.9102394634	-5.0125701922	0.0000000000
H65	5.1155536865	-7.5360813525	0.8917917734
H66	5.1155536865	-7.5360813525	-0.8917917734
H67	5.8003109931	-6.1554619163	0.0000000000
H68	7.5360813525	5.1155536865	0.8917917734
H69	7.5360813525	5.1155536865	-0.8917917734
H70	6.1554619163	5.8003109931	0.0000000000
H71	-5.8003109931	6.1554619163	0.0000000000
H72	-5.1155536865	7.5360813525	0.8917917734
H73	-5.1155536865	7.5360813525	-0.8917917734
H74	-7.5360813525	-5.1155536865	0.8917917734
H75	-7.5360813525	-5.1155536865	-0.8917917734
H76	-6.1554619163	-5.8003109931	0.0000000000

Single point energy: -2328.3685759

G4₂

O1	0.6945404805	2.3459479540	0.1706571601
O2	-2.3459479540	0.6945404805	-0.1706571601
O3	2.3459479540	-0.6945404805	-0.1706571601
O4	-0.6945404805	-2.3459479540	0.1706571601

C5	1.7963042546	2.8526090873	-0.0547924156
C6	-1.7963042546	-2.8526090873	-0.0547924156
N7	2.9386806470	2.0380660308	-0.1837168853
N8	-2.9386806470	-2.0380660308	-0.1837168853
H9	2.7632545533	1.0183673798	-0.1366789379
H10	-2.7632545533	-1.0183673798	-0.1366789379
C11	4.2132347350	2.4942587649	-0.4242337849
C12	-4.2132347350	-2.4942587649	-0.4242337849
N13	5.1943397402	1.5752676807	-0.5375749282
N14	-5.1943397402	-1.5752676807	-0.5375749282
H15	5.1052878033	0.5873134209	-0.2795213345
H16	-5.1052878033	-0.5873134209	-0.2795213345
H17	6.1213152387	1.9542093824	-0.6455813233
H18	-6.1213152387	-1.9542093824	-0.6455813233
N19	4.5233266771	3.7817021253	-0.5659134314
N20	-4.5233266771	-3.7817021253	-0.5659134314
C21	3.4501030975	4.5857578918	-0.4600431095
C22	-3.4501030975	-4.5857578918	-0.4600431095
C23	2.1242912482	4.2366104315	-0.2178670515
C24	-2.1242912482	-4.2366104315	-0.2178670515
N25	1.3194493074	5.3598252644	-0.1764216883
N26	-1.3194493074	-5.3598252644	-0.1764216883
C27	2.1387698478	6.3621726393	-0.3878657414
C28	-2.1387698478	-6.3621726393	-0.3878657414
H29	1.8598990886	7.4067780302	-0.4252850852
H30	-1.8598990886	-7.4067780302	-0.4252850852
N31	3.4491732320	5.9605710574	-0.5672238534
N32	-3.4491732320	-5.9605710574	-0.5672238534
C33	4.6117163213	6.7948873793	-0.8181339924
C34	-4.6117163213	-6.7948873793	-0.8181339924
C35	-2.8526090873	1.7963042546	0.0547924156
C36	2.8526090873	-1.7963042546	0.0547924156
N37	-2.0380660308	2.9386806470	0.1837168853
N38	2.0380660308	-2.9386806470	0.1837168853
C39	2.4942587649	-4.2132347350	0.4242337849
C40	-2.4942587649	4.2132347350	0.4242337849
N41	-1.5752676807	5.1943397402	0.5375749282
N42	1.5752676807	-5.1943397402	0.5375749282
H43	-0.5873134209	5.1052878033	0.2795213345
H44	0.5873134209	-5.1052878033	0.2795213345
H45	1.9542093824	-6.1213152387	0.6455813233
H46	-1.9542093824	6.1213152387	0.6455813233
N47	-3.7817021253	4.5233266771	0.5659134314
N48	3.7817021253	-4.5233266771	0.5659134314
C49	-4.5857578918	3.4501030975	0.4600431095
C50	4.5857578918	-3.4501030975	0.4600431095

C51	-4.2366104315	2.1242912482	0.2178670515
C52	4.2366104315	-2.1242912482	0.2178670515
N53	-5.3598252644	1.3194493074	0.1764216883
N54	5.3598252644	-1.3194493074	0.1764216883
C55	-6.3621726393	2.1387698478	0.3878657414
C56	6.3621726393	-2.1387698478	0.3878657414
H57	-7.4067780302	1.8598990886	0.4252850852
H58	7.4067780302	-1.8598990886	0.4252850852
N59	-5.9605710574	3.4491732320	0.5672238534
N60	5.9605710574	-3.4491732320	0.5672238534
C61	-6.7948873793	4.6117163213	0.8181339924
C62	6.7948873793	-4.6117163213	0.8181339924
H63	-1.0183673798	2.7632545533	0.1366789379
H64	1.0183673798	-2.7632545533	0.1366789379
H65	-7.5010518116	4.7693164110	-0.0028289782
H66	-5.4773980377	-6.1355662982	-0.8947817056
H67	-6.1355662982	5.4773980377	0.8947817056
H68	-4.7693164110	-7.5010518116	0.0028289782
H69	6.1355662982	-5.4773980377	0.8947817056
H70	7.3504346894	-4.4996282245	1.7542701557
H71	4.4996282245	7.3504346894	-1.7542701557
H72	5.4773980377	6.1355662982	-0.8947817056
H73	-7.3504346894	4.4996282245	1.7542701557
H74	-4.4996282245	-7.3504346894	-1.7542701557
H75	4.7693164110	7.5010518116	0.0028289782
H76	7.5010518116	-4.7693164110	-0.0028289782

Single point energy: -2328.3674191

G4 (Bifurcated, S_4 Symmetry)

O1	0.4698567429	2.9449923173	0.1716882409
O2	-2.9449923173	0.4698567429	-0.1716882409
O3	2.9449923173	-0.4698567429	-0.1716882409
O4	-0.4698567429	-2.9449923173	0.1716882409
C5	1.6419586785	3.3242697001	0.0169922042
C6	-1.6419586785	-3.3242697001	0.0169922042
N7	2.6760330614	2.3940871222	-0.1521160120
N8	-2.6760330614	-2.3940871222	-0.1521160120
H9	2.4191492527	1.4051120101	-0.1296013883
H10	-2.4191492527	-1.4051120101	-0.1296013883
C11	4.0136334090	2.7089764768	-0.3189798238
C12	-4.0136334090	-2.7089764768	-0.3189798238
N13	4.8528106764	1.6707668699	-0.4702289585
N14	-4.8528106764	-1.6707668699	-0.4702289585
H15	4.5191953709	0.7129758868	-0.3880598107
H16	-4.5191953709	-0.7129758868	-0.3880598107
H17	5.8389017220	1.8618052363	-0.5205189355

H18	-5.8389017220	-1.8618052363	-0.5205189355
N19	4.4739887759	3.9545370790	-0.3409421926
N20	-4.4739887759	-3.9545370790	-0.3409421926
C21	3.4999190258	4.8710228128	-0.1831145976
C22	-3.4999190258	-4.8710228128	-0.1831145976
C23	2.1311705808	4.6639721619	-0.0086323017
C24	-2.1311705808	-4.6639721619	-0.0086323017
N25	1.4560197880	5.8638812815	0.1232183208
N26	-1.4560197880	-5.8638812815	0.1232183208
C27	2.3951307534	6.7711402622	0.0294225756
C28	-2.3951307534	-6.7711402622	0.0294225756
H29	2.2441886929	7.8412843536	0.0873990842
H30	-2.2441886929	-7.8412843536	0.0873990842
N31	3.6619339012	6.2374573538	-0.1577976626
N32	-3.6619339012	-6.2374573538	-0.1577976626
C33	4.9208713875	6.9482444331	-0.2994750714
C34	-4.9208713875	-6.9482444331	-0.2994750714
C35	-3.3242697001	1.6419586785	-0.0169922042
C36	3.3242697001	-1.6419586785	-0.0169922042
N37	-2.3940871222	2.6760330614	0.1521160120
N38	2.3940871222	-2.6760330614	0.1521160120
C39	2.7089764768	-4.0136334090	0.3189798238
C40	-2.7089764768	4.0136334090	0.3189798238
N41	-1.6707668699	4.8528106764	0.4702289585
N42	1.6707668699	-4.8528106764	0.4702289585
H43	-0.7129758868	4.5191953709	0.3880598107
H44	0.7129758868	-4.5191953709	0.3880598107
H45	1.8618052363	-5.8389017220	0.5205189355
H46	-1.8618052363	5.8389017220	0.5205189355
N47	-3.9545370790	4.4739887759	0.3409421926
N48	3.9545370790	-4.4739887759	0.3409421926
C49	-4.8710228128	3.4999190258	0.1831145976
C50	4.8710228128	-3.4999190258	0.1831145976
C51	-4.6639721619	2.1311705808	0.0086323017
C52	4.6639721619	-2.1311705808	0.0086323017
N53	-5.8638812815	1.4560197880	-0.1232183208
N54	5.8638812815	-1.4560197880	-0.1232183208
C55	-6.7711402622	2.3951307534	-0.0294225756
C56	6.7711402622	-2.3951307534	-0.0294225756
H57	-7.8412843536	2.2441886929	-0.0873990842
H58	7.8412843536	-2.2441886929	-0.0873990842
N59	-6.2374573538	3.6619339012	0.1577976626
N60	6.2374573538	-3.6619339012	0.1577976626
C61	-6.9482444331	4.9208713875	0.2994750714
C62	6.9482444331	-4.9208713875	0.2994750714
H63	-1.4051120101	2.4191492527	0.1296013883

H64	1.4051120101	-2.4191492527	0.1296013883
H65	-7.5552109225	5.1274632259	-0.5873227087
H66	-5.7089242951	-6.2027239513	-0.4146410979
H67	-6.2027239513	5.7089242951	0.4146410979
H68	-5.1274632259	-7.5552109225	0.5873227087
H69	6.2027239513	-5.7089242951	0.4146410979
H70	7.5947564858	-4.9074410476	1.1822656593
H71	4.9074410476	7.5947564858	-1.1822656593
H72	5.7089242951	6.2027239513	-0.4146410979
H73	-7.5947564858	4.9074410476	1.1822656593
H74	-4.9074410476	-7.5947564858	-1.1822656593
H75	5.1274632259	7.5552109225	0.5873227087
H76	7.5552109225	-5.1274632259	-0.5873227087

Single point energy: -2328.3682674

G4 (Hoogsteen bound, C_{4h} Symmetry)

O1	0.6818228098	2.3587058315	0.0000000000
O2	-2.3587058315	0.6818228098	0.0000000000
O3	2.3587058315	-0.6818228098	0.0000000000
O4	-0.6818228098	-2.3587058315	0.0000000000
C5	1.8018755226	2.8747905551	0.0000000000
C6	-1.8018755226	-2.8747905551	0.0000000000
N7	2.9573054603	2.0666204993	0.0000000000
N8	-2.9573054603	-2.0666204993	0.0000000000
H9	2.7843800019	1.0460208660	0.0000000000
H10	-2.7843800019	-1.0460208660	0.0000000000
C11	4.2507090819	2.5353689499	0.0000000000
C12	-4.2507090819	-2.5353689499	0.0000000000
N13	5.2476192777	1.6294934836	0.0000000000
N14	-5.2476192777	-1.6294934836	0.0000000000
H15	5.1382511278	0.6100730129	0.0000000000
H16	-5.1382511278	-0.6100730129	0.0000000000
H17	6.1782352015	2.0136201859	0.0000000000
H18	-6.1782352015	-2.0136201859	0.0000000000
N19	4.5685253294	3.8297235300	0.0000000000
N20	-4.5685253294	-3.8297235300	0.0000000000
C21	3.4860304894	4.6273110000	0.0000000000
C22	-3.4860304894	-4.6273110000	0.0000000000
C23	2.1416950829	4.2658077625	0.0000000000
C24	-2.1416950829	-4.2658077625	0.0000000000
N25	1.3318511666	5.3859316955	0.0000000000
N26	-1.3318511666	-5.3859316955	0.0000000000
C27	2.1657742512	6.3983601833	0.0000000000
C28	-2.1657742512	-6.3983601833	0.0000000000
H29	1.8875436034	7.4437257814	0.0000000000
H30	-1.8875436034	-7.4437257814	0.0000000000

N31	3.4908830052	6.0064005196	0.0000000000
N32	-3.4908830052	-6.0064005196	0.0000000000
C33	4.6711769795	6.8532125248	0.0000000000
C34	-4.6711769795	-6.8532125248	0.0000000000
C35	-2.8747905551	1.8018755226	0.0000000000
C36	2.8747905551	-1.8018755226	0.0000000000
N37	-2.0666204993	2.9573054603	0.0000000000
N38	2.0666204993	-2.9573054603	0.0000000000
C39	2.5353689499	-4.2507090819	0.0000000000
C40	-2.5353689499	4.2507090819	0.0000000000
N41	-1.6294934836	5.2476192777	0.0000000000
N42	1.6294934836	-5.2476192777	0.0000000000
H43	-0.6100730129	5.1382511278	0.0000000000
H44	0.6100730129	-5.1382511278	0.0000000000
H45	2.0136201859	-6.1782352015	0.0000000000
H46	-2.0136201859	6.1782352015	0.0000000000
N47	-3.8297235300	4.5685253294	0.0000000000
N48	3.8297235300	-4.5685253294	0.0000000000
C49	-4.6273110000	3.4860304894	0.0000000000
C50	4.6273110000	-3.4860304894	0.0000000000
C51	-4.2658077625	2.1416950829	0.0000000000
C52	4.2658077625	-2.1416950829	0.0000000000
N53	-5.3859316955	1.3318511666	0.0000000000
N54	5.3859316955	-1.3318511666	0.0000000000
C55	-6.3983601833	2.1657742512	0.0000000000
C56	6.3983601833	-2.1657742512	0.0000000000
H57	-7.4437257814	1.8875436034	0.0000000000
H58	7.4437257814	-1.8875436034	0.0000000000
N59	-6.0064005196	3.4908830052	0.0000000000
N60	6.0064005196	-3.4908830052	0.0000000000
C61	-6.8532125248	4.6711769795	0.0000000000
C62	6.8532125248	-4.6711769795	0.0000000000
H63	-1.0460208660	2.7843800019	0.0000000000
H64	1.0460208660	-2.7843800019	0.0000000000
H65	-7.4863712929	4.6973876286	-0.8921047286
H66	-5.5438256855	-6.1986142291	0.0000000000
H67	-6.1986142291	5.5438256855	0.0000000000
H68	-4.6973876286	-7.4863712929	0.8921047286
H69	6.1986142291	-5.5438256855	0.0000000000
H70	7.4863712929	-4.6973876286	0.8921047286
H71	4.6973876286	7.4863712929	-0.8921047286
H72	5.5438256855	6.1986142291	0.0000000000
H73	-7.4863712929	4.6973876286	0.8921047286
H74	-4.6973876286	-7.4863712929	-0.8921047286
H75	4.6973876286	7.4863712929	0.8921047286
H76	7.4863712929	-4.6973876286	-0.8921047286

Single point energy: -2328.3672469

G4 (Hoogsteen bound, C_i Symmetry)

O1	0.8368716397	2.2798253587	0.1986881627
O2	-2.3088504938	0.8748129111	-0.4575128044
O3	2.3088504938	-0.8748129111	0.4575128044
O4	-0.8368716397	-2.2798253587	-0.1986881627
C5	1.9926801952	2.7077471782	0.1561013410
C6	-1.9926801952	-2.7077471782	-0.1561013410
N7	3.0836010969	1.8233519383	0.2806676062
N8	-3.0836010969	-1.8233519383	-0.2806676062
H9	2.8344506664	0.8239677120	0.3822262715
H10	-2.8344506664	-0.8239677120	-0.3822262715
C11	4.4084007198	2.1919342613	0.2524188098
C12	-4.4084007198	-2.1919342613	-0.2524188098
N13	5.3332541438	1.2247435963	0.4197107138
N14	-5.3332541438	-1.2247435963	-0.4197107138
H15	5.1485461129	0.2170149723	0.3863822628
H16	-5.1485461129	-0.2170149723	-0.3863822628
H17	6.2872211864	1.5296689452	0.3111813369
H18	-6.2872211864	-1.5296689452	-0.3111813369
N19	4.8235591600	3.4471653792	0.0904679895
N20	-4.8235591600	-3.4471653792	-0.0904679895
C21	3.8048270266	4.3161020055	-0.0348639338
C22	-3.8048270266	-4.3161020055	0.0348639338
C23	2.4370147587	4.0586944788	-0.0124037214
C24	-2.4370147587	-4.0586944788	0.0124037214
N25	1.7150835816	5.2269506753	-0.1699768933
N26	-1.7150835816	-5.2269506753	0.1699768933
C27	2.6239571213	6.1653613988	-0.2884113585
C28	-2.6239571213	-6.1653613988	0.2884113585
H29	2.4263986064	7.2197169915	-0.4283231890
H30	-2.4263986064	-7.2197169915	0.4283231890
N31	3.9152061210	5.6785467171	-0.2165415033
N32	-3.9152061210	-5.6785467171	0.2165415033
C33	5.1572795866	6.4261702063	-0.3090157593
C34	-5.1572795866	-6.4261702063	0.3090157593
H35	5.2280025795	6.9473629626	-1.2685927187
H36	-5.2280025795	-6.9473629626	1.2685927187
H37	5.2365042429	7.1550309416	0.5033713117
H38	-5.2365042429	-7.1550309416	-0.5033713117
H39	5.9767451387	5.7106626018	-0.2284913585
H40	-5.9767451387	-5.7106626018	0.2284913585
C41	-2.7331645283	2.0149719009	-0.2541515318
C42	2.7331645283	-2.0149719009	0.2541515318
N43	-1.8361581264	3.0906388258	-0.0932478771

N44	1.8361581264	-3.0906388258	0.0932478771
C45	2.2011465658	-4.4010008590	-0.1137833845
C46	-2.2011465658	4.4010008590	0.1137833845
N47	-1.2164578387	5.3105307910	0.2539997873
N48	1.2164578387	-5.3105307910	-0.2539997873
H49	-0.2216735366	5.1414260734	0.0712809415
H50	0.2216735366	-5.1414260734	-0.0712809415
H51	1.5269355563	-6.2627840002	-0.3593316661
H52	-1.5269355563	6.2627840002	0.3593316661
N53	-3.4652809840	4.8134438842	0.1937367652
N54	3.4652809840	-4.8134438842	-0.1937367652
C55	-4.3457810921	3.8048399316	0.0669775981
C56	4.3457810921	-3.8048399316	-0.0669775981
C57	-4.0922633265	2.4529258477	-0.1479839520
C58	4.0922633265	-2.4529258477	0.1479839520
N59	-5.2727534425	1.7376628866	-0.2211451507
N60	5.2727534425	-1.7376628866	0.2211451507
C61	-6.2151966892	2.6348393135	-0.0560247908
C62	6.2151966892	-2.6348393135	0.0560247908
H63	-7.2788921479	2.4378516768	-0.0517685391
H64	7.2788921479	-2.4378516768	0.0517685391
N65	-5.7193478667	3.9126086311	0.1220242218
N66	5.7193478667	-3.9126086311	-0.1220242218
C67	-6.4683413229	5.1393066777	0.3331575343
C68	6.4683413229	-5.1393066777	-0.3331575343
H69	-7.1316319742	5.3422003452	-0.5132042040
H70	7.1316319742	-5.3422003452	0.5132042040
H71	-7.0623838206	5.0815433200	1.2504015095
H72	7.0623838206	-5.0815433200	-1.2504015095
H73	-5.7463224216	5.9518818191	0.4254618540
H74	5.7463224216	-5.9518818191	-0.4254618540
H75	-0.8339505893	2.8331283244	-0.0633730224
H76	0.8339505893	-2.8331283244	0.0633730224

Single point energy: -2328.366841

(G4-H⁺)₁

O1	2.2923907714	0.5886970805	0.0000000000
O2	-0.0358887943	2.0233846417	0.0000000000
O3	0.4577385296	-2.2328532607	0.0000000000
O4	-2.4103826837	-0.3926253450	0.0000000000
C5	3.2921123890	-0.1848375837	0.0000000000
C6	-3.4415702233	0.2871185110	0.0000000000
N7	3.1190774535	-1.5581324365	0.0000000000
N8	-3.3372352089	1.6960332782	0.0000000000
H9	2.1303048500	-1.9027768811	0.0000000000
H10	-2.3814423766	2.0395316335	0.0000000000

C11	4.1631617092	-2.4703856922	0.0000000000
C12	-4.3945479603	2.5844189310	0.0000000000
N13	3.8614611449	-3.7721356342	0.0000000000
N14	-4.0837072884	3.8959437662	0.0000000000
H15	2.9128827046	-4.1893906802	0.0000000000
H16	-3.1180018341	4.2215859297	0.0000000000
H17	4.6568871562	-4.3921361062	0.0000000000
H18	-4.8539593419	4.5440507360	0.0000000000
N19	5.4489505751	-2.1119646100	0.0000000000
N20	-5.6598878279	2.2038469313	0.0000000000
C21	5.6279141098	-0.7900709379	0.0000000000
C22	-5.8024066185	0.8634265844	0.0000000000
C23	4.6530462823	0.2120385928	0.0000000000
C24	-4.8102755149	-0.1178575179	0.0000000000
N25	5.2508170222	1.4640106828	0.0000000000
N26	-5.3741932753	-1.3782691728	0.0000000000
C27	6.5402269220	1.2155632418	0.0000000000
C28	-6.6680154572	-1.1630989867	0.0000000000
H29	7.3215409553	1.9637890612	0.0000000000
H30	-7.4322700191	-1.9282862883	0.0000000000
N31	6.8357888319	-0.1292459131	0.0000000000
N32	-6.9934494204	0.1783263945	0.0000000000
C33	8.1527252236	-0.7559319585	0.0000000000
C34	-8.3234658311	0.7729981325	0.0000000000
C35	0.6426608241	3.1509683281	0.0000000000
C36	-0.2540395966	-3.2523932183	0.0000000000
N37	2.0014561643	3.1274911636	0.0000000000
N38	-1.6522584814	-3.1268424480	0.0000000000
C39	-2.5443277915	-4.1804559727	0.0000000000
C40	2.7866869848	4.2687225331	0.0000000000
N41	4.1078646543	4.0877809747	0.0000000000
N42	-3.8568280053	-3.8918929477	0.0000000000
H43	4.5444017385	3.1452938437	0.0000000000
H44	-4.2674726738	-2.9524613737	0.0000000000
H45	-4.4741555829	-4.6880715052	0.0000000000
H46	4.6754603741	4.9213438988	0.0000000000
N47	2.2676922999	5.4963805269	0.0000000000
N48	-2.1707377254	-5.4571267296	0.0000000000
C49	0.9372712143	5.5101297265	0.0000000000
C50	-0.8379548552	-5.6092803884	0.0000000000
C51	0.0485264928	4.4112982143	0.0000000000
C52	0.1473414884	-4.6216330113	0.0000000000
N53	-1.2642552895	4.8547603579	0.0000000000
N54	1.4049244501	-5.1957709285	0.0000000000
C55	-1.1636973440	6.1605539582	0.0000000000
C56	1.1845171750	-6.4894621237	0.0000000000

H57	-1.9989730937	6.8485043899	0.0000000000
H58	1.9465563428	-7.2570195357	0.0000000000
N59	0.1374419823	6.6220074652	0.0000000000
N60	-0.1568796180	-6.8064797364	0.0000000000
C61	0.5952305542	8.0090182820	0.0000000000
C62	-0.7598791713	-8.1321558161	0.0000000000
H63	2.4181212867	2.1448057066	0.0000000000
H64	-2.0040415990	-2.1565914473	0.0000000000
H65	0.2393299299	8.5273228915	-0.8935333588
H66	-8.2008528905	1.8564711547	0.0000000000
H67	1.6853245081	7.9967298028	0.0000000000
H68	-8.8789829302	0.4732467205	0.8925399035
H69	-1.8423395468	-8.0004759093	0.0000000000
H70	-0.4648900282	-8.6906214909	0.8925516585
H71	8.7147222255	-0.4704926621	-0.8930356654
H72	8.0017734078	-1.8357984910	0.0000000000
H73	0.2393299299	8.5273228915	0.8935333588
H74	-8.8789829302	0.4732467205	-0.8925399035
H75	8.7147222255	-0.4704926621	0.8930356654
H76	-0.4648900282	-8.6906214909	-0.8925516585
H77	0.5446135234	1.2192717933	0.0000000000

Single point energy: -2328.7797472

(G4-H⁺)₂

C1	-0.1281136777	3.7537512532	-0.2275652485
C2	0.5072974823	6.0500422107	-0.6487406811
C3	0.8909115083	4.7305567793	-0.3913352909
O4	0.0199975813	2.5282482122	-0.0179087956
N5	2.2671642920	4.6228206204	-0.3602639405
C6	7.3401066623	-1.4229598975	1.7487149394
H7	7.3699229130	-0.3588685268	1.9848538900
N8	1.6776860447	6.7533080878	-0.7799235044
C9	2.6958267082	5.8406898108	-0.5934546375
N10	-2.9915055680	5.9849879237	-0.6183030854
N11	-1.4066616118	4.3081710553	-0.3194838717
H12	7.4164360029	-1.9998639416	2.6743579940
H13	-3.6577332109	5.2843197098	-0.9100733181
H14	8.1813853807	-1.6708182590	1.0957805841
H15	-2.2030291892	3.6909117669	-0.0633847553
H16	-5.4444197792	-2.9890706626	0.7291721873
N17	-0.7415706966	6.5457166153	-0.7710464818
C18	-1.6699464043	5.6312643302	-0.5869721901
H19	-2.2338657332	-1.6958539551	-0.1426674993
H20	6.1935885970	-3.8072784200	0.7110181032
N21	2.9923817765	0.5883270988	0.0525580571
C22	4.0561450332	1.2014685354	0.6854240815

N23	3.9446331216	2.5234576913	0.9395936118
N24	5.1428088814	0.5511629180	1.0706048217
C25	5.0981841351	-0.7662431066	0.7907959205
C26	4.0876014814	-1.4820701206	0.1518022396
C27	2.9158065206	-0.7852894329	-0.2724176918
O28	1.9140877101	-1.2267394760	-0.8441154979
N29	4.4263450682	-2.8194595660	0.0469611290
C30	5.6097120546	-2.9024880302	0.6086899122
N31	6.0741942608	-1.6911567939	1.0796781789
H32	2.1529313159	1.1281018806	-0.1489987408
H33	4.7724107274	2.9446970677	1.3326477067
H34	3.2952819996	3.1348439200	0.4377234261
H35	-3.1613762878	6.9193642626	-0.9631522881
N36	-5.2416362904	-0.5402941532	0.8111589168
O37	-1.4267995356	0.5276695417	-0.4131386814
H38	-3.7710145412	-6.7631222447	-0.3330891094
C39	-4.8569487013	0.7335371670	0.7720742904
C40	-1.4478886162	-8.3309441944	-0.7927795620
C41	-4.8154833923	2.9343218956	0.9170100628
N42	-5.6107185063	1.8291726569	1.1259019033
H43	3.7341231519	6.1402963845	-0.6427171835
H44	-7.3369358047	0.7726698651	1.5558653264
H45	-1.9899391544	-8.6903992421	-1.6715385951
H46	-0.3804063365	-8.5023717896	-0.9343421317
C47	1.8016342499	8.1805320429	-1.0561601121
H48	-6.9923835224	2.0939397819	2.6975435556
C49	-2.6426331327	0.3248183109	-0.0200742377
N50	-4.5332130924	-2.7060131527	0.4032411023
H51	-1.7863450715	-8.8762062412	0.0923823635
H52	-7.6169562360	2.4615973376	1.0647354184
H53	-3.8518062373	-3.4336133792	0.1333396740
H54	3.1063985397	-5.9762459736	-1.0273493819
N55	0.8048387889	-3.7721822205	-0.6155261418
C56	1.3681604528	-5.0165114177	-0.7944502022
N57	2.7032221819	-5.0538136532	-0.9725715069
N58	0.6596473201	-6.1423667011	-0.8157999315
C59	-0.6570553231	-5.9369060670	-0.6424492254
C60	-1.3222581668	-4.7288873571	-0.4288803942
C61	-0.5500757609	-3.5387724548	-0.4040572893
O62	-0.9336744588	-2.3666913706	-0.2241639544
N63	-2.6825364624	-4.9313766782	-0.2745538110
C64	-2.8315380314	-6.2307366215	-0.3958839839
N65	-1.6434301917	-6.8975277335	-0.6187890562
H66	1.3735315261	-2.9069084263	-0.6969266514
H67	3.3038853058	-4.2677498917	-0.6955474698
N68	-3.6222036003	2.6412964173	0.4553439901

N69	-3.0344843077	-0.9788057228	0.0169547512
C70	-3.6167928901	1.2575573388	0.3631221538
H71	-5.1714705175	3.9337300684	1.1297998503
C72	-4.2869103151	-1.3911362278	0.4153444397
C73	-6.9742622105	1.7966628389	1.6458798922
H74	0.7979199218	8.5795018199	-1.2027471005
H75	2.3912491739	8.3426325773	-1.9617206724
H76	2.2742047201	8.6947084589	-0.2151007037
H77	-0.9926998540	1.4402435778	-0.2271317145

Single point energy: -2328.7769269

(G4-2H⁺)₁

C1	-2.0709997365	3.1770986655	-0.4916127498
C2	-2.8651152729	5.4344369633	-0.8067634986
C3	-1.7994507386	4.5634277307	-0.5406208759
O4	-1.2416486092	2.2419587989	-0.2859857151
N5	-0.6284954416	5.2781538385	-0.3663822104
C6	6.3060005408	2.0153372588	2.2209406269
H7	5.9848508531	3.0502854240	2.3358674274
N8	-2.3228018641	6.6932276965	-0.7995001227
C9	-0.9828769409	6.5332543545	-0.5273289328
N10	-5.6573888846	3.3555103277	-1.0871783443
N11	-3.4144098155	2.8843400974	-0.6868418794
H12	6.4198793618	1.5596526277	3.2074026091
H13	-5.7958579988	2.4138256705	-1.4234840972
H14	7.2583375231	1.9874383427	1.6875316479
H15	-3.7236696150	1.9246928034	-0.4300141571
H16	-2.3491091403	-5.1627215896	1.4144480864
N17	-4.1514378604	5.1199428980	-1.0373648717
C18	-4.3873562450	3.8266607003	-0.9527376337
H19	-0.6680085195	-2.4410148013	-0.1119527434
H20	6.1912507498	-0.6095234372	1.1405719955
N21	1.6599025131	2.2835476845	0.1337530077
C22	2.3833050638	3.2682199129	0.7953075274
N23	1.8054167181	4.4607925516	0.9339344413
N24	3.5995070213	3.0466561915	1.2943328566
C25	4.0603657116	1.8188443753	1.0715438256
C26	3.4235408828	0.7707830053	0.3769291268
C27	2.1389456101	1.0220365667	-0.0986311142
O28	1.3389418168	0.2316024193	-0.7421457833
N29	4.2464014795	-0.3429856392	0.3229639721
C30	5.3264838303	0.0194397591	0.9742464315
N31	5.2773879746	1.3123471921	1.4513088061
H32	0.6680085195	2.4410148013	-0.1119527434
H33	2.3491091403	5.1627215896	1.4144480864
H34	0.9308274603	4.7292609275	0.4503103453

H35	-6.3350327533	4.0403082147	-1.3928826454
N36	-3.5995070213	-3.0466561915	1.2943328566
O37	-1.3389418168	-0.2316024193	-0.7421457833
H38	0.3179622522	-7.3837105725	-0.4573126527
C39	-4.0603657116	-1.8188443753	1.0715438256
C40	3.0387579107	-7.9490598284	-1.0261846596
C41	-5.3264838303	-0.0194397591	0.9742464315
N42	-5.2773879746	-1.3123471921	1.4513088061
H43	-0.3179622522	7.3837105725	-0.4573126527
H44	-5.9848508531	-3.0502854240	2.3358674274
H45	2.6209852504	-8.4712681906	-1.8896567313
H46	4.0830130481	-7.7062416030	-1.2205951261
C47	-3.0387579107	7.9490598284	-1.0261846596
H48	-6.4198793618	-1.5596526277	3.2074026091
C49	-2.1389456101	-1.0220365667	-0.0986311142
N50	-1.8054167181	-4.4607925516	0.9339344413
H51	2.9735923178	-8.5864562389	-0.1414410861
H52	-7.2583375231	-1.9874383427	1.6875316479
H53	-0.9308274603	-4.7292609275	0.4503103453
H54	6.3350327533	-4.0403082147	-1.3928826454
N55	3.4144098155	-2.8843400974	-0.6868418794
C56	4.3873562450	-3.8266607003	-0.9527376337
N57	5.6573888846	-3.3555103277	-1.0871783443
N58	4.1514378604	-5.1199428980	-1.0373648717
C59	2.8651152729	-5.4344369633	-0.8067634986
C60	1.7994507386	-4.5634277307	-0.5406208759
C61	2.0709997365	-3.1770986655	-0.4916127498
O62	1.2416486092	-2.2419587989	-0.2859857151
N63	0.6284954416	-5.2781538385	-0.3663822104
C64	0.9828769409	-6.5332543545	-0.5273289328
N65	2.3228018641	-6.6932276965	-0.7995001227
H66	3.7236696150	-1.9246928034	-0.4300141571
H67	5.7958579988	-2.4138256705	-1.4234840972
N68	-4.2464014795	0.3429856392	0.3229639721
N69	-1.6599025131	-2.2835476845	0.1337530077
C70	-3.4235408828	-0.7707830053	0.3769291268
H71	-6.1912507498	0.6095234372	1.1405719955
C72	-2.3833050638	-3.2682199129	0.7953075274
C73	-6.3060005408	-2.0153372588	2.2209406269
H74	-4.0830130481	7.7062416030	-1.2205951261
H75	-2.6209852504	8.4712681906	-1.8896567313
H76	-2.9735923178	8.5864562389	-0.1414410861
H77	1.4565436875	-0.7815497732	-0.5799485668
H78	-1.4565436875	0.7815497732	-0.5799485668

Single point energy: -2329.1101789

(G4-2H⁺)₂

O1	-0.4169469163	2.3032375369	0.0000000000
O2	-2.1478506238	0.3179424616	0.0000000000
O3	2.1478506238	-0.3179424616	0.0000000000
O4	0.4169469163	-2.3032375369	0.0000000000
C5	0.4385543509	3.2295200790	0.0000000000
C6	-0.4385543509	-3.2295200790	0.0000000000
N7	1.7964700863	2.9211433686	0.0000000000
N8	-1.7964700863	-2.9211433686	0.0000000000
H9	2.0224812183	1.9290515337	0.0000000000
H10	-2.0224812183	-1.9290515337	0.0000000000
C11	2.8219417214	3.8603304186	0.0000000000
C12	-2.8219417214	-3.8603304186	0.0000000000
N13	4.0808958091	3.4035368578	0.0000000000
N14	-4.0808958091	-3.4035368578	0.0000000000
H15	4.3442373854	2.4131478207	0.0000000000
H16	-4.3442373854	-2.4131478207	0.0000000000
H17	4.8024821942	4.1085571386	0.0000000000
H18	-4.8024821942	-4.1085571386	0.0000000000
N19	2.5949755922	5.1647995298	0.0000000000
N20	-2.5949755922	-5.1647995298	0.0000000000
C21	1.2954884595	5.4844129559	0.0000000000
C22	-1.2954884595	-5.4844129559	0.0000000000
C23	0.1923529093	4.6197945960	0.0000000000
C24	-0.1923529093	-4.6197945960	0.0000000000
N25	-0.9888536339	5.3465964290	0.0000000000
N26	0.9888536339	-5.3465964290	0.0000000000
C27	-0.5989293904	6.6012058864	0.0000000000
C28	0.5989293904	-6.6012058864	0.0000000000
H29	-1.2568989112	7.4600123966	0.0000000000
H30	1.2568989112	-7.4600123966	0.0000000000
N31	0.7700656795	6.7510208813	0.0000000000
N32	-0.7700656795	-6.7510208813	0.0000000000
C33	1.5284165477	8.0017756026	0.0000000000
C34	-1.5284165477	-8.0017756026	0.0000000000
C35	-3.2233403849	1.0869649854	0.0000000000
C36	3.2233403849	-1.0869649854	0.0000000000
N37	-3.0722531846	2.4401543041	0.0000000000
N38	3.0722531846	-2.4401543041	0.0000000000
C39	4.1348429314	-3.3329433383	0.0000000000
C40	-4.1348429314	3.3329433383	0.0000000000
N41	-3.8220914038	4.6281236334	0.0000000000
N42	3.8220914038	-4.6281236334	0.0000000000
H43	-2.8401498513	4.9461481207	0.0000000000
H44	2.8401498513	-4.9461481207	0.0000000000
H45	4.5871251714	-5.2861242004	0.0000000000

H46	-4.5871251714	5.2861242004	0.0000000000
N47	-5.4019826516	2.9252351977	0.0000000000
N48	5.4019826516	-2.9252351977	0.0000000000
C49	-5.5424317768	1.6025299581	0.0000000000
C50	5.5424317768	-1.6025299581	0.0000000000
C51	-4.5257867417	0.6153539402	0.0000000000
C52	4.5257867417	-0.6153539402	0.0000000000
N53	-5.0834729031	-0.6517525419	0.0000000000
N54	5.0834729031	0.6517525419	0.0000000000
C55	-6.3756202721	-0.4330052317	0.0000000000
C56	6.3756202721	0.4330052317	0.0000000000
H57	-7.1359858275	-1.2030134700	0.0000000000
H58	7.1359858275	1.2030134700	0.0000000000
N59	-6.7186006960	0.9041706113	0.0000000000
N60	6.7186006960	-0.9041706113	0.0000000000
C61	-8.0665429096	1.4769395304	0.0000000000
C62	8.0665429096	-1.4769395304	0.0000000000
H63	-2.0851764571	2.7691797413	0.0000000000
H64	2.0851764571	-2.7691797413	0.0000000000
H65	-8.6091756579	1.1623034838	-0.8939897592
H66	-2.5880061905	-7.7465596400	0.0000000000
H67	-7.9660854353	2.5620930899	0.0000000000
H68	-1.2966040654	-8.5856667168	0.8935825823
H69	7.9660854353	-2.5620930899	0.0000000000
H70	8.6091756579	-1.1623034838	0.8939897592
H71	1.2966040654	8.5856667168	-0.8935825823
H72	2.5880061905	7.7465596400	0.0000000000
H73	-8.6091756579	1.1623034838	0.8939897592
H74	-1.2966040654	-8.5856667168	-0.8935825823
H75	1.2966040654	8.5856667168	0.8935825823
H76	8.6091756579	-1.1623034838	-0.8939897592
H77	-1.3186180086	0.8668928954	0.0000000000
H78	1.3186180086	-0.8668928954	0.0000000000

Single point energy: -2329.1053215

(G4-2H⁺)₃

C1	0.6522217847	3.1955179068	-0.0877408768
C2	0.7642832710	5.6101692915	-0.0062076152
C3	1.4015786716	4.3732957240	0.1454041562
O4	1.0178548801	1.9965866701	-0.0403652897
N5	2.7212532353	4.5537691084	0.5169330774
C6	7.6818273419	-1.7393505000	0.7694068089
H7	7.7793328164	-0.8104650759	1.3312499320
N8	1.7229498016	6.5516238190	0.2749575484
C9	2.8716233859	5.8572040630	0.5826649454
N10	-2.5119710424	4.8239718731	-0.8925244936

N11	-0.6756570769	3.4785409249	-0.4157836637
H12	7.7647705075	-2.5871441213	1.4525583668
H13	-3.1271699707	4.0087983034	-0.8692173533
H14	8.4693776039	-1.7912353527	0.0145351504
H15	-1.2538259793	2.6598738539	-0.5854442672
H16	-5.8691620790	-2.9954758959	1.2004418402
N17	-0.5124742739	5.8503164600	-0.3420373481
C18	-1.2175718754	4.7484779071	-0.5383992907
H19	-2.6822806884	-1.6416001713	0.4142503921
H20	6.3151470536	-3.6769902224	-0.7914198794
N21	3.3461669462	0.8636976817	-0.0815759074
C22	4.4671020292	1.2378900067	0.6532058599
N23	4.4440668092	2.4268027394	1.2489097610
N24	5.5461858055	0.4507875305	0.7817734830
C25	5.4493171640	-0.7144675337	0.1618825000
C26	4.3612835835	-1.1799856151	-0.6098266284
C27	3.2924784313	-0.3181754689	-0.7319880112
O28	2.1724921712	-0.5734250789	-1.4269893972
N29	4.5945855364	-2.4612723678	-1.0822442285
C30	5.7923648656	-2.7441494702	-0.6237660142
N31	6.3640761855	-1.7354197965	0.1285272666
H32	2.4416433946	1.4627489398	-0.0679780718
H33	5.2836242585	2.6706328012	1.7555305229
H34	3.7740562428	3.1860243761	1.0018927018
H35	-2.9078253510	5.7508013938	-0.9300317595
N36	-5.8310156457	-0.5934246526	0.5448571312
O37	-1.9319613447	0.5843018110	-0.3360071581
H38	-3.6792937538	-6.3607378049	0.9659657785
C39	-5.5216769727	0.6406114446	0.1535829762
C40	-1.4274385507	-7.9386864162	0.2703858995
C41	-5.6212389252	2.7555267354	-0.4407035192
N42	-6.3876012575	1.6833595314	-0.0267537818
H43	3.7856131248	6.3691239707	0.8514738250
H44	-8.1122073936	0.6315102399	0.4458833143
H45	-2.0915843098	-8.3773459284	-0.4778172739
H46	-0.3917044533	-8.1171199609	-0.0172287714
C47	1.5399921612	8.0017630573	0.2527208574
H48	-8.1146429493	2.3238940714	0.9995483683
C49	-3.1862146259	0.2695412460	-0.0692075011
N50	-4.9294529129	-2.6822414207	1.0072115469
H51	-1.6168213101	-8.3942753706	1.2448468755
H52	-8.3540904074	1.9454111248	-0.7314308590
H53	-4.1497856969	-3.3551470289	0.9633213396
H54	2.8939435558	-5.6182257197	-1.1086992653
N55	0.6972497412	-3.3613867579	-0.3534127163
C56	1.2504249451	-4.6218659795	-0.5465079834

N57	2.5217691435	-4.6888985090	-0.9816342308
N58	0.5689589710	-5.7335977033	-0.3371313159
C59	-0.6960388126	-5.5263537849	0.0602453506
C60	-1.3484561995	-4.3032899164	0.2675334786
C61	-0.6193093801	-3.1131047437	0.0498464743
O62	-1.0143588506	-1.9271493277	0.1779893248
N63	-2.6591160588	-4.5156190438	0.6627226321
C64	-2.7806284167	-5.8230803511	0.6945031007
N65	-1.6280326808	-6.4909838390	0.3416912158
H66	1.2502633948	-2.5268345557	-0.5172517482
H67	3.1501616553	-3.8934594451	-1.0888876441
N68	-4.3420148260	2.4902044483	-0.5421326022
N69	-3.4941165567	-0.9930191294	0.3375625744
C70	-4.2446391637	1.1587403477	-0.1734025749
H71	-6.0756957258	3.7143551167	-0.6537985576
C72	-4.7852897455	-1.4110037010	0.6291381907
C73	-7.8362833286	1.6526560877	0.1840862235
H74	0.4969681719	8.1995411131	0.0067533440
H75	2.1827208561	8.4556718391	-0.5050652370
H76	1.7677860060	8.4267663953	1.2326674658
H77	-1.3161286180	-0.1787260394	-0.2129616245
H78	2.3858720712	-1.2095920090	-2.1295880924

Single point energy: -2329.0853086

(G4-3H⁺)₁

C1	-0.3907565669	3.1537385907	-0.0581409629
C2	0.4704544154	5.0117054309	-1.2655731648
C3	0.7200088267	3.8898093237	-0.4438003379
O4	-0.4254769912	2.0868842595	0.7149294920
N5	2.0790502216	3.7735323890	-0.1869708518
C6	7.0924728819	-1.8794096236	1.8860661600
H7	7.4247261369	-0.9790741281	2.4013686128
N8	1.7002605515	5.5660191630	-1.5049511807
C9	2.6143203445	4.7848485943	-0.8391807602
N10	-2.9774731514	5.0084717092	-1.7246455733
N11	-1.5981790134	3.5881350756	-0.5028743918
H12	7.0909184238	-2.7189862007	2.5826159253
H13	-3.7543856785	4.3779235187	-1.5999502810
H14	7.7616074306	-2.0879359645	1.0484689092
H15	-2.4512536191	3.0291261233	-0.2087240764
H16	-5.6614363608	-3.2504819528	2.1097269781
N17	-0.7055648071	5.4334708697	-1.7202490776
C18	-1.7353988138	4.6921285690	-1.3271267529
H19	-2.8795532509	-2.3795028216	0.1213574672
H20	5.1182994656	-3.6285310422	0.8423129084
N21	3.4405232653	1.5736969403	0.9764217178

C22	4.7082856978	1.7479863919	1.5097559660
N23	5.0777042752	3.0076449141	1.8049171528
N24	5.5522279283	0.7456919711	1.7068945451
C25	5.0833498936	-0.4398372302	1.3249939126
C26	3.8061227311	-0.7271876003	0.7825241866
C27	2.9424968424	0.3474311660	0.6382061775
O28	1.6939157451	0.3460041446	0.2126510835
N29	3.6947816606	-2.0817728967	0.5174277532
C30	4.8490643698	-2.5814092708	0.8982215572
N31	5.7262955446	-1.6439388530	1.3965355451
H32	2.9017364592	2.4177849360	0.6488328038
H33	5.9817041872	3.1263959736	2.2431799995
H34	4.3958088921	3.7399249826	1.9350673795
H35	-3.0820922839	5.7844473539	-2.3638565080
N36	-5.4332967673	-0.8393820769	1.5669007557
O37	-1.8882934132	-0.1202658967	-0.4879444400
H38	-3.6349640053	-5.1160531868	-1.0313572224
C39	-5.0618761948	0.3787100714	1.1731650728
C40	-1.8032411972	-7.0981091477	-1.9028231062
C41	-4.9538906075	2.5497515446	0.8748006539
N42	-5.7309368494	1.5505919958	1.4056918688
H43	3.6727662827	5.0084597580	-0.8757613471
H44	-7.1842905885	0.8224014833	2.7094751598
H45	-2.5715210064	-7.1168658388	-2.6773238103
H46	-0.8566903940	-7.4390233878	-2.3204372595
C47	1.9737977701	6.7758091251	-2.2937094122
H48	-7.0258211693	2.5965487612	2.6859096028
C49	-3.0114421953	-0.2959879094	0.1594992875
N50	-4.8348416590	-3.0732647744	1.5553019849
H51	-2.0902176149	-7.7497051074	-1.0745786129
H52	-7.8329592160	1.7490891303	1.3335050773
H53	-4.1079833161	-3.7721179593	1.5515646454
H54	3.1916074331	-5.9712316982	-1.9440615584
N55	1.5610604913	-3.4166370329	-0.8316733367
C56	1.7707375590	-4.6938092969	-1.3262384045
N57	3.0611414038	-5.0638090666	-1.5152676687
N58	0.7958570865	-5.5458970384	-1.5776926002
C59	-0.4182200913	-5.0657054871	-1.2839379481
C60	-0.7385554343	-3.7896162086	-0.7942121379
C61	0.3152748588	-2.8812401490	-0.5750139815
O62	0.2079399440	-1.6708032810	-0.1730939444
N63	-2.1091126354	-3.6803588438	-0.6263843928
C64	-2.5871372689	-4.8459665596	-1.0164254881
N65	-1.6149829467	-5.7217371706	-1.4250400401
H66	2.3751122510	-2.8936232835	-0.4480079874
H67	3.7537426578	-4.3645960537	-1.7398455581

N68	-3.8425954754	2.1193947391	0.3142948483
N69	-3.4024618709	-1.5475544308	0.5378235632
C70	-3.8839536729	0.7417719049	0.4844284403
H71	-5.2548935603	3.5872354780	0.9426378027
C72	-4.5748901047	-1.7909194061	1.2364869326
C73	-7.0314510588	1.6938873451	2.0736234604
H74	1.1209175309	6.9521861257	-2.9481738043
H75	2.8698489662	6.6206065941	-2.8959196932
H76	2.1099514049	7.6349626815	-1.6332529892
H77	-1.2035306720	-0.8519790124	-0.3865134563
H78	0.4310809993	1.6100343233	0.7093644147
H79	1.2559330808	-0.5763656499	0.0405106391

Single point energy: -2329.3248842

(G4-3H⁺)₂

C1	-0.3102021499	3.1974891214	-0.1001024476
C2	0.4431914589	5.1807389407	-1.1773586967
C3	0.7497533377	4.0356034402	-0.4075508750
O4	-0.1752270984	2.1113398467	0.6286725968
N5	2.1131466578	3.9699160789	-0.1645621739
C6	6.9215310022	-1.8912142025	2.1512480927
H7	7.2834604206	-0.9256428038	2.5031405299
N8	1.6385469120	5.8131951875	-1.3807839993
C9	2.5937521231	5.0411194653	-0.7582368562
N10	-2.9844381360	4.9602876184	-1.7538485695
N11	-1.5373607297	3.5662663864	-0.5717982277
H12	6.7714503353	-2.5567018746	3.0034725979
H13	-3.7046825414	4.2551488131	-1.7369540116
H14	7.6490406111	-2.3231195466	1.4613522232
H15	-2.3711307182	3.0301649237	-0.2156750247
H16	-5.7719079745	-3.2904910694	1.9369974093
N17	-0.7485720282	5.5383821678	-1.6543606798
C18	-1.7297617585	4.7060110459	-1.3419208276
H19	-2.8136357580	-2.4246129154	0.2446415362
H20	5.1131024004	-3.6625363034	0.8731721803
N21	3.4524035525	1.5403955841	0.6461815840
C22	4.6258765056	1.7276867940	1.3584263996
N23	4.9319242200	2.9921089897	1.6992986414
N24	5.4356466119	0.7326115846	1.6901209742
C25	5.0187023022	-0.4637064398	1.2773334287
C26	3.8341715367	-0.7616354517	0.5675690459
C27	3.0093004245	0.3113514957	0.2541485349
O28	1.8691324239	0.2956433051	-0.3906193431
N29	3.7526590401	-2.1223610108	0.3159128381
C30	4.8410774427	-2.6148993144	0.8659751480
N31	5.6443610713	-1.6668663289	1.4595588064

H32	2.8950998283	2.3803320330	0.3704702100
H33	5.7511110335	3.1306008023	2.2750735152
H34	4.2395920609	3.7251452491	1.6658373741
H35	-3.1204832376	5.7650318464	-2.3508132444
N36	-5.4469434467	-0.8698084622	1.5303322806
O37	-1.6714802009	-0.1162758590	-0.0517419043
H38	-3.6928776418	-5.1481267524	-0.8555978108
C39	-5.0246914184	0.3545191771	1.2210057144
C40	-1.9177451587	-7.1545288879	-1.7892926481
C41	-4.8550343937	2.5297648238	0.9771533946
N42	-5.6958759563	1.5330925873	1.4095858162
H43	3.6398253926	5.3183286533	-0.7885031263
H44	-7.3176144745	0.7686571447	2.4697754944
H45	-2.7597729979	-7.1787964046	-2.4825043859
H46	-1.0145219985	-7.4847152490	-2.3010659793
C47	1.8510449348	7.0699186349	-2.1125194730
H48	-7.0748285787	2.5239365937	2.6490266128
C49	-2.8858542004	-0.3234925286	0.4141920395
N50	-4.8912855223	-3.1140577456	1.4716165751
H51	-2.1132762953	-7.8108455811	-0.9383156876
H52	-7.7650706418	1.8622286613	1.1365066556
H53	-4.1720585835	-3.8174440264	1.5475165744
H54	3.0939940735	-6.0676512730	-2.0534680398
N55	1.5237302496	-3.4955808370	-0.8835777359
C56	1.7026215972	-4.7777152443	-1.3787762287
N57	2.9736219198	-5.1580848320	-1.6279954105
N58	0.7078305183	-5.6244474015	-1.5821462863
C59	-0.4868252502	-5.1336408339	-1.2393269612
C60	-0.7749587229	-3.8533242263	-0.7403129523
C61	0.2922097991	-2.9534983695	-0.5801490375
O62	0.2268808148	-1.7346710609	-0.1906961366
N63	-2.1359699048	-3.7280890121	-0.5169361524
C64	-2.6423545749	-4.8898407619	-0.8831873138
N65	-1.6971143833	-5.7766492728	-1.3289429349
H66	2.3608379641	-2.9635835112	-0.5600287418
H67	3.6943772862	-4.4723673245	-1.7957759744
N68	-3.6972022255	2.0920482463	0.5259007493
N69	-3.3323942210	-1.5831095738	0.6721528383
C70	-3.7756020505	0.7143821419	0.6709349099
H71	-5.1496572339	3.5703664527	1.0243771133
C72	-4.5766623212	-1.8251966700	1.2399428268
C73	-7.0552039055	1.6884058873	1.9482129296
H74	0.9558269304	7.2729433135	-2.6992229887
H75	2.7079077825	6.9633706694	-2.7792119767
H76	2.0212699907	7.8900831272	-1.4116675831
H77	-0.9965516249	-0.9190619615	-0.1003470443

H78	-0.8495027634	1.4186820886	0.4436033256
H79	1.4095505515	-0.5962290392	-0.3762455123

Single point energy: -2329.3242993

(G4-4H⁺)₁

C1	1.7609170235	2.7094192467	-0.3304720363
C2	3.7331156647	3.8345642854	-0.9983675930
C3	3.1212849058	2.6375261653	-0.5352745171
O4	0.9551342358	1.7139808192	0.0650369582
N5	4.0671756682	1.6235887237	-0.4274311256
C6	4.4375750457	-6.1170170417	1.6275215571
H7	5.3165482481	-5.6414364782	2.0612089122
N8	5.0520270140	3.5245312889	-1.1690412918
C9	5.1860666066	2.2024139397	-0.8181741362
N10	1.1340096062	6.1351958019	-1.2289380343
N11	1.1419075035	3.9005256388	-0.5451160005
H12	3.9372254962	-6.7211142211	2.3853456108
H13	0.1290782861	6.1386399458	-1.3154211340
H14	4.7376730326	-6.7397379280	0.7822496301
H15	0.1394251236	3.9807295003	-0.2534936982
H16	-6.9323115464	1.6396378858	1.5971118868
N17	3.1396460819	4.9927033655	-1.2485011402
C18	1.8324313384	5.0122058636	-1.0189884461
H19	-3.9807295003	0.1394251236	0.2534936982
H20	1.7092636601	-6.1482373668	0.8821317489
N21	3.9005256388	-1.1419075035	0.5451160005
C22	5.0122058636	-1.8324313384	1.0189884461
N23	6.1351958019	-1.1340096062	1.2289380343
N24	4.9927033655	-3.1396460819	1.2485011402
C25	3.8345642854	-3.7331156647	0.9983675930
C26	2.6375261653	-3.1212849058	0.5352745171
C27	2.7094192467	-1.7609170235	0.3304720363
O28	1.7139808192	-0.9551342358	-0.0650369582
N29	1.6235887237	-4.0671756682	0.4274311256
C30	2.2024139397	-5.1860666066	0.8181741362
N31	3.5245312889	-5.0520270140	1.1690412918
H32	3.9807295003	-0.1394251236	0.2534936982
H33	6.9323115464	-1.6396378858	1.5971118868
H34	6.1386399458	-0.1290782861	1.3154211340
H35	1.6396378858	6.9323115464	-1.5971118868
N36	-4.9927033655	3.1396460819	1.2485011402
O37	-1.7139808192	0.9551342358	-0.0650369582
H38	-6.1482373668	-1.7092636601	-0.8821317489
C39	-3.8345642854	3.7331156647	0.9983675930
C40	-6.1170170417	-4.4375750457	-1.6275215571
C41	-2.2024139397	5.1860666066	0.8181741362

N42	-3.5245312889	5.0520270140	1.1690412918
H43	6.1482373668	1.7092636601	-0.8821317489
H44	-5.3165482481	5.6414364782	2.0612089122
H45	-6.7211142211	-3.9372254962	-2.3853456108
H46	-5.6414364782	-5.3165482481	-2.0612089122
C47	6.1170170417	4.4375750457	-1.6275215571
H48	-3.9372254962	6.7211142211	2.3853456108
C49	-2.7094192467	1.7609170235	0.3304720363
N50	-6.1351958019	1.1340096062	1.2289380343
H51	-6.7397379280	-4.7376730326	-0.7822496301
H52	-4.7376730326	6.7397379280	0.7822496301
H53	-6.1386399458	0.1290782861	1.3154211340
H54	-1.6396378858	-6.9323115464	-1.5971118868
N55	-1.1419075035	-3.9005256388	-0.5451160005
C56	-1.8324313384	-5.0122058636	-1.0189884461
N57	-1.1340096062	-6.1351958019	-1.2289380343
N58	-3.1396460819	-4.9927033655	-1.2485011402
C59	-3.7331156647	-3.8345642854	-0.9983675930
C60	-3.1212849058	-2.6375261653	-0.5352745171
C61	-1.7609170235	-2.7094192467	-0.3304720363
O62	-0.9551342358	-1.7139808192	0.0650369582
N63	-4.0671756682	-1.6235887237	-0.4274311256
C64	-5.1860666066	-2.2024139397	-0.8181741362
N65	-5.0520270140	-3.5245312889	-1.1690412918
H66	-0.1394251236	-3.9807295003	-0.2534936982
H67	-0.1290782861	-6.1386399458	-1.3154211340
N68	-1.6235887237	4.0671756682	0.4274311256
N69	-3.9005256388	1.1419075035	0.5451160005
C70	-2.6375261653	3.1212849058	0.5352745171
H71	-1.7092636601	6.1482373668	0.8821317489
C72	-5.0122058636	1.8324313384	1.0189884461
C73	-4.4375750457	6.1170170417	1.6275215571
H74	5.6414364782	5.3165482481	-2.0612089122
H75	6.7211142211	3.9372254962	-2.3853456108
H76	6.7397379280	4.7376730326	-0.7822496301
H77	-0.8614541501	1.4411026564	-0.1152822536
H78	0.8614541501	-1.4411026564	-0.1152822536
H79	-1.4411026564	-0.8614541501	0.1152822536
H80	1.4411026564	0.8614541501	0.1152822536

Single point energy: -2329.4395167

(G4-4H⁺)₂

C1	1.7561958622	2.6428491401	-0.3337714117
C2	3.7059507662	3.7764283053	-1.0591515239
C3	3.1175871650	2.5967661889	-0.5316781792
O4	1.0727026498	1.5924892361	0.1373543652

N5	4.0809958737	1.6090775014	-0.3672872766
C6	4.3936653233	-6.0807794644	1.7112621840
H7	5.2797088314	-5.5893736812	2.1117791621
N8	5.0327889409	3.4862586812	-1.2038252328
C9	5.1920283365	2.1876528601	-0.7822344605
N10	1.0464132425	5.9849310114	-1.4586423947
N11	1.1044843799	3.8010733383	-0.6296133723
H12	3.8960402908	-6.6412116949	2.5039351535
H13	0.0423630626	5.9526774327	-1.5520365189
H14	4.6817976553	-6.7480875814	0.8965999715
H15	0.1042036263	3.9111577643	-0.3250792518
H16	-6.7714485914	1.5320301971	1.8736497264
N17	3.0840417611	4.9010304795	-1.3862921972
C18	1.7751499174	4.8988537322	-1.1712293558
H19	-3.9111577643	0.1042036263	0.3250792518
H20	1.7112524860	-6.1641224128	0.8127373214
N21	3.8010733383	-1.1044843799	0.6296133723
C22	4.8988537322	-1.7751499174	1.1712293558
N23	5.9849310114	-1.0464132425	1.4586423947
N24	4.9010304795	-3.0840417611	1.3862921972
C25	3.7764283053	-3.7059507662	1.0591515239
C26	2.5967661889	-3.1175871650	0.5316781792
C27	2.6428491401	-1.7561958622	0.3337714117
O28	1.5924892361	-1.0727026498	-0.1373543652
N29	1.6090775014	-4.0809958737	0.3672872766
C30	2.1876528601	-5.1920283365	0.7822344605
N31	3.4862586812	-5.0327889409	1.2038252328
H32	3.9111577643	-0.1042036263	0.3250792518
H33	6.7714485914	-1.5320301971	1.8736497264
H34	5.9526774327	-0.0423630626	1.5520365189
H35	1.5320301971	6.7714485914	-1.8736497264
N36	-4.9010304795	3.0840417611	1.3862921972
O37	-1.5924892361	1.0727026498	-0.1373543652
H38	-6.1641224128	-1.7112524860	-0.8127373214
C39	-3.7764283053	3.7059507662	1.0591515239
C40	-6.0807794644	-4.3936653233	-1.7112621840
C41	-2.1876528601	5.1920283365	0.7822344605
N42	-3.4862586812	5.0327889409	1.2038252328
H43	6.1641224128	1.7112524860	-0.8127373214
H44	-5.2797088314	5.5893736812	2.1117791621
H45	-6.6412116949	-3.8960402908	-2.5039351535
H46	-5.5893736812	-5.2797088314	-2.1117791621
C47	6.0807794644	4.3936653233	-1.7112621840
H48	-3.8960402908	6.6412116949	2.5039351535
C49	-2.6428491401	1.7561958622	0.3337714117
N50	-5.9849310114	1.0464132425	1.4586423947

H51	-6.7480875814	-4.6817976553	-0.8965999715
H52	-4.6817976553	6.7480875814	0.8965999715
H53	-5.9526774327	0.0423630626	1.5520365189
H54	-1.5320301971	-6.7714485914	-1.8736497264
N55	-1.1044843799	-3.8010733383	-0.6296133723
C56	-1.7751499174	-4.8988537322	-1.1712293558
N57	-1.0464132425	-5.9849310114	-1.4586423947
N58	-3.0840417611	-4.9010304795	-1.3862921972
C59	-3.7059507662	-3.7764283053	-1.0591515239
C60	-3.1175871650	-2.5967661889	-0.5316781792
C61	-1.7561958622	-2.6428491401	-0.3337714117
O62	-1.0727026498	-1.5924892361	0.1373543652
N63	-4.0809958737	-1.6090775014	-0.3672872766
C64	-5.1920283365	-2.1876528601	-0.7822344605
N65	-5.0327889409	-3.4862586812	-1.2038252328
H66	-0.1042036263	-3.9111577643	-0.3250792518
H67	-0.0423630626	-5.9526774327	-1.5520365189
N68	-1.6090775014	4.0809958737	0.3672872766
N69	-3.8010733383	1.1044843799	0.6296133723
C70	-2.5967661889	3.1175871650	0.5316781792
H71	-1.7112524860	6.1641224128	0.8127373214
C72	-4.8988537322	1.7751499174	1.1712293558
C73	-4.3936653233	6.0807794644	1.7112621840
H74	5.5893736812	5.2797088314	-2.1117791621
H75	6.6412116949	3.8960402908	-2.5039351535
H76	6.7480875814	4.6817976553	-0.8965999715
H77	-1.6618837607	0.0928253608	-0.0589934553
H78	1.6618837607	-0.0928253608	-0.0589934553
H79	-0.0928253608	-1.6618837607	0.0589934553
H80	0.0928253608	1.6618837607	0.0589934553

Single point energy: -2329.4303013

(2G4-H⁺)₁

N1	-2.3337859761	4.3758370031	4.2935780155
C2	-3.3145692552	3.4113814950	4.2499294262
N3	-3.0431871180	2.4796576780	3.3723034783
C4	-1.8268212346	2.8384514755	2.8242962505
C5	-1.0328699556	2.1911875798	1.8256058060
O6	-1.2832337287	1.1532984579	1.2054476564
N7	0.1627098577	2.8946822857	1.5959676130
C8	0.5246633208	4.0682934003	2.2187053588
N9	1.7244778238	4.5923087486	1.8949708566
N10	-0.2261842139	4.6892561673	3.1268782550
C11	-1.3593635725	4.0196350978	3.3906770602
N12	-2.3107860008	7.3328369954	0.3775779899
C13	-3.1880743257	6.5664201100	1.1116592211

N14	-3.5237952113	5.4635439218	0.4910082006
C15	-2.8326661785	5.4997017372	-0.7060790413
C16	-2.7943602387	4.5587014322	-1.7813081481
O17	-3.3928312258	3.4809588963	-1.8966419256
N18	-1.9420750971	4.9912470159	-2.8088016498
C19	-1.2414182750	6.1780397417	-2.8096140009
N20	-0.5151529145	6.4638762113	-3.9112467319
N21	-1.2714894980	7.0540058897	-1.8093314070
C22	-2.0685145870	6.6614311833	-0.8015168447
N23	4.2212139869	4.3458369791	-2.5964219789
C24	3.6729088880	4.9985642397	-1.5109864112
N25	3.0353136589	4.1805953407	-0.7126159008
C26	3.1753225577	2.9329564156	-1.2941865622
C27	2.6856692841	1.6551078685	-0.8754379162
O28	2.0064753103	1.3815869574	0.1162348488
N29	3.0778488250	0.6415084821	-1.7753309893
C30	3.8391046883	0.8358188664	-2.9060382066
N31	4.1805781599	-0.2516755618	-3.6288592565
N32	4.2798490894	2.0259314144	-3.3059955135
C33	3.9198132481	3.0116765403	-2.4674535415
N34	2.3242139599	3.3108369791	-6.7294219893
C35	1.8243310175	4.5347607424	-6.3370085712
N36	0.6689749745	4.4287900871	-5.7294957172
C37	0.3977029945	3.0714120295	-5.7229313578
C38	-0.7210556175	2.3485907651	-5.2088036704
O39	-1.7244065929	2.7622849958	-4.6224725282
N40	-0.5668971007	0.9606171984	-5.4468680717
C41	0.5174155262	0.3582747352	-6.0526051706
N42	0.5087274481	-0.9846069078	-6.1447744311
N43	1.5512194512	1.0327325701	-6.5277881685
C44	1.4273739918	2.3573315170	-6.3358789503
N45	1.6542139953	-4.4471629862	-4.9444219812
C46	2.7025388332	-3.5462269918	-4.9909351075
N47	2.7244523564	-2.7668194151	-3.9407518423
C48	1.6639480091	-3.1845378870	-3.1596022561
C49	1.2084066277	-2.7150083279	-1.8845730669
O50	1.6609700077	-1.7982468890	-1.2019019612
N51	0.0943703453	-3.4680359346	-1.4413926421
C52	-0.4788227261	-4.5156377369	-2.1243020231
N53	-1.5264973280	-5.1453220545	-1.5632494382
N54	-0.0670674361	-4.9394980566	-3.3190429088
C55	0.9923809548	-4.2439160310	-3.7606257509
N56	-3.0297860163	-4.5901630344	-6.0044219186
C57	-1.9483943574	-3.8443301822	-6.4275605027
N58	-1.8760351059	-2.6723690785	-5.8566126919
C59	-2.9604490346	-2.6320526303	-4.9981115295

C60	-3.4450372092	-1.6632165121	-4.1212158619
O61	-2.8964793919	-0.4817439072	-3.9475375227
N62	-4.5645952696	-1.9975534421	-3.4274915763
C63	-5.2110081524	-3.2140927588	-3.5568048241
N64	-6.2968204624	-3.3857620765	-2.7976125645
N65	-4.7957475264	-4.1670062098	-4.3932350618
C66	-3.6981670603	-3.8350336937	-5.0707979910
N67	-5.2727859751	-4.2351629980	1.3885780116
C68	-4.3738050376	-5.1395501925	0.8620046125
N69	-3.1934535846	-4.6056462061	0.6786217001
C70	-3.3163864692	-3.2997407462	1.1173895165
C71	-2.3647936536	-2.2304705076	1.1298547808
O72	-1.1983939603	-2.2408321618	0.7317761044
N73	-2.9325945127	-1.0565625734	1.6642672521
C74	-4.2260065605	-0.9364658713	2.1194318581
N75	-4.6172042872	0.2652147090	2.5769767425
N76	-5.1177233990	-1.9268943106	2.0974347754
C77	-4.6053016813	-3.0523136884	1.5793968836
N78	-8.1317859774	-0.3501630665	0.8725784111
C79	-7.9909353121	-1.4549197574	0.0625733998
N80	-7.0503985012	-1.3066117908	-0.8385066904
C81	-6.5386241850	-0.0358396510	-0.6042366884
C82	-5.4805383072	0.6829503839	-1.2157839015
O83	-4.7682125126	0.2778126492	-2.1761036589
N84	-5.2810892678	1.9331597966	-0.6556191108
C85	-6.0188107052	2.4441214561	0.3969163876
N86	-5.7366063524	3.6804781253	0.8252965885
N87	-7.0136730886	1.7816999533	0.9874593559
C88	-7.2109923888	0.5755772365	0.4581354705
H89	2.3517727510	5.4580304991	-6.5338998624
H90	-0.3207282539	-1.5520953423	-5.9711176843
H91	1.3224458872	-1.4063429479	-6.5643135684
H92	-1.3032682925	0.3853007436	-5.0461586382
H93	-4.9187199927	-1.2418876472	-2.7818558413
H94	-3.5410105125	6.8743564493	2.0858215196
H95	-1.8498003462	4.3242394219	-3.5906875340
H96	0.0614728080	7.2890954875	-3.8325916537
H97	-0.2261519181	5.7450997421	-4.5844671023
H98	-4.6491220543	-6.1610084665	0.6375104829
H99	-3.9689678077	1.0267997435	2.8325355052
H100	-5.5475026399	0.2926409342	2.9670957017
H101	-2.3309023497	-0.2130705527	1.6045489559
H102	-8.6167537960	-2.3290514864	0.1787350134
H103	-4.5334993503	2.5268993301	-1.0738138909
H104	-4.8745223687	4.2073733624	0.6199350705
H105	-6.2676293848	3.9743331178	1.6326595959

H106	-1.2538720657	-4.2210462191	-7.1657334105
H107	-6.7828353378	-4.2663547795	-2.8829251101
H108	-6.6016175419	-2.6772936401	-2.1077714857
H109	-1.8604094344	-5.9567779859	-2.0606991654
H110	-1.9271027458	-4.9426581164	-0.6392234601
H111	-0.3324545439	-3.1391125580	-0.5578906323
H112	3.4063735775	-3.5245788767	-5.8122361423
H113	3.6762036472	-1.1429695029	-3.5724093793
H114	4.6155723474	-0.0353613179	-4.5143448448
H115	2.7013965547	-0.2949762612	-1.5611745254
H116	3.7793586137	6.0652648602	-1.3692765740
H117	-4.1891270007	3.4498482317	4.8846959765
H118	0.8502486213	2.4086349964	0.9912958104
H119	2.1947257582	4.3727868024	1.0080195245
H120	1.9179714704	5.4899515300	2.3150297239
H121	-3.3919621474	0.0842137680	-3.2862732162
H122	-8.7867177252	-0.2301814725	1.6326469199
H123	-1.9014441171	8.2171757374	0.6447492243
H124	3.2033471698	3.1304677616	-7.1939442853
H125	-3.2783024657	-5.5275424597	-6.2911783347
H126	4.7987733778	4.7487926244	-3.3203630648
H127	-2.2805432779	5.1598283883	4.9288982772
H128	1.5060207804	-5.2304142346	-5.5652200521
H129	-6.2136201742	-4.4291255562	1.7009002490

Single point energy: -4342.3169061

(2G4-H⁺)₂

N1	-2.3337860001	4.3758369983	4.2935779934
C2	-3.1403555554	3.2884012781	4.5507218533
N3	-2.6804211197	2.1943564592	3.9987909262
C4	-1.5170338175	2.5762452110	3.3569370203
C5	-0.5975194341	1.8101923388	2.5713216465
O6	-0.6395375725	0.6104739577	2.2941152983
N7	0.4519494524	2.6239951744	2.0906797031
C8	0.6017113805	3.9664554386	2.3557015392
N9	1.7065681978	4.5842758529	1.8799112841
N10	-0.2569903079	4.6792024574	3.0785442988
C11	-1.2765697683	3.9347419763	3.5363940536
N12	-2.3107860040	7.3328370279	0.3775780203
C13	-3.6664151241	7.1776440288	0.6126405299
N14	-4.2060227416	6.2441529428	-0.1300733347
C15	-3.1576425440	5.7615256166	-0.8927585994
C16	-3.1465333291	4.7408670646	-1.8901883701
O17	-4.0756626655	4.0418005075	-2.3060153127
N18	-1.8448998641	4.5728974188	-2.4174404591
C19	-0.7131258230	5.2477480524	-1.9999440199

N20	0.4558149482	4.9142640520	-2.5907526101
N21	-0.7326534259	6.1979106055	-1.0799915689
C22	-1.9634484725	6.4123690134	-0.5794341899
N23	4.2212140001	4.3458370042	-2.5964220004
C24	3.7585576813	4.9760805465	-1.4578501257
N25	3.1378981168	4.1434995261	-0.6569459179
C26	3.2162180065	2.9139834553	-1.2840926711
C27	2.7097173226	1.6327514261	-0.8872889547
O28	2.0881296756	1.3375754468	0.1317264912
N29	3.0131645620	0.6515394890	-1.8574835704
C30	3.7367358827	0.8681619948	-3.0077633052
N31	4.0150540593	-0.1918619413	-3.7906950280
N32	4.2023743000	2.0595704369	-3.3792654211
C33	3.9043543038	3.0157369880	-2.4892298989
N34	2.3242139504	3.3108370225	-6.7294219868
C35	1.7587774117	3.9946261873	-5.6751964521
N36	0.8654076658	3.2850243071	-5.0318651306
C37	0.8410862676	2.0718719226	-5.6915598654
C38	0.0265857012	0.9216889047	-5.4783205431
O39	-0.8439119903	0.7700674479	-4.6094399753
N40	0.3048080678	-0.0977070231	-6.4057558915
C41	1.2444988906	-0.0038072399	-7.4093991742
N42	1.4234221724	-1.1216065807	-8.1843843427
N43	1.9844695976	1.0620742865	-7.6278029565
C44	1.7465100824	2.0627548056	-6.7511605957
N45	1.6542139986	-4.4471630014	-4.9444219997
C46	2.4972801194	-3.3703388573	-5.1152468031
N47	2.4413388809	-2.5441353645	-4.1027106282
C48	1.5395027650	-3.1069274298	-3.2199873458
C49	1.0951977860	-2.6552828520	-1.9342013021
O50	1.4420391942	-1.6468593890	-1.3199753180
N51	0.1469556781	-3.5462556686	-1.3881299769
C52	-0.2686244173	-4.7196983019	-1.9755631423
N53	-1.1295087691	-5.4956516964	-1.2861782243
N54	0.1503935465	-5.1429462255	-3.1692090052
C55	1.0406148920	-4.3035763345	-3.7207763559
N56	-3.0297860973	-4.5901630075	-6.0044219898
C57	-1.8823166345	-3.9127002709	-6.3799476533
N58	-1.8171456736	-2.6894518359	-5.9179534062
C59	-2.9865951988	-2.5459724153	-5.1764227943
C60	-3.5245482286	-1.4876857378	-4.4288378328
O61	-3.0594146079	-0.3015486763	-4.2090939638
N62	-4.7358546940	-1.7277331196	-3.8487751162
C63	-5.3971072824	-2.9341847080	-3.9294287938
N64	-6.5632400334	-3.0294880968	-3.2774271867
N65	-4.9273152702	-3.9724154988	-4.6277425555

C66	-3.7589779874	-3.7272272841	-5.2191963003
N67	-5.2727860008	-4.2351629978	1.3885779963
C68	-4.4995219286	-5.0486395208	0.5851891755
N69	-3.2804173088	-4.5917747036	0.4494064073
C70	-3.2441520141	-3.4338145997	1.2055412585
C71	-2.1744386661	-2.5096611808	1.4351697262
O72	-1.0247950786	-2.5448593595	0.9913436230
N73	-2.5867977456	-1.4613505125	2.2853451691
C74	-3.8395578999	-1.3404342619	2.8465059724
N75	-4.0607376095	-0.3092585489	3.6800721543
N76	-4.8377963075	-2.1963381753	2.6248155435
C77	-4.4757131646	-3.1977570401	1.8099625537
N78	-8.1317860034	-0.3501630001	0.8725780112
C79	-8.0342495063	-1.4576104131	0.0577191388
N80	-7.3374330932	-1.2257991635	-1.0282198397
C81	-6.9537854143	0.1025487371	-0.9194407721
C82	-6.1662236717	0.9138113778	-1.7868362607
O83	-5.6367850851	0.5995014131	-2.8667917391
N84	-6.0132355581	2.2135306822	-1.2874421407
C85	-6.5509656306	2.6760052790	-0.1045645586
N86	-6.3263596394	3.9642598958	0.2178861738
N87	-7.2832681269	1.9232012934	0.7117394365
C88	-7.4404523510	0.6693610193	0.2594254152
H89	2.0390240808	5.0103944679	-5.4323490473
H90	0.6236273351	-1.7247387036	-8.3275179839
H91	1.9725453806	-0.9499639584	-9.0176549878
H92	-0.2187101428	-0.9682397398	-6.2686683628
H93	-5.1782618586	-0.8930068217	-3.3672105487
H94	-4.1905179194	7.7880067462	1.3356031427
H95	-1.7531976187	3.8230964469	-3.0969930234
H96	1.2869589316	5.1492036457	-2.0635225711
H97	0.5142690011	4.1395435220	-3.2525636859
H98	-4.8901546019	-5.9526382160	0.1382573296
H99	-3.4427075406	0.5067970717	3.7864356437
H100	-5.0126072496	-0.2216442717	4.0035033917
H101	-1.8847168294	-0.7151882314	2.4288612404
H102	-8.5047903866	-2.3964949761	0.3148407726
H103	-5.3868410903	2.8349518716	-1.8154691734
H104	-5.6729255240	4.5798159060	-0.2610096766
H105	-6.6640975683	4.2620060098	1.1205803380
H106	-1.1312556717	-4.3848853208	-6.9982689118
H107	-7.0189653420	-3.9298774547	-3.3178050463
H108	-6.8553795613	-2.3592200968	-2.5468966876
H109	-1.4547468034	-6.3035672789	-1.7978929887
H110	-1.7633965836	-5.1273483468	-0.5640188442
H111	-0.2464973139	-3.2659418789	-0.4717440170

H112	3.1078378827	-3.2493332234	-5.9993875893
H113	3.4605570446	-1.0592890082	-3.7755429065
H114	4.4704658885	0.0486012702	-4.6597395436
H115	2.5863908635	-0.2734480605	-1.6788928924
H116	3.9129531306	6.0315453675	-1.2788693298
H117	-4.0412507905	3.3679610272	5.1434980385
H118	1.1246533559	2.1534924580	1.4667899742
H119	2.2139198368	4.2490515101	1.0564112973
H120	1.6870483899	5.5878136832	1.9966661038
H121	-2.1085947193	-0.0866438492	-4.5043847192
H122	-8.6059002504	-0.2882929452	1.7627275255
H123	-1.6747224172	7.9601908812	0.8495364072
H124	3.0381539386	3.6424648658	-7.3637750034
H125	-3.2799241773	-5.5448708906	-6.2236172507
H126	4.8130562176	4.7476633305	-3.3101526833
H127	-2.4474139821	5.3143437976	4.6494434345
H128	1.6022761198	-5.2723115773	-5.5253452578
H129	-6.2168510993	-4.4103776683	1.7012563706

Single point energy: -4342.3079264

(2G4-H⁺)₃

N1	-2.3337859874	4.3758369916	4.2935779818
C2	-3.1430024556	3.2911059920	4.5573113696
N3	-2.6902356944	2.1920930927	4.0089492263
C4	-1.5295783496	2.5688212055	3.3576231233
C5	-0.6187201982	1.7982854861	2.5690864269
O6	-0.6535517359	0.5916181264	2.3145080061
N7	0.4178002476	2.6066345814	2.0580407930
C8	0.5721141638	3.9523291843	2.3094417678
N9	1.6569284138	4.5693893558	1.7960097840
N10	-0.2679021842	4.6663472121	3.0544205606
C11	-1.2854435220	3.9288623356	3.5258613424
N12	-2.3107859876	7.3328369746	0.3775779752
C13	-3.3604880425	6.6998695323	1.0087658001
N14	-3.4467733135	5.4359221265	0.6761035128
C15	-2.4063770662	5.2286164714	-0.2112229826
C16	-2.0260346435	4.0632820096	-0.9457198670
O17	-2.5343472629	2.9385284918	-0.9309312837
N18	-0.9247874502	4.3332982219	-1.7860729605
C19	-0.2650063817	5.5419433384	-1.8668583189
N20	0.8119469791	5.6281425338	-2.6730270446
N21	-0.6132781980	6.6206150288	-1.1770649918
C22	-1.6824451699	6.4023676140	-0.4019045857
N23	4.2212139521	4.3458369565	-2.5964219805
C24	3.9369813078	4.8577148258	-1.3435203213
N25	3.2443797475	4.0229947991	-0.6137082520

C26	3.0736743595	2.9079492120	-1.4128852259
C27	2.3435968962	1.7014881514	-1.1736580431
O28	1.7243350758	1.3549380010	-0.1698819541
N29	2.3787885795	0.8598259450	-2.3163473280
C30	3.0825147576	1.1185790933	-3.4738812566
N31	3.0920286321	0.1756998459	-4.4377552823
N32	3.7728858653	2.2315211816	-3.6812539387
C33	3.6923276299	3.0830723759	-2.6462959918
N34	2.3242139879	3.3108369934	-6.7294219901
C35	2.1926244944	4.2901527870	-5.7791119972
N36	1.2258987362	4.0247339878	-4.9408593640
C37	0.6994918209	2.8228586552	-5.3633631478
C38	-0.2932838140	1.9867076663	-4.7716745649
O39	-0.9093606094	2.1352061820	-3.7159537833
N40	-0.5120200088	0.8431901321	-5.5759563348
C41	0.1824432858	0.5112656101	-6.7159025606
N42	-0.1995599948	-0.6116332646	-7.3703569932
N43	1.1638912048	1.2457607922	-7.2122125046
C44	1.3656362183	2.3664766428	-6.4952777458
N45	1.6542139796	-4.4471629541	-4.9444219652
C46	2.0469489249	-3.2139177093	-5.4141401487
N47	1.5845904370	-2.2361014451	-4.6804607612
C48	0.8753771026	-2.8508908748	-3.6660687321
C49	0.1341356239	-2.2948232847	-2.5875606655
O50	-0.0527268616	-1.0804573224	-2.3481749533
N51	-0.4407874386	-3.2817819795	-1.7828806473
C52	-0.3512741285	-4.6398045022	-2.0209180567
N53	-0.9708920084	-5.4502803783	-1.1440636135
N54	0.3067311301	-5.1687410505	-3.0532716467
C55	0.9050747830	-4.2387411175	-3.8097070718
N56	-3.0297859945	-4.5901629733	-6.0044220070
C57	-2.0214250332	-3.8618299875	-6.6047203466
N58	-1.7801804526	-2.7262737426	-6.0088178751
C59	-2.6803053070	-2.6855811589	-4.9533015581
C60	-2.8751089376	-1.7874937032	-3.9103600251
O61	-2.2042906377	-0.6601586615	-3.7792799197
N62	-3.8697160444	-2.0858283381	-3.0295463218
C63	-4.6589148925	-3.2163275948	-3.1511522470
N64	-5.6687679611	-3.3717315287	-2.2971565286
N65	-4.4539980634	-4.1500334056	-4.0937342771
C66	-3.4830602676	-3.8480971339	-4.9412624963
N67	-5.2727859692	-4.2351629803	1.3885779973
C68	-4.5378877095	-4.9822014011	0.4918623107
N69	-3.3522866101	-4.4693494549	0.2736424502
C70	-3.3006488869	-3.3409506684	1.0755101991
C71	-2.2615554199	-2.3749781752	1.2497185545

O72	-1.1647865900	-2.3295981489	0.6781962402
N73	-2.6151281677	-1.4053986630	2.2004091381
C74	-3.8149100587	-1.3637904262	2.8774805258
N75	-3.9858035141	-0.3921866795	3.7912115658
N76	-4.8019656933	-2.2423020608	2.6907781109
C77	-4.4823260303	-3.1857129138	1.7948012298
N78	-8.1317859811	-0.3501630085	0.8725779885
C79	-7.9255645553	-1.4771565617	0.1107754438
N80	-6.7749055382	-1.4491975922	-0.5165274605
C81	-6.1946236030	-0.2459395255	-0.1495871686
C82	-4.9484110702	0.3411438237	-0.5150317796
O83	-4.0681147936	-0.1269233171	-1.2635251723
N84	-4.7689276384	1.5945541208	0.0767835340
C85	-5.6685620211	2.1979479475	0.9325900712
N86	-5.3503811998	3.3983729528	1.4422134487
N87	-6.8284239711	1.6467992441	1.2925068780
C88	-7.0279847537	0.4546636744	0.7227570548
H89	2.8277482641	5.1646046742	-5.7599068277
H90	-0.6941028038	-1.3509125695	-6.8682915126
H91	0.4244642610	-0.8867516682	-8.1155537243
H92	-1.1926600899	0.1928530259	-5.1871933860
H93	-4.0554699831	-1.3689128159	-2.2571089004
H94	-4.0225322906	7.2227833482	1.6851308141
H95	-0.6908256941	3.5621902844	-2.4268832660
H96	1.1310253354	6.5781729242	-2.8042090896
H97	0.9388676968	4.9791237250	-3.4626250712
H98	-4.9267384092	-5.8856711231	0.0425209837
H99	-3.4045054048	0.4561895927	3.8534936237
H100	-4.9107923516	-0.3495891097	4.1939803554
H101	-1.9117260364	-0.6555873940	2.3451882823
H102	-8.6577341645	-2.2706549218	0.0517026550
H103	-3.9091361776	2.1055448291	-0.2030758180
H104	-4.5894504867	4.0077165565	1.1095309531
H105	-6.0865556751	3.8332922511	1.9794991043
H106	-1.5088173201	-4.2258126789	-7.4851707095
H107	-6.2439542177	-4.1874668422	-2.4527799171
H108	-5.9985958839	-2.6488654619	-1.6245295780
H109	-0.9347823653	-6.4344934584	-1.3679512785
H110	-1.7533319330	-5.1119084060	-0.5656335046
H111	-0.8197143686	-2.9517250396	-0.8629479974
H112	2.6757955029	-3.1058830677	-6.2873735964
H113	2.4481663350	-0.6203996252	-4.4602857904
H114	3.4835000372	0.4778787842	-5.3176603638
H115	1.7269560906	0.0716906596	-2.2758401544
H116	4.2607741393	5.8439198850	-1.0405342050
H117	-4.0411237042	3.3761076514	5.1534073635

H118	1.0329694481	2.1438409567	1.3735670787
H119	2.2124343003	4.1998038664	1.0171747680
H120	1.6486866764	5.5738313377	1.9015782151
H121	-1.5799238051	-0.6040589767	-2.9826865989
H122	-8.9356396048	-0.1411461982	1.4482919420
H123	-2.0293460992	8.2978772283	0.4794591827
H124	2.9825493494	3.2954844728	-7.4963084532
H125	-3.3914676023	-5.4895655339	-6.2925399768
H126	4.8156701168	4.7602782237	-3.2997736277
H127	-2.4499091798	5.3202375436	4.6319007509
H128	1.9240137540	-5.3511406216	-5.3079638374
H129	-6.1845819930	-4.4566121474	1.7625160074

Single point energy: -4342.3016158

(2G4-2H⁺)₁

N1	-2.3337860000	4.3758369999	4.2935779999
C2	-3.1663370785	3.2763039574	4.3103217384
N3	-2.8879404241	2.4102594554	3.3722156705
C4	-1.8070916880	2.9544443779	2.6982438235
C5	-1.0771482021	2.5584557762	1.5808686155
O6	-1.3105513288	1.4544328829	0.9065104195
N7	-0.0693029376	3.3882220733	1.2045976211
C8	0.2295243461	4.5763852340	1.8524465654
N9	1.2558150902	5.2776356718	1.3712675113
N10	-0.4597380305	5.0114167952	2.9080388586
C11	-1.4383323462	4.1906371350	3.2722127599
N12	-2.3107860001	7.3328369999	0.3775780000
C13	-3.1265139765	6.5674888641	1.1774682192
N14	-3.2999959169	5.3606307684	0.6965804009
C15	-2.5758230668	5.3400904342	-0.4837274014
C16	-2.3826210409	4.2951846588	-1.4343879026
O17	-2.8068048323	3.1284445373	-1.3808887263
N18	-1.5988464958	4.7252675123	-2.5145218382
C19	-1.0710159392	5.9960946434	-2.6543516521
N20	-0.4070815013	6.2720786792	-3.7886059917
N21	-1.2091664458	6.9559253855	-1.7433618987
C22	-1.9650613631	6.5722426761	-0.7099264378
N23	4.2212140000	4.3458370000	-2.5964220000
C24	3.6807437210	5.0060586551	-1.5132394064
N25	2.6745726412	4.3554337091	-0.9823197907
C26	2.5506275142	3.2042747521	-1.7496586878
C27	1.6539729151	2.1087580514	-1.6748165713
O28	0.7312098290	1.9551439550	-0.8328469728
N29	1.8890834776	1.1549538037	-2.6582470315
C30	2.8891170655	1.2462529292	-3.6142213330
N31	3.0030972558	0.2700869666	-4.5164318624

N32	3.7377307568	2.2680872961	-3.6930728219
C33	3.5162703162	3.1880144860	-2.7593925183
N34	2.3242150000	3.3108370000	-6.7294220000
C35	2.0524616443	4.3896154423	-5.9252590118
N36	0.9421897907	4.2321239902	-5.2495995170
C37	0.4607305215	2.9945825640	-5.6335570230
C38	-0.6957206006	2.2758642552	-5.2077845499
O39	-1.5602879369	2.5961438816	-4.3847912129
N40	-0.7770940862	1.0314645766	-5.8653001213
C41	0.1145438109	0.5545478001	-6.8060260013
N42	-0.1681600239	-0.6404975992	-7.3669132034
N43	1.1907657788	1.2196404915	-7.1902817548
C44	1.3080189712	2.4064467294	-6.5708905248
N45	1.6542140000	-4.4471630000	-4.9444210000
C46	2.4145395992	-3.3272238234	-5.1840967478
N47	1.9513774945	-2.2862857460	-4.5425017065
C48	0.8549401380	-2.7431983269	-3.8408179394
C49	-0.0353825043	-2.0607746800	-2.9622635041
O50	-0.0282125930	-0.8701434564	-2.6274838853
N51	-1.0198133718	-2.9357632251	-2.4595081353
C52	-1.1389121247	-4.2728209794	-2.7929797368
N53	-2.1747305852	-4.9577053305	-2.2832340915
N54	-0.3088218643	-4.9044321677	-3.6149138561
C55	0.6544096096	-4.0982763726	-4.0794877453
N56	-3.0297860000	-4.5901630001	-6.0044220001
C57	-2.0099632243	-3.8188983729	-6.5184825384
N58	-2.0189382876	-2.5889535354	-6.0761073620
C59	-3.1074381480	-2.5354480944	-5.2192563534
C60	-3.6033338019	-1.5487946532	-4.3702381264
O61	-3.0645975086	-0.3567861631	-4.2414911051
N62	-4.7039400875	-1.8830844717	-3.6463533378
C63	-5.3177143805	-3.1232688644	-3.7163915328
N64	-6.4249656852	-3.2771186943	-2.9845429773
N65	-4.8509230339	-4.1147776583	-4.4739661758
C66	-3.7668922747	-3.7848318656	-5.1724922344
N67	-5.2727860000	-4.2351629999	1.3885780001
C68	-4.7964453199	-4.7541018564	0.2117683440
N69	-3.9829284137	-3.9242843371	-0.3916677704
C70	-3.9189043152	-2.8172724440	0.4327229002
C71	-3.1737948357	-1.6099453127	0.3069106857
O72	-2.3966835775	-1.2689325289	-0.5912074818
N73	-3.4180390799	-0.7557572214	1.4044139958
C74	-4.2535029554	-1.0332142134	2.4730826857
N75	-4.3567788226	-0.1012847141	3.4331436056
N76	-4.9437801224	-2.1586240287	2.5815225247
C77	-4.7251252622	-2.9927517124	1.5543579224

N78	-8.1317859999	-0.3501629999	0.8725780000
C79	-8.1083144933	-1.3757743946	-0.0488383052
N80	-7.1821292391	-1.2157346538	-0.9634527230
C81	-6.5644389879	-0.0155270135	-0.6310289941
C82	-5.4846652121	0.6862942989	-1.2312428513
O83	-4.8520529203	0.3499607035	-2.2635767096
N84	-5.1529085875	1.8512330784	-0.5430356282
C85	-5.8188925182	2.3118055032	0.5807798848
N86	-5.4173574929	3.4644415322	1.1333951473
N87	-6.8391091121	1.6705697006	1.1436251270
C88	-7.1509141068	0.5369833635	0.5129281545
H89	2.6987817156	5.2553282986	-5.8863369823
H90	-0.8159719281	-1.2913355685	-6.9194971859
H91	0.5545781550	-1.0136792498	-7.9652513727
H92	-1.5593545041	0.4549166687	-5.5663853888
H93	-5.0454650170	-1.1372823486	-2.9906869561
H94	-3.5605333710	6.9542782771	2.0890333975
H95	-1.4940408344	4.0267661987	-3.2721558159
H96	0.0046817967	7.1942845897	-3.8215768137
H97	0.0177714250	5.5272117389	-4.3597054898
H98	-5.0733149574	-5.7388685352	-0.1386458074
H99	-3.8383013521	0.7796184542	3.4042907976
H100	-4.9385670583	-0.3306452865	4.2249183441
H101	-2.8818884210	0.1090642440	1.3859938505
H102	-8.7987075800	-2.2062365581	0.0064127147
H103	-4.3276031262	2.3759307598	-0.8901500347
H104	-4.6124778469	4.0391650095	0.8551524959
H105	-5.9576452541	3.7650236936	1.9313586219
H106	-1.2929046210	-4.2240538918	-7.2192929886
H107	-6.8716474348	-4.1820967197	-3.0158200148
H108	-6.7456801852	-2.5627430117	-2.3129295112
H109	-2.1598752737	-5.9547951772	-2.4406183229
H110	-2.8271112795	-4.5551048080	-1.5962445882
H111	-1.6501030738	-2.4927065786	-1.7711987492
H112	3.2829055524	-3.3434645890	-5.8279787609
H113	2.5296571302	-0.6480410915	-4.4751124224
H114	3.7677111549	0.3813700278	-5.1668159879
H115	1.2269377777	0.3547686091	-2.6847553136
H116	4.0698485958	5.9538682031	-1.1674959727
H117	-3.9551340990	3.1727920979	5.0434148716
H118	0.4695068806	3.0654933488	0.3601005806
H119	1.7839998075	4.9791632562	0.5321616759
H120	1.4788170542	6.1442752617	1.8395709651
H121	-3.4721226431	0.1843580424	-3.5118686665
H122	-8.7685958577	-0.2426208102	1.6505815218
H123	-2.0700557706	8.3061314004	0.5107168229

H124	3.1092934659	3.2052392221	-7.3579370391
H125	-3.2212042813	-5.5629902372	-6.2058168650
H126	5.0302994870	4.6235434764	-3.1354546241
H127	-2.3280451525	5.1477523526	4.9478885688
H128	1.8403372560	-5.3849647031	-5.2749016485
H129	-5.8883968284	-4.6932501660	2.0479172342
H130	-0.7467414302	1.3632246132	0.0896271656

Single point energy: -4342.6668727

(2G4-2H⁺)_a

N1	-2.3337860000	4.3758370000	4.2935780000
C2	-3.2549646202	3.3566960685	4.3670983748
N3	-3.1576435738	2.5347442670	3.3530586061
C4	-2.1219332471	3.0291715650	2.5845146768
C5	-1.5589804173	2.5486397552	1.3662930146
O6	-1.8574045909	1.5520846336	0.6986158136
N7	-0.5083502614	3.3885829397	0.9378973292
C8	-0.0783073056	4.5348152503	1.5791024432
N9	0.9301937621	5.2177943557	1.0067290395
N10	-0.5996458832	4.9713566167	2.7134083997
C11	-1.5945944929	4.1847073238	3.1566775588
N12	-2.3107860001	7.3328370000	0.3775779999
C13	-3.2726014843	6.6152710736	1.0511397291
N14	-3.6217118741	5.5317995555	0.4045519025
C15	-2.8617152779	5.5410433309	-0.7493502134
C16	-2.7918135575	4.5957781201	-1.8169620686
O17	-3.4161330350	3.5387238281	-1.9635993117
N18	-1.8539836956	4.9969839077	-2.7856142248
C19	-1.1252434309	6.1681256142	-2.7506355192
N20	-0.3474602014	6.4446953479	-3.8177751153
N21	-1.1729638758	7.0351301419	-1.7465094189
C22	-2.0422135856	6.6664872265	-0.7918198466
N23	4.2212140000	4.3458369997	-2.5964219999
C24	3.3552016387	5.0132963658	-1.7522486788
N25	2.2927849551	4.3151352657	-1.4515426248
C26	2.4583834089	3.1170487359	-2.1278428787
C27	1.6959278784	1.9572366288	-2.2232312425
O28	0.5503735278	1.7863872973	-1.6011826894
N29	2.2091725080	0.9700217690	-3.0086815701
C30	3.4154467124	1.0768571826	-3.6868542738
N31	3.7937400794	0.0276075459	-4.4139249042
N32	4.1791372992	2.1666453643	-3.6239983269
C33	3.6706141420	3.1217479273	-2.8545268749
N34	2.3242150000	3.3108370000	-6.7294220000
C35	1.9803857532	4.4527499383	-6.0437130079
N36	0.8639298065	4.3082005047	-5.3753505778

C37	0.4486902826	3.0172346813	-5.6482892160
C38	-0.7002260388	2.2950569355	-5.2007867268
O39	-1.5967846682	2.6480413159	-4.4336316761
N40	-0.7192923108	0.9951519036	-5.7608152552
C41	0.2174896498	0.4760321358	-6.6336371445
N42	-0.0048116435	-0.7600946353	-7.1144319938
N43	1.2970846476	1.1396175078	-7.0181530816
C44	1.3448531606	2.3811663095	-6.5060046001
N45	1.6542140000	-4.4471629997	-4.9444210003
C46	2.4958735681	-3.3814731804	-5.1784335152
N47	2.1240559704	-2.3049522515	-4.5311085530
C48	0.9911556360	-2.6841059130	-3.8251329256
C49	0.1354840864	-1.9648220495	-2.9523815162
O50	0.2468238132	-0.7547332236	-2.6308049285
N51	-0.9017676039	-2.7481536581	-2.4541765826
C52	-1.1007126552	-4.0813013415	-2.7796567845
N53	-2.1565107856	-4.7191663195	-2.2712931384
N54	-0.3057608180	-4.7644244549	-3.6006552719
C55	0.6944133100	-4.0258190107	-4.0709779065
N56	-3.0297860000	-4.5901629999	-6.0044220000
C57	-2.0006249335	-3.8162233206	-6.4895741850
N58	-2.0062973910	-2.5961869122	-6.0193260337
C59	-3.1059320459	-2.5498353325	-5.1760346712
C60	-3.6259271662	-1.5637506127	-4.3375195655
O61	-3.1020947037	-0.3663357422	-4.1962003309
N62	-4.7380375435	-1.9031606951	-3.6384904186
C63	-5.3453023105	-3.1446728346	-3.7212293617
N64	-6.4583107234	-3.3034815207	-3.0017580211
N65	-4.8662669213	-4.1316477001	-4.4821258811
C66	-3.7732651929	-3.7953060193	-5.1620379216
N67	-5.2727859999	-4.2351630003	1.3885780005
C68	-4.8070072791	-4.7950606785	0.2257497445
N69	-4.0571506957	-3.9592850540	-0.4477572204
C70	-4.0180544327	-2.8050484355	0.3105391180
C71	-3.3273796138	-1.5780374285	0.1000002600
O72	-2.5941975503	-1.2658412825	-0.8562475623
N73	-3.5581051753	-0.6744450184	1.1460128742
C74	-4.3662445009	-0.9221430392	2.2424442121
N75	-4.5141126115	0.0506938195	3.1486821463
N76	-5.0100837865	-2.0721779405	2.4391060681
C77	-4.7824671903	-2.9561641333	1.4649883688
N78	-8.1317859999	-0.3501629998	0.8725779997
C79	-8.0618112404	-1.4257161468	0.0121749995
N80	-7.1834347540	-1.2537643657	-0.9472373233
C81	-6.6469073455	0.0074958370	-0.7083577516
C82	-5.6404269129	0.7492718301	-1.3792362086

O83	-5.0061266469	0.3867504631	-2.4077353727
N84	-5.3913422696	1.9794173211	-0.7855992452
C85	-6.0584623779	2.4593949293	0.3302537605
N86	-5.7595955826	3.6841580431	0.7766516774
N87	-6.9986998032	1.7714544881	0.9738719552
C88	-7.2368214691	0.5837185651	0.4230811243
H89	2.5827178910	5.3498238582	-6.0845072342
H90	-0.7255944311	-1.3747959575	-6.7294170122
H91	0.7193068626	-1.1407812811	-7.7049139087
H92	-1.5155645635	0.4322538090	-5.4703338756
H93	-5.1122821845	-1.1401509632	-3.0125072618
H94	-3.6698266130	6.9403793845	2.0024164099
H95	-1.7331675914	4.3185336093	-3.5504309656
H96	0.2183539648	7.2756623135	-3.7203487020
H97	-0.0098271522	5.6997732919	-4.4367351479
H98	-5.0432718799	-5.8100461782	-0.0626512177
H99	-4.0190978343	0.9548819976	3.1327805192
H100	-5.0702583011	-0.1889114873	3.9566311476
H101	-3.0303480652	0.2129760161	1.0728846771
H102	-8.6849536292	-2.2998165855	0.1422194261
H103	-4.6538743685	2.5707013358	-1.2151976840
H104	-4.9459096592	4.2542077986	0.5087187471
H105	-6.2500829630	3.9539165793	1.6175608856
H106	-1.2790403180	-4.2100872034	-7.1922649041
H107	-6.8987346520	-4.2117296786	-3.0326785630
H108	-6.7681188043	-2.6008328482	-2.3102986132
H109	-2.2060969705	-5.7028695719	-2.4966618796
H110	-2.8521315983	-4.3314306325	-1.6057254944
H111	-1.5692224304	-2.2651674017	-1.8133952153
H112	3.3580310170	-3.4621405316	-5.8263205539
H113	3.2042187697	-0.8165415712	-4.5082761272
H114	4.6694353339	0.1076551941	-4.9108610369
H115	1.6172293665	0.1071966548	-3.0722434055
H116	3.5701073607	6.0107759035	-1.3928566850
H117	-3.9588132178	3.2752846157	5.1838556850
H118	-0.0758639083	3.0993998891	0.0646695242
H119	1.3151471954	4.9639159993	0.0977119733
H120	1.2120017815	6.0734673728	1.4604293941
H121	-3.5800489188	0.1858044885	-3.5115342346
H122	-8.7427474073	-0.2442925777	1.6710755223
H123	-1.9105273551	8.2189381140	0.6544413213
H124	3.1089026332	3.1930734447	-7.3567192017
H125	-3.2360996153	-5.5520634360	-6.2410424631
H126	5.1150514209	4.6741009489	-2.9393960413
H127	-2.1874329605	5.1119334043	4.9716569772
H128	1.7715502548	-5.3960255962	-5.2749022831

H129	-5.8469730285	-4.6829269359	2.0907015991
H130	0.1317859711	0.9004117315	-1.7693152550

Single point energy: -4342.6642663

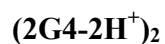
(2G4-2H⁺)_b

N1	-2.3337859999	4.3758370001	4.2935780000
C2	-3.3035791763	3.4006985077	4.3074458965
N3	-3.0698368452	2.4660625656	3.4207852508
C4	-1.8893758973	2.8342478642	2.8033719472
C5	-1.1502469982	2.2060513259	1.7592052469
O6	-1.4058219047	1.1528398628	1.1513426686
N7	0.0065116160	2.9285842968	1.4421238140
C8	0.4010627712	4.1024632224	2.0560057025
N9	1.5660025976	4.6447756944	1.6650642664
N10	-0.2963353170	4.6991086299	3.0191286505
C11	-1.4066827880	4.0248379774	3.3416111121
N12	-2.3107860000	7.3328370000	0.3775780001
C13	-3.1164122651	6.5487276779	1.1711089154
N14	-3.3585094308	5.3797355656	0.6313744136
C15	-2.6817992087	5.3952495865	-0.5751529023
C16	-2.5648773459	4.3951029614	-1.5864643981
O17	-3.0521865557	3.2542484404	-1.6142120339
N18	-1.7764499533	4.8437975913	-2.6571732930
C19	-1.1965783450	6.0935886881	-2.7482026914
N20	-0.5324886872	6.3843906889	-3.8865967595
N21	-1.2869721100	7.0171709420	-1.7991146703
C22	-2.0293104603	6.6137942826	-0.7581757002
N23	4.2212140000	4.3458370000	-2.5964220001
C24	3.7066406793	4.8871265000	-1.4390729772
N25	2.8557135440	4.0810571046	-0.8573323931
C26	2.8175541793	2.9581234221	-1.6626449747
C27	2.0726389637	1.7487666299	-1.5380479325
O28	1.2602932249	1.4082846329	-0.6739103272
N29	2.3693953173	0.8742721534	-2.6113300574
C30	3.2502166702	1.1274906157	-3.6446738923
N31	3.3946407466	0.1680837257	-4.5772559663
N32	3.9326167149	2.2521501747	-3.7576734801
C33	3.6720343563	3.1062297020	-2.7531444687
N34	2.3242150000	3.3108369999	-6.7294220000
C35	1.9998676111	4.4254462693	-5.9920376711
N36	0.8631752539	4.2857369421	-5.3577926654
C37	0.4201203057	3.0212385035	-5.6970185478
C38	-0.7483053756	2.3073353760	-5.2914532593
O39	-1.6591276349	2.6439671745	-4.5327215875
N40	-0.7772439297	1.0256940770	-5.8947512891
C41	0.1624193819	0.5207326484	-6.7692094091

N42	-0.0837640575	-0.7029393944	-7.2956788026
N43	1.2493052633	1.1772924992	-7.1252780795
C44	1.3182801603	2.4000351385	-6.5631081096
N45	1.6542140000	-4.4471629999	-4.9444209999
C46	2.4136103270	-3.2974281704	-5.0199833727
N47	2.0081073049	-2.3679791510	-4.1971262409
C48	0.9369401522	-2.9325322202	-3.5268849481
C49	0.0754761353	-2.4674562021	-2.5368074370
O50	0.1511398776	-1.2676277045	-2.0168842569
N51	-0.8782400189	-3.3474852665	-2.1242706522
C52	-1.0131043214	-4.6313897663	-2.6307799109
N53	-1.9957222311	-5.3757301865	-2.1251092152
N54	-0.2191096760	-5.1146563437	-3.5852755204
C55	0.7082833916	-4.2484053738	-3.9796132947
N56	-3.0297860000	-4.5901630000	-6.0044220000
C57	-1.9745590983	-3.8384558196	-6.4734139708
N58	-1.9037331751	-2.6508383760	-5.9306688198
C59	-2.9811901096	-2.6016524284	-5.0572085070
C60	-3.4579566452	-1.6290151777	-4.1767188394
O61	-2.8866122670	-0.4589763826	-3.9984683544
N62	-4.5785852655	-1.9534232533	-3.4816257936
C63	-5.2357632068	-3.1659089139	-3.6068989113
N64	-6.3366454356	-3.3205356055	-2.8703253668
N65	-4.8057622104	-4.1366793509	-4.4171312990
C66	-3.7106726834	-3.8122017357	-5.0987245935
N67	-5.2727860001	-4.2351630000	1.3885779999
C68	-4.6785982185	-4.8977038854	0.3424496903
N69	-3.7470379372	-4.1792785722	-0.2360714845
C70	-3.7218188693	-2.9864786117	0.4753825333
C71	-2.9213947203	-1.8265065529	0.3432246884
O72	-2.0301650749	-1.6514927772	-0.5347579236
N73	-3.2050097217	-0.8575987798	1.2879554277
C74	-4.1792867353	-0.9883538673	2.2665563947
N75	-4.3593971249	0.0165098614	3.1215263944
N76	-4.9532369007	-2.0700780374	2.3941404865
C77	-4.6718188821	-3.0098242186	1.4991576308
N78	-8.1317859999	-0.3501630000	0.8725780000
C79	-8.0550248106	-1.4102135657	-0.0037207461
N80	-7.0842119368	-1.2797243215	-0.8767248431
C81	-6.4897790736	-0.0616079784	-0.5612594121
C82	-5.3914039968	0.6295439234	-1.1325009407
O83	-4.6959271750	0.2375003069	-2.1133391015
N84	-5.1129992396	1.8289821649	-0.5000765141
C85	-5.8331741061	2.3286377217	0.5736058142
N86	-5.4815573109	3.5146528120	1.0756112275
N87	-6.8672960903	1.6901501819	1.1243083650

C88	-7.1383123399	0.5321243097	0.5289393107
H89	2.6320639857	5.3020550355	-5.9694364193
H90	-0.7194826592	-1.3515364607	-6.8330238907
H91	0.6553885426	-1.0744670073	-7.8741261078
H92	-1.5845151929	0.4669439970	-5.6355418849
H93	-4.9098536856	-1.2004615781	-2.8128638898
H94	-3.4916222138	6.8937573485	2.1242549941
H95	-1.6788272419	4.1640606868	-3.4258622353
H96	-0.0586731411	7.2770059132	-3.8714009477
H97	-0.1157548675	5.6390095190	-4.4563627920
H98	-4.9664111089	-5.9014209886	0.0606872092
H99	-3.8353105554	0.9132600065	3.1413325336
H100	-5.0675835040	-0.1398070746	3.8249484079
H101	-2.5879754691	-0.0076029111	1.2811771266
H102	-8.7446038353	-2.2416679750	0.0472542016
H103	-4.3168714355	2.3906144481	-0.8765825152
H104	-4.6432927463	4.0656105736	0.8347755028
H105	-6.0244888706	3.8185233563	1.8710819855
H106	-1.2966391400	-4.2225865621	-7.2236387003
H107	-6.8461093313	-4.1858867665	-2.9790393026
H108	-6.6569937488	-2.6027960781	-2.1958100752
H109	-2.0739531904	-6.3249677502	-2.4612481848
H110	-2.6522560446	-4.9959041126	-1.4178869008
H111	-1.5384299753	-2.9510683297	-1.4052234709
H112	3.2502636359	-3.2115530136	-5.7006188445
H113	2.9203320493	-0.7277691469	-4.4925795753
H114	4.0451233563	0.3480057301	-5.3257531302
H115	1.8472678979	0.0038247310	-2.5904926483
H116	3.9955475860	5.8666660323	-1.0839915338
H117	-4.1414124054	3.4307951373	4.9903958052
H118	0.5825396720	2.4986087093	0.7014830164
H119	2.0324514845	4.3836869727	0.7865540513
H120	1.7917203078	5.5327203650	2.0898481778
H121	-3.3543581957	0.1045494993	-3.3157047217
H122	-8.8076537270	-0.2169054861	1.6128487421
H123	-2.0011027681	8.2763880951	0.5671270724
H124	3.1420968014	3.1853885845	-7.3101491124
H125	-3.3024488503	-5.5168301060	-6.3068392852
H126	4.9322869877	4.7517764312	-3.1895101655
H127	-2.2568406736	5.1645948949	4.9215498157
H128	1.8261538288	-5.3205299751	-5.4266083109
H129	-5.9815823355	-4.5971213396	2.0129375020
H130	-0.5350019036	-1.0853787346	-1.3116779859

Single point energy:



N1	-2.3337858849	4.3758370856	4.2935782387
C2	-3.3438177811	3.4408879773	4.3558745421
N3	-3.3958805320	2.6993496077	3.2776042384
C4	-2.3603837693	3.1517836429	2.4800726803
C5	-1.9487581850	2.7384079214	1.1780883808
O6	-2.4572029140	1.8764155536	0.4491508090
N7	-0.8258088264	3.4707224256	0.7400424396
C8	-0.2478504571	4.5184509570	1.4305737331
N9	0.7589464234	5.1868991453	0.8386665850
N10	-0.6556708149	4.9250752572	2.6288444835
C11	-1.6833769956	4.2002357529	3.0972237546
N12	-2.3107856064	7.3328367017	0.3775780077
C13	-3.3301245640	6.5472690941	0.8709301492
N14	-3.6120317065	5.5302974668	0.1004433848
C15	-2.7376913716	5.6446332144	-0.9653830537
C16	-2.4651233636	4.8263072295	-2.0552939926
O17	-3.0711428628	3.6858960143	-2.3037195606
N18	-1.4936684250	5.2679597410	-2.8975296251
C19	-0.7692747794	6.4313536420	-2.6924851478
N20	0.1218208455	6.7427141306	-3.6384242393
N21	-0.9568731404	7.2151437206	-1.6325123308
C22	-1.9146900883	6.7835948853	-0.8161449786
N23	4.2212140858	4.3458368586	-2.5964219956
C24	3.4360774141	5.2183766315	-1.8725993275
N25	2.2492290468	4.7224476134	-1.6190181176
C26	2.2620525116	3.4607728283	-2.1902449222
C27	1.2446059518	2.4662119609	-2.2656811645
O28	0.0833685257	2.5304860158	-1.8293518601
N29	1.7018829845	1.3190958376	-2.9451774081
C30	2.9682889136	1.1691760323	-3.4833694922
N31	3.2882438476	0.0013368804	-4.0573725996
N32	3.8998145899	2.1168391050	-3.4489559471
C33	3.4908206465	3.2072950560	-2.7958863625
N34	2.3242152565	3.3108365869	-6.7294221982
C35	2.0659384155	4.5048356977	-6.0902407668
N36	0.9175476040	4.5032921505	-5.4576379857
C37	0.3878189335	3.2415762033	-5.6982099048
C38	-0.8021843208	2.6189877364	-5.2473674618
O39	-1.6928166482	3.1165308303	-4.5142989169
N40	-0.9308311530	1.3144800729	-5.7260621881
C41	-0.0189141858	0.6790806136	-6.5570196977
N42	-0.3163963957	-0.5456719469	-7.0090495867
N43	1.1098007268	1.2467137947	-6.9558749467
C44	1.2564661928	2.4907416629	-6.4991177839
N45	1.6542144094	-4.4471629690	-4.9444213422
C46	2.3253844405	-3.3130510368	-5.3390465136

N47	1.7806408771	-2.2299735717	-4.8444691337
C48	0.7216000389	-2.6746432624	-4.0760329537
C49	-0.2275407542	-1.9492540385	-3.2977712047
O50	-0.3073376505	-0.7251904713	-3.1344756104
N51	-1.1552590725	-2.8211251810	-2.6871174115
C52	-1.1866760195	-4.1929531212	-2.8625298699
N53	-2.1969814337	-4.8821923422	-2.3090351639
N54	-0.2965273509	-4.8647827901	-3.5850031554
C55	0.6213556160	-4.0606688698	-4.1355721464
N56	-3.0297859565	-4.5901627615	-6.0044218020
C57	-2.0615656647	-3.7636109967	-6.5269299853
N58	-2.1757964341	-2.5258036175	-6.1253987751
C59	-3.2797654491	-2.5233041837	-5.2945588232
C60	-3.8477211631	-1.5447619891	-4.4864349056
O61	-3.3982281512	-0.3138553510	-4.3768395761
N62	-4.9369820090	-1.9277907320	-3.7707270635
C63	-5.4563859529	-3.2116964172	-3.7934174056
N64	-6.5586700418	-3.4069002030	-3.0613219279
N65	-4.9126597449	-4.1942517210	-4.5106351334
C66	-3.8456720779	-3.8151326585	-5.2125119548
N67	-5.2727859267	-4.2351630945	1.3885780064
C68	-4.8438455083	-4.8096870788	0.2171843027
N69	-4.1694156906	-3.9643723141	-0.5223830559
C70	-4.1422488262	-2.7883940512	0.2048560343
C71	-3.5510589490	-1.5272556519	-0.0954307615
O72	-2.9325004095	-1.2041368878	-1.1215244983
N73	-3.7581462604	-0.6054678738	0.9495880494
C74	-4.4858867961	-0.8602424479	2.0984180880
N75	-4.6513199173	0.1354931788	2.9817223383
N76	-5.0544146734	-2.0337054408	2.3647954549
C77	-4.8328381751	-2.9375201134	1.4041435882
N78	-8.1317856949	-0.3501634080	0.8725781883
C79	-8.1001932670	-1.4222492677	0.0038948430
N80	-7.2961545913	-1.2318658418	-1.0148397114
C81	-6.7701436755	0.0385776995	-0.8070896874
C82	-5.8150554671	0.7904339904	-1.5351882366
O83	-5.2463526737	0.4660100362	-2.6081676861
N84	-5.5319417173	2.0173791377	-0.9334128636
C85	-6.1224521385	2.4845351829	0.2323542673
N86	-5.7909616338	3.7093915487	0.6645104596
N87	-7.0224655844	1.7894878826	0.9116628169
C88	-7.2862545179	0.5995045095	0.3683273271
H89	2.7588693062	5.3337428708	-6.1305837400
H90	-1.0429875230	-1.1472272638	-6.6081315734
H91	0.4459595580	-1.0040153427	-7.4886791576
H92	-1.7208486102	0.7863145117	-5.3593481657

H93	-5.3490064506	-1.1862867954	-3.1665501069
H94	-3.8235561343	6.7793121020	1.8045683408
H95	-1.2930525613	4.6412150132	-3.7017941912
H96	0.7139496560	7.5401688991	-3.4547167950
H97	0.4114085979	6.0417559904	-4.3350138034
H98	-5.0480554539	-5.8433604324	-0.0263224533
H99	-4.1954847394	1.0559723170	2.9449646645
H100	-5.1182406725	-0.1252030687	3.8384271196
H101	-3.3125993930	0.3179596353	0.8199319138
H102	-8.6931916533	-2.3097260376	0.1764792887
H103	-4.7785944980	2.5561328392	-1.3577705278
H104	-4.9770220794	4.2423159419	0.3444188228
H105	-6.1664549665	3.9461861654	1.5723418366
H106	-1.2998621554	-4.1352952628	-7.1983365744
H107	-6.9161016634	-4.3501584252	-3.0136449075
H108	-6.8837439671	-2.7038699613	-2.3847987483
H109	-2.1117041823	-5.8871846669	-2.3617343601
H110	-2.9080791448	-4.4752908689	-1.6841459615
H111	-1.8477893068	-2.3499186868	-2.0801646355
H112	3.1984457500	-3.3510475360	-5.9760445253
H113	2.6145317825	-0.7160431124	-4.3550734449
H114	4.2108733744	-0.0247644822	-4.4683330623
H115	1.0229535259	0.5434318616	-3.0119529159
H116	3.7957904870	6.1892597932	-1.5599715211
H117	-3.9961611261	3.3573762256	5.2142809585
H118	-0.4452048603	3.1792464236	-0.1755353301
H119	1.1788017114	4.9562289741	-0.0693705720
H120	1.2238995050	5.8726448323	1.4159573839
H121	-3.8691709962	0.1760623119	-3.6437028440
H122	-8.6753762959	-0.2666220206	1.7211446830
H123	-1.9206478209	8.1643310501	0.8019931434
H124	3.1351694980	3.0799875356	-7.2877452581
H125	-3.1388131432	-5.5826037231	-6.1690618677
H126	5.1870161642	4.4779575616	-2.8658943113
H127	-2.0647905163	5.0270234976	5.0193266903
H128	1.8999799766	-5.4034966255	-5.1643832592
H129	-5.7816422689	-4.6886323169	2.1359927747
H130	-2.6230593092	3.1996004757	-3.0537373961

Single point energy: -4342.6600228

(2G4-2H⁺)₃

N1	-2.3337859610	4.3758370452	4.2935780524
C2	-3.2964063648	3.3932916026	4.3877782245
N3	-3.3225322514	2.6249505973	3.3274323680
C4	-2.3187569522	3.1127068990	2.5086260237
C5	-1.8947134456	2.6961264835	1.2116194927

O6	-2.3595170695	1.7957088967	0.5034617516
N7	-0.8111519574	3.4771857534	0.7523399017
C8	-0.2721192152	4.5561373026	1.4239933428
N9	0.6996135126	5.2632007949	0.8148684939
N10	-0.6917982906	4.9641985739	2.6158429312
C11	-1.6871667309	4.2040134252	3.0982653935
N12	-2.3107858529	7.3328369218	0.3775779789
C13	-3.3420545507	6.5656384075	0.8778329173
N14	-3.6503122383	5.5528045236	0.1112323647
C15	-2.7767831671	5.6487539029	-0.9597061990
C16	-2.5279279184	4.8347722472	-2.0595209739
O17	-3.1722578506	3.7161785545	-2.3132515501
N18	-1.5470704831	5.2574751237	-2.9007164759
C19	-0.7955445069	6.4027453604	-2.6904936954
N20	0.1080816443	6.6996766096	-3.6298535898
N21	-0.9668976748	7.1875793622	-1.6302201142
C22	-1.9309766268	6.7725517252	-0.8136518578
N23	4.2212139967	4.3458370022	-2.5964219981
C24	3.4865355809	5.1596211196	-1.7624853059
N25	2.2963041052	4.6703858577	-1.5179209105
C26	2.2529366206	3.4717977041	-2.2074715649
C27	1.1994886463	2.5187728248	-2.3340775591
O28	0.0563788910	2.5700613325	-1.8594430610
N29	1.5987806266	1.4211135170	-3.1279782260
C30	2.8247483883	1.3011887850	-3.7571128865
N31	3.0526623328	0.2006444532	-4.4955971134
N32	3.7861176326	2.2137387618	-3.6701434154
C33	3.4495196388	3.2471267765	-2.8837346852
N34	2.3242141118	3.3108369179	-6.7294220022
C35	2.1177247615	4.4706969749	-6.0179300601
N36	0.9424489743	4.5051639586	-5.4378170117
C37	0.3409483677	3.3064334298	-5.7929719499
C38	-0.8899427395	2.7225535311	-5.3945923161
O39	-1.7541566370	3.2056414681	-4.6273268996
N40	-1.0790217722	1.4599946090	-5.9653725219
C41	-0.1835450468	0.8226342036	-6.8107918153
N42	-0.5439195576	-0.3674058251	-7.3385953140
N43	0.9795552166	1.3508538040	-7.1539371233
C44	1.1887018620	2.5569950916	-6.6144481964
N45	1.6542141086	-4.4471629710	-4.9444220545
C46	2.0444964312	-3.3139623431	-5.6309865914
N47	1.5169723812	-2.2221205490	-5.1387913457
C48	0.7640718332	-2.6561387656	-4.0591480853
C49	-0.1327435664	-1.9682680026	-3.2211349710
O50	-0.4284278968	-0.7350872064	-3.3003373629
N51	-0.7376696054	-2.7868812681	-2.2779241501

C52	-0.5222872964	-4.1522466032	-2.1798051319
N53	-1.1248096612	-4.8115191658	-1.1787681105
N54	0.2581653811	-4.8301808876	-3.0184536313
C55	0.8529318719	-4.0449153442	-3.9139147703
N56	-3.0297859538	-4.5901629271	-6.0044219875
C57	-1.9604108134	-3.8940391006	-6.5325805309
N58	-1.8611538615	-2.6757315602	-6.0722479819
C59	-2.9268425035	-2.5449527400	-5.1962297716
C60	-3.3423014272	-1.5012233050	-4.3779125694
O61	-2.7406361856	-0.3392472707	-4.2205062357
N62	-4.4996826115	-1.7056267441	-3.6913613296
C63	-5.2091588861	-2.8939973573	-3.7466211800
N64	-6.3423975257	-2.9738486022	-3.0501889133
N65	-4.8037485928	-3.9482107788	-4.4717777831
C66	-3.6940002930	-3.7303572771	-5.1607534430
N67	-5.2727861903	-4.2351631005	1.3885781059
C68	-4.5432755436	-4.8774570240	0.4157190113
N69	-3.6611304872	-4.0844785834	-0.1407008642
C70	-3.8120372915	-2.8690055464	0.5031749243
C71	-3.1256223792	-1.6325827195	0.3187901904
O72	-2.2304707792	-1.3607901177	-0.4959689709
N73	-3.5876263581	-0.6521854643	1.2077646893
C74	-4.5804640110	-0.8404771059	2.1486605860
N75	-4.9060932268	0.2090378051	2.9226756057
N76	-5.2390392484	-1.9868320350	2.3070708506
C77	-4.8116961897	-2.9428009222	1.4700807579
N78	-8.1317858882	-0.3501629234	0.8725779075
C79	-7.9896760512	-1.4261859615	0.0294675206
N80	-7.1205348444	-1.1998217561	-0.9253463315
C81	-6.6700418032	0.0899215449	-0.6957418613
C82	-5.6956792824	0.8709755251	-1.3757978416
O83	-5.0140881165	0.5823114930	-2.3746713812
N84	-5.5335407191	2.1263022138	-0.7706659199
C85	-6.2352136530	2.5835061099	0.3295937614
N86	-5.9899743135	3.8404311453	0.7442241096
N87	-7.1454648192	1.8577652659	0.9596925943
C88	-7.3006334952	0.6406025675	0.4214999030
H89	2.8665988210	5.2485220895	-5.9656930287
H90	-1.1015689898	-1.0420989960	-6.8076576140
H91	0.2142810145	-0.7978570006	-7.8535141540
H92	-1.9233679226	0.9695496817	-5.6710731349
H93	-4.8203937749	-0.8902078573	-3.0964488251
H94	-3.8250994926	6.8084909812	1.8142563752
H95	-1.3692987267	4.6390259600	-3.7192213761
H96	0.7054106251	7.4919987980	-3.4405590152
H97	0.3977037217	5.9990562224	-4.3270910304

H98	-4.7009629182	-5.9191231695	0.1719233452
H99	-4.3341109328	1.0606348157	2.9986242360
H100	-5.5767962053	0.0176172471	3.6526786479
H101	-3.1606279846	0.2813941453	1.0759709368
H102	-8.5524348340	-2.3388353012	0.1663536750
H103	-4.7936225545	2.6977674409	-1.1732463537
H104	-5.1642425055	4.3701272044	0.4566664651
H105	-6.4449843280	4.1009518981	1.6073473730
H106	-1.2972526108	-4.3429667670	-7.2596663517
H107	-6.8200986436	-3.8635774733	-3.0910005122
H108	-6.6256225193	-2.2860841523	-2.3262638177
H109	-0.9727312420	-5.8115572026	-1.1960320436
H110	-2.0194837626	-4.4853460017	-0.7783381945
H111	-1.3456467415	-2.3105731090	-1.5700556466
H112	2.7188312377	-3.3632639059	-6.4755783650
H113	2.3557354630	-0.5013459990	-4.7519131838
H114	3.9587820764	0.1504974957	-4.9377268998
H115	0.9059242477	0.6658573443	-3.2079051736
H116	3.8836026498	6.0855423874	-1.3693157672
H117	-3.9363569082	3.2985753891	5.2543036381
H118	-0.4368494452	3.1984629147	-0.1673919907
H119	1.1804229870	4.9799158224	-0.0474414415
H120	1.1519116276	5.9531289721	1.3978855071
H121	-1.7921413752	-0.4551112633	-3.7909730259
H122	-8.7467601544	-0.2830931541	1.6723137594
H123	-1.8970629203	8.1524114645	0.8025807839
H124	3.1449494590	3.0637574571	-7.2661787883
H125	-3.3237380833	-5.5290426917	-6.2419525894
H126	5.1815978578	4.4812146555	-2.8837155305
H127	-2.0850190964	5.0500260194	5.0053258160
H128	1.9768495109	-5.3931889269	-5.1020998200
H129	-5.9748741357	-4.6462295830	1.9892302710
H130	-2.7789488039	3.2211870691	-3.0796325228

Single point energy: -4342.6598464

(2G4-2H⁺)_c

N1	-2.3337859404	4.3758371482	4.2935780207
C2	-3.0945223174	3.2275670485	4.3717358415
N3	-2.7135914719	2.3020612428	3.5312679674
C4	-1.6352785269	2.8591561734	2.8621455482
C5	-0.7952705565	2.4005810971	1.8511997750
O6	-0.9028416595	1.2131919282	1.2968893833
N7	0.1773434720	3.2629842008	1.4500944214
C8	0.3528165951	4.5286679492	1.9870585928
N9	1.3714709042	5.2438881572	1.5087276065
N10	-0.4354225519	5.0173545446	2.9444866500

C11	-1.3794655179	4.1668153254	3.3346520989
N12	-2.3107859963	7.3328370077	0.3775780091
C13	-3.6607127549	7.2068004196	0.6690927849
N14	-4.2532188208	6.3020994004	-0.0666183557
C15	-3.2541947382	5.8212198147	-0.8929425817
C16	-3.3137017616	4.8389812398	-1.9254348472
O17	-4.2773439446	4.1723936288	-2.3112580342
N18	-2.0457965816	4.6704868389	-2.5314780337
C19	-0.8868714642	5.3303624331	-2.1700318492
N20	0.2351122778	5.0282939241	-2.8500669229
N21	-0.8359529837	6.2347212283	-1.2041713869
C22	-2.0350703406	6.4465909804	-0.6293058572
N23	4.2212141418	4.3458369878	-2.5964219753
C24	3.6676533546	5.0305184114	-1.5360485328
N25	2.7831622564	4.3107108529	-0.8854512004
C26	2.7696982308	3.0859155849	-1.5410350341
C27	1.9966062842	1.9122730993	-1.3401269654
O28	1.1281157108	1.7386988844	-0.4470465588
N29	2.2887004015	0.9133834169	-2.2580110385
C30	3.2451338698	1.0220305613	-3.2543242974
N31	3.4763710139	-0.0359611840	-4.0353417680
N32	3.9632679288	2.1233278224	-3.4670339903
C33	3.6762905909	3.0920701116	-2.6036660539
N34	2.3242139919	3.3108369943	-6.7294219966
C35	1.7555993046	3.9972916265	-5.6852905931
N36	0.8412385839	3.2965708868	-5.0594547000
C37	0.7993685681	2.0900014846	-5.7309220345
C38	-0.0328569594	0.9486816101	-5.5347722599
O39	-0.8942773975	0.7946152284	-4.6567350395
N40	0.2213983772	-0.0540760788	-6.4843370779
C41	1.1721349500	0.0352742166	-7.4789233891
N42	1.3312092980	-1.0686461572	-8.2739711551
N43	1.9421581235	1.0866654828	-7.6683801497
C44	1.7164122153	2.0771605905	-6.7802187871
N45	1.6542139718	-4.4471629761	-4.9444219735
C46	2.2437737659	-3.2539885676	-5.2848260479
N47	1.9226564901	-2.2981931788	-4.4490568470
C48	1.0984108921	-2.8904652366	-3.5114272567
C49	0.4805060969	-2.3479551344	-2.3445098118
O50	0.5609558511	-1.1948145850	-1.8957897566
N51	-0.2842459876	-3.3154547959	-1.6768543254
C52	-0.4056652317	-4.6367912045	-2.0627789777
N53	-1.1419810676	-5.4415086940	-1.2759130409
N54	0.1802930630	-5.1458633014	-3.1444150501
C55	0.9156981457	-4.2394035416	-3.8023550551
N56	-3.0297860215	-4.5901629794	-6.0044219677

C57	-1.9019358819	-3.8952957161	-6.4042405810
N58	-1.8440692373	-2.6724052547	-5.9384739536
C59	-3.0030445975	-2.5476067361	-5.1769021690
C60	-3.5467663759	-1.5009070058	-4.4213139189
O61	-3.0926694064	-0.3081299770	-4.2023476842
N62	-4.7472907823	-1.7588768267	-3.8274606470
C63	-5.3966912463	-2.9726357666	-3.9062184379
N64	-6.5539116549	-3.0847546246	-3.2432201883
N65	-4.9177898424	-4.0032122303	-4.6080416150
C66	-3.7610576499	-3.7394790421	-5.2118858942
N67	-5.2727860670	-4.2351632305	1.3885779659
C68	-4.4596140021	-4.9729790294	0.5571538090
N69	-3.3260954909	-4.3660555718	0.3108043527
C70	-3.3937817595	-3.1808643020	1.0211996032
C71	-2.4538335445	-2.1145225661	1.1410353481
O72	-1.3469862802	-1.9779399060	0.6105180270
N73	-2.9469808913	-1.1122200219	2.0058037938
C74	-4.1707927585	-1.1253402646	2.6467900355
N75	-4.4498505879	-0.0851747504	3.4544412652
N76	-5.0503950804	-2.1039614082	2.5107106603
C77	-4.6033127779	-3.0848732158	1.7075642980
N78	-8.1317859517	-0.3501629927	0.8725779532
C79	-8.0226435943	-1.4711811588	0.0779799948
N80	-7.3207115251	-1.2527478686	-1.0075465467
C81	-6.9540585904	0.0815519408	-0.9218012343
C82	-6.1854763493	0.8903704375	-1.8057636462
O83	-5.6460164185	0.5694672424	-2.8782279952
N84	-6.0617229827	2.2018529092	-1.3336089777
C85	-6.6074488751	2.6809089634	-0.1613169538
N86	-6.3899791096	3.9759504337	0.1332193994
N87	-7.3186080712	1.9306945419	0.6740939601
C88	-7.4555898822	0.6659420840	0.2425059726
H89	2.0442496723	5.0099777500	-5.4391478933
H90	0.5210949287	-1.6536057553	-8.4346394420
H91	1.8922196599	-0.8957893383	-9.0997261646
H92	-0.3017200972	-0.9257015538	-6.3498876377
H93	-5.1997401766	-0.9259834400	-3.3551117007
H94	-4.1367766190	7.8152455543	1.4263408990
H95	-2.0132522775	3.9721330323	-3.2685992501
H96	1.0901309199	5.3616359772	-2.4280191925
H97	0.2936549539	4.2607816654	-3.5272250755
H98	-4.7553528810	-5.9401409973	0.1745794096
H99	-3.8589557610	0.7462307432	3.4787990066
H100	-5.3759360729	-0.0617940066	3.8536739523
H101	-2.3256134593	-0.3155269878	2.1139937868
H102	-8.4889308541	-2.4082371410	0.3490374215

H103	-5.4775766570	2.8338333025	-1.8917147171
H104	-5.7999578461	4.5951732730	-0.4126310718
H105	-6.8071647071	4.3347390729	0.9781083559
H106	-1.1593993839	-4.3542706208	-7.0424361469
H107	-7.0230562037	-3.9768231919	-3.3092905971
H108	-6.8609978623	-2.4084455169	-2.5264540479
H109	-1.2506128506	-6.3880492830	-1.6120717760
H110	-1.8538251014	-5.0657358140	-0.6351267849
H111	-0.7172294551	-2.9808385898	-0.7991461055
H112	2.8867666619	-3.1501970067	-6.1477152017
H113	2.8517353343	-0.8569162414	-4.1178152322
H114	4.1625847799	0.1173523374	-4.7612476671
H115	1.7053654744	0.0506763176	-2.1851157657
H116	3.9556815464	6.0442379986	-1.2928813536
H117	-3.9154804342	3.1379641573	5.0704828135
H118	0.7820587428	2.9069334543	0.6675187946
H119	1.8976572270	4.9473301085	0.6722160997
H120	1.4685353385	6.1871268704	1.8566980406
H121	-2.1562848516	-0.0835811526	-4.5260220999
H122	-8.6484126342	-0.2680803572	1.7376154053
H123	-1.6602893142	7.9936613431	0.7796892740
H124	3.0331495636	3.6451844635	-7.3692105299
H125	-3.2831202243	-5.5397348943	-6.2439874145
H126	4.9779980869	4.6595886608	-3.1900165071
H127	-2.4246082734	5.2076110666	4.8629603486
H128	1.8005402665	-5.3442282883	-5.3882157582
H129	-6.1668132097	-4.5169228772	1.7673078670
H130	-0.2365334259	1.0497674414	0.5740628715

Single point energy: -4342.6593353

(2G4-2H⁺)₄

N1	-2.3337859141	4.3758368975	4.2935778291
C2	-3.4741660310	3.5946889112	4.2527380564
N3	-3.5272382594	2.8380923358	3.1861453093
C4	-2.3502239649	3.1096427025	2.5065373888
C5	-1.9242760457	2.7436557715	1.2129517801
O6	-2.5766837358	2.0598546181	0.3732535335
N7	-0.6763482810	3.2716106495	0.8825356054
C8	0.0279308430	4.1637150001	1.6761354972
N9	1.2186324243	4.5956280260	1.2406286438
N10	-0.4230342331	4.6102207361	2.8449966398
C11	-1.5858667552	4.0584229393	3.1942673662
N12	-2.3107860464	7.3328368035	0.3775779457
C13	-3.2055256327	6.5337935988	1.0629382176
N14	-3.4589903752	5.4036549334	0.4568182675
C15	-2.6983968260	5.4537476898	-0.7017070055

C16	-2.5001960977	4.5416579383	-1.7353990288
O17	-2.9856592669	3.3244783602	-1.8293900324
N18	-1.7389095806	4.9809679123	-2.7742290515
C19	-1.1123238454	6.2153917277	-2.7841150395
N20	-0.3943020372	6.5319551162	-3.8660167974
N21	-1.2077593530	7.0861935626	-1.7717805452
C22	-1.9948559360	6.6744294750	-0.7869785937
N23	4.2212138023	4.3458368089	-2.5964218976
C24	3.5260178379	5.0738513712	-1.6578847562
N25	2.3827602816	4.5150017077	-1.3477270691
C26	2.3288915397	3.3600578480	-2.1072764751
C27	1.3165132037	2.3596245822	-2.1938459086
O28	0.2352929064	2.3010578172	-1.5903855456
N29	1.6726783666	1.3505596275	-3.1112380862
C30	2.8495204160	1.3174627555	-3.8376564751
N31	3.0561447044	0.2733330729	-4.6581424992
N32	3.7849193776	2.2593095843	-3.7618732631
C33	3.4716664086	3.2325809040	-2.8936359154
N34	2.3242137902	3.3108368652	-6.7294219154
C35	2.0855910577	4.4682110572	-6.0247093668
N36	0.8897060701	4.4867105664	-5.4870941133
C37	0.3160878638	3.2847103477	-5.8635347545
C38	-0.9437701176	2.7141868747	-5.5255638152
O39	-1.8420990009	3.1760582023	-4.8082797035
N40	-1.1018746500	1.4472517722	-6.1210739961
C41	-0.1661458923	0.8067395759	-6.9115388691
N42	-0.5034302027	-0.3961651948	-7.4403125570
N43	1.0112058541	1.3318433027	-7.2029434278
C44	1.1928550385	2.5436505483	-6.6540822183
N45	1.6542140105	-4.4471628810	-4.9444219123
C46	2.0868363441	-3.3259559014	-5.6264215804
N47	1.5616545568	-2.2218143945	-5.1601672974
C48	0.7663678300	-2.6337764697	-4.1033387765
C49	-0.1627181106	-1.9238867953	-3.3163212232
O50	-0.4485179753	-0.6956674225	-3.4234165710
N51	-0.8140491346	-2.7304752182	-2.3868325084
C52	-0.6189358869	-4.0974809867	-2.2664391584
N53	-1.2685440096	-4.7408345508	-1.2816682454
N54	0.1866362661	-4.7913191929	-3.0637445002
C55	0.8273963163	-4.0215691444	-3.9440800490
N56	-3.0297859281	-4.5901627251	-6.0044219034
C57	-1.9417177647	-3.8956565836	-6.4966834648
N58	-1.8623502075	-2.6728482313	-6.0435673654
C59	-2.9622990537	-2.5378932365	-5.2111786260
C60	-3.4196561857	-1.4836981382	-4.4255361832
O61	-2.8441823808	-0.3160528413	-4.2472424240

N62	-4.6132957022	-1.6826761713	-3.8027833360
C63	-5.3109037629	-2.8757953431	-3.8670834180
N64	-6.4749319071	-2.9448029877	-3.2160264864
N65	-4.8690994735	-3.9386825437	-4.5534281450
C66	-3.7291394108	-3.7234120106	-5.1968037212
N67	-5.2727858537	-4.2351628641	1.3885779772
C68	-4.6198937456	-4.8467313567	0.3445047807
N69	-3.8340903522	-4.0191472951	-0.2991095603
C70	-3.9689434708	-2.8097729353	0.3592353434
C71	-3.3515314101	-1.5492753438	0.1054812484
O72	-2.5458473457	-1.2481008579	-0.7869887965
N73	-3.7711205962	-0.5779813526	1.0332202849
C74	-4.6646471886	-0.7999701473	2.0649146974
N75	-4.9642075661	0.2397503446	2.8641293649
N76	-5.2487277214	-1.9732936846	2.2901201917
C77	-4.8629514570	-2.9214056739	1.4214174031
N78	-8.1317858604	-0.3501629051	0.8725778766
C79	-8.0267213349	-1.4301342620	0.0266393303
N80	-7.2508706185	-1.1859808873	-1.0021673956
C81	-6.8302538126	0.1205818307	-0.8207674374
C82	-5.9441947157	0.9238734673	-1.5914945279
O83	-5.3444045915	0.6431390214	-2.6390988909
N84	-5.7728071076	2.1944021638	-1.0109246758
C85	-6.3657035042	2.6305882300	0.1582799729
N86	-6.1033229013	3.9003516241	0.5605005787
N87	-7.1960385041	1.8855189924	0.8657958550
C88	-7.3783238113	0.6625336488	0.3411952903
H89	2.8240380207	5.2537194406	-5.9466661877
H90	-1.0625377632	-1.0574203401	-6.8965415853
H91	0.2806231526	-0.8327239696	-7.9092460991
H92	-1.9747844960	0.9784717458	-5.8893704803
H93	-4.9881566900	-0.8563034932	-3.2646221133
H94	-3.6389866307	6.8485205599	2.0026140238
H95	-1.6577169114	4.3247840374	-3.5948029731
H96	0.0839899542	7.4216401415	-3.8194958666
H97	-0.0184086765	5.8139519724	-4.5085345279
H98	-4.7580837863	-5.8946694259	0.1158147410
H99	-4.4849780111	1.1450989899	2.8502298410
H100	-5.5607869135	0.0304756560	3.6511611485
H101	-3.3780961310	0.3596565406	0.8804876765
H102	-8.5436359552	-2.3597035784	0.2198127404
H103	-5.1303377236	2.8031494656	-1.5134838574
H104	-5.1796973524	4.3111058579	0.4120999325
H105	-6.4991091782	4.1041272108	1.4696693127
H106	-1.2501198166	-4.3494079292	-7.1937121965
H107	-6.9472723435	-3.8374009012	-3.2562239987

H108	-6.7642661462	-2.2668521667	-2.4909366808
H109	-1.1299544251	-5.7431265780	-1.2916526670
H110	-2.1811574593	-4.4096638110	-0.9345628428
H111	-1.4712148652	-2.2466588049	-1.7404106973
H112	2.7879828481	-3.3937069618	-6.4475197483
H113	2.3811181124	-0.4654588878	-4.8668588689
H114	3.9190906312	0.2884853130	-5.1813087180
H115	0.9701652108	0.6096629060	-3.2315303229
H116	3.9132516851	5.9945972951	-1.2435874112
H117	-4.2171908978	3.6305780308	5.0380859467
H118	-0.2697199685	2.9601897961	-0.0215587613
H119	1.5445225783	4.5314364321	0.2644346749
H120	1.6733868466	5.2655254869	1.8455517532
H121	-1.8743559233	-0.4104451295	-3.9055400455
H122	-8.6791861253	-0.2951751091	1.7210160528
H123	-2.0009111218	8.2616385860	0.6336439742
H124	3.1653929014	3.0735245201	-7.2377827643
H125	-3.3157145055	-5.5296932785	-6.2491944876
H126	5.1427518792	4.5489931924	-2.9605272061
H127	-2.0456539213	4.9903654045	5.0439935048
H128	1.9665235476	-5.3996525562	-5.0832052935
H129	-5.9009714023	-4.6717267089	2.0503330981
H130	-2.8233274622	2.7717244817	-0.9721684990

Single point energy: -4342.6556067

(2G4-2H⁺)_d

N1	-2.3337859962	4.3758369764	4.2935779738
C2	-3.2544016664	3.3659748347	4.4778466357
N3	-3.2828079585	2.5295213393	3.4687512554
C4	-2.3230366883	3.0082814927	2.5891545075
C5	-1.9119049771	2.5325348192	1.3136170427
O6	-2.3495692391	1.5485848581	0.6953953513
N7	-0.8971986115	3.3285750979	0.7596317549
C8	-0.3696222226	4.4589129545	1.3510368406
N9	0.5727849265	5.1474201014	0.6854450208
N10	-0.7629170829	4.9172393495	2.5366871066
C11	-1.7159044945	4.1566505792	3.0910695638
N12	-2.3107859758	7.3328369761	0.3775779649
C13	-3.3048058366	6.5576577767	0.9491345480
N14	-3.6723640443	5.5408709461	0.2089106881
C15	-2.8702144733	5.6428535259	-0.9249245760
C16	-2.7405246221	4.8642419062	-2.0816310036
O17	-3.3736841818	3.7904017169	-2.4434918992
N18	-1.8190191775	5.2990797095	-2.9868934390
C19	-1.0239071246	6.4109677108	-2.7993226759
N20	-0.1584440434	6.7135397483	-3.7747077911

N21	-1.1069741024	7.1828855804	-1.7129456448
C22	-2.0156449351	6.7651252697	-0.8372796647
N23	4.2212139772	4.3458369814	-2.5964219926
C24	3.3791171319	5.2308733914	-1.9559757901
N25	2.2139771122	4.6992169607	-1.6801457956
C26	2.2946906839	3.4023475731	-2.1522985650
C27	1.3283712975	2.3520719008	-2.1169857632
O28	0.1786417555	2.3600247662	-1.6642886229
N29	1.8484127421	1.1743963310	-2.6944321800
C30	3.1225713170	1.0286781183	-3.2119290055
N31	3.4427924057	-0.1904693887	-3.6866744672
N32	4.0070864031	2.0130688649	-3.2601371836
C33	3.5438415928	3.1550701804	-2.7200932793
N34	2.3242149994	3.3108370369	-6.7294219365
C35	2.1988891853	4.4651872042	-5.9866424821
N36	0.9805836505	4.6408794369	-5.5366016568
C37	0.2690512990	3.5524496939	-6.0131436346
C38	-1.0970912081	3.1890652489	-5.8365097987
O39	-1.9828361335	3.7742678163	-5.1917012088
N40	-1.3993756199	1.9977933762	-6.5045529274
C41	-0.5118459747	1.2482701807	-7.2538999260
N42	-1.0099445222	0.1528552510	-7.8549324809
N43	0.7668838748	1.5732332714	-7.4061224639
C44	1.0874932410	2.7128108386	-6.7714726611
N45	1.6542140055	-4.4471629905	-4.9444210010
C46	2.1689597177	-3.1817756651	-4.7979672672
N47	1.5843464394	-2.5063789859	-3.8390575091
C48	0.6308321731	-3.3747051198	-3.3343525866
C49	-0.3369998001	-3.2052836730	-2.3073824935
O50	-0.5264802138	-2.1765249190	-1.6343415650
N51	-1.1126272921	-4.3563739684	-2.1079505623
C52	-0.9754569100	-5.5225120567	-2.8307312877
N53	-1.8338964951	-6.5387732944	-2.5261571100
N54	-0.1013140520	-5.6848377059	-3.8023124399
C55	0.6610439660	-4.5936210558	-4.0117169639
N56	-3.0297860603	-4.5901629791	-6.0044218712
C57	-2.5031128135	-4.0961315248	-7.1883449619
N58	-2.5767104184	-2.7935273197	-7.2731384661
C59	-3.1899935138	-2.4079071101	-6.0956608678
C60	-3.5530750193	-1.1065851297	-5.6370933314
O61	-3.4003608601	-0.0161146555	-6.1986468641
N62	-4.1592158840	-1.1655675298	-4.3612359209
C63	-4.3751266831	-2.3154833798	-3.6319781725
N64	-4.9092667745	-2.1739974216	-2.3918078043
N65	-4.0474271188	-3.5220914919	-4.0621672055
C66	-3.4751139866	-3.5082713066	-5.2861998011

N67	-5.2727859888	-4.2351629804	1.3885780090
C68	-4.4234951454	-4.8515973214	0.4865384808
N69	-3.4266208294	-4.0899605803	0.1069249879
C70	-3.6203250909	-2.9005510777	0.8015869585
C71	-2.9230586468	-1.6823029998	0.8329744922
O72	-1.8382491137	-1.3182500893	0.2455119181
N73	-3.4664925662	-0.7178901839	1.6328523498
C74	-4.5869086050	-0.9031816940	2.4143714246
N75	-4.9681635298	0.1321200250	3.1691698911
N76	-5.2777140900	-2.0468467279	2.4257728554
C77	-4.7715501753	-2.9743847540	1.6136471731
N78	-8.1317859280	-0.3501630367	0.8725779058
C79	-7.6492088552	-1.0177343109	-0.2318143930
N80	-6.7202124103	-0.3452627967	-0.8672918644
C81	-6.5901005074	0.8335765983	-0.1523967272
C82	-5.7518072460	1.9721957976	-0.3754234745
O83	-4.9448776193	2.1494964538	-1.2950318475
N84	-5.9391179838	2.9547161342	0.6175838342
C85	-6.8465278020	2.8663235192	1.6517382953
N86	-6.8784132690	3.9131386525	2.5303199799
N87	-7.6352724439	1.8295225688	1.8496230604
C88	-7.4640540460	0.8516621201	0.9347558369
H89	3.0346998350	5.1300710053	-5.8192570786
H90	-1.9266644196	-0.2083890724	-7.6021339628
H91	-0.3606128593	-0.4532614392	-8.3324636658
H92	-2.3389726083	1.6245037360	-6.3585188683
H93	-4.4091539790	-0.2649973324	-3.9625147801
H94	-3.7125951202	6.7993725338	1.9211178026
H95	-1.7667778634	4.7445257736	-3.8855377556
H96	0.4452274465	7.5012151488	-3.5841878895
H97	0.1696118171	6.0116287279	-4.4578800662
H98	-4.6026794679	-5.8639912198	0.1499658235
H99	-4.3905836282	0.9830274299	3.2786018645
H100	-5.7806447650	0.0000555851	3.7541855424
H101	-3.0538581052	0.2405923938	1.4756130555
H102	-8.0275469066	-1.9893872753	-0.5191673368
H103	-5.3109399188	3.7616728378	0.5577015231
H104	-6.6101666383	4.8283168184	2.1931120565
H105	-7.6799642984	3.9069771319	3.1488262665
H106	-2.0896689480	-4.7540710222	-7.9410710337
H107	-5.1693023546	-3.0520847313	-1.9655513709
H108	-5.4610853161	-1.3609505009	-2.1039147688
H109	-1.5716856962	-7.4386967183	-2.9080132021
H110	-2.2450142773	-6.5635501840	-1.6033731731
H111	-1.8711881106	-4.2825108787	-1.4184756825
H112	2.9695233892	-2.8165771527	-5.4270754136

H113	2.8088765949	-0.9854408369	-3.5845507631
H114	4.4101889005	-0.3399543302	-3.9323694575
H115	1.2247548904	0.3710767732	-2.6652599394
H116	3.6850788972	6.2408331026	-1.7192931785
H117	-3.8667037069	3.3043552909	5.3668498835
H118	-0.5213616427	3.0078092055	-0.1481535454
H119	0.9926855786	4.8959497943	-0.2153995489
H120	0.9848310880	5.9184816465	1.1905860174
H121	-8.8719329070	-0.6481113321	1.4941708115
H122	-1.8763200242	8.1585159338	0.7671817205
H123	3.1527528375	2.9809546555	-7.2057822289
H124	-3.0950278766	-5.5575341848	-5.7187198958
H125	5.1820383908	4.5079077659	-2.8679040871
H126	-2.0901978769	5.0993991699	4.9571785372
H127	1.9503627156	-5.1523090243	-5.6069928059
H128	-6.0663036740	-4.6495607071	1.8600288446
H129	-3.9870056754	3.3451037149	-1.7787388471
H130	-1.4293336573	-1.8841049476	-0.5150433077

Single point energy: -4342.6513358

(2G4-2H⁺)_e

N1	-2.3337860000	4.3758370000	4.2935780001
C2	-3.3983248679	3.4973927742	4.3500382319
N3	-3.4535607749	2.7062406623	3.3073166152
C4	-2.3507019482	3.0631903283	2.5441160723
C5	-1.9663390416	2.6946587195	1.2391974870
O6	-2.5989490848	1.9367960356	0.4513709113
N7	-0.7900290472	3.3176788560	0.8234937048
C8	-0.1451654023	4.3207391773	1.5244429978
N9	0.9444647866	4.8795315384	0.9765826457
N10	-0.5633007134	4.7598094899	2.7075956402
C11	-1.6351386100	4.1001547662	3.1529093313
N12	-2.3107860010	7.3328370006	0.3775780001
C13	-3.2229981998	6.5590644056	1.0676661770
N14	-3.4918721360	5.4224884006	0.4785829496
C15	-2.7225802788	5.4417812576	-0.6772254625
C16	-2.5207950968	4.5117033034	-1.6939765493
O17	-3.0332735555	3.2994599570	-1.7838423470
N18	-1.7376031350	4.9139774185	-2.7278438174
C19	-1.1026239238	6.1440075295	-2.7559838205
N20	-0.3773246809	6.4410216175	-3.8354675023
N21	-1.1988847813	7.0347577182	-1.7578533430
C22	-1.9983505188	6.6504223074	-0.7750871752
N23	4.2212140001	4.3458369999	-2.5964219999
C24	3.3827614679	5.2216015691	-1.9401309907
N25	2.2394097522	4.6700784247	-1.6142310157

C26	2.3313576802	3.3672498954	-2.0718217753
C27	1.3909569814	2.2989843001	-1.9961011310
O28	0.2503860432	2.2899210284	-1.5096738106
N29	1.9098027539	1.1253868548	-2.5710299163
C30	3.1723097190	0.9944949040	-3.1234439031
N31	3.5068989068	-0.2272382640	-3.5711366003
N32	4.0341578121	1.9977298824	-3.2148593499
C33	3.5663748228	3.1377765023	-2.6792432378
N34	2.3242150002	3.3108369994	-6.7294220000
C35	2.0817661082	4.4523217260	-5.9998558915
N36	0.9136094638	4.4225139666	-5.4060379541
C37	0.3582432174	3.2069853946	-5.7704428985
C38	-0.8854872949	2.6095316427	-5.4127002878
O39	-1.7644958647	3.0613481632	-4.6596753999
N40	-1.0546474149	1.3595854628	-6.0254939434
C41	-0.1438592265	0.7696392771	-6.8803621040
N42	-0.4722845693	-0.4083203517	-7.4377751706
N43	1.0325377661	1.3105060265	-7.1901345199
C44	1.2185627117	2.5039019477	-6.6124132520
N45	1.6542140000	-4.4471630002	-4.9444210001
C46	2.2844398925	-3.2550545142	-4.6855309545
N47	1.6715321626	-2.5446172397	-3.7700768723
C48	0.5770969164	-3.3121632350	-3.4049863909
C49	-0.4800956041	-3.0634386287	-2.4815745459
O50	-0.6209680506	-2.0568221839	-1.7586514980
N51	-1.4043345082	-4.1122501743	-2.4416802308
C52	-1.3488779571	-5.2413455755	-3.2327041598
N53	-2.3830325405	-6.1237408340	-3.0636423341
N54	-0.3743621349	-5.4881380613	-4.0838948545
C55	0.5519645052	-4.5084059531	-4.1252610330
N56	-3.0297859998	-4.5901630002	-6.0044220003
C57	-2.2123273861	-3.8678206995	-6.8512648974
N58	-2.2590753078	-2.5832111010	-6.6050658159
C59	-3.1575048736	-2.4534678995	-5.5627867025
C60	-3.6225396229	-1.2839393552	-4.8823782169
O61	-3.2992106017	-0.1106395082	-5.0593285738
N62	-4.5808550872	-1.6233246735	-3.8962212502
C63	-5.0012180526	-2.8981382616	-3.5986536009
N64	-5.9187716525	-3.0561873302	-2.6258573922
N65	-4.5291275783	-3.9912208871	-4.1985422224
C66	-3.6536788503	-3.6945618306	-5.1789085489
N67	-5.2727860000	-4.2351630000	1.3885780000
C68	-4.4760526159	-4.8016919836	0.4012240286
N69	-3.6212540693	-3.9632110089	-0.1269075392
C70	-3.8450341692	-2.7715218954	0.5490352404
C71	-3.2886509550	-1.4911234597	0.4245064772

O72	-2.3897612869	-1.0264905097	-0.3744846491
N73	-3.7959132859	-0.5495526431	1.2829399759
C74	-4.7566283770	-0.8159044355	2.2403054234
N75	-5.0935482159	0.1902485345	3.0547483019
N76	-5.3353630382	-2.0114723155	2.3646209512
C77	-4.8677888200	-2.9246755704	1.5122705803
N78	-8.1317859995	-0.3501629997	0.8725780001
C79	-8.0214054299	-1.3938045054	-0.0136089893
N80	-7.2336837208	-1.1036356852	-1.0185861410
C81	-6.8217340805	0.1945555844	-0.7862866302
C82	-5.9328655614	1.0277483028	-1.5312317930
O83	-5.3113877637	0.7780060493	-2.5630906295
N84	-5.7987911109	2.2918173763	-0.9088415501
C85	-6.4044745634	2.6817437489	0.2677251549
N86	-6.1660358075	3.9451952066	0.7028873046
N87	-7.2167929243	1.8987261867	0.9575230771
C88	-7.3844777087	0.6913821029	0.3854873638
H89	2.7943372386	5.2638434665	-5.9508159293
H90	-1.2392549803	-1.0183806755	-7.1367886029
H91	0.2344828882	-0.8093380743	-8.0368607312
H92	-1.9172631506	0.8505404428	-5.7746084409
H93	-4.9697789265	-0.8120015021	-3.3881495627
H94	-3.6581121822	6.8956759936	1.9989565465
H95	-1.6358803414	4.2228894301	-3.5332314977
H96	0.1069373499	7.3276784384	-3.7922273668
H97	0.0107697173	5.7093940388	-4.4617702086
H98	-4.5775739023	-5.8422407875	0.1233927280
H99	-4.5909972960	1.0877140127	3.0815584287
H100	-5.7821474224	-0.0099307769	3.7656037596
H101	-3.4301102889	0.4109006733	1.1338928590
H102	-8.5418839807	-2.3298263999	0.1338619932
H103	-5.1839200454	2.9332142686	-1.4041379222
H104	-5.2617588889	4.3899241936	0.5351811113
H105	-6.5718622342	4.1343316065	1.6100520027
H106	-1.6198657063	-4.3457366006	-7.6190415170
H107	-6.3408462227	-3.9727325908	-2.5877026600
H108	-6.4284788195	-2.2759523624	-2.1901472533
H109	-2.3116754303	-6.9331510827	-3.6687569931
H110	-3.3129573075	-5.7045676490	-3.0427173168
H111	-2.1448116805	-4.0606853918	-1.7298012601
H112	3.1869141742	-2.9656134465	-5.2069201805
H113	2.8653792280	-1.0222677695	-3.5111113948
H114	4.4476423911	-0.3467317449	-3.9157111599
H115	1.2954991979	0.3151730484	-2.5207938713
H116	3.6740999381	6.2414314663	-1.7286311859
H117	-4.0886077131	3.4923787286	5.1827114198

H118	-0.3853084943	2.9909866791	-0.0766245684
H119	1.2512452469	4.7686759383	0.0024106629
H120	1.3801735066	5.6073271457	1.5254346408
H121	-1.7910505816	-1.6537086535	-0.9425249683
H122	-8.7235498005	-0.3133677198	1.6919445484
H123	-1.9924975976	8.2626705854	0.6184012158
H124	3.1321925664	3.1180977055	-7.3059214626
H125	-3.2113417979	-5.5828559840	-6.0507099289
H126	5.1660446954	4.5263955444	-2.9092272705
H127	-2.0614157305	5.0424764376	5.0044178436
H128	1.9514165833	-5.1680011659	-5.5891430170
H129	-5.9517207002	-4.7060148481	1.9723097826
H130	-2.8942111898	2.7393676253	-0.9492449304

Single point energy: -4342.6495562

(2G4-2H⁺)₅

N1	-2.3337859998	4.3758369982	4.2935779931
C2	-3.2207027482	3.3339764297	4.4500925360
N3	-3.1656804988	2.4874497915	3.4527321880
C4	-2.1833215957	2.9860514093	2.6130327542
C5	-1.7219186881	2.5283245591	1.3453648795
O6	-2.1389131526	1.5601344078	0.6893143126
N7	-0.6915393695	3.3462505429	0.8465664894
C8	-0.2272720357	4.4957828678	1.4575289378
N9	0.7234479597	5.2093427482	0.8341064651
N10	-0.6935023128	4.9508843327	2.6170512051
C11	-1.6451807770	4.1619352623	3.1297896852
N12	-2.3107860032	7.3328370288	0.3775780205
C13	-3.3194661613	6.7274246344	1.0957297790
N14	-3.7343851484	5.6083393296	0.5520998287
C15	-2.9567721495	5.4675164030	-0.5894817893
C16	-2.8651468679	4.4074175962	-1.5293526794
O17	-3.5060236573	3.3296896155	-1.5519752904
N18	-1.9200000213	4.6524513546	-2.5163114592
C19	-1.1255039755	5.7829592611	-2.5888744582
N20	-0.3077919095	5.8640612822	-3.6521894411
N21	-1.1707220552	6.7588712861	-1.6945436154
C22	-2.0688294317	6.5423655435	-0.7222662127
N23	4.2212140000	4.3458370044	-2.5964220002
C24	3.4887363636	5.1467806579	-1.7485537271
N25	2.3173970236	4.6303249724	-1.4724546598
C26	2.2848054857	3.4258540232	-2.1519868198
C27	1.2569910265	2.4379738774	-2.2328534564
O28	0.1290971163	2.4663185554	-1.7197088850
N29	1.6607457493	1.3397344777	-3.0125408169
C30	2.8609828284	1.2541414042	-3.6897819548

N31	3.0766335192	0.1647341660	-4.4482372074
N32	3.8029992467	2.1932458317	-3.6476300979
C33	3.4679773626	3.2247746348	-2.8575997862
N34	2.3242139502	3.3108370227	-6.7294219870
C35	1.6447514094	4.1200522721	-5.8546672688
N36	0.5176062514	3.5936740599	-5.4417309476
C37	0.4517131289	2.3648384024	-6.0832612807
C38	-0.4792092102	1.2911262836	-5.9748958006
O39	-1.4966116787	1.2504012798	-5.2576434516
N40	-0.1323014794	0.2022081021	-6.7882777903
C41	0.9800168929	0.1555272947	-7.6033626094
N42	1.1644676421	-0.9866453587	-8.3295737730
N43	1.8634899470	1.1261156009	-7.6877435218
C44	1.5713875500	2.1769279585	-6.8977240813
N45	1.6542139987	-4.4471630014	-4.9444219996
C46	2.0006439205	-3.2723901421	-5.5754614244
N47	1.4824555709	-2.2225778963	-4.9850129405
C48	0.7757388575	-2.7340709822	-3.9099843340
C49	0.0080936359	-2.0666337335	-2.9092467969
O50	-0.2111528577	-0.8514870858	-2.8043995370
N51	-0.5294647874	-2.9853778853	-1.9866517860
C52	-0.3404458113	-4.3535237915	-2.0257331960
N53	-0.8701347758	-5.0820195768	-1.0244412230
N54	0.3450707503	-4.9771885602	-2.9790825514
C55	0.8794078350	-4.1220332164	-3.8608494634
N56	-3.0297860969	-4.5901630080	-6.0044219900
C57	-2.1425734406	-3.7832561337	-6.7020750537
N58	-2.0861008788	-2.5540567939	-6.2553228435
C59	-2.9848132573	-2.5360774700	-5.1954668003
C60	-3.3915224051	-1.5332998648	-4.3044334947
O61	-3.0742910424	-0.2917768239	-4.1954328769
N62	-4.3249426028	-1.9371469866	-3.3787264656
C63	-4.8677903115	-3.2070280460	-3.3091092054
N64	-5.7933411007	-3.4130939370	-2.3660534342
N65	-4.5068519528	-4.1796645061	-4.1370767356
C66	-3.5867109108	-3.8064800597	-5.0277910538
N67	-5.2727860012	-4.2351629979	1.3885779964
C68	-4.4055512219	-4.9693971356	0.6055474438
N69	-3.3455050216	-4.2802734474	0.2688931254
C70	-3.5107367492	-3.0485750486	0.8741540068
C71	-2.6802671286	-1.8847328502	0.8478612064
O72	-1.6107983221	-1.7144123726	0.2587112248
N73	-3.2477631918	-0.8414640145	1.6057833785
C74	-4.4283351456	-0.9214388072	2.3091272382
N75	-4.8318113175	0.1883546299	2.9651372329
N76	-5.2051705623	-1.9999454875	2.3309091977

C77	-4.6998216945	-3.0050447711	1.5952751619
N78	-8.1317860044	-0.3501630006	0.8725780113
C79	-7.7746603630	-1.3844257746	0.0382962689
N80	-6.7087816977	-1.1278564096	-0.6763169171
C81	-6.3372152388	0.1526205739	-0.2875851148
C82	-5.2893039197	0.9949162072	-0.6376675212
O83	-4.3645786318	0.6758437144	-1.5200574718
N84	-5.2608036925	2.2036000358	-0.0243772340
C85	-6.1987300383	2.6186084263	0.9012027207
N86	-6.0460438544	3.8518411179	1.3913390889
N87	-7.2167800500	1.8468864270	1.2826923149
C88	-7.2302047638	0.6617390440	0.6822533995
H89	2.0331391872	5.0857905896	-5.5615233445
H90	0.3521546344	-1.5365172526	-8.5739335273
H91	1.8627972861	-0.9034443814	-9.0578349636
H92	-0.6975015174	-0.6434490662	-6.6713810876
H93	-4.5815688651	-1.2257278695	-2.6931384642
H94	-3.7050457524	7.1608980740	2.0079690953
H95	-1.7262166389	3.8672086000	-3.1341540750
H96	0.3601106570	6.6206554552	-3.6421769248
H97	-0.1493698072	5.0569303956	-4.2609810942
H98	-4.6089491224	-5.9948034638	0.3280965051
H99	-4.1858068636	0.9669933532	3.1687304157
H100	-5.6078180211	0.0452364414	3.5964475061
H101	-2.7772796559	0.0724466023	1.4842552094
H102	-8.3476724978	-2.3008292590	-0.0012456154
H103	-4.5295061428	2.8658149006	-0.3894175803
H104	-5.2567992307	4.4630038626	1.1346892674
H105	-6.7393218430	4.1743665268	2.0510839711
H106	-1.5697858227	-4.1717870798	-7.5332117093
H107	-6.1842971381	-4.3409575065	-2.2984693845
H108	-6.0994765411	-2.6628065466	-1.7376620492
H109	-0.7532505467	-6.0806749388	-1.1269890866
H110	-1.6871245521	-4.7542178420	-0.4960130592
H111	-0.9761335198	-2.5640553058	-1.1517802047
H112	2.6292816934	-3.2534120283	-6.4548387836
H113	2.4073921015	-0.5968257755	-4.5966235961
H114	3.9825441516	0.1042909354	-4.8889925863
H115	0.9901757094	0.5531915316	-3.0382392586
H116	3.8717703151	6.0853251787	-1.3717855321
H117	-3.8687762060	3.2554685365	5.3121384259
H118	-0.3132910087	3.0604506510	-0.0726626588
H119	1.2056023408	4.9379097435	-0.0325932957
H120	1.0874071473	5.9921163773	1.3576880093
H121	-2.3254395260	0.1490400784	-4.7738285249
H122	-8.9193228237	-0.3245443539	1.5076602579

H123	-1.8434117577	8.2022350635	0.5968391044
H124	3.2145423402	3.4974209060	-7.1716471216
H125	-3.2414101735	-5.5646252041	-6.1759095140
H126	5.1700676536	4.5025103323	-2.9095192123
H127	-2.1463629415	5.1155583664	4.9572414549
H128	1.9740472284	-5.3783822864	-5.1755989145
H129	-6.0928800580	-4.5843560581	1.8664239413
H130	-3.6839512442	1.3893412104	-1.6276751565

Single point energy: -4342.6479694

(2G4-2H⁺)_f

N1	-2.3337860002	4.3758369993	4.2935779997
C2	-3.0510705278	3.2227820071	4.5282485276
N3	-2.7223961252	2.2665107177	3.6996163012
C4	-1.7257720699	2.8062093031	2.9076641679
C5	-1.0779767928	2.2808362200	1.7519133619
O6	-1.2633903498	1.2025674415	1.1853156529
N7	-0.1525922130	3.2160903312	1.2235003423
C8	0.0519243845	4.4956839678	1.6977032356
N9	0.9027323190	5.2911215053	1.0173885271
N10	-0.5823730619	4.9935259983	2.7488183724
C11	-1.4535108125	4.1180988642	3.2800903153
N12	-2.3107859999	7.3328370021	0.3775780001
C13	-3.0928013501	6.5020647472	1.1562022520
N14	-3.1916301674	5.2886338248	0.6842015606
C15	-2.4376268391	5.3040773553	-0.4768091199
C16	-2.0072434117	4.2877696074	-1.3242747095
O17	-2.2868574756	3.0155704852	-1.1659304678
N18	-1.2406949762	4.6898787418	-2.3807570448
C19	-0.8482100829	6.0047171498	-2.5832738432
N20	-0.1555450413	6.2357473232	-3.7076991689
N21	-1.1340900011	6.9792304602	-1.7276421960
C22	-1.8939780536	6.5908143124	-0.7022567770
N23	4.2212140003	4.3458370001	-2.5964219999
C24	3.5089518644	5.1132830612	-1.7020499947
N25	2.3688670931	4.5625892567	-1.3677652088
C26	2.3364789984	3.3603688883	-2.0573108972
C27	1.3379358916	2.3514543155	-2.1219248255
O28	0.2248561549	2.3778825437	-1.5416471896
N29	1.7083970957	1.2783907614	-2.9243304315
C30	2.8849030613	1.2254653430	-3.6532511563
N31	3.0931235758	0.1513869022	-4.4265645218
N32	3.8076358254	2.1888117731	-3.6381575095
C33	3.4909756016	3.2011903778	-2.8254925300
N34	2.3242139992	3.3108369992	-6.7294219995
C35	1.7528402408	4.1222753039	-5.7822123249

N36	0.6372576596	3.6314997333	-5.2903677986
C37	0.4737143378	2.4189962847	-5.9558170451
C38	-0.4821266495	1.3697141414	-5.7887866144
O39	-1.4298791156	1.3334340187	-4.9894261610
N40	-0.2346419955	0.2889442475	-6.6540242414
C41	0.8112301864	0.2196452591	-7.5490365829
N42	0.8994688709	-0.9104020168	-8.3015664326
N43	1.7203481226	1.1637453179	-7.6824868459
C44	1.5177304414	2.2083999443	-6.8587029886
N45	1.6542139998	-4.4471630001	-4.9444219998
C46	2.0315373411	-3.2663275305	-5.5441348492
N47	1.5361918251	-2.2191405227	-4.9286868365
C48	0.8094924226	-2.7399523517	-3.8703716953
C49	0.0679066158	-2.0845509320	-2.8435869014
O50	-0.0959752737	-0.8618048487	-2.6907479770
N51	-0.5045907156	-3.0111072627	-1.9578734015
C52	-0.3613554135	-4.3836779007	-2.0425343943
N53	-0.9228603652	-5.1304125235	-1.0755715485
N54	0.3170188733	-4.9972374699	-3.0096620948
C55	0.8776597221	-4.1316887801	-3.8599692241
N56	-3.0297860005	-4.5901629997	-6.0044220007
C57	-2.1529501862	-3.7663662273	-6.6937149131
N58	-2.1234148620	-2.5347029232	-6.2476009803
C59	-3.0297911192	-2.5351137240	-5.1914685598
C60	-3.4728183583	-1.5471995027	-4.3025413825
O61	-3.2029705036	-0.2826976948	-4.2190350098
N62	-4.3830900350	-1.9596706587	-3.3709242944
C63	-4.9063528120	-3.2348842995	-3.3151709064
N64	-5.8333091740	-3.4714927268	-2.3847678981
N65	-4.5274422579	-4.2054330920	-4.1500569669
C66	-3.6076488185	-3.8175681047	-5.0275934480
N67	-5.2727860000	-4.2351629994	1.3885780005
C68	-4.4729392891	-4.9763282691	0.5453251084
N69	-3.3667987857	-4.3471241790	0.2397358703
C70	-3.4355812894	-3.1475780151	0.9228978256
C71	-2.5099169121	-2.0618070740	0.9813638876
O72	-1.4215212163	-1.9414558398	0.4107666769
N73	-2.9804269510	-1.0388718703	1.8241397542
C74	-4.1679655232	-1.0699042463	2.5248137739
N75	-4.4653183716	0.0030716929	3.2801886008
N76	-5.0317233264	-2.0778453839	2.4694978481
C77	-4.6134860878	-3.0632385044	1.6594941341
N78	-8.1317859989	-0.3501630015	0.8725779996
C79	-7.9836939124	-1.4319509272	0.0370857327
N80	-6.8822407151	-1.3655876769	-0.6702316108
C81	-6.2823898255	-0.1818448828	-0.2735260620

C82	-5.0538900122	0.4123953783	-0.6660866003
O83	-4.2249663587	0.0059679785	-1.4925484373
N84	-4.8219347262	1.6175417769	0.0262287713
C85	-5.6727924275	2.1806768444	0.9576284042
N86	-5.3074797085	3.3496521193	1.5177966822
N87	-6.8187909593	1.6283916133	1.3189246551
C88	-7.0515011603	0.4657313636	0.6913429685
H89	2.2074895535	5.0601252408	-5.4931005449
H90	0.0735721894	-1.4765229161	-8.4366397043
H91	1.5398690371	-0.8573336998	-9.0827604375
H92	-0.8216572387	-0.5406920852	-6.5244137375
H93	-4.5445812861	-1.2612301220	-2.6032683934
H94	-3.5622871492	6.8580103863	2.0628330872
H95	-0.8750641746	3.9688421054	-3.0054620740
H96	0.0740576472	7.1929275247	-3.9337313316
H97	-0.0193337873	5.4915204348	-4.3924973689
H98	-4.7545801731	-5.9631639758	0.2040938375
H99	-3.7859706143	0.7480682074	3.4736435265
H100	-5.2951693602	-0.0751034335	3.8490457738
H101	-2.3904272599	-0.1946024021	1.8156207910
H102	-8.7186846282	-2.2235353260	-0.0107902548
H103	-3.9300414243	2.0594633491	-0.1844362263
H104	-4.5050784508	3.9044290578	1.2233887338
H105	-5.9807397356	3.7614528977	2.1466146798
H106	-1.5655342115	-4.1440328916	-7.5197028174
H107	-6.2091284402	-4.4075274601	-2.3493311605
H108	-6.2090223688	-2.7317286573	-1.7677951798
H109	-0.8314376711	-6.1273740273	-1.2152922853
H110	-1.7406590679	-4.8051365341	-0.5422965303
H111	-0.9277737874	-2.6127649675	-1.0955691802
H112	2.6656482793	-3.2411854493	-6.4195023359
H113	2.4287131078	-0.6217719208	-4.5743330308
H114	3.9781018123	0.1230491883	-4.9120580085
H115	1.0483965336	0.4709441214	-2.9344435268
H116	3.8837756307	6.0590842661	-1.3350503977
H117	-3.7930778299	3.1566348396	5.3121061792
H118	0.2717130835	2.9212600496	0.3389062379
H119	1.4493662567	4.9808232557	0.2061869128
H120	1.1350995233	6.1662260059	1.4637009205
H121	-2.4008038525	0.1237235094	-4.6835157520
H122	-8.8986926984	-0.1767433734	1.5087496559
H123	-2.1085825109	8.3114390689	0.5391855071
H124	3.1826842996	3.4751948083	-7.2385865756
H125	-3.2219552164	-5.5679531688	-6.1775843845
H126	5.1515787039	4.5304642832	-2.9483199316
H127	-2.3289338131	5.2053251575	4.8726619068

H128	1.9458162953	-5.3806909767	-5.2019675682
H129	-6.1354422915	-4.5334383602	1.8229224021
H130	-1.5227461963	2.4292756024	-1.4505674160

Single point energy: -4342.6364122

(2G4-2H⁺)_g

N1	-2.3337859999	4.3758369996	4.2935779993
C2	-3.2706180635	3.3710260984	4.4012045172
N3	-3.2588113784	2.5741868778	3.3619499396
C4	-2.2547876682	3.0680369822	2.5467330696
C5	-1.8120928271	2.6434343526	1.2595562630
O6	-2.2557534821	1.7223969721	0.5655409442
N7	-0.7514503457	3.4490507450	0.7915268199
C8	-0.2435971259	4.5503529748	1.4484110739
N9	0.7158269806	5.2706393479	0.8366859891
N10	-0.6815768467	4.9679507209	2.6314971002
C11	-1.6620657401	4.1908277245	3.1157317928
N12	-2.3107859999	7.3328369997	0.3775779998
C13	-3.3418733587	6.6113838689	0.9572081778
N14	-3.6994218431	5.5527197663	0.2718379935
C15	-2.8502744576	5.5554039740	-0.8283488491
C16	-2.6834673361	4.6661767201	-1.9054506896
O17	-3.2886378129	3.5896564309	-2.2573097443
N18	-1.6920596818	5.0279718411	-2.7835865206
C19	-0.9135774262	6.1584556656	-2.6684657026
N20	-0.0340652087	6.3623628609	-3.6632949581
N21	-1.0333552325	7.0142702594	-1.6635555478
C22	-1.9752488383	6.6681413814	-0.7801886292
N23	4.2212139990	4.3458369985	-2.5964220000
C24	3.5069670614	5.1656868730	-1.7512667720
N25	2.3112822817	4.6936184097	-1.4979175365
C26	2.2438035905	3.4970898767	-2.1900857331
C27	1.1761044554	2.5537144930	-2.2967126795
O28	0.0441226614	2.6313585045	-1.8006578492
N29	1.5443122948	1.4461037258	-3.0818449774
C30	2.7535722704	1.3136692989	-3.7350127991
N31	2.9438860074	0.2175663926	-4.4916037226
N32	3.7338935371	2.2131395747	-3.6683376017
C33	3.4291504845	3.2544037249	-2.8780397372
N34	2.3242150002	3.3108369999	-6.7294219997
C35	1.6507861365	4.1425660926	-5.8697474801
N36	0.4774243970	3.6780582473	-5.5134114659
C37	0.3788340461	2.4581122314	-6.1781966246
C38	-0.6041084547	1.4249427147	-6.1329093093
O39	-1.6626314863	1.4236931270	-5.4799877326
N40	-0.2598374490	0.3242961617	-6.9348739227

C41	0.8813314280	0.2357956388	-7.7045203490
N42	1.0415442478	-0.8971669833	-8.4412335899
N43	1.8076548114	1.1696872969	-7.7368677878
C44	1.5235024548	2.2214131726	-6.9458600403
N45	1.6542140013	-4.4471629982	-4.9444210006
C46	1.9964614569	-3.3192836101	-5.6625904796
N47	1.4316098396	-2.2362496615	-5.1854766097
C48	0.6949967924	-2.6756502721	-4.0985765301
C49	-0.1343014630	-1.9496022472	-3.1939557496
O50	-0.3810749812	-0.7341759684	-3.2001897130
N51	-0.6986686163	-2.8060926133	-2.2291687456
C52	-0.4528114158	-4.1604291457	-2.1275330179
N53	-0.9913262768	-4.8163299601	-1.0774642349
N54	0.3000812368	-4.8409599843	-2.9841426077
C55	0.8352715853	-4.0501997274	-3.9226227950
N56	-3.0297860021	-4.5901629981	-6.0044219969
C57	-2.1998168299	-3.8057165744	-6.7927598345
N58	-2.2159028199	-2.5351025309	-6.4766701605
C59	-3.1051292217	-2.4582961311	-5.4129919210
C60	-3.5892205193	-1.3781840200	-4.6534280616
O61	-3.3950116258	-0.1111400362	-4.7162407039
N62	-4.4912144329	-1.7338146956	-3.6789500851
C63	-4.9173362831	-3.0220741510	-3.4317432404
N64	-5.8164749313	-3.1590225932	-2.4409754587
N65	-4.4994576524	-4.0614308946	-4.1417724698
C66	-3.6213734572	-3.7386760235	-5.0982189594
N67	-5.2727860008	-4.2351629996	1.3885780009
C68	-4.5095764392	-4.8825959749	0.4429446836
N69	-3.5955299959	-4.0958199928	-0.0691876613
C70	-3.7505938622	-2.8884734881	0.5862319622
C71	-3.0214229716	-1.6638715982	0.4594295554
O72	-2.0808782825	-1.4021840356	-0.2937014712
N73	-3.5117996509	-0.6851908642	1.3409580356
C74	-4.5465234252	-0.8658329355	2.2310785981
N75	-4.8930649091	0.1894644834	2.9956879976
N76	-5.2306508815	-2.0021595385	2.3491985107
C77	-4.7872765873	-2.9546372753	1.5126233959
N78	-8.1317859978	-0.3501630017	0.8725779973
C79	-7.6239926017	-1.1300237643	-0.1384128658
N80	-6.6460877325	-0.5516954091	-0.7953098084
C81	-6.5054213158	0.6872666337	-0.1782452636
C82	-5.6269892134	1.7818835818	-0.4335775693
O83	-4.7734108263	1.8725967131	-1.3342083628
N84	-5.8193912684	2.8385230335	0.4712882573
C85	-6.7764401790	2.8623215431	1.4637080856
N86	-6.8077038258	3.9731568568	2.2521595004

N87	-7.6160413675	1.8745397055	1.6872215540
C88	-7.4261568051	0.8250811028	0.8649627110
H89	2.0875082162	5.0770101832	-5.5439864989
H90	0.2291840684	-1.4458886008	-8.6848177625
H91	1.7741135013	-0.8521420480	-9.1372640744
H92	-0.8593119966	-0.4997914470	-6.8517726058
H93	-4.8153366767	-0.9704079824	-3.0833091438
H94	-3.7848659224	6.9247539440	1.8926537488
H95	-1.4709854802	4.3321539796	-3.4978106886
H96	0.6346810579	7.1101042277	-3.5544389760
H97	0.1132069728	5.6403972047	-4.3623243682
H98	-4.6655775657	-5.9228071501	0.1901121225
H99	-4.2843000473	1.0126139352	3.1079403018
H100	-5.5648038357	-0.0101818807	3.7231935917
H101	-3.0718691474	0.2439881595	1.2173884691
H102	-8.0236194161	-2.1137335162	-0.3451302329
H103	-5.1622570657	3.6196272237	0.4064706548
H104	-6.4413981361	4.8416417904	1.8870077613
H105	-7.6251700094	4.0508961508	2.8430859012
H106	-1.6113065204	-4.2417225275	-7.5886945166
H107	-5.9634973015	-4.0976274580	-2.0978598144
H108	-5.9779911561	-2.3761110515	-1.8065635167
H109	-0.8384687533	-5.8157672568	-1.1064815860
H110	-1.8851911159	-4.5057365245	-0.6803795648
H111	-1.2470689925	-2.3344589406	-1.4853832253
H112	2.6584424878	-3.3611058637	-6.5165643259
H113	2.2517199192	-0.5102843309	-4.6820500357
H114	3.8471436044	0.1370448725	-4.9347205300
H115	0.8358553945	0.6972961047	-3.1537895419
H116	3.9216793641	6.0837896303	-1.3577651316
H117	-3.9221469460	3.2829199363	5.2595686169
H118	-0.3799636023	3.1791950135	-0.1344560182
H119	1.2028391637	4.9932297067	-0.0241976823
H120	1.1449793805	5.9822377945	1.4107788277
H121	-2.5656835971	0.3446283209	-5.1709969147
H122	-8.8806898646	-0.5845706264	1.5106833982
H123	-1.8640603234	8.1661903669	0.7364767161
H124	3.2442168463	3.4525990748	-7.1249203131
H125	-3.1779607508	-5.5890583696	-6.0661952541
H126	5.1819185459	4.4665351505	-2.8891205257
H127	-2.1092313862	5.0702428922	4.9938628401
H128	2.0061319341	-5.3853685678	-5.0818950270
H129	-5.9810580855	-4.6502246590	1.9797518125
H130	-3.9112565544	3.0041845438	-1.6508269688

Single point energy: -4342.625823

(2G4-3H⁺)₁

N1	-2.3337861092	4.3758371423	4.2935774849
C2	-3.1476357834	3.2879623992	4.5366795388
N3	-3.0389030331	2.3593967509	3.6166847422
C4	-2.0885321176	2.8528041374	2.7295388285
C5	-1.5576809084	2.3257868098	1.5274393506
O6	-1.8829796072	1.2323296402	0.9865402448
N7	-0.6086978559	3.1554770621	0.9422583681
C8	-0.2259033555	4.3865514183	1.4561030693
N9	0.6612013990	5.1187175857	0.7714010065
N10	-0.7310036592	4.8997848437	2.5747209141
C11	-1.6317367725	4.1062089172	3.1504710514
N12	-2.3107859130	7.3328369118	0.3775779119
C13	-3.2519210022	6.5066317405	0.9486470883
N14	-3.4391238750	5.3985909618	0.2782733393
C15	-2.5794137281	5.4976692162	-0.8042219621
C16	-2.2565673811	4.6377946188	-1.8432084625
O17	-2.7792854717	3.4369136413	-2.0101303442
N18	-1.3320563841	5.0935184408	-2.7287812334
C19	-0.7082514260	6.3289368271	-2.6222821630
N20	0.1536609725	6.6409649182	-3.5887247948
N21	-0.9601897743	7.1705586032	-1.6207410947
C22	-1.8674895073	6.7198978510	-0.7643329505
N23	4.2212137459	4.3458369332	-2.5964220432
C24	3.5007965168	5.0963332727	-1.6955802727
N25	2.3661111405	4.5254588156	-1.3747057478
C26	2.3450635281	3.3355177897	-2.0802652129
C27	1.3635803175	2.3074605852	-2.1369663679
O28	0.2603206367	2.2565993971	-1.5565739673
N29	1.7621985145	1.2614146869	-2.9854507963
C30	2.9423784282	1.2386599628	-3.7138410138
N31	3.1728266412	0.1869636804	-4.5099342794
N32	3.8458484774	2.2129453988	-3.6752498832
C33	3.5022039048	3.2051154502	-2.8488850342
N34	2.3242147475	3.3108370633	-6.7294219620
C35	2.1123251022	4.4351817778	-5.9666463796
N36	0.9957844295	4.3785630103	-5.2806610436
C37	0.4405526394	3.1509174882	-5.6177153081
C38	-0.7156493763	2.4850748185	-5.1483738914
O39	-1.5464864311	2.9003491213	-4.2993409093
N40	-0.8874475584	1.2370152293	-5.7458549641
C41	-0.0445771697	0.6911833305	-6.7060943574
N42	-0.4005423998	-0.4780073287	-7.2589955533
N43	1.0625266667	1.2906705294	-7.1121539310
C44	1.2556510530	2.4806820612	-6.5386412082
N45	1.6542139179	-4.4471628585	-4.9444213528

C46	2.2155027458	-3.2742554403	-5.3939980767
N47	1.6726194817	-2.2226038350	-4.8319164554
C48	0.7249292824	-2.7297807448	-3.9624026108
C49	-0.1595875449	-2.0687284034	-3.0634494610
O50	-0.2951305010	-0.8587898029	-2.8383752542
N51	-0.9597480404	-3.0113454743	-2.3708659172
C52	-0.8927451120	-4.3893233345	-2.5109045293
N53	-1.7158726819	-5.1287085506	-1.7470399080
N54	-0.0734258502	-4.9909559036	-3.3528681390
C55	0.7031550625	-4.1235211801	-4.0203637446
N56	-3.0297859927	-4.5901626876	-6.0044222374
C57	-2.0874708122	-3.7640263960	-6.5801751867
N58	-2.1566251869	-2.5307161896	-6.1529917633
C59	-3.2070416366	-2.5313600854	-5.2531342200
C60	-3.7399623103	-1.5590058853	-4.4198221962
O61	-3.2948284263	-0.3205796250	-4.3436045080
N62	-4.7900719675	-1.9469997164	-3.6435173520
C63	-5.3222808956	-3.2280264578	-3.6596520287
N64	-6.3825504314	-3.4384744608	-2.8728080858
N65	-4.8143754076	-4.2031221751	-4.4083405363
C66	-3.7829318941	-3.8207648949	-5.1579250098
N67	-5.2727860922	-4.2351628069	1.3885775433
C68	-4.7105974075	-4.6432839770	0.2005909119
N69	-3.8601948858	-3.7778423187	-0.2901368220
C70	-3.8502637936	-2.7396157977	0.6275146071
C71	-3.1706279370	-1.5279993489	0.6846157635
O72	-2.3218425985	-1.1233518494	-0.2376851997
N73	-3.4304665708	-0.7472049903	1.7668992158
C74	-4.3169269738	-1.1038850193	2.7746066673
N75	-4.4632213759	-0.2315379514	3.7703973941
N76	-4.9982595071	-2.2515316796	2.7548730402
C77	-4.7344805093	-3.0101608032	1.6967908755
N78	-8.1317861746	-0.3501629005	0.8725778892
C79	-8.0699388559	-1.4050716259	-0.0128900469
N80	-7.1381753074	-1.2530845924	-0.9243252799
C81	-6.5653653994	-0.0189272026	-0.6327610764
C82	-5.5229380723	0.7046009478	-1.2611088941
O83	-4.8553661148	0.3585452711	-2.2686463173
N84	-5.2560724472	1.9197267729	-0.6273744624
C85	-5.9400918934	2.4017835023	0.4834412520
N86	-5.5909919887	3.5975484341	0.9680693985
N87	-6.9172367422	1.7259474890	1.0733713617
C88	-7.1828739136	0.5578338371	0.4863398056
H89	2.8112606460	5.2600591833	-5.9621752095
H90	-1.0756062852	-1.1183669567	-6.8337011840
H91	0.2791956759	-0.8669375567	-7.8980274563

H92	-1.6883249026	0.7007770398	-5.4192237467
H93	-5.1534428203	-1.2218246164	-2.9949602366
H94	-3.7668543824	6.7802102334	1.8593300198
H95	-1.1276679987	4.4525521233	-3.5198067251
H96	0.6207789123	7.5347778961	-3.5228469171
H97	0.4632410314	5.9309050855	-4.2685160501
H98	-4.9609200655	-5.5953175812	-0.2484661018
H99	-3.9701405050	0.6760152411	3.7793830875
H100	-5.0807349730	-0.4884680571	4.5285128087
H101	-2.9192751188	0.1689185251	1.7780484887
H102	-8.7407336689	-2.2499804619	0.0637302206
H103	-4.5063474985	2.4762409039	-1.0376936636
H104	-4.8089469642	4.1734025794	0.6327562700
H105	-6.1290799652	3.9199317155	1.7603300575
H106	-1.3803858701	-4.1344740142	-7.3100109870
H107	-6.8438877418	-4.3346312324	-2.9443734546
H108	-6.7577659897	-2.7030401475	-2.2605005736
H109	-1.6270421380	-6.1319753670	-1.8147882331
H110	-2.4480628269	-4.7019284821	-1.1841833054
H111	-1.5533688088	-2.6041116002	-1.6532098120
H112	3.0143713781	-3.2619264408	-6.1228394347
H113	2.5447838105	-0.6185320990	-4.6214011630
H114	4.0668931870	0.1798146158	-4.9797352341
H115	1.1033639020	0.4707548583	-3.0342914022
H116	3.8644203569	6.0403670345	-1.3135714164
H117	-3.7906789802	3.2405511855	5.4050577255
H118	-0.2043856910	2.8309814726	0.0400754081
H119	1.2278229069	4.7996998252	-0.0345534128
H120	0.9782074590	5.9496978522	1.2531806678
H121	-3.7390355102	0.1845649597	-3.6111158345
H122	-8.8003157616	-0.2235789381	1.6224074862
H123	-2.0215343212	8.2459460648	0.7071090044
H124	3.1002706863	3.1396450280	-7.3562247285
H125	-3.1830645860	-5.5713262450	-6.2053597132
H126	5.1489475600	4.5468521434	-2.9475959278
H127	-2.1865063346	5.1689882442	4.9051574390
H128	1.9390695121	-5.3874885595	-5.1891147045
H129	-5.9163222146	-4.7581462541	1.9707896380
H130	-2.3507842969	2.9691149293	-2.7835997557
H131	-1.9248147957	-0.2290226404	-0.0363603928

Single point energy: -4342.9319605

$(2G4-3H^+)_2$

N1	-2.3337859999	4.3758369999	4.2935779999
C2	-3.2558185107	3.3660010766	4.4623247384
N3	-3.2640776419	2.5274217542	3.4542269398

C4	-2.2834392520	3.0012192606	2.5953999274
C5	-1.8599358261	2.5420688680	1.3215062944
O6	-2.3114056601	1.5815663867	0.6682962530
N7	-0.8200009000	3.3286760334	0.7996976574
C8	-0.3061788321	4.4619813548	1.4025548323
N9	0.6382265887	5.1651474644	0.7527956463
N10	-0.7269729884	4.9154106038	2.5769382332
C11	-1.6872139210	4.1511658765	3.1111175838
N12	-2.3107859998	7.3328370003	0.3775780003
C13	-3.2854169944	6.5226011894	0.9157860076
N14	-3.5394098565	5.4675610969	0.1849705382
C15	-2.6899329628	5.5859948057	-0.9031597380
C16	-2.4038161262	4.7553088073	-1.9766788367
O17	-2.9647187522	3.5794530245	-2.1802686659
N18	-1.4686652686	5.2118328791	-2.8513274821
C19	-0.7947029401	6.4146824488	-2.6965056053
N20	0.0657941748	6.7369264973	-3.6643039643
N21	-0.9987914581	7.2172831136	-1.6545241337
C22	-1.9173756149	6.7670625193	-0.8068992542
N23	4.2212139998	4.3458369999	-2.5964220000
C24	3.4281359327	5.2330537461	-1.9016294113
N25	2.2404557654	4.7439665584	-1.6407569616
C26	2.2574052767	3.4683742775	-2.1737654307
C27	1.2375396544	2.4759355104	-2.2023647043
O28	0.0734295786	2.5326300707	-1.7739328398
N29	1.6938602179	1.2995485601	-2.8273689372
C30	2.9532348480	1.1195558939	-3.3746048184
N31	3.1987653593	-0.0841593725	-3.9270684325
N32	3.8832543384	2.0604999718	-3.3802177741
C33	3.4902885003	3.1925161617	-2.7677758835
N34	2.3242149995	3.3108369996	-6.7294219997
C35	2.0780177571	4.4705473895	-6.0270431652
N36	0.9437269537	4.4341543260	-5.3699597429
C37	0.4095135215	3.1868025469	-5.6647754679
C38	-0.7729435478	2.5448728589	-5.2227908503
O39	-1.6467416696	2.9931667931	-4.4416252037
N40	-0.9142574387	1.2667947953	-5.7737247517
C41	-0.0351011239	0.6846882184	-6.6780788458
N42	-0.3680438883	-0.5046026159	-7.2011872868
N43	1.0906035043	1.2660135690	-7.0583393028
C44	1.2570779997	2.4820822840	-6.5295105840
N45	1.6542140000	-4.4471629997	-4.9444209999
C46	1.8641489147	-3.0949039081	-5.0895080344
N47	1.1400196485	-2.3732008772	-4.2673411438
C48	0.4151597035	-3.3058424883	-3.5389030777
C49	-0.5828999812	-3.1464665354	-2.5401550111

O50	-1.0712775174	-2.0723315908	-2.1297759640
N51	-1.0442060309	-4.3728741571	-2.0405208941
C52	-0.6032770559	-5.6107732409	-2.4724099287
N53	-1.1632447453	-6.6983542580	-1.8813700365
N54	0.2744432130	-5.7702040778	-3.4436529071
C55	0.7365758106	-4.6077066136	-3.9368535676
N56	-3.0297860004	-4.5901629999	-6.0044219996
C57	-2.1338132841	-3.7449494196	-6.6251541408
N58	-2.1527785985	-2.5319302087	-6.1384942653
C59	-3.1222725629	-2.5651231943	-5.1516467085
C60	-3.5970540763	-1.6187707811	-4.2527031868
O61	-3.1616008035	-0.3783186902	-4.1751573993
N62	-4.5902211846	-2.0362708706	-3.4205777418
C63	-5.1257423691	-3.3147726817	-3.4412134749
N64	-6.1243692602	-3.5524998311	-2.5857408908
N65	-4.6753240035	-4.2646591433	-4.2574462329
C66	-3.7007705522	-3.8531345792	-5.0647226389
N67	-5.2727859999	-4.2351629998	1.3885779999
C68	-4.4554213560	-4.8426750956	0.4500453535
N69	-3.4858232095	-4.0710196645	0.0217561001
C70	-3.6644918471	-2.8802191667	0.7209064682
C71	-2.9772445530	-1.6608617320	0.7259100927
O72	-1.9289724120	-1.2872166499	0.0647922731
N73	-3.4687876919	-0.7074681475	1.5694914202
C74	-4.5449586862	-0.9088053574	2.4130622148
N75	-4.8893152725	0.1062242301	3.2073251980
N76	-5.2355498907	-2.0534667453	2.4363421128
C77	-4.7733720790	-2.9708959010	1.5922498753
N78	-8.1317859993	-0.3501630004	0.8725779991
C79	-7.9538787047	-1.4733137398	0.0967686375
N80	-6.9715325217	-1.3477394139	-0.7639298305
C81	-6.4819240573	-0.0641461171	-0.5469085753
C82	-5.4243034435	0.6513894353	-1.1539109422
O83	-4.6594308500	0.2381533037	-2.0660159470
N84	-5.2655154268	1.9285720189	-0.6283584274
C85	-6.0496595677	2.4704729813	0.3833812245
N86	-5.7902898322	3.7220634190	0.7746468010
N87	-7.0427961885	1.8038074532	0.9581507354
C88	-7.2061974365	0.5745334501	0.4684797376
H89	2.7680661272	5.3029166797	-6.0440440742
H90	-1.0679087892	-1.1324766997	-6.7956883090
H91	0.3079486890	-0.8917705329	-7.8447392227
H92	-1.7468248513	0.7569107223	-5.4869690931
H93	-4.9148227000	-1.3220131817	-2.7337343831
H94	-3.7716232970	6.7666603349	1.8503561335
H95	-1.2635245361	4.5827172546	-3.6481078213

H96	0.5928478875	7.5906011165	-3.5426103999
H97	0.3758461902	6.0314673877	-4.3448756994
H98	-4.6320124080	-5.8597740732	0.1262181317
H99	-4.3243586832	0.9697889791	3.2938213517
H100	-5.6512146751	-0.0573989361	3.8507601529
H101	-3.0397754102	0.2443054334	1.4332055034
H102	-8.5833468511	-2.3454955715	0.2088377886
H103	-4.4732070435	2.4586480427	-0.9898658075
H104	-4.9745738555	4.2728151145	0.4839990808
H105	-6.3789347812	4.0789413269	1.5144622700
H106	-1.4999995399	-4.0861377534	-7.4327009021
H107	-6.5951655957	-4.4434246000	-2.6640596020
H108	-6.5014501949	-2.8118607714	-1.9757577382
H109	-0.7270914550	-7.5837944729	-2.1082590566
H110	-1.5308041423	-6.6189508171	-0.9428591712
H111	-1.8124768140	-4.3240870355	-1.3574191987
H112	2.5673930241	-2.7053442362	-5.8138551368
H113	2.5042789698	-0.8287682115	-3.9344373025
H114	4.1392656206	-0.2629280216	-4.2474944598
H115	1.0279110276	0.5310849925	-2.8366452016
H116	3.7848307015	6.2129915614	-1.6144938853
H117	-3.8834092091	3.3050874678	5.3409049676
H118	-0.4583860834	3.0328911024	-0.1196128109
H119	1.0861912310	4.9112618555	-0.1328593795
H120	1.0531796270	5.9195844932	1.2818472591
H121	-1.6699491211	-1.8078958191	-0.7780478942
H122	-8.8513643511	-0.2009277696	1.5689661902
H123	-1.9663298201	8.2059403175	0.7579988157
H124	3.1098921824	3.1249395994	-7.3401027494
H125	-3.2248033401	-5.5546154115	-6.2464778598
H126	5.1892185054	4.4772519381	-2.8624586779
H127	-2.1018650792	5.0974390397	4.9647316425
H128	2.1400331369	-5.1955991704	-5.4239504117
H129	-6.0266511948	-4.6655320483	1.9096008251
H130	-2.5328430971	3.1086248467	-2.9458042103
H131	-3.5871803064	0.1098311944	-3.4162449608

Single point energy: -4342.9292385

(2G4-3H⁺)₃

N1	-2.3337860000	4.3758370000	4.2935780000
C2	-3.4820200981	3.6190799383	4.1655400236
N3	-3.4500685856	2.8269869767	3.1240365644
C4	-2.2083965629	3.0528141208	2.5543731330
C5	-1.6526799672	2.6002335000	1.3461348563
O6	-2.1927988532	1.8643599359	0.4702174254
N7	-0.3649929978	3.0965222890	1.1262877580

C8	0.2852534904	4.0071238127	1.9478170738
N9	1.5338554210	4.3648813411	1.6045046471
N10	-0.2754510801	4.5124815287	3.0354841817
C11	-1.4889457596	4.0092844562	3.2847812494
N12	-2.3107860000	7.3328370000	0.3775780000
C13	-3.1899530899	6.5498341146	1.1015101676
N14	-3.4008283534	5.3759353164	0.5649825073
C15	-2.6283815128	5.3807317496	-0.5866214698
C16	-2.3961887324	4.4283526852	-1.5664635721
O17	-2.8782806361	3.1977479790	-1.6137803575
N18	-1.6102132578	4.8129550954	-2.6101098769
C19	-1.0407315589	6.0744827631	-2.6985006192
N20	-0.3264542497	6.3605423362	-3.7859750186
N21	-1.1864382680	6.9996147087	-1.7411168861
C22	-1.9625565381	6.6199351209	-0.7393404652
N23	4.2212140000	4.3458370000	-2.5964220000
C24	3.4584916844	4.9039465223	-1.5905643328
N25	2.4763045167	4.1321923810	-1.1988502722
C26	2.5975204520	2.9924010836	-1.9801509860
C27	1.8608037607	1.8192256160	-2.0785428037
O28	0.7772652881	1.5623346614	-1.3688206794
N29	2.3119669440	0.9027212912	-2.9770231066
C30	3.4341492983	1.0942966524	-3.7728181731
N31	3.7716321379	0.0931475300	-4.5799609086
N32	4.1449752975	2.2230155182	-3.7432445599
C33	3.7015440702	3.1063783530	-2.8588181211
N34	2.3242150000	3.3108370000	-6.7294220000
C35	2.0237240945	4.4381721428	-6.0043371216
N36	0.9595320485	4.2761916966	-5.2554528714
C37	0.5347191975	2.9834270050	-5.5165745490
C38	-0.5569630186	2.2380082296	-4.9965182124
O39	-1.3919779316	2.5733695708	-4.1381293115
N40	-0.6228285433	0.9569982818	-5.5682893914
C41	0.2418774236	0.4626486480	-6.5330614507
N42	-0.0026487568	-0.7618550684	-7.0170729814
N43	1.2848321517	1.1452484639	-6.9839574391
C44	1.3695708199	2.3708743018	-6.4534342413
N45	1.6542140000	-4.4471630000	-4.9444210000
C46	2.5138689325	-3.3899701311	-5.1562205700
N47	2.1631880271	-2.3186979671	-4.4868871683
C48	1.0244761917	-2.6960722041	-3.7853811910
C49	0.1811324972	-1.9876740687	-2.8990138015
O50	0.3080998535	-0.7785883994	-2.5618879905
N51	-0.8675182362	-2.7626807271	-2.4124755827
C52	-1.0854383213	-4.0893237382	-2.7647659249
N53	-2.1480842979	-4.7247840485	-2.2710979798

N54	-0.3023004072	-4.7609578983	-3.6031861289
C55	0.7065654522	-4.0291825060	-4.0602594785
N56	-3.0297860000	-4.5901630000	-6.0044220000
C57	-2.0067340432	-3.8097950020	-6.4896132474
N58	-2.0102322525	-2.5954526347	-6.0033060971
C59	-3.1030641757	-2.5641515294	-5.1514831630
C60	-3.6248343851	-1.5921417386	-4.3075793434
O61	-3.1067234720	-0.3885879619	-4.1632510211
N62	-4.7320356488	-1.9437579897	-3.6030833909
C63	-5.3323671231	-3.1912320636	-3.6899669052
N64	-6.4326807034	-3.3704105080	-2.9570516273
N65	-4.8518448232	-4.1630972689	-4.4648117587
C66	-3.7674872337	-3.8128257361	-5.1483306959
N67	-5.2727860000	-4.2351630000	1.3885780000
C68	-4.7194233533	-4.8145737653	0.2771150785
N69	-3.9717501217	-3.9709036417	-0.3879200869
C70	-4.0200083883	-2.7902645834	0.3251165682
C71	-3.3816203643	-1.5414451296	0.0865372072
O72	-2.6226623938	-1.2234805599	-0.8468597963
N73	-3.7104714193	-0.6038602963	1.0812558393
C74	-4.5643397927	-0.8402388972	2.1471629774
N75	-4.8127487487	0.1820614163	2.9835358242
N76	-5.1544085611	-2.0098343863	2.3647808084
C77	-4.8372274337	-2.9321409407	1.4449631847
N78	-8.1317860000	-0.3501630000	0.8725780000
C79	-8.0017320236	-1.4566307077	0.0632047064
N80	-7.1472188724	-1.2732011231	-0.9156457898
C81	-6.6986013513	0.0292494359	-0.7434057742
C82	-5.7340620826	0.7873234184	-1.4503449382
O83	-5.0568230342	0.4307433969	-2.4451635436
N84	-5.5715478311	2.0671198509	-0.9145622578
C85	-6.2520447115	2.5638454653	0.1877336714
N86	-6.0124412539	3.8443580987	0.5507046285
N87	-7.1401722310	1.8539195437	0.8587196226
C88	-7.3163620813	0.6221443318	0.3641904649
H89	2.6135286064	5.3414706109	-6.0783533313
H90	-0.7547354085	-1.3646012836	-6.6700633426
H91	0.6148867789	-1.0863792438	-7.7469705793
H92	-1.3998413473	0.3874293312	-5.2381798093
H93	-5.1279044587	-1.1921402677	-2.9978752294
H94	-3.6459205981	6.9105688998	2.0138820226
H95	-1.4404245676	4.0654624653	-3.3336032615
H96	0.0775472114	7.2874818903	-3.8153718380
H97	0.0572346744	5.6231863077	-4.4030016193
H98	-4.8960915537	-5.8490688774	0.0165294524
H99	-4.3676192906	1.1014602940	2.9256767159

H100	-5.3727235693	-0.0342497760	3.7958838393
H101	-3.2581267371	0.3107692070	0.9701765233
H102	-8.5642932393	-2.3620745021	0.2445528819
H103	-4.8926324697	2.6560450452	-1.3941990879
H104	-5.0901888188	4.2699742496	0.4479029454
H105	-6.5093978529	4.1161215437	1.3898569077
H106	-1.2923251174	-4.1943448287	-7.2048751588
H107	-6.8956846289	-4.2659537116	-3.0260485554
H108	-6.7569638405	-2.6672495574	-2.2785879970
H109	-2.1982201371	-5.7071007095	-2.5053023515
H110	-2.8112896361	-4.3521925645	-1.5652152007
H111	-1.5334385604	-2.2792976214	-1.7779186782
H112	3.3732245672	-3.4733934782	-5.8076636980
H113	3.2335168769	-0.7894454270	-4.6010566040
H114	4.5959734940	0.2140301525	-5.1522556068
H115	1.7251804064	0.0404195752	-3.0528396003
H116	3.6834931222	5.8817859272	-1.1854636560
H117	-4.2960168131	3.6976583936	4.8738652717
H118	0.1156152822	2.7131755790	0.3130662435
H119	1.8797181108	4.2522624719	0.6484086498
H120	1.9739555009	5.0507139155	2.2033592634
H121	0.3647268347	0.6825326833	-1.6104079264
H122	-8.7514382036	-0.2478328361	1.6665014052
H123	-2.0497155278	8.2923724153	0.5723728294
H124	3.0609747684	3.2139665717	-7.4170975997
H125	-3.2391122883	-5.5478541740	-6.2595461001
H126	5.0576446339	4.7360325118	-3.0142900202
H127	-2.1068362327	5.0068101857	5.0530069834
H128	1.7628048618	-5.3929306227	-5.2888582703
H129	-5.8510096039	-4.6905780080	2.0838523392
H130	-2.6482879647	2.6525484622	-0.7738436893
H131	-3.5963904025	0.1562634433	-3.4894410105

Single point energy: -4342.9270672

(2G4-3H⁺)_a

N1	-2.3337860000	4.3758370001	4.2935769999
C2	-3.1482808814	3.2774708244	4.4497575152
N3	-2.8536233362	2.3256363051	3.6009724123
C4	-1.7820451897	2.8060614718	2.8727427447
C5	-1.0829628399	2.2406654370	1.7705633399
O6	-1.2745162735	1.1560852824	1.1948865191
N7	-0.0731877813	3.1049472220	1.3113282317
C8	0.2035696211	4.3595404345	1.8274681221
N9	1.2002377057	5.0601008091	1.2600322330
N10	-0.4688418190	4.8937828910	2.8387384377
C11	-1.4316299013	4.0853027674	3.3026682286

N12	-2.3107860000	7.3328370000	0.3775780000
C13	-3.1211099134	6.4894867556	1.1096196110
N14	-3.1466466559	5.2666223265	0.6466742449
C15	-2.3147858937	5.3005573614	-0.4621228234
C16	-1.8331942355	4.3264163895	-1.3201326609
O17	-2.1176699523	3.0391123194	-1.2112434839
N18	-1.0226246576	4.7521602175	-2.3273936087
C19	-0.6250563434	6.0757495601	-2.4728910504
N20	0.1222402484	6.3772700100	-3.5296694981
N21	-0.9756345331	7.0260792906	-1.6050537258
C22	-1.7964875421	6.6039445850	-0.6565730636
N23	4.2212140000	4.3458369998	-2.5964220000
C24	3.4498046116	5.0941806364	-1.7354074199
N25	2.3797330377	4.4503659904	-1.3379628831
C26	2.4607765566	3.2130256258	-1.9562205632
C27	1.5896045625	2.0956287329	-1.9268424972
O28	0.4960133106	1.9735218098	-1.3339754511
N29	2.1052045438	1.0280278724	-2.6859714427
C30	3.2879697009	1.0524877989	-3.4123692757
N31	3.6432950821	-0.0577624865	-4.0714350078
N32	4.0669332848	2.1185078614	-3.4824647545
C33	3.6170898811	3.1322396239	-2.7383020671
N34	2.3242150000	3.3108370000	-6.7294220000
C35	2.0976930398	4.4067652630	-5.9368527385
N36	1.0860645599	4.2272469061	-5.1229440503
C37	0.6256861835	2.9515509210	-5.4042491190
C38	-0.4079990639	2.1822036919	-4.8151674946
O39	-1.1573241101	2.4893050767	-3.8671398718
N40	-0.5266898291	0.9225392886	-5.4259665832
C41	0.2583779872	0.4640534087	-6.4742171116
N42	-0.0224306655	-0.7468063211	-6.9824030213
N43	1.2548225679	1.1641004769	-6.9862255095
C44	1.3853751491	2.3706490388	-6.4211335452
N45	1.6542140000	-4.4471629998	-4.9444210000
C46	2.3771370905	-3.2780625974	-5.0360937687
N47	1.9570325225	-2.3583742896	-4.2091013956
C48	0.9135354272	-2.9492084893	-3.5212171990
C49	0.0463780858	-2.4959276068	-2.5360897490
O50	0.0882056098	-1.2872045395	-2.0219991968
N51	-0.8944702575	-3.3885272371	-2.1197111174
C52	-1.0097518535	-4.6774794773	-2.6225817164
N53	-1.9920888624	-5.4276230021	-2.1233876017
N54	-0.2009740752	-5.1509362076	-3.5691010744
C55	0.7123858587	-4.2728253957	-3.9689811857
N56	-3.0297860000	-4.5901630000	-6.0044220000
C57	-1.9390597669	-3.8560906449	-6.4067579613

N58	-1.8527630461	-2.6938866630	-5.8120148914
C59	-2.9584264839	-2.6463230861	-4.9773910161
C60	-3.4263230953	-1.7032600311	-4.0704399307
O61	-2.8121254756	-0.5666417698	-3.8070870488
N62	-4.5836159891	-2.0126395187	-3.4298747672
C63	-5.2831380412	-3.1930559163	-3.6345081340
N64	-6.4186083376	-3.3316737335	-2.9507915111
N65	-4.8530567187	-4.1419310548	-4.4682838751
C66	-3.7241431496	-3.8301259254	-5.0958345468
N67	-5.2727859999	-4.2351630001	1.3885780000
C68	-4.7867627530	-4.8259898536	0.2466771812
N69	-3.8526510315	-4.1087460333	-0.3326935196
C70	-3.7118755584	-2.9908920836	0.4829169258
C71	-2.8783135429	-1.8552986651	0.3832168598
O72	-2.0647072162	-1.6295528632	-0.5600317001
N73	-3.0359659130	-0.9646252398	1.4326213869
C74	-3.9212541488	-1.1571215725	2.4881235949
N75	-3.9519096692	-0.2518379481	3.4649050556
N76	-4.7416213091	-2.2052321320	2.5711184316
C77	-4.5866634727	-3.0654982802	1.5716794200
N78	-8.1317860000	-0.3501630000	0.8725780000
C79	-8.0849928122	-1.3709757197	-0.0515405214
N80	-7.0820167004	-1.2559900891	-0.8897316788
C81	-6.4367814641	-0.0869046913	-0.4998375120
C82	-5.2874834673	0.5620872638	-1.0045670189
O83	-4.5743406912	0.1930584713	-1.9754232380
N84	-4.9643699705	1.7203345875	-0.3004651029
C85	-5.6965732345	2.2223752127	0.7700924492
N86	-5.2938926852	3.3711072971	1.3251522067
N87	-6.7723468707	1.6136753156	1.2511031476
C88	-7.0860411983	0.4916654387	0.5998691562
H89	2.6993530669	5.3022040918	-6.0102226862
H90	-0.7078619831	-1.3836308631	-6.5735947904
H91	0.5265142062	-1.0322798496	-7.7803226905
H92	-1.2755470074	0.3408765668	-5.0574521072
H93	-4.9111671936	-1.2940488778	-2.7459238993
H94	-3.6709134188	6.8425141503	1.9713962860
H95	-0.8238348148	4.0369585345	-3.0591665400
H96	0.3781673849	7.3479087056	-3.6477461524
H97	0.4775560840	5.6437120203	-4.1647752041
H98	-5.1510642616	-5.7833197492	-0.1006109593
H99	-3.4703572002	0.6646194846	3.4604606985
H100	-4.6032557550	-0.4484501280	4.2127796493
H101	-2.4058831373	-0.1335248487	1.4338344314
H102	-8.8205392938	-2.1638761614	-0.0582856335
H103	-4.1109511493	2.1937269823	-0.5958425324

H104	-4.4716701580	3.9166061590	1.0487375757
H105	-5.8483426775	3.6960176573	2.1046398182
H106	-1.2472955598	-4.2317004415	-7.1487182976
H107	-6.9706873912	-4.1605451215	-3.1243746254
H108	-6.7344497243	-2.6231369011	-2.2711167516
H109	-2.0549169401	-6.3853357710	-2.4402974891
H110	-2.6755437475	-5.0396591064	-1.4535322666
H111	-1.5689626261	-3.0011727235	-1.4195566208
H112	3.1999926498	-3.1701822548	-5.7303392002
H113	3.0569220899	-0.8933352599	-4.0926084511
H114	4.5278194176	-0.0290986993	-4.5576321719
H115	1.5508519531	0.1763694708	-2.6460927238
H116	3.7328446701	6.0938117042	-1.4347542303
H117	-3.9261815742	3.2397321752	5.2000387436
H118	0.4072852778	2.7663451768	0.4712611479
H119	1.6237397858	4.8111068853	0.3598508305
H120	1.3844494747	5.9696605637	1.6585395593
H121	-3.2847687623	-0.0415902357	-3.0991658584
H122	-8.8286323408	-0.2136753880	1.5944158479
H123	-2.1562116528	8.3208853162	0.5389768934
H124	3.0272261700	3.2231905168	-7.4528887631
H125	-3.3199440906	-5.4939655408	-6.3594746423
H126	5.1193170955	4.6042765088	-2.9857667974
H127	-2.3027472473	5.1911071378	4.8927637907
H128	1.8454371700	-5.3165066087	-5.4287505981
H129	-5.9494879720	-4.6255152360	2.0326159844
H130	-1.3896500127	2.4798082041	-1.5902879139
H131	-0.6123131766	-1.1388953356	-1.3183916168

Single point energy: -4342.9255755

(2G4-3H⁺)_b

N1	-2.3337859886	4.3758369969	4.2935779877
C2	-3.1628611380	3.2737808980	4.3130449410
N3	-2.8708705691	2.3937283090	3.3903189354
C4	-1.7769090766	2.9338650864	2.7295800866
C5	-1.0130855044	2.5187206979	1.6451239548
O6	-1.2312976897	1.3985670909	0.9887169817
N7	-0.0011443787	3.3468739753	1.2714301456
C8	0.2798336506	4.5491033801	1.9046566221
N9	1.3021445288	5.2548143563	1.4240514873
N10	-0.4362359843	4.9970175398	2.9369046022
C11	-1.4192098094	4.1793734131	3.2945346299
N12	-2.3107859917	7.3328369828	0.3775779848
C13	-3.2677361782	6.6989006124	1.1421053969
N14	-3.5219992837	5.4761936551	0.7382177172
C15	-2.6926822174	5.2950285944	-0.3632614089

C16	-2.4907394216	4.1747653033	-1.2084017029
O17	-3.0183895595	3.0353806611	-1.1180856655
N18	-1.5780657801	4.4290991870	-2.2258301546
C19	-0.9329132823	5.6440442251	-2.4255896679
N20	-0.1450291709	5.7325735915	-3.5027642690
N21	-1.0758194882	6.6780876272	-1.6074351610
C22	-1.9452135588	6.4555684667	-0.6158721768
N23	4.2212139840	4.3458369861	-2.5964219886
C24	3.6726185629	5.0088538127	-1.5193003127
N25	2.6614443190	4.3626821764	-0.9911945256
C26	2.5462269642	3.2035088385	-1.7487605642
C27	1.6299281327	2.1245060568	-1.6840673512
O28	0.6707160476	2.0079166358	-0.8716796759
N29	1.8643647420	1.1530065090	-2.6473728886
C30	2.8898365507	1.2127969786	-3.5786820442
N31	3.0231439528	0.2013662878	-4.4443043601
N32	3.7448293683	2.2305301014	-3.6628796362
C33	3.5261497715	3.1723072951	-2.7463253745
N34	2.3242139895	3.3108370091	-6.7294219865
C35	1.7454290955	4.0842380190	-5.7589240199
N36	0.6771228214	3.5312155860	-5.2334867933
C37	0.5444272271	2.3218888637	-5.9013300738
C38	-0.3681190432	1.2419077180	-5.7275255698
O39	-1.2962345722	1.1709832543	-4.8947874745
N40	-0.1185551245	0.1877259925	-6.6146746190
C41	0.9076617203	0.1672665697	-7.5398892325
N42	1.0206930745	-0.9530855985	-8.3065981218
N43	1.7798346174	1.1435317472	-7.6822491421
C44	1.5658943791	2.1720537416	-6.8436313523
N45	1.6542139981	-4.4471629861	-4.9444219930
C46	2.0586503282	-3.2549847459	-5.4994014662
N47	1.5826396193	-2.2204759730	-4.8492200413
C48	0.8444858523	-2.7596092035	-3.8102454256
C49	0.1083458374	-2.1233950249	-2.7707959419
O50	-0.0357918971	-0.9042390787	-2.5644051706
N51	-0.5022359628	-3.0652299473	-1.9274643376
C52	-0.3847149288	-4.4389933945	-2.0516021955
N53	-0.9805896365	-5.1951326174	-1.1109977948
N54	0.2945291526	-5.0310410179	-3.0265720448
C55	0.8829453827	-4.1531290570	-3.8484821535
N56	-3.0297860036	-4.5901629968	-6.0044219962
C57	-2.0724449569	-3.7950479043	-6.6158742874
N58	-1.9928624802	-2.5869708476	-6.1153913591
C59	-2.9518680344	-2.5728546583	-5.1098018189
C60	-3.3611119610	-1.5978129897	-4.1938020641
O61	-2.9783920759	-0.3818171397	-3.9913174202

N62	-4.3728412086	-1.9942617083	-3.3509269261
C63	-4.9797031619	-3.2374959546	-3.3781269138
N64	-5.9760242016	-3.4378059385	-2.5069589004
N65	-4.6060693519	-4.1896721075	-4.2208839956
C66	-3.6170790367	-3.8225550086	-5.0360250388
N67	-5.2727859872	-4.2351629930	1.3885780012
C68	-4.4536101641	-4.9127524245	0.5118680966
N69	-3.4228752740	-4.1945897281	0.1433291287
C70	-3.5589187568	-2.9995330792	0.8250006657
C71	-2.7283262836	-1.8391141248	0.8338559925
O72	-1.6954768623	-1.6020343709	0.2013972792
N73	-3.2445232157	-0.8641940454	1.7184269274
C74	-4.3944198256	-0.9864315304	2.4728677209
N75	-4.7401499391	0.0795039733	3.2324224659
N76	-5.1753115363	-2.0508057022	2.4382243009
C77	-4.7031539716	-3.0111911159	1.6204540067
N78	-8.1317860004	-0.3501629990	0.8725779908
C79	-7.8142005680	-1.3595062767	-0.0074697634
N80	-6.7355926690	-1.1160091557	-0.7087570127
C81	-6.3156101905	0.1301095956	-0.2618796295
C82	-5.2433942250	0.9484492581	-0.5815355556
O83	-4.3355349230	0.6346855245	-1.4850975315
N84	-5.1588852701	2.1262950322	0.0947889886
C85	-6.0885190240	2.5379765735	1.0352339325
N86	-5.8849665883	3.7367996968	1.5935868225
N87	-7.1336504543	1.7903628497	1.3767501677
C88	-7.1920613321	0.6304464802	0.7301151793
H89	2.1551056954	5.0461829680	-5.4824720848
H90	0.1934448388	-1.5072368982	-8.4821201083
H91	1.6533743049	-0.8604834896	-9.0923039801
H92	-0.6729586648	-0.6629750735	-6.4779791792
H93	-4.6582470217	-1.2987176516	-2.6628265480
H94	-3.7438142077	7.1948633794	1.9770117546
H95	-1.4009773059	3.6583230747	-2.8678272585
H96	0.2618952665	6.6364741727	-3.6967182841
H97	-0.0065260871	4.9446391654	-4.1472435364
H98	-4.6656510710	-5.9244772732	0.1938878628
H99	-4.0624072391	0.8257251182	3.3968326620
H100	-5.4463055693	-0.0974740426	3.9338667254
H101	-2.6711906066	-0.0275907476	1.7908426681
H102	-8.4262010423	-2.2479813414	-0.0881907927
H103	-4.3471123111	2.7316007427	-0.1644740137
H104	-5.1109646694	4.3541117102	1.3168164244
H105	-6.6092064383	4.0844031803	2.2074141493
H106	-1.4687273777	-4.1748982152	-7.4290361761
H107	-6.4658648260	-4.3196669855	-2.5557311732

H108	-6.2878548974	-2.6940822172	-1.8795321362
H109	-0.9096129394	-6.1929613965	-1.2576289259
H110	-1.7870998484	-4.8416665007	-0.5864743210
H111	-0.9756615163	-2.6590819400	-1.1050822770
H112	2.6963074255	-3.2123683827	-6.3714983436
H113	2.4093165994	-0.6226539463	-4.5219517774
H114	3.8113680071	0.2677410945	-5.0731428457
H115	1.1996636142	0.3523420777	-2.6605948182
H116	4.0622693346	5.9571967192	-1.1748601487
H117	-3.9614683530	3.1801714947	5.0370054413
H118	0.5234035639	3.0372878741	0.4142715349
H119	1.8338002029	4.9569268028	0.5879381458
H120	1.5340888630	6.1150656573	1.9014813109
H121	-2.1923205094	0.0548512182	-4.5167114486
H122	-8.9285576493	-0.3178935006	1.4978231822
H123	-1.9943745773	8.2904678992	0.4686962616
H124	3.1445227797	3.5302801389	-7.2806433470
H125	-3.2773745459	-5.5438681820	-6.2390344086
H126	5.0575085434	4.6059107070	-3.1040291670
H127	-2.3283253742	5.1443109406	4.9535866150
H128	1.9393700184	-5.3761039241	-5.2279205723
H129	-6.0672144804	-4.6162568754	1.8868998084
H130	-3.6594620375	1.3489614024	-1.6120200448
H131	-0.6101039836	1.2628952933	0.2214928104

Single point energy: -4342.9238846

(2G4-3H⁺)_c

N1	-2.3337859999	4.3758370001	4.2935780002
C2	-3.3371190360	3.4311980801	4.3552094399
N3	-3.3102870960	2.6035653642	3.3393739547
C4	-2.2089012621	3.0061434488	2.5946112456
C5	-1.7728059275	2.6457971689	1.3087023416
O6	-2.3476955092	1.8403301632	0.5141828494
N7	-0.6330483842	3.3350196547	0.9021876272
C8	-0.0659009587	4.3905955811	1.5973847568
N9	0.9897510916	5.0150921316	1.0623021021
N10	-0.5451383463	4.8250616555	2.7586183210
C11	-1.5816221724	4.1084507258	3.1894885264
N12	-2.3107859999	7.3328369998	0.3775779998
C13	-3.1891082485	6.5498355652	1.0980067907
N14	-3.4269496050	5.3883943947	0.5434358090
C15	-2.6715728673	5.3992733347	-0.6206200222
C16	-2.4376742916	4.4454919313	-1.5999901469
O17	-2.9093041710	3.2040743592	-1.6331610024
N18	-1.6715919851	4.8366105494	-2.6527275244
C19	-1.0873416604	6.0922298570	-2.7320786136

N20	-0.3862725346	6.3858198723	-3.8253095993
N21	-1.2131615937	7.0086337375	-1.7607622952
C22	-1.9881856115	6.6313396251	-0.7595526501
N23	4.2212140001	4.3458370000	-2.5964219999
C24	3.4754489367	5.1704529545	-1.7852582004
N25	2.3258136405	4.6358048178	-1.4526550543
C26	2.3196626898	3.3952183227	-2.0643751471
C27	1.3275140264	2.3755290913	-2.0647352285
O28	0.2109628980	2.3614591459	-1.5206665361
N29	1.7445687355	1.2590929480	-2.8083137336
C30	2.9526911129	1.1471932488	-3.4743852417
N31	3.1697632255	-0.0126322726	-4.1226744521
N32	3.8612551283	2.1085984907	-3.4961444408
C33	3.4999188016	3.1889355540	-2.7804786232
N34	2.3242149998	3.3108370002	-6.7294220000
C35	2.0414650667	4.4420719221	-6.0013952838
N36	0.9018377720	4.3469244622	-5.3601239352
C37	0.4089034637	3.0972780069	-5.6933100819
C38	-0.7682156021	2.4191885367	-5.2732967443
O39	-1.6453270821	2.7855249793	-4.4728445210
N40	-0.8713589525	1.1569609437	-5.8875328720
C41	0.0327800549	0.6235691284	-6.7910050070
N42	-0.2710761207	-0.5646375610	-7.3436585348
N43	1.1520209387	1.2359528712	-7.1377730765
C44	1.2796665989	2.4430841494	-6.5672548955
N45	1.6542140000	-4.4471630000	-4.9444210000
C46	1.8790268877	-3.0976754852	-5.0883268686
N47	1.1674322756	-2.3692635959	-4.2622160165
C48	0.4340662808	-3.2944560574	-3.5329823154
C49	-0.5600163155	-3.1284684888	-2.5328880373
O50	-1.0276538596	-2.0465016088	-2.1165391523
N51	-1.0412138623	-4.3490429243	-2.0407564713
C52	-0.6188451994	-5.5913625769	-2.4799201970
N53	-1.1991109117	-6.6741805347	-1.8978164226
N54	0.2584596981	-5.7575972558	-3.4491347764
C55	0.7371719081	-4.5991419964	-3.9365625405
N56	-3.0297860000	-4.5901630001	-6.0044219999
C57	-2.1246963274	-3.7616956416	-6.6371724443
N58	-2.1439816779	-2.5358943293	-6.1832812465
C59	-3.1255406135	-2.5406972003	-5.2058755990
C60	-3.6189958320	-1.5677311354	-4.3429890225
O61	-3.1837388935	-0.3268486499	-4.3030447168
N62	-4.6235895811	-1.9629953933	-3.5123532461
C63	-5.1530040846	-3.2448148761	-3.5019586679
N64	-6.1587154018	-3.4687950098	-2.6508463488
N65	-4.6904438821	-4.2159035654	-4.2850136438

C66	-3.7073903302	-3.8256897447	-5.0923753747
N67	-5.2727860000	-4.2351630001	1.3885780000
C68	-4.4472428816	-4.8326117066	0.4500602634
N69	-3.5075924478	-4.0394145511	-0.0043842336
C70	-3.7146006193	-2.8409648809	0.6725115686
C71	-3.0725330591	-1.5961628162	0.6265703470
O72	-2.0656826112	-1.1873017811	-0.0684898261
N73	-3.5840541437	-0.6394356921	1.4618389682
C74	-4.6336847261	-0.8603384187	2.3369264664
N75	-4.9846822545	0.1595978786	3.1233189215
N76	-5.2848738797	-2.0246335775	2.3926374830
C77	-4.8087331644	-2.9497712899	1.5611304930
N78	-8.1317860002	-0.3501629999	0.8725779999
C79	-7.9502018845	-1.4717024164	0.0972529133
N80	-7.0187175180	-1.3130365976	-0.8130590649
C81	-6.5755953130	-0.0086359953	-0.6336515453
C82	-5.5798796561	0.7428237388	-1.3029866101
O83	-4.8396911890	0.3553819009	-2.2420969196
N84	-5.4616548688	2.0349992221	-0.7970159696
C85	-6.1946339464	2.5463220339	0.2646456744
N86	-5.9583522771	3.8174253493	0.6369673204
N87	-7.1264624598	1.8468221378	0.8947693764
C88	-7.2727288061	0.6099991834	0.4110083577
H89	2.7031397767	5.2969467175	-5.9896490908
H90	-0.9805820024	-1.1892006800	-6.9575550491
H91	0.4060756386	-0.9293953692	-7.9978391865
H92	-1.6993714718	0.6269489178	-5.6286188828
H93	-4.9815406589	-1.2216918614	-2.8699083342
H94	-3.6257337941	6.8987602120	2.0241561387
H95	-1.5414544786	4.1180192937	-3.4121715449
H96	0.0447228388	7.3011760233	-3.8306140547
H97	0.0034621906	5.6545487056	-4.4482530079
H98	-4.5960567108	-5.8602733405	0.1460614315
H99	-4.4320145097	1.0300619437	3.1867593132
H100	-5.7217481390	-0.0116985664	3.7933366500
H101	-3.1768788673	0.3054798548	1.3286618929
H102	-8.5368959155	-2.3675432901	0.2476184114
H103	-4.7552640500	2.6195443328	-1.2479576039
H104	-5.0525935137	4.2792463396	0.5152058562
H105	-6.5052113261	4.1219122664	1.4320562223
H106	-1.4838397007	-4.1252447654	-7.4293171957
H107	-6.6228359843	-4.3641554825	-2.7173423860
H108	-6.5411540203	-2.7252613388	-2.0476106540
H109	-0.7759153500	-7.5639296512	-2.1330238887
H110	-1.5532882557	-6.5972090770	-0.9539378382
H111	-1.8137477642	-4.2941697792	-1.3639456068

H112	2.5820477171	-2.7162057613	-5.8171189833
H113	2.4956545998	-0.7750968229	-4.0978769430
H114	4.0749071557	-0.1433596147	-4.5497228075
H115	1.0863168321	0.4840393907	-2.8243213045
H116	3.8342522615	6.1416455196	-1.4726368766
H117	-4.0480380139	3.4076370893	5.1700961540
H118	-0.2249371128	3.0394752037	-0.0069445876
H119	1.3814308094	4.8425346832	0.1254298713
H120	1.3903983148	5.7545563816	1.6229060094
H121	-1.7218378056	-1.7495488219	-0.8680522728
H122	-8.8260424173	-0.2213231909	1.5983226412
H123	-2.0197085482	8.2787881997	0.5930144253
H124	3.1209523039	3.1647128776	-7.3362618117
H125	-3.2276935383	-5.5589264892	-6.2254037480
H126	5.1563213155	4.5205898643	-2.9427012452
H127	-2.1208634193	5.0744420565	4.9952266166
H128	2.1274050860	-5.2001689149	-5.4294300932
H129	-6.0082467983	-4.6787884803	1.9249428265
H130	-2.6122594853	2.6298654149	-0.8338689680
H131	-3.6252047391	0.2164485778	-3.5976122296

Single point energy: -4342.9210486

(2G4-3H⁺)_d

N1	-2.3337862294	4.3758370176	4.2935777548
C2	-3.0009200345	3.1754382919	4.4864123902
N3	-2.6651024165	2.2434545867	3.6288241276
C4	-1.7058805678	2.8552179572	2.8253134624
C5	-0.9706185219	2.4293920537	1.7147804438
O6	-0.9419210153	1.2821421361	1.1132177115
N7	-0.1523316960	3.3647735061	1.1488395258
C8	0.0123623679	4.6432033209	1.6466729942
N9	0.8622532083	5.4444763968	1.0029436906
N10	-0.6518708120	5.0878898657	2.7169472976
C11	-1.4835089791	4.1901929145	3.2342974341
N12	-2.3107860976	7.3328371548	0.3775779522
C13	-3.2365058851	6.6847933663	1.1679065187
N14	-3.5372131666	5.4841195820	0.7316848192
C15	-2.7723902891	5.3329809181	-0.4200882387
C16	-2.6220809385	4.2370515495	-1.3054500986
O17	-3.1561727428	3.0984815355	-1.2185163065
N18	-1.7672578641	4.5110536837	-2.3607571784
C19	-1.1053503436	5.7159359556	-2.5504808339
N20	-0.3629533438	5.8199741304	-3.6599379592
N21	-1.1989777957	6.7309601090	-1.7005442606
C22	-2.0188612033	6.4896449888	-0.6713912956
N23	4.2212142400	4.3458367998	-2.5964218441

C24	3.6026881039	5.0881500569	-1.6155362483
N25	2.4785303536	4.5445744117	-1.2162987457
C26	2.3657868767	3.3789857756	-1.9595260614
C27	1.3430875382	2.3946141003	-1.9953050889
O28	0.2788515708	2.3844925564	-1.3458128603
N29	1.6366922781	1.3603520801	-2.8939851357
C30	2.7672043514	1.3071073074	-3.6886764667
N31	2.9178967929	0.2581018120	-4.5137079183
N32	3.7056754936	2.2480798736	-3.6888730555
C33	3.4542130712	3.2322336415	-2.8174393419
N34	2.3242141383	3.3108368807	-6.7294219653
C35	1.6791854536	4.1022048199	-5.8137228008
N36	0.5511987723	3.5824412046	-5.3898102587
C37	0.4459645488	2.3762678187	-6.0702427838
C38	-0.4949966745	1.3119172342	-5.9679369780
O39	-1.4876583984	1.2583394102	-5.2107829953
N40	-0.1914957095	0.2477523226	-6.8265602373
C41	0.9023225796	0.2077385962	-7.6709261981
N42	1.0505857095	-0.9143698876	-8.4322622621
N43	1.8022651364	1.1649061006	-7.7399117209
C44	1.5448606482	2.1972212913	-6.9171849993
N45	1.6542139963	-4.4471632205	-4.9444222464
C46	2.0185899488	-3.2771150814	-5.5739275380
N47	1.4781172145	-2.2207794630	-5.0172092519
C48	0.7333339033	-2.7173300576	-3.9632171578
C49	-0.0654231032	-2.0253292579	-3.0062098581
O50	-0.2882878926	-0.8111872063	-2.9051706940
N51	-0.6541978569	-2.9289268776	-2.0953021997
C52	-0.4752234773	-4.3029647165	-2.0996289995
N53	-1.1049350622	-4.9890231712	-1.1246959479
N54	0.2541890268	-4.9379800253	-3.0030453983
C55	0.8329203277	-4.1069977094	-3.8912342235
N56	-3.0297860842	-4.5901629906	-6.0044221258
C57	-2.1202777173	-3.7913875282	-6.6829519910
N58	-2.0857435512	-2.5542302438	-6.2547371569
C59	-3.0269122602	-2.5221713351	-5.2339319186
C60	-3.4647654121	-1.5093710198	-4.3717090316
O61	-3.1394180396	-0.2695932765	-4.2559546097
N62	-4.4416175069	-1.9036755709	-3.4829440741
C63	-4.9927317855	-3.1712183481	-3.4273670085
N64	-5.9535030986	-3.3745522509	-2.5134751162
N65	-4.5941868354	-4.1531666490	-4.2207712474
C66	-3.6347296332	-3.7917092490	-5.0748387897
N67	-5.2727858346	-4.2351631150	1.3885779799
C68	-4.2949028019	-4.4799840454	0.4487244044
N69	-3.3576544273	-3.5625572497	0.4371031672

C70	-3.7301014967	-2.6751899082	1.4354555886
C71	-3.1339342422	-1.4547428835	1.8676221691
O72	-2.1284344119	-0.9038945320	1.3940690330
N73	-3.8434943798	-0.8664882826	2.9314269646
C74	-4.9885253962	-1.3946202093	3.4977401256
N75	-5.5514848929	-0.6860037646	4.5168663661
N76	-5.5740734011	-2.4940616814	3.0660835691
C77	-4.9149456902	-3.0838180495	2.0487118733
N78	-8.1317860147	-0.3501630184	0.8725779658
C79	-7.8670489105	-1.3219127957	-0.0654632396
N80	-6.8018507330	-1.0703700514	-0.7848481272
C81	-6.3392722915	0.1454218931	-0.2974375534
C82	-5.2747204652	0.9717816839	-0.6346719648
O83	-4.4137338719	0.6988055441	-1.5940916659
N84	-5.1504166665	2.1176462412	0.0867808469
C85	-6.0300392579	2.4972156434	1.0851159024
N86	-5.7858459324	3.6677017514	1.6837562215
N87	-7.0661848063	1.7419561860	1.4456969509
C88	-7.1719248557	0.6162261458	0.7459521961
H89	2.0909317414	5.0506579974	-5.4969759580
H90	0.2218352962	-1.4308212581	-8.6956729068
H91	1.7475713345	-0.8276528311	-9.1624687399
H92	-0.7631185046	-0.5947127197	-6.7208944493
H93	-4.7465135295	-1.1804242517	-2.8324703169
H94	-3.6542509570	7.1540767251	2.0479398779
H95	-1.5655400721	3.7276169833	-2.9787525644
H96	0.0967264753	6.7044939613	-3.8214045760
H97	-0.2137468670	5.0325851908	-4.3002858402
H98	-4.3266394519	-5.3501147565	-0.1928804409
H99	-4.9545320085	-0.1081523726	5.0939846725
H100	-6.2743901902	-1.1839383939	5.0225636322
H101	-3.4774175190	0.0314259650	3.2660871472
H102	-8.5032740707	-2.1904946012	-0.1714920002
H103	-4.3574438891	2.7442541066	-0.2109840563
H104	-5.0332625354	4.3029413147	1.3797770498
H105	-6.4778585169	3.9952396363	2.3442081300
H106	-1.5156372172	-4.1912448999	-7.4857465851
H107	-6.4563173871	-4.2491238201	-2.5701279309
H108	-6.3149182985	-2.6028947444	-1.9474822951
H109	-0.8986499107	-5.9735438382	-1.0375831267
H110	-1.6865803165	-4.5215600928	-0.4319850368
H111	-1.1828893689	-2.4995895775	-1.3393362191
H112	2.6793328896	-3.2685984004	-6.4298759986
H113	2.2670071721	-0.5239052410	-4.6263025430
H114	3.7801343704	0.2338115446	-5.0392579875
H115	0.9409086949	0.6010507050	-2.9398308993

H116	4.0275653117	6.0094858541	-1.2412396985
H117	-3.7246890893	3.0608430694	5.2822662260
H118	0.2254937875	3.0858431543	0.2075035817
H119	1.4432318302	5.1302374951	0.2040450681
H120	1.0117650297	6.3602877249	1.4026693081
H121	-2.3568910574	0.1735115606	-4.8036313596
H122	-8.9133713889	-0.3236074641	1.5168743673
H123	-1.9773210935	8.2824381686	0.4861417489
H124	3.2007353479	3.5037471310	-7.1972670932
H125	-3.2468698027	-5.5627613816	-6.1851477493
H126	5.1283867189	4.5280360029	-3.0068353587
H127	-2.3761549395	5.1977143139	4.8829747911
H128	1.9851267515	-5.3801571376	-5.1562615116
H129	-6.0373440774	-4.8474632866	1.6444784116
H130	-3.7473177427	1.4269130069	-1.7239714178
H131	-1.5129074084	0.5259055066	1.4697219783

Single point energy: -4342.9164895

(2G4-3H⁺)_e

N1	-2.3337859959	4.3758369838	4.2935779757
C2	-3.1706833758	3.3001972812	4.4932597568
N3	-3.0515350188	2.4010614550	3.5481704063
C4	-2.0734808137	2.9035407078	2.7060740335
C5	-1.5651907946	2.4135410348	1.4760477646
O6	-1.9058326061	1.3914546861	0.8588207761
N7	-0.5776325068	3.2676870917	0.9460390534
C8	-0.1888037565	4.4727752421	1.4970862748
N9	0.7013103403	5.2311452952	0.8241430665
N10	-0.6873704540	4.9473574425	2.6281462576
C11	-1.6051647105	4.1313538737	3.1670655553
N12	-2.3107860138	7.3328369552	0.3775780258
C13	-3.1832677442	6.4225228739	0.9353937522
N14	-3.2987552632	5.3191670629	0.2426560653
C15	-2.4607707618	5.5027490182	-0.8450139184
C16	-2.0049905708	4.6296119001	-1.8272150090
O17	-2.3679629369	3.3710470597	-1.9131721871
N18	-1.1199804449	5.1604821485	-2.7308951634
C19	-0.6798167016	6.4751667051	-2.6640008835
N20	0.1213693932	6.8958036551	-3.6664626815
N21	-0.9939495729	7.2930902009	-1.6720669325
C22	-1.8453576870	6.7742854968	-0.7866345387
N23	4.2212139586	4.3458369973	-2.5964220015
C24	3.4342684809	5.2191573145	-1.8783868919
N25	2.2564645232	4.7191733282	-1.5956297745
C26	2.2750763406	3.4449391834	-2.1346629116
C27	1.2639847126	2.4543091530	-2.1825635955

O28	0.0949206329	2.5281318960	-1.7354137573
N29	1.6991946160	1.2858785311	-2.8035305933
C30	2.9445983729	1.1195470292	-3.3900192019
N31	3.1680522305	-0.0626194763	-3.9914688723
N32	3.8746034910	2.0640257576	-3.3955037483
C33	3.4988135916	3.1840661964	-2.7582281428
N34	2.3242150024	3.3108370095	-6.7294220011
C35	1.7307984871	4.1075734334	-5.7767829802
N36	0.6691199670	3.5578295460	-5.2302555958
C37	0.5596824856	2.3271223166	-5.8706896909
C38	-0.3228410591	1.2286852082	-5.6540478126
O39	-1.2074733597	1.1392001610	-4.7837100698
N40	-0.0734128724	0.1613976617	-6.5314962892
C41	0.9425212051	0.1365134326	-7.4654538908
N42	1.0720979724	-1.0090446642	-8.1993658459
N43	1.8020907357	1.1182662772	-7.6310093046
C44	1.5785649067	2.1636959751	-6.8132240702
N45	1.6542139972	-4.4471629977	-4.9444209978
C46	1.8721091319	-3.0979998029	-5.0844708037
N47	1.1975327510	-2.3797438678	-4.2164803441
C48	0.4936508533	-3.3133080195	-3.4677277979
C49	-0.4594709332	-3.1542727071	-2.4235325698
O50	-0.8946931092	-2.0806557883	-1.9611430148
N51	-0.9351708003	-4.3832027756	-1.9425959226
C52	-0.5317527535	-5.6188221427	-2.4138829014
N53	-1.0933937494	-6.7053556213	-1.8288222123
N54	0.3164755229	-5.7752879670	-3.4123737493
C55	0.7773111447	-4.6112113845	-3.9005130588
N56	-3.0297860151	-4.5901629881	-6.0044219686
C57	-2.0846794356	-3.7887797474	-6.6231980110
N58	-2.0050751329	-2.5824532874	-6.1159786741
C59	-2.9583845052	-2.5801758293	-5.1025454554
C60	-3.3847821060	-1.6124811717	-4.1862257572
O61	-3.0382000019	-0.3770554487	-4.0304968772
N62	-4.3545927717	-2.0159087306	-3.3123198837
C63	-4.9514652736	-3.2589257200	-3.3405028945
N64	-5.9159549953	-3.4948828608	-2.4440332591
N65	-4.5933152299	-4.2065239382	-4.2068614200
C66	-3.6152650491	-3.8302642416	-5.0265296343
N67	-5.2727860051	-4.2351629951	1.3885779986
C68	-4.4494573797	-4.8724175821	0.4732424515
N69	-3.4032061538	-4.1629201922	0.1267430745
C70	-3.5355624745	-2.9846980285	0.8545641083
C71	-2.7591286010	-1.8256577790	0.9414874234
O72	-1.6411665639	-1.5208702992	0.3619900074
N73	-3.2202830984	-0.8705384490	1.8026326967

C74	-4.3648061193	-1.0108414950	2.5670116308
N75	-4.6899693956	0.0071156186	3.3651302062
N76	-5.1332530990	-2.1012763426	2.5159328115
C77	-4.6946024547	-3.0209557002	1.6624714996
N78	-8.1317859282	-0.3501629648	0.8725779690
C79	-7.9423381385	-1.4806250850	0.1152651465
N80	-6.8459616988	-1.4215533930	-0.6021289000
C81	-6.2998467087	-0.1831040558	-0.3011118306
C82	-5.0875200438	0.4236710200	-0.7204901790
O83	-4.2118943680	-0.0412199778	-1.4662140215
N84	-4.9209577153	1.6997254301	-0.1520285448
C85	-5.8087508665	2.3065384000	0.7180275001
N86	-5.5062181219	3.5390956790	1.1701162843
N87	-6.9187181501	1.7232925032	1.1390467172
C88	-7.0981399691	0.5034404140	0.6126554808
H89	2.1369023641	5.0777092101	-5.5233278650
H90	0.2360788515	-1.5481032585	-8.3872732565
H91	1.7011861245	-0.9198945065	-8.9893397505
H92	-0.6395656062	-0.6828878453	-6.3932358103
H93	-4.5339218357	-1.3241636743	-2.5442826495
H94	-3.7043045988	6.6357315564	1.8589033897
H95	-0.7112187694	4.5413848769	-3.4437728774
H96	0.3282471521	7.8867519331	-3.6817093877
H97	0.1050992893	6.4169109531	-4.5572767868
H98	-4.6806521528	-5.8624656203	0.1035231094
H99	-4.1057218038	0.8546449155	3.4550999810
H100	-5.5252036688	-0.0968230108	3.9236925444
H101	-2.7393446520	0.0498994998	1.6987427579
H102	-8.6466218249	-2.3011198699	0.1282737894
H103	-4.0341829077	2.1462709421	-0.3742245477
H104	-4.7876279467	4.1265445825	0.7471815381
H105	-6.2403467646	3.9870292507	1.7011568589
H106	-1.4889431259	-4.1622850774	-7.4452048999
H107	-6.4243918262	-4.3612476644	-2.5539213865
H108	-6.2806042916	-2.7582391153	-1.8182962735
H109	-0.6890921021	-7.5976778569	-2.0831523075
H110	-1.4691546535	-6.6343581924	-0.8932508498
H111	-1.6941884511	-4.3405212379	-1.2491360433
H112	2.5308679798	-2.7051446593	-5.8472393196
H113	2.4966040860	-0.8314735060	-3.9382926757
H114	4.1118672701	-0.2438626388	-4.3032821258
H115	1.0126055090	0.5349337295	-2.8478668471
H116	3.7873794907	6.2006870339	-1.5922693450
H117	-3.8356818990	3.2415118908	5.3439772002
H118	-0.1933351602	2.9696158891	0.0422305555
H119	1.2057722943	4.9447481332	-0.0189950483

H120	1.0631426005	6.0226244333	1.3382292830
H121	-2.2322046172	0.0037845006	-4.5135249079
H122	-8.9213735125	-0.1525717876	1.4745650175
H123	-2.0794219140	8.2539573281	0.7305614751
H124	3.1326734931	3.5327842647	-7.2973844469
H125	-3.2927191470	-5.5341997642	-6.2588860346
H126	5.1828651031	4.4890334438	-2.8802528814
H127	-2.1890129451	5.1483291173	4.9318365599
H128	2.1002659605	-5.1950052979	-5.4613172998
H129	-6.0902933519	-4.6189967455	1.8452368133
H130	-1.5927129329	2.7853877562	-2.1479426614
H131	-1.4532291556	-1.9149711841	-0.5642871852

Single point energy: -4342.9070324

(2G4-3H⁺)_f

N1	-2.3337859998	4.3758369998	4.2935779994
C2	-3.2019110507	3.3225169448	4.4965295452
N3	-3.1023936931	2.4013966529	3.5680084313
C4	-2.1034742460	2.8648835078	2.7189453997
C5	-1.5393264364	2.3190904493	1.5401439260
O6	-1.8668898312	1.2340650701	0.9902185861
N7	-0.5483046299	3.1266470187	0.9908431962
C8	-0.1504396614	4.3453925719	1.5199500296
N9	0.7839914310	5.0519553707	0.8752189468
N10	-0.6738317196	4.8680192365	2.6261341164
C11	-1.6133638417	4.0954802925	3.1667627530
N12	-2.3107860000	7.3328370000	0.3775779999
C13	-3.2864464854	6.5463440966	0.9670296993
N14	-3.5058393981	5.4140581367	0.3431355898
C15	-2.6185488718	5.4398863731	-0.7281073245
C16	-2.3157178381	4.5141931424	-1.7370981607
O17	-2.7884545564	3.3405019919	-2.0041350725
N18	-1.3419501944	4.9160456010	-2.6161605178
C19	-0.7254170276	6.1524002450	-2.5738164398
N20	0.1384133379	6.4167326118	-3.5677839722
N21	-0.9603287693	7.0406801432	-1.6187046660
C22	-1.8720504109	6.6439652162	-0.7283587437
N23	4.2212139995	4.3458369995	-2.5964220000
C24	3.4933060460	5.0962561195	-1.7025390518
N25	2.3807913505	4.4987986623	-1.3532072707
C26	2.3863937778	3.2937446889	-2.0315692489
C27	1.4386615345	2.2313578909	-2.0409800084
O28	0.3580432895	2.1592459432	-1.4298269814
N29	1.8537444112	1.1780546280	-2.8703975575
C30	3.0108689616	1.1824229473	-3.6319301072
N31	3.2433860142	0.1289408576	-4.4280565700

N32	3.8885336168	2.1805659873	-3.6302920830
C33	3.5326302617	3.1790263986	-2.8145290685
N34	2.3242149998	3.3108370000	-6.7294220000
C35	1.7185697802	4.0948322224	-5.7773274523
N36	0.6394920152	3.5503258548	-5.2625155280
C37	0.5353665006	2.3242300727	-5.9137059936
C38	-0.3562925240	1.2259681724	-5.7341436554
O39	-1.2929562832	1.1498801343	-4.9118108915
N40	-0.0691564466	0.1555018050	-6.5909888325
C41	0.9694395707	0.1358503721	-7.5017476362
N42	1.1179441489	-1.0030953409	-8.2396259537
N43	1.8216154120	1.1252274234	-7.6510478797
C44	1.5787199003	2.1652219359	-6.8332097233
N45	1.6542140031	-4.4471629996	-4.9444210015
C46	2.1803658521	-3.2493257530	-5.3656090971
N47	1.6842771596	-2.2359189835	-4.6994238205
C48	0.8047050234	-2.7976337381	-3.7938004255
C49	-0.0252413788	-2.1885715492	-2.8102345627
O50	-0.1392998359	-0.9933577453	-2.5162473836
N51	-0.7946380359	-3.1687504300	-2.1361058029
C52	-0.7376234902	-4.5348472083	-2.3565264229
N53	-1.5459642689	-5.3159782156	-1.6157641299
N54	0.0423041027	-5.0896098545	-3.2666611982
C55	0.7745875942	-4.1834258046	-3.9329411244
N56	-3.0297860004	-4.5901629998	-6.0044220001
C57	-2.0043523436	-3.8313986024	-6.5455143792
N58	-1.9427864218	-2.6116182948	-6.0692498447
C59	-2.9858198457	-2.5491335321	-5.1547952936
C60	-3.4324663011	-1.5335412618	-4.2909328048
O61	-3.0236978932	-0.3384656940	-4.0781798110
N62	-4.5262009666	-1.8856569376	-3.5257359048
C63	-5.1745680178	-3.1022339745	-3.6031998357
N64	-6.2600163988	-3.2527823203	-2.8129208358
N65	-4.7652293040	-4.0854821236	-4.3847164629
C66	-3.6856885594	-3.7774346909	-5.1138187980
N67	-5.2727860022	-4.2351630001	1.3885780024
C68	-4.5320736373	-4.7478768010	0.3451604305
N69	-3.6198510963	-3.9184942450	-0.0919960505
C70	-3.7533699600	-2.7978768280	0.7095306393
C71	-3.1066667395	-1.5656939677	0.7307956074
O72	-2.1620543079	-1.2306173103	-0.1186819032
N73	-3.5077900182	-0.6982453287	1.6951626295
C74	-4.5163837387	-0.9804149144	2.6047938141
N75	-4.7890669271	-0.0267023743	3.4984184750
N76	-5.1959283049	-2.1282109129	2.5920690557
C77	-4.7831997777	-2.9798155205	1.6569645886

N78	-8.1317860000	-0.3501630000	0.8725780000
C79	-7.5549657532	-1.1502326079	-0.0856791651
N80	-6.5233925790	-0.5925495419	-0.6786117023
C81	-6.4170084955	0.6570128355	-0.0716765689
C82	-5.4802602518	1.7240346658	-0.2498508918
O83	-4.4999144027	1.7586935483	-1.0145924893
N84	-5.7587413401	2.8152562374	0.5925442543
C85	-6.8037386271	2.8737477359	1.4942905791
N86	-6.9025649107	4.0042148880	2.2465465476
N87	-7.6550210551	1.8869258624	1.6815137014
C88	-7.4170286369	0.8220608181	0.8942473451
H89	2.1330065125	5.0557408259	-5.5030603700
H90	0.2928907631	-1.5510044463	-8.4453902327
H91	1.7673245508	-0.9094140966	-9.0118787391
H92	-0.6120832206	-0.7004705426	-6.4449163865
H93	-4.8554706941	-1.1778150281	-2.8661617612
H94	-3.7987690711	6.8726385437	1.8620123849
H95	-1.0399648358	4.2256764080	-3.3105488927
H96	0.5144380882	7.3527500101	-3.6285899804
H97	0.2004965200	5.7958121174	-4.3656271153
H98	-4.7100225686	-5.7423444747	-0.0424078917
H99	-4.2134385844	0.8282922189	3.5742729697
H100	-5.4677634069	-0.2469321937	4.2145838875
H101	-3.0025251874	0.2228920433	1.6918828364
H102	-7.9458962266	-2.1372243014	-0.2954707312
H103	-5.0917797406	3.5911878605	0.5523341595
H104	-6.5402358436	4.8722777800	1.8751145173
H105	-7.7639611847	4.0857038504	2.7734096446
H106	-1.3369632600	-4.2444061370	-7.2899566353
H107	-6.8583469037	-4.0426063298	-3.0157203232
H108	-6.6680938083	-2.4371696670	-2.3708796163
H109	-1.3895891710	-6.3122524666	-1.6624321234
H110	-2.1665855452	-4.9134432224	-0.9190022084
H111	-1.3810570009	-2.7995282951	-1.3930927794
H112	2.9149481392	-3.1875063642	-6.1563234706
H113	2.6307093125	-0.6938502138	-4.4917759630
H114	4.1354651136	0.1230875114	-4.9015550406
H115	1.2144658023	0.3699318454	-2.8813717280
H116	3.8338023415	6.0595947039	-1.3484311455
H117	-3.8764052477	3.2937021444	5.3413910425
H118	-0.1178431433	2.7850761619	0.1055556095
H119	1.3135186266	4.7554104813	0.0369134462
H120	1.0961670893	5.8830676147	1.3587783424
H121	-2.1880309332	0.1125526156	-4.5612566510
H122	-8.9490463700	-0.5538545761	1.4346268116
H123	-1.9978262174	8.2495460015	0.6727909463

H124	3.1637969719	3.5195307383	-7.2549946981
H125	-3.2791166865	-5.5432765613	-6.2391527805
H126	5.1382850061	4.5648560516	-2.9643650517
H127	-2.1760608291	5.1586066994	4.9155951333
H128	1.9207805100	-5.3706019641	-5.2625001215
H129	-5.9838869234	-4.7177446779	1.9249818367
H130	-3.4918210790	2.9012667285	-1.4106706331
H131	-1.8205122686	-0.3022083186	0.0086985909

Single point energy: -4342.905034

(2G4-3H⁺)_g

N1	-2.3337859872	4.3758369954	4.2935779750
C2	-3.2332401103	3.3468895426	4.4650186901
N3	-3.1981608652	2.4899720307	3.4732582978
C4	-2.2136915390	2.9744915851	2.6257079940
C5	-1.7474906978	2.4999846318	1.3727468318
O6	-2.1415858424	1.5053416063	0.7398132923
N7	-0.7359219396	3.3222766572	0.8475389413
C8	-0.2693374609	4.4809451701	1.4366713651
N9	0.6522002718	5.2113696425	0.7832205757
N10	-0.7155907150	4.9364926289	2.6006388036
C11	-1.6608060381	4.1499267599	3.1286130500
N12	-2.3107859738	7.3328369811	0.3775779623
C13	-3.2845692091	6.5411833136	0.9636069634
N14	-3.5687923852	5.4571479271	0.2831077613
C15	-2.7298476288	5.5206843627	-0.8238276935
C16	-2.4849288611	4.6368308220	-1.8853517212
O17	-2.9872896210	3.4873149515	-2.1952090512
N18	-1.5322470060	5.0645961680	-2.7789769991
C19	-0.8837047883	6.2808471568	-2.6966413892
N20	-0.0373232630	6.5781208803	-3.7011670807
N21	-1.0625726427	7.1248915837	-1.6930250229
C22	-1.9464725973	6.7006455253	-0.7864530408
N23	4.2212139870	4.3458369881	-2.5964219917
C24	3.4700969896	5.2179509349	-1.8404184363
N25	2.2861488969	4.7344789402	-1.5548428014
C26	2.2658208915	3.4798548966	-2.1336345687
C27	1.2252344035	2.5086418701	-2.1733266626
O28	0.0761789090	2.5771994951	-1.7168193109
N29	1.6433687331	1.3447584490	-2.8426280816
C30	2.8693354708	1.1758055504	-3.4574223730
N31	3.0592070509	0.0065667133	-4.1106989512
N32	3.8176494061	2.0967995878	-3.4572595322
C33	3.4687076191	3.2095128605	-2.7823605243
N34	2.3242149625	3.3108370232	-6.7294219437
C35	1.6647904444	4.1019413881	-5.8161784375

N36	0.5813313981	3.5417913367	-5.3308271591
C37	0.5273925402	2.3064351637	-5.9651304630
C38	-0.3475628106	1.1961642310	-5.7911887373
O39	-1.2900674699	1.1130440015	-4.9790627548
N40	-0.0237975607	0.1191193268	-6.6269567053
C41	1.0452621915	0.1025314118	-7.5010203213
N42	1.2406325193	-1.0561301634	-8.2074766388
N43	1.8899814860	1.0987955035	-7.6351408629
C44	1.6043866349	2.1506968879	-6.8435853922
N45	1.6542140044	-4.4471629895	-4.9444209998
C46	1.8277981266	-3.0929109833	-5.1145148771
N47	1.0939581966	-2.3777946019	-4.2947103105
C48	0.4011474051	-3.3172713164	-3.5443543557
C49	-0.5972162785	-3.1666597610	-2.5450456595
O50	-1.1088641752	-2.0986381897	-2.1498966512
N51	-1.0299527073	-4.3960843715	-2.0270902326
C52	-0.5639571129	-5.6289589256	-2.4446724563
N53	-1.1021261380	-6.7209602756	-1.8410840776
N54	0.3164341161	-5.7820923539	-3.4147711776
C55	0.7498816749	-4.6159065292	-3.9258297051
N56	-3.0297860004	-4.5901630043	-6.0044219986
C57	-2.0328093968	-3.8184409640	-6.5789057278
N58	-1.9820958313	-2.5934278186	-6.1162358597
C59	-3.0086018470	-2.5393128489	-5.1814343919
C60	-3.4733948667	-1.5156532192	-4.3370856272
O61	-3.1003132728	-0.3011583764	-4.1711516167
N62	-4.5477074464	-1.8681211717	-3.5529461557
C63	-5.1639862891	-3.1033752276	-3.5839475011
N64	-6.2225645602	-3.2529353145	-2.7643564408
N65	-4.7429459291	-4.0959008027	-4.3518122713
C66	-3.6858298898	-3.7778613660	-5.1100741248
N67	-5.2727859979	-4.2351630000	1.3885780012
C68	-4.4589200335	-4.8559909906	0.4551312449
N69	-3.4768392476	-4.0980076854	0.0309884350
C70	-3.6426385919	-2.9036765697	0.7266872823
C71	-2.9285833137	-1.6990438823	0.7446987246
O72	-1.8610540946	-1.3528035531	0.1001734526
N73	-3.4058235295	-0.7400644450	1.5889722579
C74	-4.4993612018	-0.9194267050	2.4133961686
N75	-4.8412069532	0.1042821480	3.1992059892
N76	-5.2110760423	-2.0510236815	2.4305048547
C77	-4.7567085831	-2.9769320376	1.5914760205
N78	-8.1317859945	-0.3501629940	0.8725779952
C79	-7.6267139714	-1.1336412049	-0.1371763276
N80	-6.6327580826	-0.5706257498	-0.7865283900
C81	-6.4751368186	0.6670804429	-0.1638185057

C82	-5.5636212735	1.7482771363	-0.3981237463
O83	-4.6731100714	1.8295302835	-1.2604484223
N84	-5.7670963287	2.8077269827	0.5062567894
C85	-6.7393975092	2.8441493896	1.4838274209
N86	-6.7767900430	3.9539350718	2.2715000431
N87	-7.5840317054	1.8583003624	1.7022704967
C88	-7.4054802417	0.8146038966	0.8719895361
H89	2.0434322288	5.0782839275	-5.5451685238
H90	0.4170408425	-1.5806037581	-8.4766376323
H91	1.9218987201	-0.9569919748	-8.9523649336
H92	-0.5701611734	-0.7366677866	-6.4886458477
H93	-4.8939616676	-1.1443557882	-2.9184966809
H94	-3.7429228010	6.8247733231	1.9011275715
H95	-1.2301843648	4.3771067439	-3.4745193104
H96	0.3466082944	7.5128637699	-3.7208409844
H97	-0.0402012271	6.0313890283	-4.5518477854
H98	-4.6482827954	-5.8707768240	0.1313168609
H99	-4.2530134552	0.9507540434	3.3042107502
H100	-5.6099841938	-0.0506511590	3.8366589456
H101	-2.9499664892	0.2023045230	1.4617730988
H102	-8.0405511541	-2.1122975781	-0.3413658667
H103	-5.1040010369	3.5843111717	0.4420775146
H104	-6.4172828768	4.8251334264	1.9054193939
H105	-7.6025060403	4.0328008882	2.8522704982
H106	-1.3784998331	-4.2272792234	-7.3369904808
H107	-6.8047975996	-4.0675418372	-2.9025055362
H108	-6.6033783976	-2.4420878748	-2.2866638627
H109	-0.6478673218	-7.5999506381	-2.0566561777
H110	-1.4740357969	-6.6373737747	-0.9046281765
H111	-1.8013503285	-4.3535190875	-1.3468759357
H112	2.4984862812	-2.6956897265	-5.8647098277
H113	2.4059679828	-0.7684414437	-4.0060291831
H114	4.0071094985	-0.1906393936	-4.3998999015
H115	0.9385502309	0.6136893797	-2.9011324664
H116	3.8513022058	6.1818261977	-1.5317298618
H117	-3.8779313004	3.2868238919	5.3309413788
H118	-0.3705677413	3.0348794342	-0.0741396579
H119	1.1367239725	4.9425352640	-0.0797213225
H120	1.0430752596	5.9778498170	1.3133044544
H121	-2.2571000842	0.1034288768	-4.6476591814
H122	-8.9089065466	-0.5610921785	1.4857785573
H123	-1.9502716259	8.2162274317	0.7157540893
H124	3.1685539026	3.5354306514	-7.2407507108
H125	-3.2821120949	-5.5422949753	-6.2402879981
H126	5.1810620861	4.4737431248	-2.8918920644
H127	-2.1315739138	5.1139874544	4.9560410164

H128	2.1530280316	-5.1907336612	-5.4176691796
H129	-6.0335053888	-4.6547069852	1.9082594300
H130	-3.6564844946	2.9967803780	-1.5983989419
H131	-1.6433639931	-1.8421739347	-0.7727666552

Single point energy: -4342.9005827

(2G4-3H⁺)₄

N1	-2.3337860001	4.3758370000	4.2935770000
C2	-3.2499150437	3.3521131233	4.3534503707
N3	-3.0518696173	2.4681679749	3.4080895394
C4	-1.9415170104	2.9166221910	2.7196897391
C5	-1.2935769463	2.3923412520	1.5661482105
O6	-1.5865559675	1.4013166525	0.8886668611
N7	-0.1877838022	3.1957905624	1.2022036212
C8	0.1887436731	4.3731716592	1.8234632306
N9	1.2351603465	5.0445965308	1.3093850349
N10	-0.4460727230	4.8768459901	2.8705961401
C11	-1.4723150771	4.1079643232	3.2663285313
N12	-2.3107860003	7.3328370000	0.3775780002
C13	-3.1562250546	6.3980964308	0.9387429236
N14	-3.1043879027	5.2337614322	0.3463825835
C15	-2.1811235829	5.4017270731	-0.6697102189
C16	-1.5982310655	4.5012291224	-1.5530933888
O17	-1.8848617359	3.2249264127	-1.5951556274
N18	-0.6834523051	5.0421912741	-2.4215348882
C19	-0.3342614970	6.3854320725	-2.4137032529
N20	0.5308541208	6.7849550633	-3.3693011054
N21	-0.7948258151	7.2469135309	-1.5220907174
C22	-1.6829775489	6.7241667090	-0.6752042101
N23	4.2212140001	4.3458369999	-2.5964219999
C24	3.5056727227	5.0383264637	-1.6456313440
N25	2.4394479676	4.3864708270	-1.2549360665
C26	2.4752212932	3.1949516756	-1.9612173714
C27	1.5432450211	2.1369690510	-2.0410386389
O28	0.4356049509	2.0555007663	-1.4559347049
N29	1.9654922071	1.1204271904	-2.9025265592
C30	3.1063609772	1.1759542535	-3.6886601857
N31	3.3319117141	0.1738326364	-4.5498550435
N32	3.9521358429	2.2003218746	-3.6652957286
C33	3.5931584132	3.1486493007	-2.7970014650
N34	2.3242150003	3.3108369999	-6.7294220003
C35	2.0120587535	4.1875475577	-5.7127795799
N36	0.9680541855	3.8269973810	-5.0048607556
C37	0.5576458995	2.6353820850	-5.5949877563
C38	-0.3261817437	1.6433575276	-5.1803400979
O39	-1.0226061353	1.6783730273	-4.0711084661

N40	-0.4156251527	0.5512073120	-5.9978210672
C41	0.3610404702	0.3779873422	-7.1352000453
N42	0.1017999194	-0.7142917601	-7.8623539276
N43	1.3113895064	1.2373050193	-7.4831378794
C44	1.3883475193	2.3068871353	-6.6942493214
N45	1.6542140000	-4.4471629999	-4.9444210000
C46	2.3385358535	-3.3255886614	-5.3548297232
N47	1.8189994148	-2.2207783415	-4.8776976995
C48	0.7546443761	-2.6361895718	-4.0917729199
C49	-0.1963619223	-1.9028164416	-3.3466926879
O50	-0.2533190678	-0.6428589820	-3.2534492988
N51	-1.1156305798	-2.7121929307	-2.6915825272
C52	-1.1464023464	-4.0967766551	-2.8030259436
N53	-2.1143914326	-4.7629822488	-2.1697404435
N54	-0.2738015540	-4.7945668359	-3.5306064469
C55	0.6406818359	-4.0296738235	-4.1210376097
N56	-3.0297860002	-4.5901630000	-6.0044219999
C57	-2.0391215840	-3.7868398604	-6.5290564595
N58	-2.1159189196	-2.5338067851	-6.1464488821
C59	-3.2360883126	-2.5047890303	-5.3191325576
C60	-3.7971588609	-1.5263427247	-4.5051316704
O61	-3.3198777864	-0.3037204583	-4.3710115790
N62	-4.8993764303	-1.8886637219	-3.7992744392
C63	-5.4503053575	-3.1588000140	-3.8304295067
N64	-6.5629304023	-3.3378202840	-3.1176010083
N65	-4.9071571102	-4.1497721136	-4.5391089052
C66	-3.8325915620	-3.7874282202	-5.2314959712
N67	-5.2727859999	-4.2351629999	1.3885780000
C68	-4.9566018222	-4.7415781489	0.1506219534
N69	-4.2473749540	-3.8978839398	-0.5610661852
C70	-4.0789024059	-2.7914131351	0.2553827370
C71	-3.3719059142	-1.5758432700	0.0430733099
O72	-2.7489490471	-1.2178542567	-0.9773863834
N73	-3.4435114244	-0.7371651182	1.1687056452
C74	-4.1153374913	-1.0417602675	2.3437960704
N75	-4.0856864627	-0.1543407251	3.3425885830
N76	-4.7912387101	-2.1716055623	2.5306409325
C77	-4.7150324230	-2.9896719624	1.4816851063
N78	-8.1317860000	-0.3501630000	0.8725779999
C79	-8.2044456815	-1.3455234640	-0.0825531418
N80	-7.3494544331	-1.1795584402	-1.0639591728
C81	-6.6794790980	-0.0047671772	-0.7431100285
C82	-5.6500646959	0.6998424708	-1.4108422382
O83	-5.1153766349	0.4207807970	-2.5154874511
N84	-5.2371892233	1.8330985646	-0.7072760984
C85	-5.7754324176	2.2601332561	0.4994248274

N86	-5.2901582595	3.3892650573	1.0377335795
N87	-6.7546973461	1.6186331473	1.1141394713
C88	-7.1557548966	0.5192917503	0.4684546473
H89	2.6061475619	5.0754271301	-5.5415516975
H90	-0.6345028125	-1.3601892204	-7.5913090933
H91	0.6230624130	-0.8614197571	-8.7159356297
H92	-1.0447586393	-0.2032669802	-5.7192965474
H93	-5.2894802669	-1.1468105494	-3.1769579140
H94	-3.7874412212	6.6434885630	1.7821186685
H95	-0.2255274626	4.4325720712	-3.1073182991
H96	0.6660325662	7.7837824937	-3.4635575552
H97	0.6594033962	6.2091544724	-4.1911824479
H98	-5.2638484872	-5.7303536287	-0.1617554801
H99	-3.6849259189	0.7913409009	3.2858358731
H100	-4.5638167231	-0.4349120592	4.1871199854
H101	-2.8405126992	0.1011366929	1.1289643640
H102	-8.9096008149	-2.1611222228	0.0019578209
H103	-4.4384308676	2.3242502984	-1.0986182435
H104	-4.4422458100	3.8616282975	0.7208399894
H105	-5.6101965867	3.5838526917	1.9760347364
H106	-1.2855791314	-4.1911306632	-7.1916086069
H107	-6.9614822245	-4.2665019773	-3.1055290258
H108	-6.9123507637	-2.6249530387	-2.4630120489
H109	-2.0568920390	-5.7707294036	-2.2260652354
H110	-2.8951853782	-4.3442963858	-1.6360780006
H111	-1.7775863623	-2.2258498261	-2.0472668641
H112	3.2071443827	-3.3884893190	-5.9964351865
H113	2.7560115493	-0.6781733544	-4.6223090531
H114	4.2271773903	0.1960658963	-5.0191308631
H115	1.3079987593	0.3314375233	-2.9942643434
H116	3.8230423907	6.0067782653	-1.2832161686
H117	-4.0211070466	3.3112873674	5.1106300028
H118	0.3211776330	2.8485860175	0.3858882097
H119	1.7094447404	4.7658004763	0.4474869359
H120	1.5552418582	5.8474361647	1.8312851041
H121	-3.8125781285	0.1903910790	-3.6541856298
H122	-8.6986869451	-0.2608573346	1.7062822878
H123	-2.1925488509	8.2980954725	0.6633558979
H124	3.0769784293	3.3980502845	-7.4024464527
H125	-3.1756140197	-5.5763054825	-6.1841405916
H126	5.1231485335	4.6063700439	-2.9769725842
H127	-2.2303187634	5.1294474280	4.9618024558
H128	1.9010318159	-5.4109145504	-5.1338129335
H129	-5.7780782152	-4.7074305329	2.1274954279
H130	-1.0559871852	2.6440358559	-1.6783152419
H131	-1.0563364555	0.7554041545	-3.6566848019

Single point energy: -4342.8948988

(2G4-3H⁺)_n

N1	-2.3337860000	4.3758370002	4.2935770002
C2	-3.2781106494	3.3767191589	4.3348892228
N3	-3.1302370355	2.5271777734	3.3499340305
C4	-2.0264239182	2.9719439955	2.6501869263
C5	-1.4250089376	2.4735720629	1.4601622180
O6	-1.7511486011	1.5069743564	0.7629462420
N7	-0.3198227073	3.2718673205	1.0832136809
C8	0.0971224596	4.4215939306	1.7281253136
N9	1.1310946218	5.0991872518	1.1925079548
N10	-0.4833811270	4.8927589664	2.8205412219
C11	-1.5111997709	4.1292979815	3.2278921941
N12	-2.3107860000	7.3328370000	0.3775780000
C13	-3.1718779805	6.4157393204	0.9442275312
N14	-3.1946560046	5.2704720184	0.3150451076
C15	-2.3100331534	5.4309980778	-0.7344570117
C16	-1.8032159750	4.5332859898	-1.6679796085
O17	-2.1433067514	3.2701721739	-1.7326596209
N18	-0.9035759504	5.0579246943	-2.5629159557
C19	-0.5020551420	6.3859389631	-2.5347561220
N20	0.3401134530	6.7888042775	-3.5187455539
N21	-0.8834719135	7.2359637025	-1.5976463761
C22	-1.7541587757	6.7299202085	-0.7205303395
N23	4.2212140000	4.3458369999	-2.5964220001
C24	3.4365856772	5.1383782770	-1.7885017786
N25	2.3109258857	4.5540588969	-1.4576565447
C26	2.3745521040	3.3064209175	-2.0564706746
C27	1.4249382690	2.2596159898	-2.1177949389
O28	0.2737988732	2.2415454721	-1.6283215865
N29	1.9162312177	1.1490519643	-2.8141968739
C30	3.1305312888	1.1023767802	-3.4823121546
N31	3.4393265163	-0.0233375429	-4.1472367635
N32	3.9867288443	2.1124097299	-3.4902694521
C33	3.5712390065	3.1537369814	-2.7605323575
N34	2.3242150000	3.3108370000	-6.7294220000
C35	1.7816938890	3.9012858172	-5.6095945707
N36	0.7590746839	3.2453015170	-5.1150957574
C37	0.6188158996	2.1489656653	-5.9638005764
C38	-0.2164135122	1.0102538721	-5.9182375990
O39	-1.0383492128	0.6881818544	-5.0126820577
N40	-0.0503775509	0.1541324471	-7.0051877339
C41	0.8835502046	0.3354289743	-8.0082160527
N42	0.9324253629	-0.5996132184	-8.9871807053
N43	1.7419557721	1.3393015096	-8.0117346217

C44	1.5794035857	2.1906599994	-6.9905480798
N45	1.6542140001	-4.4471630000	-4.9444210000
C46	2.1998929850	-3.2663460876	-5.4007660621
N47	1.6155866402	-2.2026619384	-4.9072831398
C48	0.6301025053	-2.7074336184	-4.0686867329
C49	-0.2864002363	-2.1124709463	-3.2169089393
O50	-0.4223233194	-0.8131656562	-2.9807711647
N51	-1.0843429271	-2.9415396264	-2.4951800765
C52	-1.0198078195	-4.3245095558	-2.6050951256
N53	-1.8742412882	-5.0542791178	-1.9026192593
N54	-0.1343342319	-4.9446733465	-3.4031976683
C55	0.6454071359	-4.1212364642	-4.0760190141
N56	-3.0297860000	-4.5901630000	-6.0044220000
C57	-2.0602718877	-3.8366362976	-6.6432052682
N58	-2.1175672272	-2.5558655875	-6.3672326443
C59	-3.2028108702	-2.4484097851	-5.4988883336
C60	-3.8083716849	-1.3688182086	-4.8521225586
O61	-3.5027172691	-0.0993564250	-4.9095296352
N62	-4.8802867941	-1.6541303589	-4.0666583546
C63	-5.3837764271	-2.9320113553	-3.9040080480
N64	-6.4439103572	-3.0791740843	-3.1108485202
N65	-4.8485918962	-3.9978315786	-4.5151838364
C66	-3.7951102341	-3.7131227548	-5.2694843413
N67	-5.2727860001	-4.2351630002	1.3885779999
C68	-4.7846529463	-4.8504839445	0.2638517253
N69	-3.9883171239	-4.0625408552	-0.4192459389
C70	-3.9464525236	-2.8792191428	0.3010775766
C71	-3.2372200474	-1.6711115335	0.0784917579
O72	-2.4728264793	-1.3954947539	-0.8708134250
N73	-3.4735615708	-0.7300521431	1.0864243311
C74	-4.2975371886	-0.9374475034	2.1813188471
N75	-4.4275961188	0.0414560764	3.0801344004
N76	-4.9761486732	-2.0638250936	2.3821687958
C77	-4.7485526847	-2.9738158075	1.4377737149
N78	-8.1317860000	-0.3501630000	0.8725779999
C79	-8.1892163984	-1.3546664664	-0.0694932832
N80	-7.3632629983	-1.1540537469	-1.0693434024
C81	-6.7398582137	0.0473893274	-0.7699239446
C82	-5.7483358124	0.7830668141	-1.4713495214
O83	-5.2002235384	0.5351800152	-2.5577104704
N84	-5.3805968264	1.9468458516	-0.7680386353
C85	-5.9218305974	2.3636650846	0.4348721813
N86	-5.4892349179	3.5316360616	0.9497714298
N87	-6.8566143884	1.6868996538	1.0755372900
C88	-7.2117695723	0.5614004626	0.4408400052
H89	2.1987481210	4.8109751118	-5.1983779240

H90	0.1145601375	-1.1543662704	-9.2015880794
H91	1.5329639259	-0.3770506575	-9.7721066395
H92	-0.6126169522	-0.7028428983	-6.9687772164
H93	-5.2168233303	-0.8473950683	-3.4718465333
H94	-3.7568409559	6.6589608564	1.8209519746
H95	-0.4829686890	4.4212849262	-3.2493127139
H96	0.5053254340	7.7883258366	-3.5527954315
H97	0.3015161030	6.3227368513	-4.4160899003
H98	-5.0386810278	-5.8699099586	0.0075057813
H99	-3.9281291289	0.9414140596	3.0694932041
H100	-5.0015648513	-0.1822368788	3.8808856270
H101	-2.9184573332	0.1390855909	1.0159367405
H102	-8.8585513964	-2.1974120108	0.0349648891
H103	-4.6280639191	2.4778095480	-1.1958222383
H104	-4.6202839117	3.9768937601	0.6583848615
H105	-5.8073392329	3.7128505554	1.8915315616
H106	-1.3394680784	-4.2990932635	-7.3043360166
H107	-6.7773790828	-4.0250849392	-2.9852750088
H108	-6.8107748476	-2.3398335797	-2.4866237814
H109	-1.7766964004	-6.0575665048	-1.9883765298
H110	-2.6815903762	-4.6563692211	-1.3708432607
H111	-1.7474565145	-2.4468151597	-1.8063502862
H112	3.0334850625	-3.2574540881	-6.0908799885
H113	2.7554222689	-0.7416238543	-4.3940470097
H114	4.3328681208	-0.0217753723	-4.6197849461
H115	1.2955696296	0.3397263422	-2.8147088961
H116	3.7506942320	6.1256870994	-1.4778646049
H117	-4.0334156384	3.3292955652	5.1074697947
H118	0.1464371045	2.9521456679	0.2312858196
H119	1.5533122695	4.8701626569	0.2912310617
H120	1.4700707244	5.8912987120	1.7189178388
H121	-2.5654649633	0.0864406328	-5.1931785840
H122	-8.6883262045	-0.2742861147	1.7142195364
H123	-2.1410826370	8.2834048967	0.6857970722
H124	3.0986438456	3.6484037173	-7.2883712643
H125	-3.2078539761	-5.5806044528	-6.1168771435
H126	5.1592744254	4.5536467144	-2.9177246490
H127	-2.1963581602	5.1030290046	4.9845248303
H128	1.9744050954	-5.3855586514	-5.1536630271
H129	-5.8776804344	-4.6453836882	2.0888636977
H130	-1.3468796061	2.6719107502	-1.8680668906
H131	-0.5904986860	-0.2628022775	-3.8091909867

Single point energy: -4342.8914128

(2G4-3H⁺)_i

N1	-2.3337860000	4.3758369999	4.2935779998
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C2	-3.2656789010	3.3660454393	4.3988008588
N3	-3.1990917020	2.5183182253	3.4026927285
C4	-2.1500111109	2.9751565800	2.6182767035
C5	-1.6731909143	2.5441586779	1.3566193659
O6	-2.1693543758	1.6435450054	0.6282920876
N7	-0.5636707968	3.2761863050	0.9301464484
C8	-0.0703785224	4.4016705793	1.5740125114
N9	0.9421869301	5.0683409535	1.0015655437
N10	-0.5800219137	4.8716779540	2.7079017731
C11	-1.5837897396	4.1255724622	3.1756684627
N12	-2.3107859998	7.3328369999	0.3775779999
C13	-3.1767247501	6.4151166685	0.9280771471
N14	-3.2675554963	5.3022024404	0.2430107239
C15	-2.4127659123	5.4904558930	-0.8382155495
C16	-1.9178465344	4.6241667848	-1.8154027572
O17	-2.2260494725	3.3570801403	-1.9143543062
N18	-1.0293415648	5.1761781812	-2.7035592751
C19	-0.6154331305	6.4978942940	-2.6344259874
N20	0.1896340797	6.9320225001	-3.6230768563
N21	-0.9627936991	7.3091123474	-1.6461786974
C22	-1.8202073404	6.7733949186	-0.7776775425
N23	4.2212139996	4.3458369999	-2.5964220000
C24	3.4609909091	5.1597388228	-1.7867176479
N25	2.2940068271	4.6349419851	-1.4999556247
C26	2.2940093357	3.4009432322	-2.1325418873
C27	1.2980606845	2.4012896415	-2.2174155823
O28	0.1449168457	2.4497287885	-1.6984468959
N29	1.7013932375	1.2926729070	-2.9442939555
C30	2.9176914073	1.1994541742	-3.6044723180
N31	3.1604651994	0.0958643253	-4.3212687931
N32	3.8471474791	2.1548815781	-3.5691133751
C33	3.4954033156	3.1993746052	-2.8199324783
N34	2.3242140000	3.3108370002	-6.7294219997
C35	1.7454725349	4.1011016756	-5.7624049253
N36	0.6571308162	3.5772418894	-5.2419931807
C37	0.5109373733	2.3621212130	-5.9099446462
C38	-0.4070471383	1.2798735549	-5.7283122690
O39	-1.3275339657	1.1956037436	-4.8917791932
N40	-0.1612054210	0.2241931615	-6.6194543668
C41	0.8616240353	0.1939502580	-7.5459106056
N42	0.9602056838	-0.9221896003	-8.3188445966
N43	1.7447052866	1.1606624976	-7.6839545918
C44	1.5398708105	2.1896846089	-6.8442201790
N45	1.6542139999	-4.4471629999	-4.9444219999
C46	2.0281707115	-3.2643657903	-5.5415508936
N47	1.5430615434	-2.2165939217	-4.9182539422

C48	0.8284868611	-2.7373771540	-3.8517932612
C49	0.0874494359	-2.0813997219	-2.8268506183
O50	-0.0946203048	-0.8599991921	-2.6716561637
N51	-0.4833697168	-3.0054978066	-1.9346623579
C52	-0.3390630051	-4.3812295918	-2.0172790578
N53	-0.9024637597	-5.1198897827	-1.0442360434
N54	0.3338876046	-4.9909099269	-2.9863371684
C55	0.8938925076	-4.1306924790	-3.8456945421
N56	-3.0297860001	-4.5901630002	-6.0044219999
C57	-2.1117918520	-3.7669073050	-6.6394476703
N58	-2.0346671515	-2.5665046148	-6.1214217274
C59	-2.9540348978	-2.5881046226	-5.0794993439
C60	-3.3358862449	-1.6481189952	-4.1198576689
O61	-2.9620136304	-0.4290606783	-3.8968514410
N62	-4.2978087128	-2.0876004450	-3.2400284742
C63	-4.8939412764	-3.3357571356	-3.2782221328
N64	-5.8561685589	-3.5803603729	-2.3824039919
N65	-4.5435582250	-4.2576469830	-4.1641039717
C66	-3.5930881730	-3.8525987548	-5.0033325330
N67	-5.2727859998	-4.2351629999	1.3885780000
C68	-4.4367331063	-4.9088413852	0.5233096020
N69	-3.3699327793	-4.2116975310	0.2261270972
C70	-3.4945372676	-3.0433512892	0.9544742708
C71	-2.6754230290	-1.8788184732	0.9753685037
O72	-1.6647949108	-1.6178497410	0.3144870994
N73	-3.2017879671	-0.9113672701	1.8637799256
C74	-4.3753581127	-1.0320241022	2.5853594547
N75	-4.7584069752	0.0320258609	3.3212652490
N76	-5.1536741222	-2.1006979964	2.5276259467
C77	-4.6684228743	-3.0481541108	1.7052460356
N78	-8.1317859998	-0.3501630001	0.8725779999
C79	-7.8294320256	-1.4799364504	0.1419245697
N80	-6.6901876805	-1.3968435496	-0.4963405716
C81	-6.2069548814	-0.1363331309	-0.1729011227
C82	-4.9873484559	0.4931503719	-0.3704103839
O83	-3.9799995242	-0.0659899062	-1.0180267179
N84	-4.8529696783	1.7436088080	0.1464570780
C85	-5.8717702462	2.3827137207	0.8427092384
N86	-5.6438255618	3.6498942050	1.1975518193
N87	-7.0163339147	1.7806622975	1.1491215313
C88	-7.1197932346	0.5468217055	0.6678397949
H89	2.1845500528	5.0475680222	-5.4765444144
H90	0.1299119910	-1.4729263985	-8.4889989285
H91	1.5950740977	-0.8367957657	-9.1032849858
H92	-0.7192596345	-0.6228806994	-6.4785580733
H93	-4.5029293411	-1.4456045682	-2.4764787807

H94	-3.7133977105	6.6292617552	1.8426240973
H95	-0.6186618781	4.5661517532	-3.4262755543
H96	0.3975043108	7.9226065082	-3.6389124285
H97	0.2425890364	6.4276248147	-4.4981306025
H98	-4.6664031986	-5.9006700441	0.1582881545
H99	-4.1604331658	0.8560278160	3.4434407515
H100	-5.5171116548	-0.1275821832	3.9692124250
H101	-2.6923771688	-0.0273384560	1.8606098448
H102	-8.4984777779	-2.3298013627	0.1177417711
H103	-3.8781144582	2.0896131516	0.2168603261
H104	-4.8382487569	4.1756824026	0.8444575262
H105	-6.3922722685	4.1332899122	1.6754823654
H106	-1.5335079997	-4.1219139051	-7.4818189753
H107	-6.3034434765	-4.4850064566	-2.4263262692
H108	-6.1587270193	-2.8806641676	-1.6994239009
H109	-0.8048160743	-6.1197470977	-1.1588792232
H110	-1.7112326257	-4.7765498221	-0.5152363602
H111	-0.9357869854	-2.5907822061	-1.1049061249
H112	2.6533784888	-3.2377273095	-6.4233758460
H113	2.4822958488	-0.6532461487	-4.5148656626
H114	4.0694785966	0.0463820904	-4.7600111761
H115	1.0396242083	0.4893296865	-2.9534607445
H116	3.8227992187	6.1183815760	-1.4400975754
H117	-3.9562319497	3.3109960630	5.2295611701
H118	-0.1565167192	2.9746158058	0.0303057304
H119	1.3751414848	4.8425484053	0.0959522875
H120	1.3269881137	5.8294162046	1.5440387219
H121	-2.2142548438	0.0155831495	-4.4488553493
H122	-8.9714947858	-0.1830809404	1.4149571725
H123	-2.1014347991	8.2622245648	0.7232559644
H124	3.1542150295	3.5106209602	-7.2733132992
H125	-3.2705677232	-5.5435553017	-6.2473127329
H126	5.1715642875	4.5123521169	-2.9037279778
H127	-2.1380224706	5.0892710505	4.9853789691
H128	1.9509020521	-5.3795153697	-5.2038010171
H129	-6.0897608462	-4.6152512230	1.8497668268
H130	-3.0996433467	0.3397358880	-0.8311231289
H131	-1.3945213299	2.8044581775	-2.1082836890

Single point energy: -4342.8898457

(2G4-4H⁺)₁

N1	-2.3337859962	4.3758369990	4.2935779997
C2	-3.2216305064	3.3331758369	4.4664735876
N3	-3.0679927705	2.3830156161	3.5748639691
C4	-2.0106400381	2.8176115448	2.7840700975
C5	-1.3807861507	2.2410321896	1.6619020555

O6	-1.6782486641	1.1547926113	1.0951593160
N7	-0.3314392947	3.0233827001	1.1736332465
C8	0.0633939450	4.2462099255	1.7095788215
N9	1.0960025698	4.8786497724	1.1388706657
N10	-0.5444580845	4.8026558252	2.7437163350
C11	-1.5372746214	4.0579372644	3.2340525556
N12	-2.3107859980	7.3328369920	0.3775780077
C13	-3.2547177382	6.5175303887	0.9629940233
N14	-3.3832574172	5.3630694998	0.3594975995
C15	-2.4805034192	5.4212307786	-0.6904520691
C16	-2.1067744007	4.5217831834	-1.6723813832
O17	-2.6054512958	3.3022223123	-1.7879816345
N18	-1.1551841857	4.9496306801	-2.5505064505
C19	-0.5803554873	6.2159234016	-2.5006305763
N20	0.3065254154	6.5102979245	-3.4496754069
N21	-0.8869566864	7.0973957548	-1.5536633996
C22	-1.8061120737	6.6670501646	-0.7004480715
N23	4.2212140005	4.3458370016	-2.5964219982
C24	3.3437955217	4.9560777458	-1.7292760161
N25	2.3765518993	4.1663424048	-1.3367373123
C26	2.6345549887	2.9592603187	-1.9655965575
C27	1.9932490928	1.7324067452	-1.9646464042
O28	0.8937414933	1.4705599069	-1.2771394323
N29	2.5563942568	0.7564236535	-2.7299715347
C30	3.7117694727	0.9447575378	-3.4839263733
N31	4.1430682741	-0.1023098272	-4.1809661485
N32	4.3546531964	2.1122526771	-3.5161664070
C33	3.8004018517	3.0529913111	-2.7637505074
N34	2.3242150046	3.3108369979	-6.7294219998
C35	2.0874892872	4.4169293648	-5.9499495922
N36	1.1077576031	4.2322463111	-5.0962146822
C37	0.6664518211	2.9382276593	-5.3448009150
C38	-0.3481404231	2.1624724646	-4.7436855103
O39	-1.0836476505	2.4946788045	-3.7779857373
N40	-0.4723998266	0.9003648981	-5.3251718117
C41	0.3023202791	0.4353395245	-6.3854366899
N42	0.0398710303	-0.7839510211	-6.8646485083
N43	1.2853720673	1.1448074470	-6.9186369809
C44	1.4122063520	2.3569254972	-6.3793289458
N45	1.6542139937	-4.4471629989	-4.9444210156
C46	2.5528427736	-3.4084186317	-5.0766330431
N47	2.2815041520	-2.4043067613	-4.2775393438
C48	1.1569309088	-2.8136833318	-3.5718966024
C49	0.3888445418	-2.1783784461	-2.5739964117
O50	0.5630068567	-1.0275831959	-2.0950098927
N51	-0.6616699479	-2.9840006354	-2.1197341555

C52	-0.9443664179	-4.2644319453	-2.5906052101
N53	-1.9899362427	-4.9153174029	-2.0709367676
N54	-0.2457215117	-4.8459186532	-3.5487359960
C55	0.7691227448	-4.0974492328	-3.9760285326
N56	-3.0297860152	-4.5901630172	-6.0044220172
C57	-2.0089631814	-3.8036684097	-6.4830403563
N58	-1.9436400589	-2.6342709484	-5.8988501415
C59	-2.9876352403	-2.6410610707	-4.9892629420
C60	-3.4342424701	-1.7287914953	-4.0485404074
O61	-2.8712634381	-0.5519935428	-3.8293121873
N62	-4.5151607083	-2.1043110083	-3.3095146938
C63	-5.1702098703	-3.3182876278	-3.4761817973
N64	-6.2352115809	-3.5320640720	-2.6981907310
N65	-4.7589003410	-4.2341599373	-4.3481206015
C66	-3.6948080763	-3.8668439014	-5.0528954752
N67	-5.2727859927	-4.2351629737	1.3885780000
C68	-4.5796234346	-4.6950320878	0.2985971869
N69	-3.6582263148	-3.8587724556	-0.1043392944
C70	-3.7344818187	-2.7936579723	0.7723183196
C71	-3.0375990925	-1.6024626438	0.8750017147
O72	-2.0601906889	-1.2472796469	0.0607394584
N73	-3.4103816487	-0.7746790035	1.8885335967
C74	-4.4220996419	-1.0801205614	2.7938274157
N75	-4.6666209086	-0.1694043770	3.7339909946
N76	-5.1206213046	-2.2141308641	2.7239340877
C77	-4.7505916715	-3.0130499829	1.7302270198
N78	-8.1317860036	-0.3501629953	0.8725780000
C79	-7.9446216688	-1.4696084321	0.0921750178
N80	-6.8991082154	-1.3735562069	-0.6964380441
C81	-6.3793071040	-0.1103075524	-0.4292254463
C82	-5.2537355528	0.5682512653	-0.9442013017
O83	-4.4163703922	0.1293784179	-1.7810261742
N84	-5.0963598941	1.8430755709	-0.3992759791
C85	-5.9472450681	2.4125652165	0.5447693126
N86	-5.6902749918	3.6612483785	0.9481427710
N87	-6.9862915516	1.7656122469	1.0515397338
C88	-7.1532572117	0.5452885893	0.5410296551
H89	2.6610515138	5.3268902562	-6.0656993636
H90	-0.7167728193	-1.3828733681	-6.5177333307
H91	0.5534788113	-1.0522602265	-7.6933642581
H92	-1.2192888088	0.3178462586	-4.9504905131
H93	-4.8163807085	-1.4250357821	-2.5866233666
H94	-3.8189287962	6.8375433084	1.8288194348
H95	-0.8657287298	4.2604211989	-3.2635419216
H96	0.6544490275	7.4594804756	-3.4870195374
H97	0.5792582854	5.8081593054	-4.1490040621

H98	-4.7949887246	-5.6564747521	-0.1491446556
H99	-4.1409306421	0.7137864808	3.7771304826
H100	-5.3636625009	-0.3879999733	4.4342354489
H101	-2.8988818772	0.1256500687	1.9371627092
H102	-8.6168326417	-2.3156639701	0.1456642051
H103	-4.3125026789	2.3840087206	-0.7608320955
H104	-4.8705364257	4.2086320254	0.6691439395
H105	-6.3591458487	4.0644772380	1.5902335050
H106	-1.3513531374	-4.1484248008	-7.2699763411
H107	-6.8032124024	-4.3434694181	-2.9045799740
H108	-6.5764748992	-2.8109863985	-2.0497208683
H109	-2.0753712387	-5.8888688339	-2.3312283702
H110	-2.5426885576	-4.5356838401	-1.2946507521
H111	-1.2094175803	-2.5904657365	-1.3567048457
H112	3.3809191212	-3.4566604448	-5.7711591740
H113	3.5953966402	-0.9723251417	-4.2269837502
H114	5.0006458409	0.0019566919	-4.7078517476
H115	2.0673646877	-0.1556106445	-2.7216059418
H116	3.4765183347	5.9844816554	-1.4197294826
H117	-3.9494032565	3.3344045085	5.2669745758
H118	0.1870524448	2.6200447515	0.3955383613
H119	1.5523926265	4.5652438254	0.2774897740
H120	1.4105520512	5.7235745087	1.5968561922
H121	-3.3418370184	-0.0546911129	-3.1038062972
H122	-8.9009892186	-0.1770884223	1.5099494247
H123	-2.0744706126	8.2810650255	0.6504086949
H124	2.9875373176	3.2397658775	-7.4929428118
H125	-3.2916653102	-5.5127013627	-6.3354299763
H126	5.0729377965	4.7426194847	-2.9788897114
H127	-2.2123250258	5.1718053519	4.9091031631
H128	1.7159136505	-5.3559313872	-5.3890740622
H129	-5.9864751163	-4.7346635005	1.9081639659
H130	-2.1809741726	2.8088364964	-2.5437132099
H131	-1.7041534257	-0.3446002400	0.2924155031
H132	0.5833094273	0.5355603495	-1.4329120379

Single point energy: -4343.1190004

(2G4-4H⁺)₂

N1	-2.3337860012	4.3758369988	4.2935780006
C2	-3.0573834827	3.2048246813	4.4026330323
N3	-2.7025322856	2.2940519570	3.5310364340
C4	-1.6704810406	2.8944896195	2.8194568850
C5	-0.9036089053	2.5043552322	1.7354621491
O6	-1.0455234488	1.3436066958	1.1265797103
N7	0.0234128517	3.3998071997	1.2943391700
C8	0.2133966331	4.6530750059	1.8581243627

N9	1.1525479354	5.4249396357	1.3094586721
N10	-0.5202138515	5.0846116921	2.8810350895
C11	-1.4163902279	4.2001101772	3.3021179195
N12	-2.3107859994	7.3328369965	0.3775779979
C13	-3.1640886473	6.4810240207	1.0421417402
N14	-3.2264605775	5.2876687195	0.5054083727
C15	-2.3749799432	5.3578958022	-0.5882933985
C16	-1.9813162858	4.4415291975	-1.5495211599
O17	-2.3790927684	3.1799197875	-1.5802927037
N18	-1.1206696070	4.8985846415	-2.5000898282
C19	-0.6377157078	6.2035886224	-2.5361352066
N20	0.1705053305	6.5150937433	-3.5441654108
N21	-0.9622668885	7.1047718782	-1.6098553173
C22	-1.8038567368	6.6506848374	-0.6934292560
N23	4.2212140001	4.3458369907	-2.5964219998
C24	3.5419640076	5.1072100624	-1.6709200388
N25	2.5234802164	4.4738112009	-1.1381602072
C26	2.5403353159	3.2190792067	-1.7349852758
C27	1.6895414818	2.1019265369	-1.5791928326
O28	0.6643914384	2.0125207713	-0.8474802358
N29	2.0763682365	1.0177316179	-2.3573948855
C30	3.1780672035	1.0072510446	-3.2068743299
N31	3.4172399526	-0.1400294095	-3.8544809525
N32	3.9580532881	2.0630107898	-3.3846362315
C33	3.6079538439	3.1173070968	-2.6392640253
N34	2.3242149982	3.3108369996	-6.7294219984
C35	2.0607472001	4.4288460810	-5.9757820266
N36	1.0824131348	4.2418287987	-5.1210372330
C37	0.6744888028	2.9315776599	-5.3372095967
C38	-0.3258693761	2.1470457776	-4.7242798021
O39	-1.0945532097	2.4891191269	-3.7863231241
N40	-0.4094364830	0.8663814520	-5.2729409674
C41	0.3791977105	0.3972097490	-6.3195737008
N42	0.1512404064	-0.8418757163	-6.7724485466
N43	1.3436203510	1.1172790275	-6.8677514611
C44	1.4390594148	2.3439310220	-6.3543532443
N45	1.6542139927	-4.4471629917	-4.9444209905
C46	2.1112533014	-3.1552775551	-4.8538047597
N47	1.5139167408	-2.4636928334	-3.9119814450
C48	0.6171264017	-3.3576290655	-3.3420976791
C49	-0.3540792029	-3.1988156473	-2.3204828547
O50	-0.6428395402	-2.1342530051	-1.7201979713
N51	-1.0418245840	-4.3840225785	-2.0383362184
C52	-0.8232451314	-5.5910017815	-2.6847501493
N53	-1.5810569193	-6.6451060411	-2.2858355065
N54	0.0262050879	-5.7310732627	-3.6827255819

C55	0.7048800048	-4.6077823803	-3.9673930406
N56	-3.0297859993	-4.5901629987	-6.0044220001
C57	-1.9876582753	-3.8217569620	-6.4701945936
N58	-1.9077547806	-2.6558332663	-5.8819518384
C59	-2.9638376214	-2.6427180793	-4.9869149092
C60	-3.4090218836	-1.7201180557	-4.0539313426
O61	-2.8362492606	-0.5507759350	-3.8339674502
N62	-4.5092913711	-2.0763881638	-3.3343558034
C63	-5.1805190928	-3.2805214298	-3.5050380084
N64	-6.2561945874	-3.4771683622	-2.7381012684
N65	-4.7725988414	-4.2052220935	-4.3698206883
C66	-3.6937462781	-3.8544258111	-5.0614449522
N67	-5.2727859924	-4.2351629961	1.3885779913
C68	-4.5451452618	-4.7634521881	0.3360118956
N69	-3.5240259863	-4.0212498733	-0.0207309283
C70	-3.5699131678	-2.9394303033	0.8519216785
C71	-2.7800194218	-1.7960124256	0.9896200523
O72	-1.7465814241	-1.3888757591	0.3294924534
N73	-3.1600690092	-0.9513116848	2.0037309288
C74	-4.2331420032	-1.1771033801	2.8526083461
N75	-4.4499419637	-0.2561079257	3.7960567039
N76	-5.0169563806	-2.2420604165	2.7332125796
C77	-4.6558318794	-3.0671140110	1.7519257145
N78	-8.1317859987	-0.3501629992	0.8725779989
C79	-8.0022374331	-1.4227674551	0.0188867640
N80	-6.9433377684	-1.3364126716	-0.7525742323
C81	-6.3521860909	-0.1294427326	-0.3961103492
C82	-5.1933344577	0.5227867510	-0.8745740455
O83	-4.3909414761	0.1107481846	-1.7538419391
N84	-4.9644813206	1.7455883357	-0.2388334931
C85	-5.7750221441	2.2877607127	0.7537513522
N86	-5.4211067055	3.4731580505	1.2747665054
N87	-6.8510657238	1.6712179233	1.2139564542
C88	-7.0927455193	0.5011165706	0.6152801052
H89	2.6141495135	5.3486132715	-6.1095093418
H90	-0.6229900295	-1.4278974455	-6.4457481195
H91	0.6383270809	-1.0906663358	-7.6230833748
H92	-1.1403952049	0.2718019018	-4.8866279197
H93	-4.8084184155	-1.3927269295	-2.6136080337
H94	-3.7173946992	6.8045754239	1.9136672422
H95	-0.8570503364	4.2086564146	-3.2268081926
H96	0.4821219888	7.4748973067	-3.6165970960
H97	0.4893375208	5.7936341703	-4.2071734480
H98	-4.8240604548	-5.7026236376	-0.1230645472
H99	-3.8675056790	0.5791899782	3.8602248992
H100	-5.1900383659	-0.4233591578	4.4645650169

H101	-2.5868891887	-0.1156542337	2.1160583028
H102	-8.7241655195	-2.2284381312	0.0082082154
H103	-4.1591652188	2.2699477865	-0.5768473538
H104	-4.6537143653	4.0515236576	0.9212818209
H105	-6.1070091043	3.8998638438	1.8836537064
H106	-1.3263939522	-4.1783878492	-7.2487631775
H107	-6.8274361510	-4.2868215686	-2.9436057692
H108	-6.5976601538	-2.7488686064	-2.0965533463
H109	-1.3038019177	-7.5401100359	-2.6732916941
H110	-1.9205964056	-6.6783867699	-1.3335919495
H111	-1.8073889673	-4.3194116835	-1.3555424674
H112	2.8877026731	-2.7861243312	-5.5104865263
H113	2.7989440408	-0.9491799054	-3.7635512882
H114	4.2499938841	-0.1870217291	-4.4252158681
H115	1.5108908144	0.1761890383	-2.2656998878
H116	3.8509113313	6.1154175806	-1.4289547672
H117	-3.8321168684	3.0918687039	5.1498998429
H118	0.5330479680	3.1111545508	0.4327373365
H119	1.6997058581	5.1256646310	0.4890759266
H120	1.3506362415	6.3088794870	1.7600101068
H121	-3.2845994886	-0.0572768910	-3.0955474070
H122	-8.8929570580	-0.1789213229	1.5198724441
H123	-2.1471363858	8.3124517832	0.5843690429
H124	3.0021331344	3.2313722515	-7.4788476960
H125	-3.3098973425	-5.5038686797	-6.3447572743
H126	5.0794035313	4.5967495979	-3.0739399940
H127	-2.3793182338	5.1710000375	4.9218794130
H128	2.0239216274	-5.1836252052	-5.5350834183
H129	-6.0501294444	-4.6715330861	1.8715391727
H130	-1.9608247287	2.6922964979	-2.3456311825
H131	-1.4094760682	-1.9087515944	-0.5154229887
H132	-0.4326057314	1.2524350657	0.3488493466

Single point energy: -4343.1174665

(2G4-4H⁺)₃

N1	-2.3337859954	4.3758369986	4.2935779806
C2	-3.1160255974	3.2418291251	4.3579101716
N3	-2.8330190100	2.3659071450	3.4256044412
C4	-1.7913216356	2.9531208945	2.7165548533
C5	-1.0485082417	2.5724240005	1.6128237086
O6	-1.2450372415	1.4393767523	0.9649701730
N7	-0.0765720647	3.4347704889	1.2085702582
C8	0.1821260886	4.6486203661	1.8280154619
N9	1.1715577517	5.3860055612	1.3254321371
N10	-0.5242399527	5.0717566446	2.8733573577
C11	-1.4586255868	4.2149133023	3.2627566180

N12	-2.3107859618	7.3328369978	0.3775779887
C13	-3.1433154486	6.3178356882	0.7822572830
N14	-3.0661647951	5.2492120480	0.0210881035
C15	-2.1318773807	5.5883360998	-0.9528342087
C16	-1.5871926054	4.8520367911	-2.0406410493
O17	-1.8410969460	3.6604683354	-2.3428668687
N18	-0.6692535306	5.5961676617	-2.7877254762
C19	-0.3232104179	6.9104371901	-2.5229147165
N20	0.5750573492	7.4871075146	-3.3632885377
N21	-0.7847319961	7.5855639136	-1.4908689316
C22	-1.6613797238	6.8926895634	-0.7484567900
N23	4.2212139766	4.3458369964	-2.5964219858
C24	3.5886173843	5.0662288047	-1.6070223124
N25	2.5783385167	4.4195797618	-1.0765608660
C26	2.5528397642	3.2014490235	-1.7405334486
C27	1.6950486931	2.0837582564	-1.6017844572
O28	0.7176956082	1.9552179390	-0.8247271843
N29	2.0298595990	1.0423536358	-2.4642692470
C30	3.0792989914	1.0744367816	-3.3734139791
N31	3.2369369091	-0.0204838196	-4.1382583904
N32	3.8720713984	2.1225093870	-3.5206587134
C33	3.5807973721	3.1343250001	-2.6888635775
N34	2.3242150060	3.3108369919	-6.7294219597
C35	2.0128461703	4.3230520454	-5.8402982924
N36	1.0122735167	4.0337302616	-5.0422048591
C37	0.6306504991	2.7539710903	-5.4287741368
C38	-0.3301404884	1.8616863337	-4.9486319471
O39	-1.1636322413	1.9458323090	-3.9616518722
N40	-0.3876414797	0.6631759002	-5.6173080156
C41	0.4149615578	0.3276096224	-6.6959573916
N42	0.1967310642	-0.8660404196	-7.2599595119
N43	1.3646247093	1.1348936171	-7.1492941507
C44	1.4368861938	2.2947286926	-6.5005475707
N45	1.6542139969	-4.4471629991	-4.9444210044
C46	1.9790942155	-3.1135655356	-4.9765867860
N47	1.3552129026	-2.4086870201	-4.0609521630
C48	0.5775664164	-3.3386555821	-3.3808406517
C49	-0.3628975631	-3.1937420546	-2.3268202090
O50	-0.7248103486	-2.1205738112	-1.7859949320
N51	-0.9274722474	-4.4128780684	-1.9350060332
C52	-0.6129398955	-5.6414527653	-2.4964225339
N53	-1.2480664295	-6.7267213165	-1.9902747250
N54	0.2165562842	-5.7782469898	-3.5126533167
C55	0.7651917179	-4.6209081104	-3.9128675967
N56	-3.0297860123	-4.5901629815	-6.0044220091
C57	-2.0442383582	-3.8035090054	-6.5595377174

N58	-1.9558605915	-2.6182680604	-6.0079551611
C59	-2.9535958839	-2.6209613547	-5.0406080010
C60	-3.3657148915	-1.7056215487	-4.0857795600
O61	-2.8073917425	-0.5223950459	-3.9246495108
N62	-4.4040380928	-2.0863832637	-3.2917212015
C63	-5.0523781622	-3.3069610095	-3.4048491037
N64	-6.0775295081	-3.5266721124	-2.5774979720
N65	-4.6705192928	-4.2318049033	-4.2800159847
C66	-3.6499600440	-3.8537778983	-5.0404407268
N67	-5.2727860007	-4.2351630032	1.3885779983
C68	-4.4900444859	-4.8073822382	0.3987757265
N69	-3.4666014946	-4.0673817815	0.0460275173
C70	-3.5684590163	-2.9406542374	0.8537166469
C71	-2.7952287726	-1.7847543163	0.9716306779
O72	-1.7298226053	-1.4042740679	0.3436852207
N73	-3.2239902940	-0.8985891111	1.9281155567
C74	-4.3344831225	-1.0925394395	2.7357129474
N75	-4.6034457715	-0.1274603310	3.6193251090
N76	-5.1035265978	-2.1703777672	2.6338905624
C77	-4.6905816381	-3.0386028240	1.7124465833
N78	-8.1317860082	-0.3501630007	0.8725779911
C79	-7.9297155660	-1.4919196492	0.1325556805
N80	-6.8572582523	-1.4306677008	-0.6220283436
C81	-6.3286106507	-0.1695297394	-0.3767798247
C82	-5.1830383251	0.4788354394	-0.8999581579
O83	-4.3373225700	0.0196810072	-1.7125550695
N84	-5.0197677591	1.7680311557	-0.4000065984
C85	-5.8791680174	2.3816766551	0.5037740111
N86	-5.5685802751	3.6387221865	0.8648717136
N87	-6.9389934287	1.7719072884	1.0125578175
C88	-7.1220063363	0.5274080295	0.5477067338
H89	2.5654637370	5.2531257206	-5.8361575719
H90	-0.5666443398	-1.4665891363	-6.9399014196
H91	0.6748445047	-1.0618196977	-8.1296161030
H92	-1.0871013051	0.0055273450	-5.2729913873
H93	-4.6644395038	-1.4046520202	-2.5468086038
H94	-3.7884965677	6.4294442435	1.6433559968
H95	-0.1739788461	5.1051150731	-3.5420966883
H96	0.7056758605	8.4832846655	-3.2287135998
H97	0.6295531792	7.1682284760	-4.3213222933
H98	-4.7315285669	-5.7765205745	-0.0173568141
H99	-4.0314721759	0.7180012324	3.6669365217
H100	-5.3788832166	-0.2655760026	4.2533191526
H101	-2.6709131172	-0.0463484169	2.0145643659
H102	-8.6130780476	-2.3288117317	0.1868137927
H103	-4.2317927209	2.2915779436	-0.7764127481

H104	-4.7904719182	4.1522306109	0.4434226931
H105	-6.2714033714	4.1452603347	1.3865859106
H106	-1.4289283594	-4.1644180817	-7.3732238081
H107	-6.6278581675	-4.3588388616	-2.7466645288
H108	-6.4197846130	-2.8049221780	-1.9266661824
H109	-0.9116576598	-7.6215761773	-2.3272812442
H110	-1.5756381136	-6.7174052562	-1.0336211133
H111	-1.6878015914	-4.3628612509	-1.2455822419
H112	2.6845323820	-2.7240311681	-5.6984505183
H113	2.6723301029	-0.8570489543	-3.9831614542
H114	4.0891918737	-0.0813046196	-4.6789681329
H115	1.4614928866	0.2013864084	-2.3845937176
H116	3.9214038777	6.0555067604	-1.3228729205
H117	-3.8753435418	3.1255955926	5.1203433791
H118	0.4611689276	3.1303677429	0.3712217585
H119	1.7167568308	5.0852697747	0.5050205836
H120	1.4028203213	6.2441904919	1.8085858529
H121	-3.1968404671	-0.0219336441	-3.1622282874
H122	-8.9186581222	-0.1518559315	1.4802475063
H123	-2.2390770405	8.2619655005	0.7763244607
H124	3.0303576224	3.3318135049	-7.4568087629
H125	-3.3060051835	-5.5180973952	-6.3071927868
H126	5.0709904798	4.6066717812	-3.0833601173
H127	-2.3319492036	5.1451515192	4.9548649090
H128	2.0650381446	-5.1895672535	-5.4993392687
H129	-6.0608793550	-4.6605899239	1.8635049523
H130	-1.4271529247	-1.9058398343	-0.5184354176
H131	-0.6048342275	1.3192272004	0.2162504292
H132	-1.2805485842	2.8209034678	-3.3956590499

Single point energy: -4343.1164446

(2G4-4H⁺)_a

N1	-2.3337860003	4.3758370004	4.2935780004
C2	-2.9780785147	3.1916233687	4.0035208187
N3	-2.4082446934	2.5077193277	3.0367833681
C4	-1.3157124724	3.2879479767	2.6681510987
C5	-0.3388304014	3.1305472725	1.6415363760
O6	-0.2702267740	2.2088485189	0.7973199395
N7	0.5938916267	4.1766565138	1.6253602660
C8	0.5903924697	5.2522440652	2.4979614887
N9	1.5733858983	6.1759881214	2.3385157505
N10	-0.3367983864	5.4319399345	3.4161166946
C11	-1.2514295807	4.4487103588	3.4521012412
N12	-2.3107859841	7.3328369774	0.3775779704
C13	-3.2427476314	6.6638278643	1.1457236704
N14	-3.5624699757	5.4883487770	0.6556279460

C15	-2.8059059455	5.3837122706	-0.5068440495
C16	-2.6849486286	4.3484019615	-1.4606537481
O17	-3.2596052447	3.2262805336	-1.4513992785
N18	-1.8139610566	4.6795368920	-2.4994344680
C19	-1.1531873692	5.8981473372	-2.6258914446
N20	-0.4433258735	6.1114441569	-3.7417685699
N21	-1.2235134377	6.8479839528	-1.7102026094
C22	-2.0418399197	6.5445458774	-0.7019544685
N23	4.2212139998	4.3458369924	-2.5964220012
C24	3.4842383283	4.9059896494	-1.5623618478
N25	2.6040106864	4.0870891788	-1.0402544172
C26	2.7668880053	2.9080913106	-1.7565889827
C27	2.1142333968	1.6682419634	-1.7042900873
O28	1.1421859888	1.2431240002	-0.9732641072
N29	2.5856042676	0.7336813826	-2.6014865202
C30	3.6396015887	0.9545151037	-3.4713254668
N31	4.0040165704	-0.0814153803	-4.2503994199
N32	4.2488064682	2.1256345932	-3.5740117762
C33	3.7906286672	3.0489084055	-2.7232104395
N34	2.3242149555	3.3108370169	-6.7294219593
C35	1.9087997395	4.3185490102	-5.8912207688
N36	0.8722544335	3.9868128645	-5.1652795863
C37	0.5698856040	2.6937066289	-5.5559341355
C38	-0.4124282441	1.7920230460	-5.1729550508
O39	-1.3249191237	2.0370087675	-4.2507628764
N40	-0.3987300570	0.5871105333	-5.8051935700
C41	0.5127647574	0.2523899361	-6.7977328855
N42	0.3746764728	-0.9581647518	-7.3423114935
N43	1.4815302961	1.0815455172	-7.1848352626
C44	1.4690670402	2.2524434792	-6.5564276341
N45	1.6542140148	-4.4471630106	-4.9444209945
C46	2.0831235092	-3.1389827897	-4.8827388891
N47	1.5049268146	-2.4429279845	-3.9289316281
C48	0.6419411840	-3.3510748110	-3.3221356511
C49	-0.3156550737	-3.1981752772	-2.2780443453
O50	-0.6085471756	-2.1408078087	-1.6727936698
N51	-0.9777995207	-4.3942972266	-1.9777450811
C52	-0.7476380373	-5.6037919587	-2.6124407940
N53	-1.4748737986	-6.6676006627	-2.1851529356
N54	0.0905693077	-5.7423810242	-3.6199284672
C55	0.7361435274	-4.6081940376	-3.9362142019
N56	-3.0297860010	-4.5901629931	-6.0044220102
C57	-1.9695629627	-3.9672739519	-6.6274282577
N58	-1.7876378448	-2.7350473905	-6.2130845916
C59	-2.7938571941	-2.5335751999	-5.2752501547
C60	-3.1274974233	-1.4128890904	-4.4826210557

O61	-2.5433730711	-0.2985803221	-4.4537658957
N62	-4.2405282927	-1.6424754714	-3.6718473902
C63	-4.9744167950	-2.8243091104	-3.6469968651
N64	-6.0398946217	-2.8858505823	-2.8360690687
N65	-4.6530008491	-3.8818558421	-4.3720932118
C66	-3.5854834052	-3.6839093638	-5.1486669374
N67	-5.2727859992	-4.2351629954	1.3885780014
C68	-4.5202490838	-4.7553002410	0.3468444928
N69	-3.5023825611	-4.0020598901	0.0072128372
C70	-3.5716268161	-2.9198609306	0.8752801144
C71	-2.7965323576	-1.7582002747	1.0048951209
O72	-1.7864647837	-1.3298554979	0.3303523572
N73	-3.1893925521	-0.9165119222	2.0234039940
C74	-4.2429831503	-1.1799263153	2.8829565062
N75	-4.4684310276	-0.2736243293	3.8532957136
N76	-5.0259459742	-2.2400793578	2.7527578932
C77	-4.6647989940	-3.0609957653	1.7614833636
N78	-8.1317859856	-0.3501629879	0.8725779933
C79	-7.9000707032	-1.2555181012	-0.1377823279
N80	-6.8944185015	-0.9230616464	-0.9063103157
C81	-6.4416866963	0.2799054029	-0.3904680366
C82	-5.4207722947	1.1468707557	-0.7536868935
O83	-4.5932749147	0.9421462173	-1.7635211238
N84	-5.2828376418	2.2667047150	0.0072387840
C85	-6.1156959336	2.5751580752	1.0732141396
N86	-5.8688961245	3.7273000335	1.7028132565
N87	-7.1009436001	1.7673729272	1.4642345488
C88	-7.2221093985	0.6676535390	0.7268651589
H89	2.4069854096	5.2788904847	-5.8699485226
H90	-0.3808316029	-1.5942946034	-7.0511600760
H91	0.9423176679	-1.1725810205	-8.1518445872
H92	-1.1451247191	-0.0747560472	-5.5125403082
H93	-4.5331288077	-0.8532730312	-3.0992713078
H94	-3.6494173610	7.1000901968	2.0478715648
H95	-1.7149187242	3.9773524586	-3.2293368338
H96	0.0056538816	7.0156852089	-3.8025189170
H97	-0.0970030931	5.3468238942	-4.3256741608
H98	-4.7813576607	-5.6970329356	-0.1177830813
H99	-3.7614313809	0.4158280122	4.0782166715
H100	-5.1268658604	-0.5321363723	4.5779230701
H101	-2.6621367915	-0.0442062939	2.1258079345
H102	-8.5140493450	-2.1386520006	-0.2571584935
H103	-4.5136764997	2.9074706930	-0.2818642458
H104	-5.1305747095	4.3707312041	1.3878752081
H105	-6.5400227228	4.0300398033	2.3968232013
H106	-1.3790750588	-4.4719751518	-7.3800452661

H107	-6.6356667683	-3.6935493507	-2.9587917542
H108	-6.3697330629	-2.0980471165	-2.2713725654
H109	-1.1937845125	-7.5615148173	-2.5714670754
H110	-1.8010801624	-6.6949165368	-1.2284543827
H111	-1.7504545540	-4.3268862418	-1.3049804566
H112	2.8179544683	-2.7594268124	-5.5807443328
H113	3.6690062063	-1.0147706270	-4.0442792254
H114	4.8705167558	0.0131997724	-4.7654654261
H115	2.1057501089	-0.1707808257	-2.6152346281
H116	3.6495243558	5.9283533614	-1.2483106033
H117	-3.8704246758	2.8989009592	4.5411603831
H118	1.2730972104	4.1622377906	0.8581514135
H119	2.4616403289	5.8942412966	1.9459090677
H120	1.6291803072	6.8707619966	3.0744147433
H121	-1.9400869656	1.2579683246	-4.1373133163
H122	-8.8905390327	-0.3707929668	1.5454543834
H123	-1.9666161161	8.2744470714	0.5244922203
H124	3.0675332731	3.3600455373	-7.4178266406
H125	-3.3902299937	-5.5161951081	-6.2027450852
H126	5.0132400447	4.7613183567	-3.0740624207
H127	-2.5452806650	5.0226404952	5.0442299602
H128	2.0091638118	-5.1825396620	-5.5444692570
H129	-6.0432873939	-4.6867884531	1.8684516753
H130	-3.9696146711	1.7139122800	-1.8786365827
H131	-1.4088112487	-1.8640980964	-0.4966047775
H132	0.6882082778	1.8468780156	-0.2416538044

Single point energy: -4343.1075148

(2G4-4H⁺)_b

N1	-2.3337860000	4.3758370000	4.2935779999
C2	-3.0956061473	3.2285838507	4.3804268850
N3	-2.7418062157	2.3051076154	3.5209106353
C4	-1.6728372584	2.8748074259	2.8370321626
C5	-0.8672947786	2.4528814755	1.7936676240
O6	-1.0101715996	1.2850286278	1.1940021781
N7	0.1109482952	3.3113528115	1.3955700481
C8	0.3155981034	4.5608066210	1.9624530533
N9	1.3205717907	5.2885654397	1.4766991676
N10	-0.4545099105	5.0249546193	2.9432403532
C11	-1.3950844414	4.1729106910	3.3273816913
N12	-2.3107860000	7.3328370001	0.3775780000
C13	-3.0749417145	6.2855825464	0.8320308798
N14	-2.8992530055	5.1785783388	0.1457510772
C15	-1.9679949030	5.5239404808	-0.8281319083
C16	-1.3423173336	4.7614899982	-1.8534987480

O17	-1.4781630958	3.5327074789	-2.0648643570
N18	-0.4832735594	5.5294977837	-2.6454609633
C19	-0.2277408986	6.8755036029	-2.4499671979
N20	0.6614197220	7.4582006246	-3.3018306383
N21	-0.7548506819	7.5764056097	-1.4689057907
C22	-1.6001771685	6.8700738184	-0.7012556351
N23	4.2212139999	4.3458369998	-2.5964219999
C24	3.6488554528	5.0227360357	-1.5412343260
N25	2.7340089024	4.3154975890	-0.9229005010
C26	2.7134161627	3.1019084719	-1.5939556465
C27	1.9405284603	1.9334780974	-1.3830259609
O28	1.0690482147	1.7284998607	-0.5059038565
N29	2.2439493647	0.9251560450	-2.2993464391
C30	3.1936234568	1.0260730231	-3.3057065547
N31	3.3319033515	-0.0474530111	-4.1079245282
N32	3.9119216493	2.1146053173	-3.5093324917
C33	3.6456308383	3.1009692347	-2.6386240373
N34	2.3242149998	3.3108369996	-6.7294220000
C35	2.0476679539	4.3109825965	-5.8166940969
N36	1.1269843379	3.9819795831	-4.9419861824
C37	0.7679100763	2.6879542242	-5.3016000461
C38	-0.1007530195	1.7492550383	-4.7445054994
O39	-0.8439464654	1.7934825729	-3.6860494594
N40	-0.1583966263	0.5489919709	-5.4113255843
C41	0.5657617386	0.2516643080	-6.5532861596
N42	0.3709033731	-0.9520079189	-7.1086509871
N43	1.4357425553	1.1015648682	-7.0801568680
C44	1.5038546548	2.2619665025	-6.4339650926
N45	1.6542140000	-4.4471629998	-4.9444209999
C46	1.9546390204	-3.1057411103	-4.9621249411
N47	1.3690670158	-2.4281934459	-4.0021808166
C48	0.6432962389	-3.3840710045	-3.3002491466
C49	-0.2641386722	-3.2764679695	-2.2235301483
O50	-0.6676883152	-2.2099607777	-1.6611475689
N51	-0.7794081611	-4.5030390570	-1.8100035308
C52	-0.4519094818	-5.7227256954	-2.3881204256
N53	-1.0165254873	-6.8270915867	-1.8552823666
N54	0.3296596158	-5.8265810674	-3.4495256237
C55	0.8297529355	-4.6580153416	-3.8658233716
N56	-3.0297859999	-4.5901629995	-6.0044219999
C57	-1.9646006913	-3.9099408056	-6.5522693320
N58	-1.6858717712	-2.7950997223	-5.9260459697
C59	-2.6428997682	-2.7238086076	-4.9206093104
C60	-2.8126441214	-1.8940339901	-3.8361672285
O61	-1.9994840466	-0.8750992620	-3.5560508668
N62	-3.8693138240	-2.1495921169	-3.0127324635

C63	-4.7353014986	-3.2126240163	-3.2175679292
N64	-5.7853241788	-3.3519184205	-2.4105965129
N65	-4.5337928311	-4.1166366344	-4.1842538312
C66	-3.5156753872	-3.8398511402	-4.9764524480
N67	-5.2727859999	-4.2351629999	1.3885780000
C68	-4.4699046057	-4.8201778957	0.4232414732
N69	-3.3810557935	-4.1376504347	0.1579629321
C70	-3.4599070616	-3.0373381823	1.0046901280
C71	-2.6303268928	-1.9381268372	1.2098910014
O72	-1.4936195045	-1.6154273799	0.6628058270
N73	-3.0509907425	-1.0570870414	2.1673366984
C74	-4.2190235969	-1.2021538743	2.9010508506
N75	-4.4839764088	-0.2403521324	3.7894833553
N76	-5.0397607578	-2.2318480352	2.7261961667
C77	-4.6346854092	-3.0928255844	1.7954885032
N78	-8.1317859999	-0.3501630002	0.8725779999
C79	-7.8784602016	-1.5429466283	0.2407514368
N80	-6.7133712751	-1.5571152926	-0.3642555813
C81	-6.1775778883	-0.3001784426	-0.1312920687
C82	-4.9306607350	0.2606291489	-0.5112961440
O83	-3.9756534628	-0.2696399537	-1.1231107673
N84	-4.8059795967	1.5892419497	-0.0881830052
C85	-5.7622621603	2.2916635975	0.6296661581
N86	-5.4655287657	3.5693386489	0.9397143108
N87	-6.9011925454	1.7494286371	1.0299015178
C88	-7.0600977352	0.4786884419	0.6280956587
H89	2.5622279042	5.2618659562	-5.8556895616
H90	-0.3605450557	-1.5830377902	-6.7691325144
H91	0.7785672027	-1.0978153109	-8.0233627851
H92	-0.7784255923	-0.1471236001	-4.9890326903
H93	-4.0279820328	-1.4701634718	-2.2192940161
H94	-3.7487252406	6.4028671810	1.6701776888
H95	0.0385839111	5.0329372904	-3.3783632939
H96	0.7111499757	8.4680957103	-3.2213529021
H97	0.7172510471	7.1094200956	-4.2500821905
H98	-4.7472536991	-5.7553259508	-0.0448016097
H99	-3.9082515620	0.6016935987	3.8419324064
H100	-5.3132001345	-0.3346327670	4.3604839944
H101	-2.4669767600	-0.2308850552	2.2941406749
H102	-8.5927005234	-2.3552239805	0.2538937517
H103	-3.9540445096	2.0594657289	-0.3851559321
H104	-4.6558297672	4.0473382888	0.5392848849
H105	-6.2286473335	4.1271986714	1.2999108593
H106	-1.4392201602	-4.2920375359	-7.4180898603
H107	-6.4365533884	-4.0834845226	-2.6681179407
H108	-6.0697433670	-2.6746261921	-1.6791524225

H109	-0.6908792740	-7.7152150420	-2.2191887692
H110	-1.3521710571	-6.8303007383	-0.9016253414
H111	-1.5323627746	-4.4674187402	-1.1104632286
H112	2.6098956679	-2.6880092586	-5.7145259859
H113	2.8122239141	-0.9041154716	-3.9309295576
H114	4.1351805684	-0.0624969756	-4.7216599135
H115	1.7323180134	0.0548178503	-2.1802462884
H116	3.9500083001	6.0282563734	-1.2797862593
H117	-3.8958537919	3.1400227042	5.1035846037
H118	0.7107395746	2.9687261767	0.6186638285
H119	1.8916023049	4.9715338256	0.6810496332
H120	1.5120776421	6.1747175127	1.9253254953
H121	-1.5026328414	-1.0729873970	-2.7115664099
H122	-8.9809293433	-0.0923179595	1.3626947443
H123	-2.3114037475	8.2867475063	0.7202864313
H124	2.9697496349	3.3588052682	-7.5100469972
H125	-3.4450501814	-5.4454092502	-6.3590923085
H126	5.0064547486	4.6559441748	-3.1569193167
H127	-2.3826576611	5.1800076956	4.9097428950
H128	2.0527978580	-5.1707795737	-5.5325815060
H129	-6.1169799598	-4.6215558990	1.7950026597
H130	-1.2646864084	-2.0645295063	-0.2173423520
H131	-0.3406529055	1.1528497826	0.4752222117
H132	-0.9607548868	2.6731047891	-3.1324388857

Single point energy: -4343.1048372

(2G4-4H⁺)_c

N1	-2.3337859697	4.3758370141	4.2935780741
C2	-3.0809758771	3.2943417193	3.8759554457
N3	-2.5438476619	2.6478230501	2.8655735619
C4	-1.3696349825	3.3465106647	2.6007825298
C5	-0.3906509858	3.2015572787	1.5756289553
O6	-0.3971793311	2.3765929157	0.6342211906
N7	0.6375658077	4.1490497588	1.6780461755
C8	0.7140042621	5.1305068133	2.6534321519
N9	1.7810428020	5.9684322434	2.6005295136
N10	-0.2169393084	5.3083627624	3.5683170193
C11	-1.2204773116	4.4187196874	3.4920067203
N12	-2.3107859382	7.3328369667	0.3775779386
C13	-3.2626028284	6.5467287872	1.0090914632
N14	-3.4602885010	5.3885220799	0.4279845235
C15	-2.5966626215	5.4054688360	-0.6615994721
C16	-2.3085077613	4.4816995638	-1.6688790832
O17	-2.7577466812	3.2916702317	-1.9109362805
N18	-1.3761343376	4.9050504655	-2.5879602131
C19	-0.7613113429	6.1474622395	-2.5693615064

N20	0.0866051825	6.4202959952	-3.5669806210
N21	-0.9881996553	7.0339920690	-1.6113753129
C22	-1.8823500353	6.6306621462	-0.7123923024
N23	4.2212139747	4.3458369519	-2.5964220064
C24	3.4945920575	4.9047136849	-1.5548116464
N25	2.5928208717	4.0983133906	-1.0503391364
C26	2.7308006634	2.9277359677	-1.7865238408
C27	2.0512004645	1.7019334585	-1.7541643028
O28	1.0606591626	1.2952373984	-1.0369018399
N29	2.5094971636	0.7658991428	-2.6541940834
C30	3.5728789560	0.9756077570	-3.5166222948
N31	3.9233953012	-0.0625480793	-4.2947908117
N32	4.2038674353	2.1378100064	-3.6063110647
C33	3.7623888980	3.0594938254	-2.7457900926
N34	2.3242149601	3.3108368910	-6.7294221642
C35	1.9191629488	4.3388231145	-5.9113522601
N36	0.8363355867	4.0593582304	-5.2280583577
C37	0.4992953087	2.7756534687	-5.6364548575
C38	-0.5116776146	1.8953750648	-5.2795598314
O39	-1.4237677492	2.1733105741	-4.3707152594
N40	-0.5127767088	0.6929242570	-5.9138162044
C41	0.4216424958	0.3242883508	-6.8691759989
N42	0.2732736512	-0.8836813882	-7.4147649072
N43	1.4292874413	1.1222625359	-7.2202917031
C44	1.4202664736	2.2942167302	-6.5958405409
N45	1.6542139939	-4.4471629462	-4.9444209636
C46	2.0869542922	-3.1411975726	-4.8980318658
N47	1.5169553502	-2.4348868104	-3.9461141041
C48	0.6527942840	-3.3347299163	-3.3264221780
C49	-0.3016459430	-3.1700627113	-2.2784615793
O50	-0.5906208507	-2.1112385285	-1.6772968365
N51	-0.9670045563	-4.3643797468	-1.9701526662
C52	-0.7438348772	-5.5778192504	-2.5978333623
N53	-1.4734153365	-6.6368851578	-2.1626909290
N54	0.0907599234	-5.7262299946	-3.6068088210
C55	0.7397886519	-4.5964944478	-3.9311744032
N56	-3.0297858112	-4.5901632450	-6.0044223793
C57	-2.0357755816	-3.9512476157	-6.7129861218
N58	-1.8583417889	-2.7062435297	-6.3372296764
C59	-2.7977313527	-2.5094378644	-5.3332966288
C60	-3.1001194118	-1.3702382231	-4.5491936625
O61	-2.5569306815	-0.2375572757	-4.5961349283
N62	-4.1316617630	-1.5967779654	-3.6444459804
C63	-4.8320308828	-2.7895054081	-3.5277749505
N64	-5.8159585707	-2.8146792775	-2.6099138766
N65	-4.5516325358	-3.8613547353	-4.2495660267

C66	-3.5486370813	-3.6745327180	-5.1210472892
N67	-5.2727860103	-4.2351629765	1.3885780127
C68	-4.4791462666	-4.7749735375	0.3883219136
N69	-3.4757546227	-4.0060588969	0.0408468676
C70	-3.5992693707	-2.8901981325	0.8594924781
C71	-2.8650683497	-1.7009710615	0.9611330165
O72	-1.8418586942	-1.2693247169	0.3030566809
N73	-3.3102403857	-0.8310769139	1.9309270165
C74	-4.3842842986	-1.0860503039	2.7659129596
N75	-4.6712831432	-0.1426041248	3.6839669614
N76	-5.1259357511	-2.1777069689	2.6665636761
C77	-4.7123795707	-3.0271840797	1.7224039641
N78	-8.1317859550	-0.3501628818	0.8725778584
C79	-7.6163222386	-1.1071982540	-0.1488081457
N80	-6.5629015660	-0.5631413887	-0.7147327788
C81	-6.3844230482	0.6364433454	-0.0333904732
C82	-5.4312213375	1.6872550639	-0.1876097072
O83	-4.4789670331	1.7392745059	-0.9950901432
N84	-5.6479828575	2.7356111578	0.7184731505
C85	-6.6609863483	2.7723043560	1.6587887262
N86	-6.6873680773	3.8547764804	2.4912588108
N87	-7.5379995816	1.8053083660	1.8140231802
C88	-7.3624497889	0.7823755064	0.9592764309
H89	2.4627451136	5.2735452460	-5.8701681296
H90	-0.4857342510	-1.5216109080	-7.1341359259
H91	0.8804646180	-1.1225151679	-8.1877017075
H92	-1.2772653906	0.0431837729	-5.6193189325
H93	-4.4007708945	-0.7998313267	-3.0712199241
H94	-3.7725060944	6.8957509710	1.8970134374
H95	-1.1808187899	4.2492482491	-3.3438595722
H96	0.4305163064	7.3683489476	-3.6406107380
H97	0.2644456937	5.7346584777	-4.3016451952
H98	-4.7006526699	-5.7431430538	-0.0410185921
H99	-3.9923259893	0.5737720796	3.9074779289
H100	-5.3589018784	-0.3821073834	4.3873496173
H101	-2.8256034842	0.0685042681	1.9929004763
H102	-8.0693765558	-2.0471775309	-0.4344962353
H103	-4.9678209988	3.5001701934	0.6946770146
H104	-6.3563130207	4.7404858924	2.1288943756
H105	-7.5376329118	3.9247295568	3.0405191136
H106	-1.4857948383	-4.4555760716	-7.4959559001
H107	-6.4517174266	-3.5989160635	-2.6558315257
H108	-6.0808373698	-1.9750421520	-2.0896366177
H109	-1.1943830218	-7.5343793708	-2.5417668072
H110	-1.8012668711	-6.6547741580	-1.2064453114
H111	-1.7324533251	-4.2938970872	-1.2889715949

H112	2.8193514736	-2.7729330819	-5.6045459093
H113	3.5410656662	-0.9839373501	-4.1154010954
H114	4.7870222434	0.0152232382	-4.8167100144
H115	2.0181683459	-0.1327856790	-2.6730026289
H116	3.6847363859	5.9159260634	-1.2196219660
H117	-4.0264064642	3.0552145647	4.3453510983
H118	1.3181250506	4.1519135400	0.9122887348
H119	2.6520355932	5.6450828695	2.2011086187
H120	1.8757947780	6.5910849609	3.3948024521
H121	-2.0503896204	1.4133177726	-4.2231825524
H122	-8.9651867941	-0.5402343825	1.4170617140
H123	-2.0387083678	8.2787658729	0.6205281220
H124	3.0975476335	3.3270152806	-7.3853661163
H125	-3.3768517316	-5.5294799297	-6.1590137588
H126	5.0268772899	4.7490569801	-3.0615705439
H127	-2.5113747651	4.9731029835	5.0927142107
H128	1.9998421522	-5.1879214497	-5.5430854199
H129	-6.0460927946	-4.6860391837	1.8644652582
H130	-3.4873068193	2.8538554155	-1.3280592760
H131	-1.4476461399	-1.8143322919	-0.4923098526
H132	0.5995068599	1.9276081643	-0.3408298452

Single point energy: -4343.1019398

(2G4-4H⁺)_d

N1	-2.3337860001	4.3758370002	4.2935780003
C2	-3.0767476316	3.2152674530	4.3766463193
N3	-2.8055367399	2.3541013323	3.4275112817
C4	-1.8117177276	2.9759609852	2.6800388359
C5	-1.1472369539	2.6446319687	1.5110626204
O6	-1.3571921937	1.5257756638	0.8446042690
N7	-0.2337352665	3.5464296986	1.0513391796
C8	0.0307284054	4.7567142188	1.6824709276
N9	0.9490235025	5.5425922715	1.1176797340
N10	-0.6020333377	5.1273338208	2.7912097038
C11	-1.4924128904	4.2429877236	3.2259398181
N12	-2.3107859999	7.3328369998	0.3775780000
C13	-3.1307773056	6.5380550831	1.1394997570
N14	-3.3204953631	5.3566071943	0.6012914390
C15	-2.6142434830	5.3934538339	-0.5884360465
C16	-2.4224396874	4.3938776467	-1.5800345690
O17	-2.7974593570	3.2077054309	-1.5886614980
N18	-1.6622927289	4.9000891721	-2.6553301231
C19	-1.1022382617	6.1669130369	-2.7300333168
N20	-0.4279620751	6.4613528861	-3.8642560130
N21	-1.2265775070	7.0623640273	-1.7709655874
C22	-1.9940709878	6.6346083642	-0.7557840327

N23	4.2212139999	4.3458370003	-2.5964219997
C24	3.4207085089	5.1848231746	-1.8456590475
N25	2.3468030610	4.5925764553	-1.3840235873
C26	2.4530266723	3.2827777353	-1.8317805234
C27	1.5547718112	2.2058563248	-1.7662680698
O28	0.3592871337	2.2167625043	-1.3174456543
N29	2.0468461974	1.0401412525	-2.3446429249
C30	3.2663940332	0.9464034275	-3.0083098760
N31	3.5884285986	-0.2550559053	-3.5053958478
N32	4.0706918662	1.9888228255	-3.1680597409
C33	3.6361690329	3.1040796436	-2.5731037248
N34	2.3242150000	3.3108369999	-6.7294220004
C35	2.1029588473	4.3091650145	-5.8015799478
N36	1.1816122038	4.0131984363	-4.9187930011
C37	0.7533236459	2.7429193187	-5.2828982608
C38	-0.1903018702	1.8697409744	-4.7663756164
O39	-0.9925892211	1.9976440706	-3.7196149955
N40	-0.3861454900	0.7139366154	-5.4724759148
C41	0.3105716568	0.3860419237	-6.6271851920
N42	-0.0053406278	-0.7577694791	-7.2310883890
N43	1.2702861658	1.1718218009	-7.1168170372
C44	1.4478280451	2.2987658832	-6.4452183826
N45	1.6542139998	-4.4471630005	-4.9444210001
C46	2.0784767637	-3.1401784846	-4.9036333326
N47	1.4863366658	-2.4347085915	-3.9658876086
C48	0.6280825231	-3.3366070107	-3.3467883739
C49	-0.3235556686	-3.1692003652	-2.3048029557
O50	-0.6263387847	-2.0970510288	-1.7279390778
N51	-0.9719396724	-4.3645558792	-1.9725209123
C52	-0.7291753329	-5.5863019844	-2.5814659036
N53	-1.4366262039	-6.6489663576	-2.1252162638
N54	0.1010784018	-5.7352831215	-3.5956556488
C55	0.7355926251	-4.6028570135	-3.9353583967
N56	-3.0297859999	-4.5901629999	-6.0044220000
C57	-2.0295111209	-3.8111156487	-6.5405484006
N58	-1.9428997606	-2.6247395328	-5.9890636202
C59	-2.9574088116	-2.6118932290	-5.0389786621
C60	-3.3761048082	-1.6879741819	-4.0910880821
O61	-2.8055816925	-0.5094819760	-3.9045699932
N62	-4.4356998939	-2.0499413507	-3.3194015819
C63	-5.0948797469	-3.2643957000	-3.4443129869
N64	-6.1393534190	-3.4671503909	-2.6402861311
N65	-4.7027698237	-4.1998633586	-4.3083563197
C66	-3.6645974024	-3.8403829339	-5.0515373381
N67	-5.2727859999	-4.2351630000	1.3885779999
C68	-4.4934607872	-4.7898365369	0.3875000228

N69	-3.4759532336	-4.0398865493	0.0364520568
C70	-3.5807247384	-2.9213655202	0.8564609026
C71	-2.8206845813	-1.7577876433	0.9792495082
O72	-1.7588636437	-1.3579498326	0.3522201091
N73	-3.2572773087	-0.8808454899	1.9391191751
C74	-4.3645776285	-1.0896602072	2.7473481504
N75	-4.6424126436	-0.1298532273	3.6331737629
N76	-5.1187432034	-2.1777195423	2.6457609223
C77	-4.6999788142	-3.0355963068	1.7187250945
N78	-8.1317859999	-0.3501629999	0.8725780000
C79	-7.9735153722	-1.4541291908	0.0654607599
N80	-6.9018296527	-1.3857792721	-0.6903923500
C81	-6.3281054850	-0.1573466984	-0.3760889427
C82	-5.1739892670	0.4967048215	-0.8709207481
O83	-4.3587668066	0.0463134567	-1.7276542661
N84	-4.9653968358	1.7465477859	-0.2945127871
C85	-5.7977492607	2.3105289415	0.6665465776
N86	-5.4861290222	3.5211899579	1.1450886464
N87	-6.8738195039	1.6962817271	1.1467639619
C88	-7.0952091479	0.5038387111	0.5949047727
H89	2.6501225831	5.2422656787	-5.8414949955
H90	-0.7226716337	-1.3923476105	-6.8575525253
H91	0.4432938144	-0.9521171930	-8.1173035084
H92	-1.1003063250	0.0850364477	-5.0978701697
H93	-4.7008474256	-1.3565969497	-2.5780100781
H94	-3.5555271403	6.8846879063	2.0714124599
H95	-1.6186042273	4.2963292238	-3.4687337653
H96	-0.0170197546	7.3859892313	-3.8909106226
H97	0.0648352547	5.7162243816	-4.3503866915
H98	-4.7329911291	-5.7547179603	-0.0393747024
H99	-4.0820478343	0.7217881365	3.6764673813
H100	-5.4314249689	-0.2633572903	4.2511580564
H101	-2.7249236976	-0.0158963935	2.0228866556
H102	-8.6850974263	-2.2688535299	0.0736006490
H103	-4.1831948336	2.2998332884	-0.6805548952
H104	-4.6859622870	4.0974277871	0.8560207448
H105	-6.1832946408	3.9397979411	1.7464388151
H106	-1.4010240320	-4.1752820559	-7.3425079125
H107	-6.6934333320	-4.2964588429	-2.8114702188
H108	-6.4799672839	-2.7389398250	-1.9910821230
H109	-1.1475947605	-7.5497612753	-2.4893159753
H110	-1.7748761043	-6.6537244736	-1.1722180344
H111	-1.7297305877	-4.3002278207	-1.2806347434
H112	2.8310220000	-2.7700645207	-5.5873649743
H113	2.9327521589	-1.0395931974	-3.5045987841
H114	4.5036467677	-0.3568517538	-3.9237138257

H115	1.4589514391	0.2118090848	-2.2615233132
H116	3.6910476427	6.2183912091	-1.6725771897
H117	-3.8021293865	3.0706028409	5.1667749410
H118	0.1884902801	3.3323399354	0.1343146440
H119	1.4345198355	5.2904638439	0.2492830493
H120	1.1706108983	6.4110136674	1.5869029404
H121	-3.2196420384	-0.0073857838	-3.1486132736
H122	-8.9088095091	-0.1581708933	1.4940088264
H123	-2.0801706918	8.3043598003	0.5523495826
H124	2.9508772300	3.3459533255	-7.5269609331
H125	-3.3094157651	-5.5156881246	-6.3109789249
H126	5.1365897106	4.5634242181	-2.9751848976
H127	-2.3301247380	5.1401641375	4.9604616977
H128	2.0274266492	-5.1914583219	-5.5229033368
H129	-6.0625077260	-4.6656256546	1.8562388892
H130	-0.5636661128	2.3047625709	-2.8736362960
H131	-1.4233544912	-1.8745159297	-0.4772660455
H132	-0.8346549712	1.4833280372	0.0068660231

Single point energy: -4343.0961959

(2G4-4H⁺)_e

N1	-2.3337860000	4.3758369999	4.2935780000
C2	-2.9894809839	3.1633300271	4.4006427620
N3	-2.4937482962	2.2411175176	3.6193337939
C4	-1.4432924010	2.8648163228	2.9695696818
C5	-0.5905790134	2.4651283244	1.9573705997
O6	-0.6177545896	1.2713894974	1.3961800067
N7	0.3092446127	3.3996798494	1.5245811386
C8	0.3827884862	4.6905954445	2.0379552885
N9	1.3057457030	5.4935606772	1.4980451286
N10	-0.4351791586	5.1200611452	2.9911608344
C11	-1.3146056040	4.2082152467	3.3997442038
N12	-2.3107860000	7.3328370000	0.3775780000
C13	-3.0610067128	6.4429306591	1.1198343781
N14	-2.9878827550	5.2087999208	0.6889241030
C15	-2.1579636482	5.2888056980	-0.4221791191
C16	-1.5818663286	4.3325748209	-1.2402843447
O17	-1.7433680528	3.0323391340	-1.0795988685
N18	-0.7966706765	4.8069653354	-2.2578554831
C19	-0.5326172022	6.1613467816	-2.4512482661
N20	0.1967733541	6.4814897924	-3.5230860440
N21	-0.9652017811	7.0935733568	-1.6126934616
C22	-1.7469750644	6.6295722288	-0.6459281884
N23	4.2212140000	4.3458370000	-2.5964220000
C24	3.5211107727	5.0969603441	-1.6724612107
N25	2.5230799260	4.4428360449	-1.1264492300

C26	2.5798284062	3.1789617325	-1.7090168554
C27	1.7621296013	2.0465738902	-1.5743220937
O28	0.7008692315	1.9462918905	-0.8640767302
N29	2.1919252049	0.9622231302	-2.3281185334
C30	3.3135391131	0.9746694478	-3.1563862083
N31	3.6470114442	-0.1536760663	-3.7800814300
N32	4.0499838110	2.0653608827	-3.3417293740
C33	3.6579170577	3.1016433232	-2.6114019635
N34	2.3242150000	3.3108370000	-6.7294220000
C35	2.0160397454	4.2738710529	-5.7976685419
N36	1.0417861348	3.9292596066	-4.9859412074
C37	0.6777770436	2.6557826872	-5.4132651912
C38	-0.2410527672	1.7172933453	-4.9577810425
O39	-1.0239430141	1.8890664923	-3.9038604765
N40	-0.3015404948	0.5468635555	-5.6454603381
C41	0.4846964164	0.2677816430	-6.7545174203
N42	0.2865172523	-0.9100975501	-7.3440789339
N43	1.4072125054	1.1215500512	-7.2035639547
C44	1.4675708298	2.2574418521	-6.5220587465
N45	1.6542140000	-4.4471630000	-4.9444210000
C46	2.2894804712	-3.2368040010	-5.0795589003
N47	1.8986026138	-2.3513929437	-4.1965698498
C48	0.9603611457	-3.0165690898	-3.4236797489
C49	0.1961903132	-2.6504443083	-2.3280462909
O50	0.2318372515	-1.4579067656	-1.7532470934
N51	-0.6312113928	-3.6067529799	-1.8275667172
C52	-0.7343619108	-4.8894955541	-2.3562382271
N53	-1.5904229038	-5.7095898233	-1.7557008890
N54	-0.0140444657	-5.2825799795	-3.4083242267
C55	0.7940546892	-4.3458633542	-3.8822605845
N56	-3.0297860000	-4.5901629999	-6.0044220000
C57	-1.9937490964	-3.9593551333	-6.6587412998
N58	-1.6940223334	-2.7912284569	-6.1371908299
C59	-2.5991247884	-2.6354950175	-5.0889155768
C60	-2.7807045161	-1.6045000675	-4.1397412038
O61	-2.0706375478	-0.5577580601	-4.0283126372
N62	-3.8282685607	-1.8468875824	-3.2600675002
C63	-4.6360638764	-2.9794826084	-3.3024048609
N64	-5.6345333128	-3.0913505706	-2.4253377190
N65	-4.4457590329	-3.9740705573	-4.1643097310
C66	-3.4471141881	-3.7516300927	-5.0095734346
N67	-5.2727859999	-4.2351629999	1.3885780000
C68	-4.5769969156	-4.9482225818	0.4371221222
N69	-3.4602791676	-4.3610871688	0.0795251202
C70	-3.4116110486	-3.2046182422	0.8466607183
C71	-2.4704511724	-2.1548203974	0.8982063517

O72	-1.4142446643	-2.0334373269	0.2181916335
N73	-2.7999433289	-1.1902843736	1.8496117067
C74	-3.9270845536	-1.2272444599	2.6635270466
N75	-4.0818508137	-0.2378577299	3.5537714847
N76	-4.8352968055	-2.1851827295	2.5840075594
C77	-4.5333442798	-3.1246854092	1.6845186489
N78	-8.1317860000	-0.3501630000	0.8725779999
C79	-7.9127049371	-1.3897028282	0.0045015623
N80	-6.7573738536	-1.2893355806	-0.6064985885
C81	-6.1945660140	-0.1235643469	-0.1283696816
C82	-4.9486572751	0.4929721664	-0.4348056693
O83	-4.0414367504	0.1266054821	-1.2015694960
N84	-4.7919503998	1.6906913887	0.2958838244
C85	-5.7145624963	2.2207510315	1.1804524966
N86	-5.3734537915	3.3883449357	1.7957995975
N87	-6.8561944358	1.6358116461	1.4704284135
C88	-7.0449859472	0.4833874138	0.7991074607
H89	2.5449198745	5.2177823979	-5.7721982750
H90	-0.4293697058	-1.5743208856	-7.0063797064
H91	0.7789100302	-1.0845272402	-8.2110258339
H92	-0.9752195727	-0.1569182076	-5.2542284551
H93	-3.9936294768	-1.1350599285	-2.5267631277
H94	-3.6445231987	6.7761856625	1.9681097390
H95	-0.4204429938	4.1461753272	-2.9382906087
H96	0.2950269521	7.4639180634	-3.7479673284
H97	0.4381926970	5.7663320169	-4.2074034620
H98	-4.9410831843	-5.8924397989	0.0550167083
H99	-3.4424051106	0.5536379156	3.6285810954
H100	-4.8773758190	-0.3068970918	4.1734332266
H101	-2.1366798618	-0.4257371452	1.9431102974
H102	-8.6386342455	-2.1782844856	-0.1399196913
H103	-3.9305717243	2.1923534332	0.1030158371
H104	-4.6715472720	3.9865734353	1.3661351788
H105	-6.1548938989	3.8566541633	2.2388981258
H106	-1.5088740754	-4.4066954107	-7.5161045019
H107	-6.2388860628	-3.8874155874	-2.5831033653
H108	-5.9788520226	-2.3453619957	-1.7974366033
H109	-1.6618958755	-6.6563960341	-2.1054082583
H110	-2.2458391363	-5.3575571422	-1.0420741895
H111	-1.1521615481	-3.3346415741	-0.9707777548
H112	3.0380031501	-3.0709356088	-5.8431483012
H113	3.0222902402	-0.9696788245	-3.8473998820
H114	4.4876934284	-0.1186441123	-4.3425738301
H115	1.6569418761	0.0999506924	-2.2110200508
H116	3.8022120272	6.1169002683	-1.4445768033
H117	-3.8272851337	3.0326811069	5.0728358161

H118	0.8600346210	3.1461341267	0.6980001475
H119	1.8637700081	5.2033484878	0.6915190649
H120	1.4353882219	6.4093998976	1.9080607671
H121	-0.4019771763	-1.4240323871	-0.9765670927
H122	-8.9612632611	-0.1922546760	1.4330355930
H123	-2.2623431963	8.3391878444	0.5027549897
H124	3.0050137948	3.3812871389	-7.4784108949
H125	-3.4680369611	-5.4664407586	-6.2628070967
H126	5.0828124842	4.6108952341	-3.0613847307
H127	-2.4802597534	5.1916680548	4.8785563269
H128	1.8311760958	-5.2902496509	-5.4797269565
H129	-6.1157536366	-4.5283933305	1.8678006391
H130	-0.9180095880	2.5213202597	-1.3113047984
H131	-0.0216474056	1.2240311234	0.6033288013
H132	-1.6214745294	1.0939379366	-3.7614709775

Single point energy: -4343.0960031

(2G4-4H⁺)_r

N1	-2.3337859999	4.3758370000	4.2935780000
C2	-3.3651408397	3.4639143600	4.3078647114
N3	-3.3311899917	2.6545641920	3.2776264555
C4	-2.2058572667	3.0334031598	2.5636502049
C5	-1.6789961742	2.5591715700	1.3460797109
O6	-2.1406855892	1.6359364201	0.6131236120
N7	-0.5118163367	3.2217895693	0.9720180654
C8	0.0491964199	4.2844975395	1.6704657336
N9	1.1601619362	4.8457416210	1.1724976706
N10	-0.4708609512	4.7624553920	2.7947247311
C11	-1.5615586219	4.1055724011	3.1938404890
N12	-2.3107860000	7.3328370000	0.3775780000
C13	-3.1680061600	6.3795724795	0.8904086215
N14	-3.2123362587	5.2732606320	0.1877363102
C15	-2.3348961610	5.5142352218	-0.8657748338
C16	-1.7720059757	4.6817453302	-1.8258384531
O17	-2.0247666464	3.3979720233	-1.9162115831
N18	-0.8892608336	5.2754585804	-2.6920329169
C19	-0.5214316474	6.6122297479	-2.5976004331
N20	0.2901061787	7.0863622250	-3.5570760704
N21	-0.9183117404	7.3924066169	-1.6034620289
C22	-1.7833632249	6.8157281806	-0.7736025442
N23	4.2212139999	4.3458370000	-2.5964220000
C24	3.3965835328	5.1382195221	-1.8272597885
N25	2.2567662396	4.5540383941	-1.5422973665
C26	2.3452162216	3.3043593810	-2.1386060665
C27	1.4288337701	2.2352720302	-2.1957134397
O28	0.2666708466	2.1704925708	-1.7053020479

N29	1.9428725052	1.1345029525	-2.8883237189
C30	3.1964554205	1.0850595007	-3.4907929050
N31	3.5431482468	-0.0473175558	-4.1114403609
N32	4.0348541638	2.1113839642	-3.4833670834
C33	3.5769609542	3.1566609076	-2.7935707715
N34	2.3242150000	3.3108370000	-6.7294220000
C35	1.9482978135	4.2957110732	-5.8385342231
N36	0.8236230141	4.0383926309	-5.2111635888
C37	0.4282754260	2.8105395262	-5.7305136453
C38	-0.6192274291	1.9502731324	-5.4338491298
O39	-1.5336601677	2.1975542367	-4.5198749493
N40	-0.6590334174	0.7841516612	-6.1352586737
C41	0.2793735440	0.4310615702	-7.0937323547
N42	0.0952690257	-0.7447441367	-7.6989127878
N43	1.3194872988	1.2087225763	-7.3865203414
C44	1.3547441844	2.3435030559	-6.6947839882
N45	1.6542140000	-4.4471630001	-4.9444210000
C46	2.1591030809	-3.1999421599	-5.2293662228
N47	1.7090088384	-2.2664473319	-4.4280316683
C48	0.8651520757	-2.9340657386	-3.5537875991
C49	0.0923649339	-2.5261882064	-2.4765444643
O50	0.0183386977	-1.2763730980	-2.0520590606
N51	-0.6218582015	-3.4986768955	-1.8470328066
C52	-0.6040752965	-4.8356675753	-2.2318236194
N53	-1.3573457981	-5.6684990975	-1.5189829497
N54	0.1245953765	-5.2691380155	-3.2611643862
C55	0.8219099027	-4.3153780828	-3.8630052065
N56	-3.0297860001	-4.5901630000	-6.0044220000
C57	-2.1392624068	-3.9104382843	-6.8111083862
N58	-1.9759403438	-2.6583892604	-6.4525163671
C59	-2.8215640668	-2.5010340591	-5.3606023961
C60	-3.1099038052	-1.3753254131	-4.5569245013
O61	-2.6295198403	-0.2177768648	-4.6564697416
N62	-4.0362234681	-1.6571039911	-3.5514617852
C63	-4.6560258246	-2.8880010363	-3.3645078050
N64	-5.5472324103	-2.9808596202	-2.3684423456
N65	-4.3886460089	-3.9441479258	-4.1131799818
C66	-3.4923356543	-3.7002843004	-5.0755004905
N67	-5.2727860000	-4.2351630000	1.3885780000
C68	-4.4679376954	-4.9958828398	0.5641795011
N69	-3.4016508519	-4.3472173009	0.1634968820
C70	-3.4953553653	-3.1057234283	0.7774120701
C71	-2.6851250119	-1.9512028910	0.6831281529
O72	-1.6549944032	-1.8091429917	-0.0267832311
N73	-3.1501937580	-0.9046665435	1.4814218113
C74	-4.2931153386	-0.9592575623	2.2675955802

N75	-4.6499945420	0.1378932923	2.9587304562
N76	-5.0807567349	-2.0227548199	2.3231263829
C77	-4.6468628275	-3.0346160235	1.5684522671
N78	-8.1317860000	-0.3501630001	0.8725780000
C79	-7.5849893648	-1.2764596954	0.0156391567
N80	-6.4938570113	-0.8591122281	-0.5760161579
C81	-6.3119633506	0.4304258086	-0.0997907015
C82	-5.2720785001	1.3441754568	-0.2261443070
O83	-4.1726119034	1.1254644227	-0.9095242889
N84	-5.4489932874	2.5414814133	0.4239383532
C85	-6.5615261512	2.8160829087	1.2118134520
N86	-6.6367991664	4.0422137600	1.7624029355
N87	-7.5091877519	1.9231903145	1.4476929625
C88	-7.3490861105	0.7714606657	0.8011034160
H89	2.5554019193	5.1799555697	-5.6967736588
H90	-0.6586830406	-1.3858598033	-7.4250208562
H91	0.7138651739	-0.9817057627	-8.4633769444
H92	-1.4200872339	0.1312050128	-5.8623381679
H93	-4.2794879281	-0.8774561119	-2.9463752655
H94	-3.7267834997	6.5676834555	1.7977483760
H95	-0.4495939268	4.7122740618	-3.4307744157
H96	0.4627122092	8.0845444621	-3.5643370538
H97	0.4225441631	6.5724293919	-4.4184180321
H98	-4.7210736087	-6.0151974427	0.3043261477
H99	-4.0697039658	0.9791304575	3.0757132702
H100	-5.3884155276	-0.0123524049	3.6344303842
H101	-2.6454087197	-0.0146914253	1.3823116368
H102	-8.0464302158	-2.2437430307	-0.1331019761
H103	-4.7092039480	3.2476359588	0.3497391080
H104	-6.0914348746	4.8105870638	1.3975727595
H105	-7.5027762273	4.2728685043	2.2358306813
H106	-1.6524888019	-4.3928400869	-7.6482191859
H107	-6.0511711872	-3.8541319107	-2.3038184720
H108	-5.8261160307	-2.1844682205	-1.7894974723
H109	-1.3346429989	-6.6498882893	-1.7644822320
H110	-2.0384050270	-5.3134156889	-0.8332423092
H111	-1.1708426313	-3.1804429283	-1.0219807416
H112	2.8631230329	-3.0447796064	-6.0364795145
H113	2.9072485557	-0.8440708163	-4.2011039971
H114	4.4837031344	-0.0955815977	-4.4795418274
H115	1.3624152653	0.2978417183	-2.8559087277
H116	3.6952007839	6.1270662749	-1.5053517067
H117	-4.1000664240	3.4452685182	5.1015628140
H118	-0.0684307699	2.8716682222	0.1141254680
H119	1.5046573704	4.6957775963	0.2192192798
H120	1.5644940755	5.5915303953	1.7233993726

H121	-0.5702295819	-1.1893732541	-1.2495925554
H122	-8.9884949655	-0.4433387290	1.4083363012
H123	-2.1479149616	8.2665405385	0.7397539190
H124	3.1299533819	3.3221454360	-7.3453456446
H125	-3.3563784660	-5.5414858993	-6.1293101166
H126	5.1719649753	4.5569570051	-2.8787672192
H127	-2.1114454890	5.0464916769	5.0208881882
H128	1.9008424502	-5.3217450850	-5.3950144693
H129	-6.0712594541	-4.5685341330	1.9160775597
H130	-1.1840841654	2.8636622117	-2.0813655842
H131	-3.3488787699	1.5095697536	-0.4542462859
H132	-2.1477379667	1.4226625547	-4.4002326139

Single point energy: -4343.0957589

(2G4-4H⁺)_g

N1	-2.3337859977	4.3758369991	4.2935779969
C2	-3.0755854114	3.2839753889	3.8945153873
N3	-2.5336619014	2.6209867101	2.8977373007
C4	-1.3608132821	3.3187919504	2.6236824597
C5	-0.3772710041	3.1574154278	1.6034885743
O6	-0.3762841577	2.3180329999	0.6782219014
N7	0.6485706489	4.1112097723	1.6939561787
C8	0.7185668742	5.1089901559	2.6519386061
N9	1.7848730394	5.9475864818	2.5891993342
N10	-0.2168670651	5.3019825500	3.5594727405
C11	-1.2174581867	4.4071149064	3.4951833900
N12	-2.3107859973	7.3328369978	0.3775779957
C13	-3.2741092947	6.5450642983	0.9874631131
N14	-3.4478218517	5.3800883630	0.4111290495
C15	-2.5525049063	5.3897121708	-0.6516913645
C16	-2.2258974153	4.4416155475	-1.6321799143
O17	-2.6584410280	3.2455353986	-1.8527683867
N18	-1.2664210926	4.8512142057	-2.5315252636
C19	-0.6874596746	6.1074002503	-2.5278779285
N20	0.1851566205	6.3732429724	-3.5235827223
N21	-0.9398882006	7.0095582274	-1.5953696682
C22	-1.8459783208	6.6168421473	-0.6954537563
N23	4.2212139975	4.3458369961	-2.5964219995
C24	3.5342803036	4.8768926428	-1.5141893496
N25	2.6363426013	4.0649872429	-1.0105360377
C26	2.7334498978	2.9204769966	-1.7929934127
C27	2.0415514859	1.7014823730	-1.7835254980
O28	1.0868108864	1.2641896857	-1.0334449218
N29	2.4525416783	0.7989721563	-2.7356754150
C30	3.4745600214	1.0347476843	-3.6376065802
N31	3.7630313986	0.0322352248	-4.4864907392

N32	4.1301807218	2.1840477351	-3.6939563789
C33	3.7344271608	3.0748564737	-2.7809602515
N34	2.3242149943	3.3108370010	-6.7294219928
C35	1.7984683253	4.0433686919	-5.6908480960
N36	0.8140314255	3.4335898997	-5.0664629038
C37	0.6832142363	2.2234026787	-5.7412185328
C38	-0.1783735198	1.1041950488	-5.5222420902
O39	-1.0225812982	0.9674414572	-4.6149612539
N40	0.0331603227	0.0820934615	-6.4592828978
C41	0.9742445452	0.1212792481	-7.4714686664
N42	1.0737019258	-0.9887866982	-8.2595782205
N43	1.7946454250	1.1324263034	-7.6595164431
C44	1.6151244494	2.1363124210	-6.7830303655
N45	1.6542140019	-4.4471629957	-4.9444209983
C46	2.0004275935	-3.1149458190	-4.9762460657
N47	1.3976052445	-2.3982485513	-4.0537245395
C48	0.6053053071	-3.3174334262	-3.3715018873
C49	-0.3537963753	-3.1551715830	-2.3271648571
O50	-0.7153996894	-2.0870365268	-1.7885933261
N51	-0.9420475724	-4.3718477448	-1.9496635029
C52	-0.6458032866	-5.6017353155	-2.5118645325
N53	-1.3139438527	-6.6776542219	-2.0196803871
N54	0.1923582183	-5.7517632567	-3.5173902736
C55	0.7665541104	-4.6015573164	-3.9085767009
N56	-3.0297860000	-4.5901629999	-6.0044220014
C57	-1.9553626265	-3.8482159166	-6.4657334653
N58	-1.8639902141	-2.6566563278	-5.9252017233
C59	-2.9457835963	-2.5938694533	-5.0547875376
C60	-3.3978415462	-1.6073126021	-4.1653139530
O61	-2.9382670064	-0.4406628191	-3.8662467615
N62	-4.5451085147	-1.9360636679	-3.4774566098
C63	-5.2409596614	-3.1185798322	-3.6501389878
N64	-6.3762033860	-3.2604520401	-2.9324894093
N65	-4.8216365166	-4.0857208932	-4.4479791948
C66	-3.6968887099	-3.7932748281	-5.1081621914
N67	-5.2727859992	-4.2351629988	1.3885779998
C68	-4.4968043002	-4.7626194358	0.3689072873
N69	-3.5094361176	-3.9813022523	0.0009787627
C70	-3.6260609877	-2.8696847409	0.8276599881
C71	-2.8976899104	-1.6756436225	0.9222626039
O72	-1.8874181275	-1.2376168602	0.2491117163
N73	-3.3241555603	-0.8167032221	1.9079550670
C74	-4.3776115857	-1.0850379236	2.7645925806
N75	-4.6451434845	-0.1528260031	3.6979458945
N76	-5.1135759744	-2.1825502136	2.6749178742
C77	-4.7162048628	-3.0220041466	1.7156437438

N78	-8.1317859993	-0.3501629994	0.8725779994
C79	-7.5289855646	-1.1444915318	-0.0760625696
N80	-6.4746600927	-0.5891784468	-0.6322965301
C81	-6.3801444094	0.6544043998	-0.0122999266
C82	-5.4381538247	1.7211251945	-0.1582543450
O83	-4.4360283019	1.7560254831	-0.8987263757
N84	-5.7360399038	2.8068627209	0.6810138482
C85	-6.8031697731	2.8608023994	1.5586944843
N86	-6.9087096253	3.9816120251	2.3295067165
N87	-7.6601251075	1.8751888234	1.7157873062
C88	-7.4088460851	0.8161218920	0.9258124231
H89	2.1918842236	5.0198989082	-5.4410894235
H90	0.2346476797	-1.5288244307	-8.4311057382
H91	1.6565133680	-0.8574246696	-9.0795480108
H92	-0.5041345192	-0.7777752512	-6.3115833280
H93	-4.8816538091	-1.2482731349	-2.7982256323
H94	-3.8118025233	6.8975249023	1.8575427028
H95	-0.9768903946	4.1694169925	-3.2385944242
H96	0.4442727479	7.3458500290	-3.6371725121
H97	0.1824382158	5.7878479566	-4.3505534362
H98	-4.7160158090	-5.7323503319	-0.0582786884
H99	-3.9719840565	0.5760237632	3.8985059551
H100	-5.3160146370	-0.3971783540	4.4155000485
H101	-2.8427962071	0.0854567372	1.9665905079
H102	-7.9180834524	-2.1275505204	-0.3065123693
H103	-5.0628533235	3.5775815612	0.6648795911
H104	-6.5848333182	4.8605107075	1.9456775482
H105	-7.7824123227	4.0473947547	2.8406328058
H106	-1.2773612275	-4.2514164422	-7.2060396315
H107	-6.9827553296	-4.0241056903	-3.2063701240
H108	-6.8113966781	-2.4407949320	-2.5261474670
H109	-0.9832685647	-7.5747463986	-2.3565159506
H110	-1.6235481537	-6.6695497345	-1.0568210044
H111	-1.7130990100	-4.3065050149	-1.2750748311
H112	2.6878969259	-2.7368689977	-5.7220253386
H113	3.3667233227	-0.8876473507	-4.3372254389
H114	4.5957206248	0.1235831137	-5.0538448258
H115	1.9294579896	-0.0792653012	-2.7860541761
H116	3.7487851034	5.8731843502	-1.1504226908
H117	-4.0179299306	3.0470828599	4.3714332711
H118	1.3384788838	4.0974911099	0.9363508337
H119	2.6560390488	5.6184667763	2.1949253410
H120	1.8788150000	6.5797592939	3.3758589888
H121	-2.0807183162	-0.0649918336	-4.3098315240
H122	-8.9739356339	-0.5493224765	1.3996583306
H123	-2.0497100258	8.2819515710	0.6204658797

H124	3.0575270775	3.5894811870	-7.3708061611
H125	-3.3207386113	-5.5095343454	-6.3178019806
H126	5.0112343376	4.7584811831	-3.0794299421
H127	-2.5152852016	4.9863957617	5.0816177432
H128	2.0457396153	-5.1959932409	-5.5038574552
H129	-6.0297866890	-4.6960070240	1.8808512759
H130	-3.4036514039	2.8284649497	-1.2752575425
H131	-1.5249277409	-1.7737412416	-0.5608615370
H132	0.6361352498	1.8807529066	-0.3307068673

Single point energy: -4343.0903559

(2G4-4H⁺)_n

N1	-2.3337860000	4.3758370000	4.2935780000
C2	-2.9671171860	3.1764139627	4.0534771337
N3	-2.3858712410	2.4518930259	3.1219814286
C4	-1.2933934416	3.2218616455	2.7237493802
C5	-0.2990252049	3.0227150552	1.7140752964
O6	-0.1883609233	2.0630786428	0.9220513587
N7	0.6139676024	4.0884840755	1.6563499179
C8	0.5876149611	5.2038934386	2.4741335339
N9	1.5578389739	6.1331670815	2.2774951421
N10	-0.3465843082	5.4123292492	3.3793350722
C11	-1.2478782376	4.4192079849	3.4529015186
N12	-2.3107860000	7.3328369996	0.3775779997
C13	-3.2815633534	6.7088985460	1.1379614020
N14	-3.5341042589	5.4812808231	0.7432861884
C15	-2.6871963291	5.2850179627	-0.3456120699
C16	-2.4511369697	4.1650747709	-1.1779028446
O17	-3.0062899313	3.0280673873	-1.0971054445
N18	-1.4914160807	4.4078586320	-2.1556763606
C19	-0.8692292473	5.6377870379	-2.3506255475
N20	-0.0703772636	5.7973072296	-3.4075157864
N21	-1.0543694131	6.6796210011	-1.5513415324
C22	-1.9395534323	6.4478227307	-0.5906536969
N23	4.2212140000	4.3458369999	-2.5964220000
C24	3.4912885387	4.8796496848	-1.5442701068
N25	2.6679262811	4.0252222361	-0.9869211096
C26	2.8565262456	2.8514166242	-1.7047795223
C27	2.2599445230	1.5878500909	-1.6343533653
O28	1.3390911466	1.1072513644	-0.8618389262
N29	2.7419014569	0.6745490353	-2.5479896553
C30	3.7491589570	0.9428395184	-3.4585230159
N31	4.1261434351	-0.0696520740	-4.2679864845
N32	4.3106068032	2.1332435695	-3.5717741920
C33	3.8387748583	3.0361741617	-2.7087996795
N34	2.3242150000	3.3108370001	-6.7294219999

C35	2.1689591122	4.2891461313	-5.7865611094
N36	1.3573076856	3.9161573022	-4.8275555594
C37	0.9512974763	2.6421483680	-5.1685044238
C38	0.0342826979	1.7635398789	-4.5275069385
O39	-0.6209213932	1.9350172654	-3.4884611395
N40	-0.0686050373	0.5496975803	-5.2434674515
C41	0.5888927992	0.2505357474	-6.4239856162
N42	0.3812632448	-0.9735779331	-6.9615853022
N43	1.4176700976	1.0831753214	-7.0236513510
C44	1.5496618734	2.2445719453	-6.3639425337
N45	1.6542140001	-4.4471629999	-4.9444210000
C46	1.9555935556	-3.0970998410	-4.9091293283
N47	1.3945368887	-2.4617758687	-3.9082714608
C48	0.6898183385	-3.4507036582	-3.2354330681
C49	-0.2578715177	-3.3740564909	-2.1976857585
O50	-0.7341880430	-2.3117154739	-1.6800498354
N51	-0.7481357113	-4.6110794855	-1.7928487902
C52	-0.3995049027	-5.8155723150	-2.3921999637
N53	-0.9464455066	-6.9406160064	-1.8763167467
N54	0.3725514474	-5.8851352928	-3.4617829681
C55	0.8666206684	-4.7029118750	-3.8508236600
N56	-3.0297859997	-4.5901630000	-6.0044220002
C57	-1.7920981083	-4.0706246131	-6.3232675862
N58	-1.4892022820	-2.9934514561	-5.6471843745
C59	-2.5969537318	-2.7712449098	-4.8415321023
C60	-2.8766144163	-1.8416628851	-3.8620643953
O61	-2.0771830640	-0.8833748811	-3.4091633038
N62	-4.1337541012	-1.9012389256	-3.3171751106
C63	-5.0734016300	-2.8644948442	-3.6617109802
N64	-6.2696485163	-2.8035614734	-3.0807043669
N65	-4.7952051024	-3.8390130847	-4.5317438272
C66	-3.5966393999	-3.7537631148	-5.0844396193
N67	-5.2727860000	-4.2351630000	1.3885780000
C68	-4.4733829888	-4.7752814162	0.3937242408
N69	-3.4286338739	-4.0397223284	0.0972521668
C70	-3.5267385215	-2.9491068026	0.9561399934
C71	-2.7404599250	-1.8054002047	1.1309247826
O72	-1.6712790205	-1.4153625370	0.5092211144
N73	-3.1599863934	-0.9451595434	2.1138959852
C74	-4.2682209571	-1.1795591951	2.9138140413
N75	-4.5239359233	-0.2632168652	3.8601955273
N76	-5.0627243876	-2.2301313796	2.7478611063
C77	-4.6675586819	-3.0661187819	1.7860516948
N78	-8.1317860003	-0.3501629996	0.8725780005
C79	-7.8512783776	-1.3094820718	-0.0721333831
N80	-6.7764192780	-1.0494087595	-0.7785107483

C81	-6.3226819269	0.1688733396	-0.2852994830
C82	-5.2420891802	0.9897148925	-0.5946551509
O83	-4.3266686114	0.7067136319	-1.5106533303
N84	-5.1314916756	2.1406978520	0.1161302883
C85	-6.0380744472	2.5261898038	1.0908479654
N86	-5.8145249385	3.7025737090	1.6778781244
N87	-7.0757861652	1.7601460092	1.4426470673
C88	-7.1752994101	0.6328335983	0.7493424593
H89	2.6621575609	5.2483653248	-5.8655263409
H90	-0.3121444594	-1.6114540361	-6.5804058458
H91	0.6793854195	-1.0866007119	-7.9213827499
H92	-0.7197845126	-0.1177235426	-4.8393973540
H93	-4.3649321422	-1.1592729486	-2.6519686725
H94	-3.7665477922	7.2139870532	1.9621520987
H95	-1.2259655220	3.6016238633	-2.7418297784
H96	0.3416116197	6.7185539164	-3.4786863973
H97	0.3826743256	5.0252099031	-3.9183497991
H98	-4.7213160914	-5.7209072645	-0.0707148959
H99	-3.8424308985	0.4544702391	4.0787799140
H100	-5.2407001503	-0.4774124197	4.5424331827
H101	-2.6220003211	-0.0795910820	2.2383439628
H102	-8.4851801681	-2.1776125269	-0.1976727631
H103	-4.3032461483	2.7461453145	-0.1442418947
H104	-5.0520327932	4.3337317944	1.3796299958
H105	-6.5278884076	4.0455222035	2.3087483717
H106	-1.1661950394	-4.5345856189	-7.0746272571
H107	-6.9672522040	-3.4667588725	-3.3943428526
H108	-6.4932748864	-2.1249015479	-2.3404857544
H109	-0.6032696507	-7.8115276868	-2.2660985478
H110	-1.2182399366	-6.9764709715	-0.9027794624
H111	-1.5182698259	-4.5836955448	-1.1157379373
H112	2.5774372093	-2.6418692809	-5.6681016460
H113	3.9078347267	-1.0267413439	-4.0270043305
H114	4.9511197971	0.0908468346	-4.8330465426
H115	2.2617558606	-0.2259594389	-2.5855753759
H116	3.6197850615	5.9103198407	-1.2408214594
H117	-3.8603122660	2.9027028260	4.5995033409
H118	1.2981025630	4.0523020117	0.8945138857
H119	2.4479293242	5.8506697650	1.8903043105
H120	1.6005636010	6.8639661509	2.9779904293
H121	-1.3891885688	-1.2770670359	-2.7741152434
H122	-8.9384135391	-0.3159425591	1.4866620097
H123	-1.9977672523	8.2927307787	0.4562335732
H124	2.8755594967	3.3706576932	-7.5777715956
H125	-3.4853729930	-5.3842700712	-6.4427331021
H126	4.9577990291	4.8007983145	-3.1233294015

H127	-2.5593869398	5.0602762961	5.0053063703
H128	2.0519523407	-5.1438761459	-5.5645820085
H129	-6.0713878243	-4.6741666854	1.8335182645
H130	-3.6614411833	1.4526841440	-1.6104385975
H131	-1.3734538360	-1.9688095419	-0.2903311340
H132	0.8525383328	1.7072843981	-0.1782405098
Single point energy: -4343.0836329			

(2G4-4H⁺)_i

N1	-2.3337860205	4.3758369828	4.2935779596
C2	-3.4775804011	3.6223353570	4.1263493987
N3	-3.4846100443	2.9407154326	3.0030134736
C4	-2.2626498017	3.2357714732	2.4098020696
C5	-1.7480095753	2.9435819246	1.1295577793
O6	-2.3501295873	2.3494034210	0.1734634998
N7	-0.4592829624	3.4253982208	0.9375117938
C8	0.2195496891	4.2322320248	1.8433687291
N9	1.4562223797	4.6202615236	1.5176123329
N10	-0.3176420760	4.6377995551	2.9896560258
C11	-1.5195953913	4.1124495256	3.2203382271
N12	-2.3107860071	7.3328369273	0.3775779514
C13	-3.2200209274	6.3914454804	0.8167632587
N14	-3.2560383887	5.3092973380	0.0798902482
C15	-2.3111888864	5.5465589826	-0.9131379760
C16	-1.7499745160	4.7405998616	-1.9026411031
O17	-1.9424717025	3.4602543884	-2.1034739280
N18	-0.8698688219	5.3709885054	-2.7488396068
C19	-0.4942691694	6.7009391173	-2.5998999053
N20	0.3253926870	7.2119078226	-3.5380665237
N21	-0.8744766101	7.4398050597	-1.5706203703
C22	-1.7441124889	6.8359704139	-0.7633782536
N23	4.2212140018	4.3458369951	-2.5964220017
C24	3.5604549142	5.0158514885	-1.5919800317
N25	2.4870146012	4.3778045858	-1.1904448443
C26	2.4608081672	3.2192226862	-1.9496857094
C27	1.5084624790	2.1668376348	-1.9929679290
O28	0.4541485156	2.0486111252	-1.3468359245
N29	1.8618576932	1.1858464091	-2.9429407187
C30	2.9761950324	1.2400433581	-3.7677343671
N31	3.1417034393	0.2529789057	-4.6672531040
N32	3.8435080641	2.2409063398	-3.7412690238
C33	3.5432856967	3.1767918435	-2.8273909505
N34	2.3242149163	3.3108369164	-6.7294219314
C35	1.9639716071	4.2225178530	-5.7551223410
N36	0.8606695115	3.9094961693	-5.1145839458
C37	0.4673875957	2.7088854059	-5.6969940922

C38	-0.5480549588	1.8071375881	-5.4116602073
O39	-1.4894681294	1.8484578478	-4.4930629900
N40	-0.6000290815	0.6969883222	-6.2063344220
C41	0.2823281596	0.4588911659	-7.2498573369
N42	0.0685579338	-0.6399882756	-7.9810734650
N43	1.2977467568	1.2688793124	-7.5217326690
C44	1.3679596157	2.3313912018	-6.7289389520
N45	1.6542140240	-4.4471630130	-4.9444210127
C46	2.1685219772	-3.2874867192	-5.4819624522
N47	1.5564230135	-2.2117801768	-5.0459308652
C48	0.6118794337	-2.6865441299	-4.1475144229
C49	-0.4395590521	-2.0313217856	-3.4742893912
O50	-0.7721061883	-0.8127314034	-3.5703458913
N51	-1.1811857683	-2.8931849026	-2.6642819149
C52	-1.0102705734	-4.2737911225	-2.6192317586
N53	-1.8217302556	-4.9737649127	-1.8165878815
N54	-0.0969308033	-4.9067626343	-3.3424254354
C55	0.6721303725	-4.0851911484	-4.0605173944
N56	-3.0297858747	-4.5901632713	-6.0044223139
C57	-2.0294994978	-3.7435051988	-6.4413124572
N58	-2.1314995131	-2.5236314963	-5.9727831605
C59	-3.2765842543	-2.5632416726	-5.1853515898
C60	-3.8250148277	-1.6588008390	-4.2823383985
O61	-3.3385004235	-0.5059518740	-3.9035877919
N62	-5.0080757726	-2.0464417485	-3.7051704207
C63	-5.5976543722	-3.2837182849	-3.9334054824
N64	-6.7880718004	-3.5090566791	-3.3574465006
N65	-5.0151981194	-4.2273353657	-4.6596286112
C66	-3.8777578061	-3.8432708008	-5.2332499337
N67	-5.2727859917	-4.2351630123	1.3885779986
C68	-4.9192530851	-4.7444542922	0.1612388684
N69	-4.2308576114	-3.8920307334	-0.5604483774
C70	-4.1009375539	-2.7750368978	0.2509623978
C71	-3.5875171260	-1.4948051782	-0.0269426223
O72	-3.1517286178	-1.0673066789	-1.1337033347
N73	-3.6547593228	-0.6310049022	1.0707404088
C74	-4.3054870216	-0.9283144990	2.2639648455
N75	-4.3644803251	0.0358574328	3.1945670734
N76	-4.8820576335	-2.1024842413	2.4882440703
C77	-4.7414447021	-2.9720170342	1.4808610745
N78	-8.1317860438	-0.3501630923	0.8725780126
C79	-7.7286876947	-1.2925856330	-0.0566955031
N80	-6.7373006639	-0.8965225429	-0.8192405787
C81	-6.4646006462	0.3916943564	-0.3722338325
C82	-5.4650968364	1.3088798991	-0.6865739282
O83	-4.4647070637	1.1941777290	-1.5252778655

N84	-5.5367355930	2.5097934183	-0.0282641053
C85	-6.5245116650	2.8163198974	0.8965931926
N86	-6.5253985586	4.0576794666	1.4011815815
N87	-7.4305563275	1.9318638160	1.2932176076
C88	-7.3548393809	0.7600892687	0.6692782846
H89	2.5661934655	5.1003991568	-5.5632968635
H90	-0.7094953916	-1.2596281802	-7.7957752597
H91	0.6730961223	-0.8153721960	-8.7731841543
H92	-1.2203954273	-0.0560256283	-5.9064441349
H93	-5.3753895203	-1.4622401540	-2.9519570584
H94	-3.8247147241	6.5708487450	1.6960553509
H95	-0.3636904286	4.8066260335	-3.4443308306
H96	0.5178646381	8.2052092896	-3.4780374761
H97	0.3965047487	6.7822134229	-4.4502590807
H98	-5.1896559332	-5.7487902326	-0.1372243929
H99	-4.0508238317	1.0012027510	3.0562478039
H100	-4.7939242155	-0.2136534452	4.0757613006
H101	-3.2102263141	0.2807722306	0.9411984112
H102	-8.2152249550	-2.2573691980	-0.1155251389
H103	-4.7240570248	3.1261139069	-0.1221939332
H104	-5.9304047962	4.7810368824	1.0233959163
H105	-7.2816371653	4.3167386292	2.0219876527
H106	-1.2531982069	-4.0959650519	-7.1076415257
H107	-7.2707273937	-4.3657348722	-3.5986879507
H108	-7.3131193650	-2.7636721026	-2.9218152393
H109	-1.6727822226	-5.9740151436	-1.7931228495
H110	-2.6777938296	-4.5843553792	-1.4097825262
H111	-1.8868587699	-2.4384845682	-2.0745169678
H112	2.9941045950	-3.3031667591	-6.1812387196
H113	2.5519430513	-0.5832166833	-4.7282107480
H114	4.0288532402	0.2467891108	-5.1529225047
H115	1.1978317460	0.4160387155	-3.0266376754
H116	3.9198332544	5.9580203682	-1.2004251509
H117	-4.2633276417	3.6135516228	4.8702953774
H118	0.0263628515	3.0556238101	0.0990390882
H119	1.8413390125	4.5141684387	0.5707271094
H120	1.9429000952	5.1904747844	2.1965476576
H121	-2.3142329417	-0.5455788795	-3.7751780676
H122	-8.9068498427	-0.4245557334	1.5228950907
H123	-2.1553842766	8.2589439960	0.7621489810
H124	3.1211606577	3.3679725754	-7.3543043296
H125	-3.1789474998	-5.5521103955	-6.2906516273
H126	5.1184362323	4.5969247413	-2.9954835863
H127	-2.0794461708	4.9232468732	5.1079575229
H128	2.0050613804	-5.3878926167	-5.0856898814
H129	-5.7583708954	-4.7273618877	2.1303442453

H130	-2.1275298059	2.9314591739	-1.1930004166
H131	-3.9924315049	0.2921571869	-1.5077531802
H132	-1.3452639036	2.4842697504	-3.7573990473

Single point energy: -4343.0609514

(2G4-4H⁺)₄

N1	-2.3337860005	4.3758369947	4.2935779924
C2	-3.4316794588	3.5433412359	4.2673276992
N3	-3.4466069362	2.7620961077	3.2124510016
C4	-2.2830642018	3.0796371897	2.5268852144
C5	-1.7817861609	2.6177078558	1.2931222387
O6	-2.3164428327	1.7750469802	0.5185740374
N7	-0.5590718274	3.1989103415	0.9605360484
C8	0.0750528998	4.1827736006	1.7090419759
N9	1.2415341537	4.6650882971	1.2589765005
N10	-0.4251692899	4.6639392552	2.8412103727
C11	-1.5687210187	4.0789214192	3.1982857248
N12	-2.3107860034	7.3328369910	0.3775779965
C13	-3.2090910927	6.3848478055	0.8267311806
N14	-3.2379138112	5.2925041088	0.1022745046
C15	-2.3034139981	5.5315409495	-0.9015555117
C16	-1.7169183585	4.7100933229	-1.8632051690
O17	-1.9887392045	3.4390361834	-2.0228368469
N18	-0.7852411633	5.3106214300	-2.6752321001
C19	-0.3999581297	6.6359942291	-2.5307028820
N20	0.4692790209	7.1279826346	-3.4391988964
N21	-0.8261031683	7.3992300461	-1.5381598609
C22	-1.7347349336	6.8211066830	-0.7547656427
N23	4.2212140002	4.3458369990	-2.5964219984
C24	3.4417359281	5.1228702010	-1.7677758451
N25	2.3165670790	4.5335233165	-1.4406929268
C26	2.3759623581	3.2953115006	-2.0613221085
C27	1.4323512915	2.2523463160	-2.1362280362
O28	0.2737175173	2.2278050840	-1.6322872896
N29	1.8976169679	1.1633220387	-2.8735004078
C30	3.1059377629	1.1306450314	-3.5558779278
N31	3.3962386885	0.0442911240	-4.2844727578
N32	3.9704546504	2.1388399544	-3.5402761035
C33	3.5686235547	3.1584517984	-2.7812009578
N34	2.3242149928	3.3108369936	-6.7294219970
C35	1.8733042855	4.1478447732	-5.7296417362
N36	0.8301978790	3.6872818595	-5.0802841595
C37	0.5649631501	2.4652277318	-5.6944875176
C38	-0.2629466529	1.3966262251	-5.3534367607
O39	-1.0463995628	1.3705699290	-4.3051263446
N40	-0.2081762238	0.3078107533	-6.1899634509

C41	0.6414479867	0.2381364899	-7.2876512077
N42	0.5467639737	-0.8485988589	-8.0753353956
N43	1.5359431374	1.1749899201	-7.5560736082
C44	1.4838806043	2.2295510500	-6.7462727141
N45	1.6542140021	-4.4471630006	-4.9444210004
C46	2.1973272246	-3.2994926183	-5.4742391041
N47	1.7004203719	-2.2133114240	-4.9302956905
C48	0.8073199325	-2.6763666699	-3.9766501005
C49	-0.0747264897	-1.9835094794	-3.1242848270
O50	-0.2216373970	-0.7322482720	-3.0327883698
N51	-0.8279947441	-2.8382900978	-2.3245844246
C52	-0.7730282682	-4.2249191193	-2.3818227801
N53	-1.5575524392	-4.9176512047	-1.5408882120
N54	0.0198767133	-4.8819358700	-3.2183700205
C55	0.7749026752	-4.0746065414	-3.9650175575
N56	-3.0297860011	-4.5901629790	-6.0044219881
C57	-2.0185621158	-3.6997673464	-6.3077221745
N58	-2.0992313081	-2.5617600738	-5.6601158350
C59	-3.2456704168	-2.6983767623	-4.8820004363
C60	-3.7775835264	-1.9390428622	-3.8401732311
O61	-3.2466197589	-0.8403752602	-3.3691317298
N62	-4.9414553899	-2.4191034514	-3.2884429829
C63	-5.5287526960	-3.6147713279	-3.6789313878
N64	-6.6996260058	-3.9481984217	-3.0984384989
N65	-4.9696986515	-4.4294713464	-4.5589775409
C66	-3.8531122625	-3.9580269055	-5.1099748880
N67	-5.2727859978	-4.2351630019	1.3885780019
C68	-4.8508230093	-4.7544426061	0.1869756685
N69	-4.0950287632	-3.9176267531	-0.4847653289
C70	-3.9992736265	-2.8010642193	0.3332516932
C71	-3.3533032700	-1.5660260904	0.1383857986
O72	-2.6966717983	-1.1935665884	-0.8773912576
N73	-3.4932586682	-0.7089450085	1.2271202300
C74	-4.2546403901	-0.9837109215	2.3542817852
N75	-4.3563010711	-0.0340173792	3.2943886980
N76	-4.9006715492	-2.1330156960	2.5251286242
C77	-4.7253658310	-2.9864214715	1.5159312608
N78	-8.1317859922	-0.3501629967	0.8725779931
C79	-7.6114219166	-1.2231842220	-0.0623570837
N80	-6.5719278739	-0.7546185449	-0.7105519938
C81	-6.3946335090	0.5218383469	-0.1800316592
C82	-5.3859077026	1.4745972300	-0.3165162466
O83	-4.3329158667	1.3363288404	-1.0806449485
N84	-5.5411645024	2.6212191162	0.4258278743
C85	-6.6083710104	2.8263941536	1.2919162880
N86	-6.6763603266	4.0121608607	1.9222321527

N87	-7.5238681897	1.9000598933	1.5252768989
C88	-7.3777258147	0.7906582519	0.8049707820
H89	2.3716497947	5.0860836173	-5.5244491804
H90	-0.2784910878	-1.4307858819	-8.0618669165
H91	1.0879844837	-0.8350497152	-8.9320493332
H92	-0.7801526125	-0.5110031762	-5.9509323785
H93	-5.3567407610	-1.8875089487	-2.5137832670
H94	-3.8090208491	6.5674671695	1.7085497764
H95	-0.3210098787	4.7314902509	-3.3896408363
H96	0.6426697644	8.1255753056	-3.3851650267
H97	0.5201160510	6.7155082442	-4.3607154961
H98	-5.1257451291	-5.7510171286	-0.1319920431
H99	-3.9994481086	0.9241429089	3.2091320806
H100	-4.8621266932	-0.2903157157	4.1318730817
H101	-2.9981217148	0.1920473994	1.1388853326
H102	-8.0499879365	-2.2015771752	-0.2080284787
H103	-4.8100974286	3.3370570967	0.3528141810
H104	-6.1511856707	4.8114950585	1.5996152055
H105	-7.5118763367	4.1916721709	2.4667322559
H106	-1.2435576678	-3.9622109267	-7.0157366140
H107	-7.1711401082	-4.7587358359	-3.4839580089
H108	-7.2894070119	-3.2351658034	-2.6923321082
H109	-1.4889232811	-5.9242675435	-1.6209235908
H110	-2.4240084102	-4.5293103678	-1.1575083565
H111	-1.4510865716	-2.3679968317	-1.6527380751
H112	2.9535997461	-3.3288750729	-6.2472534783
H113	2.7511488678	-0.7311561781	-4.4718979023
H114	4.3136152184	0.0291766747	-4.7098253496
H115	1.2545069178	0.3584434300	-2.9101039248
H116	3.7596502202	6.1032211720	-1.4387764549
H117	-4.1760512574	3.5566252509	5.0523040206
H118	-0.1184648400	2.8402314745	0.1012397210
H119	1.5734186210	4.5659876524	0.2938779916
H120	1.6784980890	5.3644999654	1.8449669570
H121	-3.1884772210	-0.8365555573	-2.3464307675
H122	-8.9423094832	-0.4947185911	1.4652475609
H123	-2.1484576410	8.2568363710	0.7637474069
H124	3.0948848572	3.4769523921	-7.3677959435
H125	-3.1813605371	-5.5082746812	-6.4086334361
H126	5.1597430017	4.5590512370	-2.9150683852
H127	-2.0740718688	5.0098249759	5.0408221054
H128	1.9327821098	-5.3990383266	-5.1549788511
H129	-5.8077854437	-4.7194550478	2.1007485630
H130	-1.1465153384	2.8783436060	-2.1135089018
H131	-3.4964750997	1.7139599829	-0.6566104139
H132	-1.0128101088	0.4747629333	-3.8335208469

Single point energy: -4343.0606158

Table S2. The Electron density (ρ), Laplacian ($\nabla^2\rho$) in a.u., and Ellipticity (ϵ) for selected BCP's

Structure	BCP	ρ	$\nabla^2\rho$	ϵ
G4₁	N7...H ₂ N-	0.009	0.028	1.067
	O6... H ₂ N-	0.025	0.074	0.009
	O6... H-N1	0.023	0.080	0.103
G4₂	N7...H ₂ N-	0.017	0.072	0.023
	O6... H-N1	0.032	0.124	0.058
(G4-H⁺)₁	N7...H ₂ N- (A)	0.017	0.078	0.135
	N7...H ₂ N- (B)	0.024	0.090	0.042
	N7...H ₂ N- (C)	0.026	0.087	0.129
	N7...H ₂ N- (D)	0.016	0.070	0.045
	O6... H-N1 (A)	0.035	0.103	0.051
	O6... H-N1 (B)	0.031	0.134	0.101
	O6... H-N1 (C)	0.070	0.131	0.033
	O6... H-N1 (D)	0.005	0.034	0.030
	H _s ...O6	0.017	0.102	0.050
	O6...O6	0.001	0.009	0.646
(G4-2H⁺)₁	N7...H ₂ N-	0.031	0.092	0.039
	N7...H-N1	0.032	0.096	0.035
	O6... H-N1	0.021	0.079	0.007
	H _d ...O6	0.066	0.159	0.080
	O6...O6	0.012	0.048	0.121
(G4-3H⁺)₁	N7...H-N1 (A)	0.017	0.107	0.109
	N7...H-N1 (B)	0.032	0.102	0.015
	N7...H-N1 (C)	0.023	0.130	0.085
	N7...H-N1 (D)	0.038	0.113	0.023
	H _{t1} ...O6 (A)	0.022	0.112	0.101
	H _{t2} ...O6 (B)	0.047	0.128	0.123
	H _{t3} ...O6 (C)	0.044	0.116	0.086
	O6...O6	0.007	0.028	0.270
(G4-4H⁺)₁	N7...H-N1 (A)	0.020	0.081	0.028
	N7...H-N1 (B)	0.022	0.077	0.100
	H _{q1} ...O6 (A)	0.015	0.080	0.047
	H _{q2} ...O6 (B)	0.026	0.094	0.102
Cont'd				

Structure	BCP	ρ	$\nabla^2\rho$	ε
(2G4-H⁺)₃				
G2—G6	O6...O6	0.0351	0.1315	0.0226
G1—G5	N7...N3	0.0053	0.0188	0.6710
	C4...N2	0.0040	0.0149	0.8764
G1—G6	N2...N7	0.0029	0.0111	0.1381
	O6...O6	0.0017	0.0106	1.4092
G2—G6	N7...C5	0.0028	0.0101	1.4284
G2—G7	N2...C8	0.0049	0.0144	0.4070
G3—G7	C5...N3	0.0030	0.0103	1.0668
G3—G8	N2...C8	0.0018	0.0077	0.4881
G4—G8	O6...C6	0.0006	0.0034	0.3726
	C5...N3	0.0022	0.0087	2.7722
	N3...N2	0.0008	0.0043	0.4165
G4—G5	N1...C6	0.0006	0.0030	1.7763
	N2...C8	0.0024	0.1008	0.4927

