Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information to

DFT study of the mechanism of hydrogen evolution catalysed by molecular Ni, Co and Fe catalysts containing a diamine-tripyridine ligand

*Ke Ye, Ying-Ying Li, Rong-Zhen Liao**

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S1. Overlaid structure of 1-H2O from geometry optimization and from crystal structure.

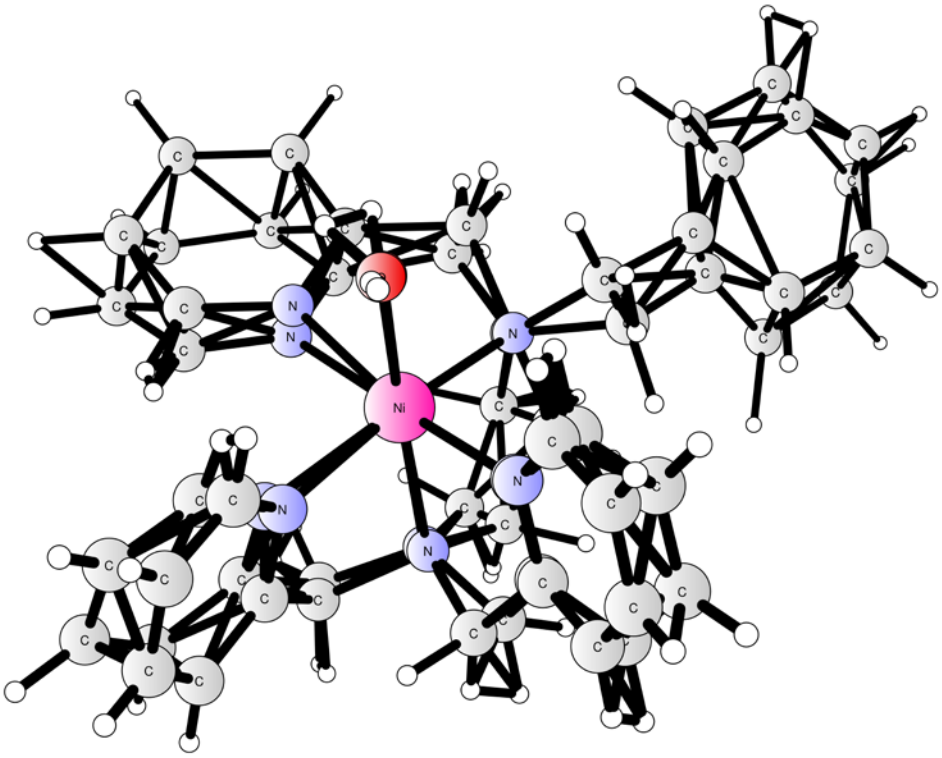

Fig. S1 Overlaid structure of 1-H2O from geometry optimization and from crystal structure.

Ni

S2. Structures of 1 with the square pyramidal structure.

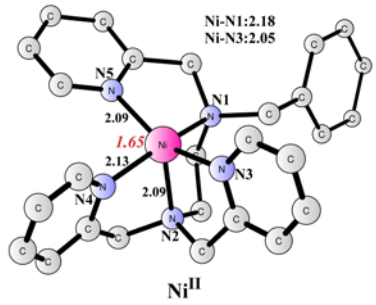

Fig. S2 Optimized isomers of ***1*** *with the square pyramidal structure. Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin density on Ni is shown in red italic.*

S3. Structures of 1 in the protonated form.

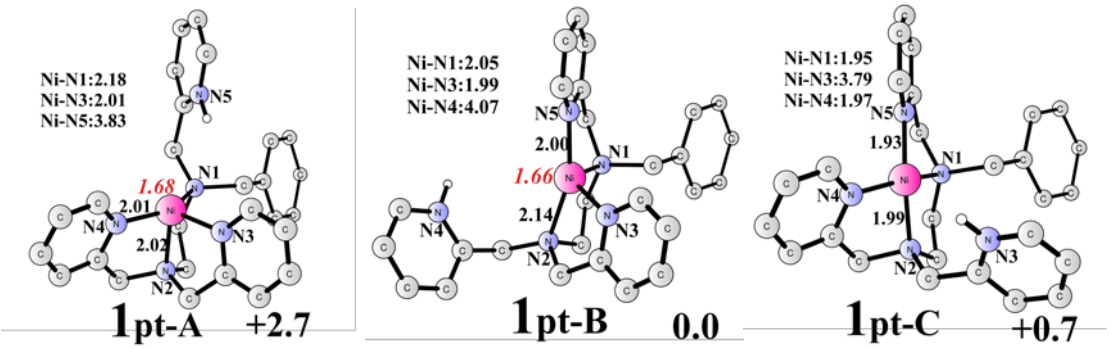

Fig. S3 Optimized isomers of $\mathbf{1}_{pt}$*. Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin densities on Ni are shown in red italic. Energies of* $\mathbf{1}_{pt\text{-}A}$ *and* $\mathbf{1}_{pt\text{-}C}$ *are given relative to* $\mathbf{1}_{pt\text{-}B}$*.*

Table S1. Relative energies (in kcal mol^{-1}) of different spin states of the three isomers.

	$\mathbf{1}_{pt\text{-}A}$	$\mathbf{1}_{pt\text{-}B}$	$\mathbf{1}_{pt\text{-}C}$
singlet	+26.5	+5.2	+0.7
triplet	+2.7	0.0	+3.3
quintet	+76.6	+75.1	+76.4

S4. Structures of 2_{dp}-H_2O.

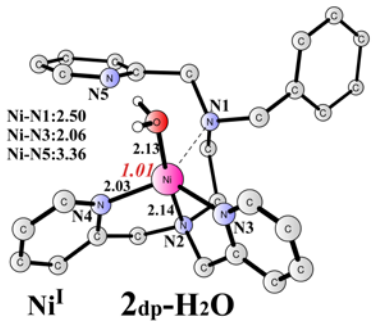

Fig. S4 Optimized structure of ***2_{dp}-H_2O****. Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin density on Ni is shown in red italic. For* ***2_{dp}-H_2O*** *the doublet state is the ground state, and the quartet state is 15.4* kcal mol^{-1} *higher.*

S5. Structures of 2(Ni^{I} HNPy).

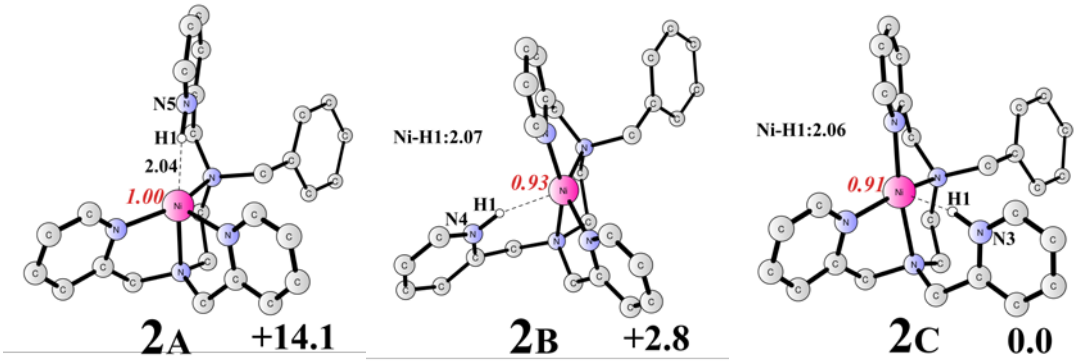

Fig. S5 Optimized isomers of ***2****(Ni^{I} HNPy). Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin densities on Ni are shown in red italic. Energies of* ***2_A*** *and* ***2_B*** *are given relative to* ***2_C****.*

Table S2. Relative energies (in kcal mol^{-1}) of different spin states of the three isomers.

	2_A	**2_B**	**2_C**
doublet	+14.1	+2.8	0.0
quartet	+47.0	+15.7	+16.8

S6. Structures of 2 (Ni^{III}-H).

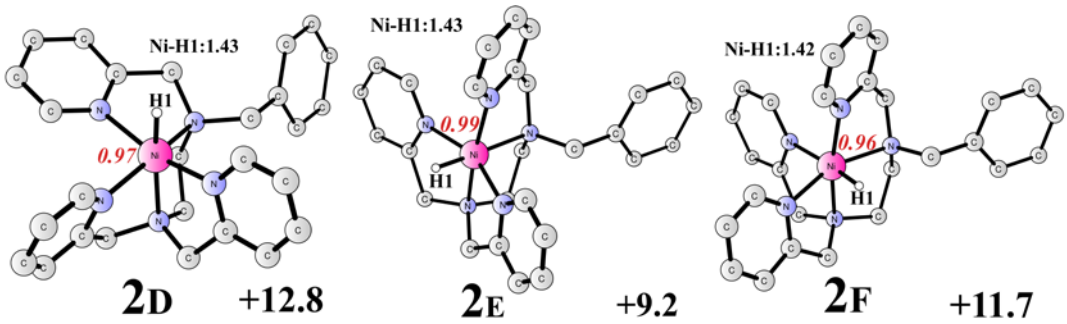

*Fig. S6 Optimized isomers of **2**(Ni^{III}-H). Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin densities on Ni are shown in red italic. Energies of $\mathbf{2_D}$, $\mathbf{2_E}$ and $\mathbf{2_F}$ are given relative to $\mathbf{2_C}$.*

Table S3. Relative energies (in kcal mol^{-1}) of different spin states of the three isomers.

	$\mathbf{2_D}$	$\mathbf{2_E}$	$\mathbf{2_F}$
doublet	+12.8	+9.2	+11.7
quartet	+37.0	+35.5	+35.7

Co

S7. Structure of 1'-H_2O.

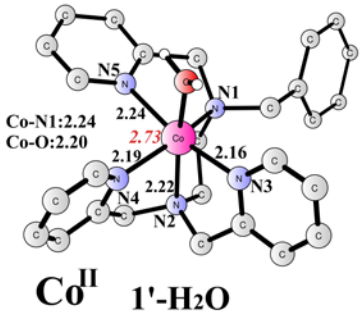

*Fig. S7 Optimized structure of **1'-H_2O**. Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin density on Co is shown in red italic. For **1'-H_2O** the quartet state is the ground state, and the doublet state is 9.6* kcal mol^{-1} *higher.*

S8. Structure of 2'$_{dp}$.

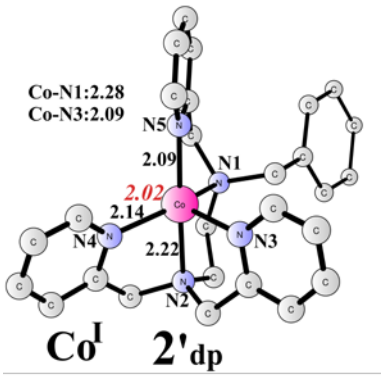

*Fig. S8 Optimized structure of **2'$_{dp}$**. Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin density on Co is shown in red italic. For **2'$_{dp}$** the triplet state is the ground state, and the singlet state is 17.7* kcal mol^{-1} *higher.*

S9. Structure of $2'_{dp}$-H_2O.

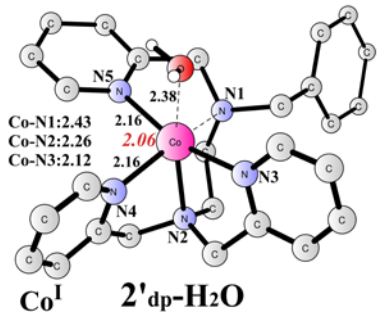

Fig. S9 Optimized structure of ***2'$_{dp}$-H_2O****. Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin density on Co is shown in red italic. For* ***2'$_{dp}$-H_2O*** *the triplet state is the ground state, and the singlet state is 18.2* kcal mol^{-1} *higher.*

S10. Structures of $1'_{pt}$.

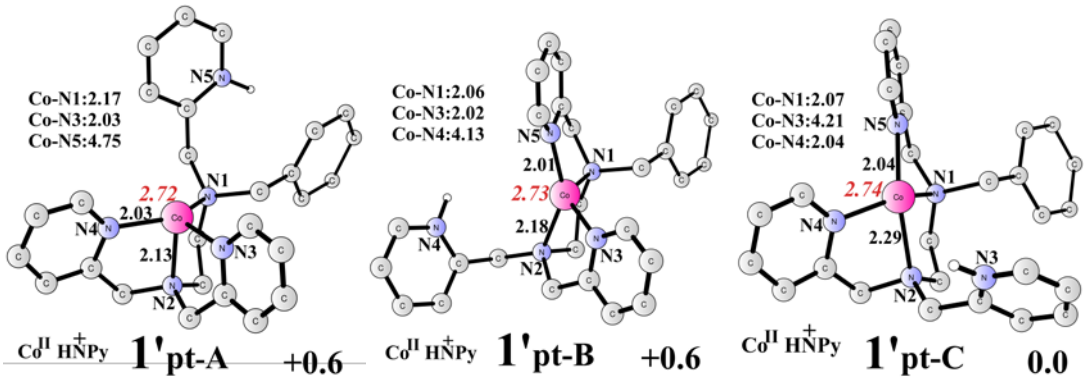

Fig. S10 Optimized isomers of ***1'$_{pt}$****. Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin densities on Co are shown in red italic. Energies of* ***1'$_{pt\text{-}A}$*** *and* ***1'$_{pt\text{-}B}$*** *are given relative to* ***1'$_{pt\text{-}C}$****.*

Table S4. Relative energies (in kcal mol^{-1}) of different spin states of the three isomers.

	1'$_{pt\text{-}A}$	**1'$_{pt\text{-}B}$**	**1'$_{pt\text{-}C}$**
doublet	+17.5	+10.5	+1.5
quartet	+0.6	+0.6	0.0

S11. Structures of 2'(Co^{I} HNPy).

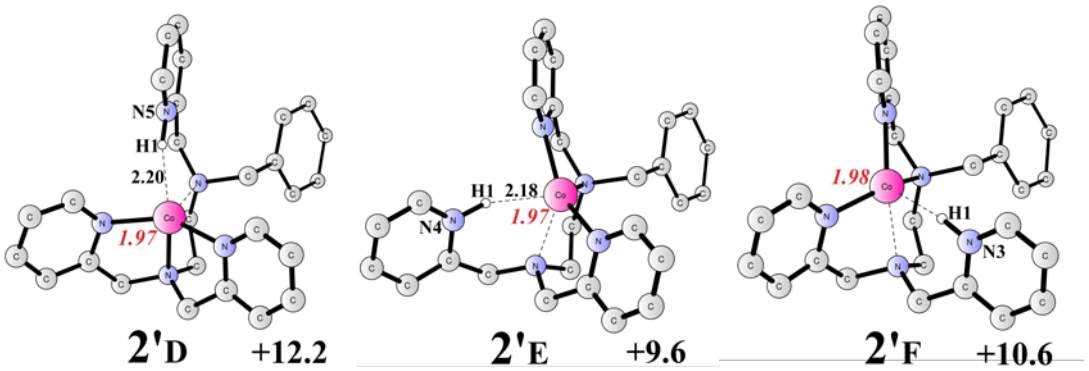

*Fig. S11 Optimized isomers of **2'**. Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin densities on Co are shown in red italic. Energies of **2'$_D$**, **2'$_E$** and **2'$_F$** are given relative to **2'$_B$**.*

Table S4. Relative energies (in kcal mol^{-1}) of different spin states of the three isomers.

	2'$_D$	**2'$_E$**	**2'$_F$**
singlet	+29.9	+19.1	+16.5
triplet	+12.2	+9.6	+10.6

S12. Structures of 3'$_{dp}$.

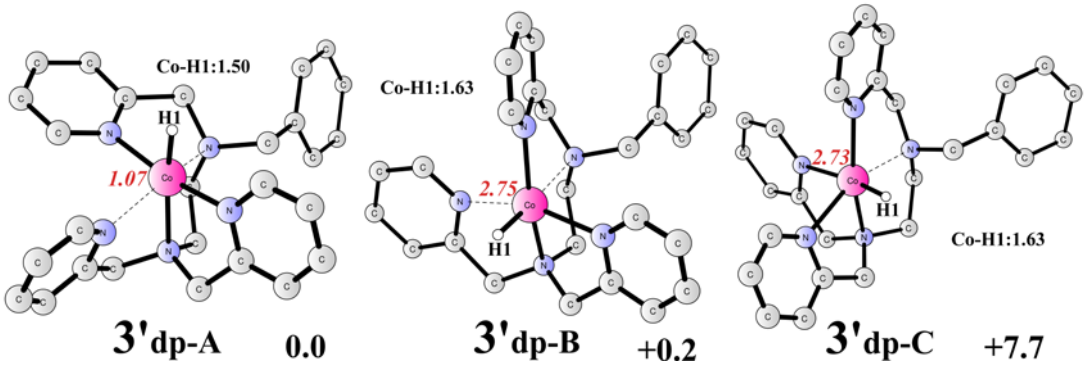

*Fig. S12 Optimized isomers of **3'$_{dp}$**. Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin densities on Co are shown in red italic. Energies of **3'$_{dp-B}$** and **3'$_{dp-C}$** are given relative to **3'$_{dp-A}$**.*

Table S4. Relative energies (in kcal mol^{-1}) of different spin states of the three isomers.

	3'$_{dp-A}$	**3'$_{dp-B}$**	**3'$_{dp-C}$**
doublet	0.0	+0.8	+7.8
quartet	+5.2	+0.2	+7.7

Fe

S13. Structure of 1''-H_2O.

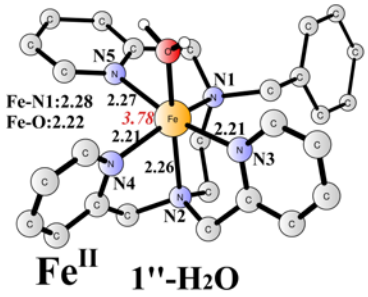

*Fig. S13 Optimized structure of **1''-H_2O**. Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin density on Fe is shown in red italic. For **1''-H_2O** the quintet state is the ground state, and the singlet state and triplet are 15.6 and 15.3* kcal mol^{-1} *higher.*

S14. Structures of 1''$_{pt}$.

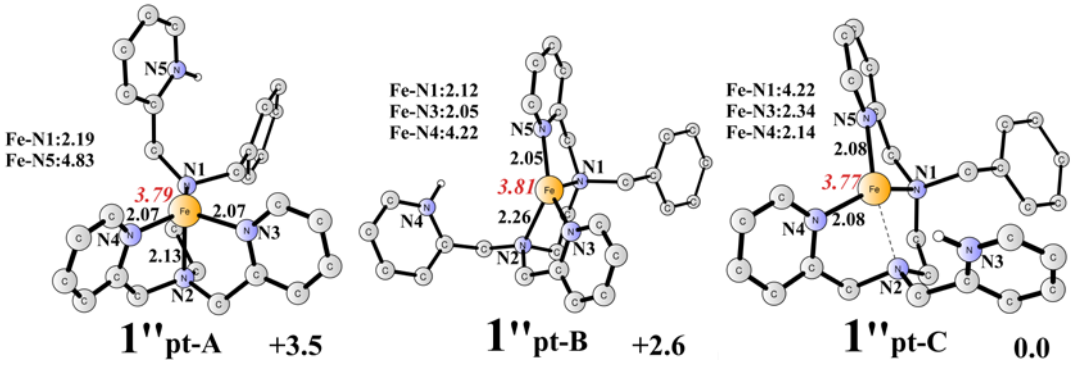

*Fig. S14 Optimized isomers of **1''$_{pt}$**. Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin densities on Fe are shown in red italic. Energies of **1''$_{pt-A}$** and **1''$_{pt-B}$** are given relative to **1''$_{pt-C}$**.*

Table S5. Relative energies (in kcal mol^{-1}) of different spin states of the three isomers.

	1''$_{pt-A}$	**1''$_{pt-B}$**	**1''$_{pt-C}$**
singlet	+31.8	+27.3	+30.5
triplet	+24.0	+17.5	+11.7
quintet	+3.5	+2.6	0.0

S15. Structures of 2’’(Fe^{I} HNPy).

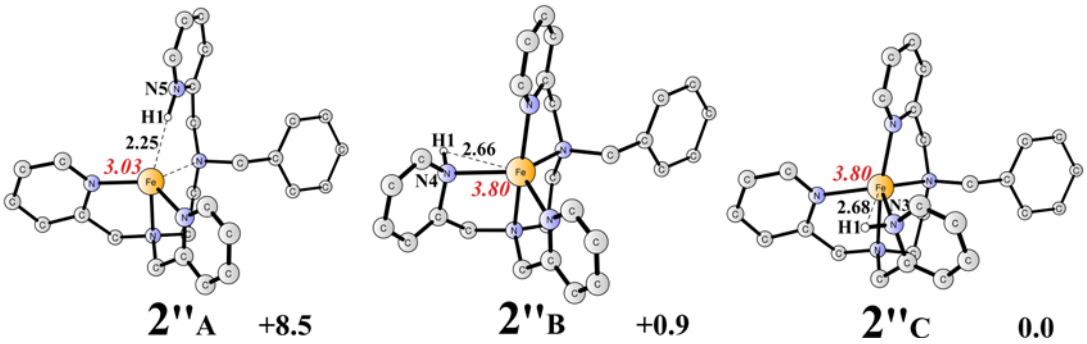

Fig. S15 Optimized isomers of 2’’ (Fe^{I} HNPy). Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin densities on Fe are shown in red italic. Energies of 2’’$_A$ and 2’’$_B$ are given relative to 2’’$_C$.

Table S6. Relative energies (in kcal mol^{-1}) of different spin states of the three isomers.

	2”$_A$	**2”$_B$**	**2”$_C$**
doublet	+35.0	+24.8	+17.4
quartet	+8.5	+6.2	+6.6
sextet	+11.8	+0.9	0.0

S16. Structures of 2’’(Fe^{III}-H).

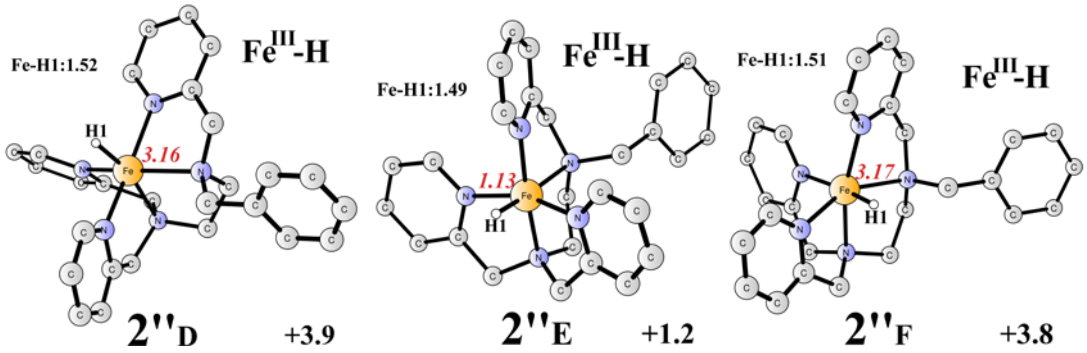

*Fig. S16 Optimized isomers of **2’’** (Fe^{III}-H). Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin densities on Fe are shown in red italic. Energies of **2”$_D$** , **2”$_E$** and **2”$_F$** are given relative to **2”$_C$**.*

Table S7. Relative energies (in kcal mol^{-1}) of different spin states of the three isomers.

	2”$_D$	**2”$_E$**	**2”$_F$**
doublet	+4.3	+1.2	+5.0
quartet	+3.9	+4.5	+3.8
sextet	+8.4	+10.0	+13.0

S17. Structures of $2''_{dp}$-H_2O

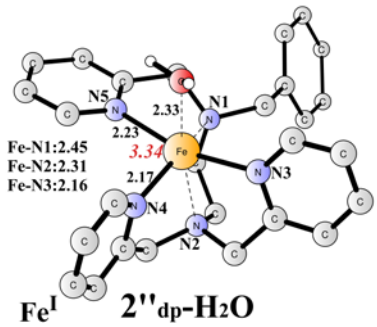

Fig. S17 Optimized structure of ***$2''_{dp}$-H_2O****. Distances are given in Ångstroms. For clarity, unimportant hydrogen atoms are not shown. Spin density on Fe is shown in red italic. For* ***$2''_{dp}$-H_2O*** *the quartet state is the ground state, and the doublet 14.2* kcal mol^{-1} *higher.*

S18. Cartesian coordinates for all optimized structures.

Ni

1-H_2O (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1567.13337251 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.834259	-0.761392	1.558946
2	6	0	1.943469	0.010226	2.165387
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4	1	0	2.216783	-0.377542	3.155893
5	6	0	1.168369	-2.211553	1.512404
6	1	0	2.256876	-2.316853	1.476247
7	1	0	0.835979	-2.717519	2.426731
8	6	0	-0.499151	-0.533872	2.188442
9	1	0	-1.076160	-1.453272	2.065645
10	1	0	-0.399796	-0.364411	3.267975
11	28	0	0.750696	-0.041927	-0.449528
12	6	0	3.144463	-0.023602	1.234119
13	6	0	4.454065	0.046811	1.706411
14	6	0	3.889912	-0.181882	-0.960937
15	6	0	5.508828	0.008312	0.792879
16	1	0	4.644429	0.123072	2.772212
17	6	0	5.222921	-0.114287	-0.567456
18	1	0	3.621904	-0.277982	-2.008415
19	1	0	6.536152	0.060596	1.139180
20	1	0	6.012216	-0.162370	-1.309369
21	6	0	0.590693	-2.883289	0.286610
22	6	0	0.310964	-4.249698	0.265085
23	6	0	-0.151272	-4.830847	-0.914633
24	1	0	0.456233	-4.847225	1.159427
25	6	0	-0.052764	-2.665659	-1.931187
26	6	0	-0.337198	-4.021874	-2.036705
27	1	0	-0.371221	-5.892880	-0.954787
28	1	0	-0.220783	-1.997964	-2.769614
29	1	0	-0.705905	-4.427677	-2.972109
30	7	0	2.868895	-0.130533	-0.086792
31	7	0	0.412680	-2.101219	-0.798938
32	6	0	-1.239949	0.634253	1.543953
33	1	0	-2.241364	0.721260	1.980994

34	1	0	-0.715788	1.567966	1.760851
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37	1	0	-1.797036	1.640598	-1.621914
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44	6	0	-4.379735	-0.608720	1.194987
45	6	0	-5.940383	0.880191	-0.571958
46	1	0	-4.219831	0.886763	-1.858038
47	6	0	-5.700555	-0.300479	1.523123
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51	1	0	-6.123567	-0.657108	2.456961
52	1	0	-7.511144	0.683273	0.891329
53	6	0	-0.386008	2.724967	-0.440168
54	6	0	-0.531656	4.112965	-0.450938
55	6	0	0.604061	4.918500	-0.396462
56	1	0	-1.523411	4.550618	-0.501500
57	6	0	1.923064	2.921393	-0.304654
58	6	0	1.858082	4.309497	-0.322938
59	1	0	0.512589	5.999994	-0.405642
60	1	0	2.877529	2.411731	-0.243189
61	1	0	2.769324	4.895276	-0.275261
62	7	0	0.827451	2.134555	-0.362563
63	8	0	0.763580	0.331795	-2.606681
64	1	0	1.217292	-0.242326	-3.239334
65	1	0	0.972317	1.241649	-2.861590

1-H_2O (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1567.09332723 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.614494	-0.918553	-1.948118
2	6	0	-1.786361	-0.224819	-2.488635
3	1	0	-1.495595	0.803851	-2.734290
4	1	0	-2.162066	-0.675876	-3.419238
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6	1	0	-1.839624	-2.622609	-1.963460
7	1	0	-0.166507	-2.962091	-2.332778
8	6	0	0.716973	-0.532389	-2.442442
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11	28	0	-0.667314	0.166146	0.148448
12	6	0	-2.910816	-0.192114	-1.460159
13	6	0	-4.249880	-0.326006	-1.822015
14	6	0	-3.511470	0.006739	0.802566
15	6	0	-5.238680	-0.282215	-0.837600
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17	6	0	-4.862861	-0.118102	0.495598
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19	1	0	-6.284741	-0.384759	-1.108537
20	1	0	-5.599587	-0.089475	1.290639
21	6	0	-0.595778	-2.725923	-0.237385
22	6	0	-0.477096	-4.065289	0.139473
23	6	0	-0.345341	-4.390901	1.486477
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39	6	0	2.246229	-0.656512	0.327590
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51	1	0	6.199930	-0.901559	-2.180262
52	1	0	7.528823	0.237148	-0.416657
53	6	0	0.495285	2.691679	0.365868
54	6	0	0.658965	4.072411	0.430420
55	6	0	-0.460399	4.895564	0.317813
56	1	0	1.650408	4.491537	0.566289
57	6	0	-1.801761	2.922072	0.066839
58	6	0	-1.711617	4.306591	0.132357
59	1	0	-0.357206	5.974799	0.366501
60	1	0	-2.755847	2.434814	-0.080805
61	1	0	-2.609379	4.906235	0.032815
62	7	0	-0.720755	2.119601	0.185253
63	8	0	-1.844226	0.420431	3.654375
64	1	0	-2.234985	-0.084409	4.381103
65	1	0	-1.694934	1.297951	4.030963

2_{dp}-H_2O (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1567.38493820 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.726126	1.128045	1.496814
2	6	0	-1.864892	0.482150	2.179131
3	1	0	-1.550757	-0.526364	2.468883
4	1	0	-2.137010	1.006259	3.107103
5	6	0	-0.860374	2.600988	1.474039
6	1	0	-1.926822	2.827664	1.353495
7	1	0	-0.539514	3.057616	2.422365
8	6	0	0.585417	0.690452	2.030917
9	1	0	1.317789	1.454003	1.758342
10	1	0	0.568483	0.653596	3.131016
11	28	0	-0.883028	0.595561	-0.569889
12	6	0	-3.068381	0.354793	1.265938
13	6	0	-4.371087	0.400573	1.755383
14	6	0	-3.834704	-0.056931	-0.879259
15	6	0	-5.440561	0.198508	0.881391
16	1	0	-4.543537	0.589179	2.810667
17	6	0	-5.161459	-0.040382	-0.464539
18	1	0	-3.579079	-0.228073	-1.920469
19	1	0	-6.463399	0.230437	1.242042
20	1	0	-5.955184	-0.202968	-1.185820
21	6	0	-0.114666	3.217754	0.305368
22	6	0	0.424039	4.501573	0.368150

23	6	0	1.016314	5.047547	-0.771411
24	1	0	0.373487	5.065719	1.294369
25	6	0	0.514016	3.001960	-1.915844
26	6	0	1.058009	4.282725	-1.937273
27	1	0	1.438601	6.047003	-0.747176
28	1	0	0.538053	2.361783	-2.792460
29	1	0	1.510913	4.663359	-2.846321
30	7	0	-2.792854	0.140927	-0.044774
31	7	0	-0.064289	2.471636	-0.821594
32	6	0	1.030995	-0.676238	1.496131
33	1	0	1.969823	-0.950933	2.002385
34	1	0	0.293543	-1.434652	1.776418
35	7	0	1.165233	-0.714245	0.027486
36	6	0	1.268105	-2.108169	-0.470224
37	1	0	1.550054	-2.046232	-1.524959
38	1	0	2.070957	-2.655447	0.044768
39	6	0	2.327995	0.082242	-0.482089
40	1	0	2.235881	0.080223	-1.572117
41	1	0	2.179600	1.115013	-0.162517
42	6	0	3.716078	-0.384665	-0.075930
43	6	0	4.434376	-1.288998	-0.873096
44	6	0	4.321593	0.090546	1.097523
45	6	0	5.706228	-1.723599	-0.498503
46	1	0	4.002419	-1.644135	-1.805621
47	6	0	5.592828	-0.342439	1.477811
48	1	0	3.805229	0.825319	1.711197
49	6	0	6.286381	-1.255573	0.682033
50	1	0	6.247851	-2.418852	-1.132982
51	1	0	6.045273	0.040972	2.387570
52	1	0	7.277762	-1.589637	0.972457
53	6	0	-0.006113	-2.923590	-0.392612
54	6	0	-0.166628	-3.941498	0.551796
55	6	0	-1.327016	-4.716529	0.537443
56	1	0	0.618742	-4.133136	1.276223
57	6	0	-2.058537	-3.427163	-1.338714
58	6	0	-2.294853	-4.457918	-0.430186
59	1	0	-1.464743	-5.514531	1.260621
60	1	0	-2.784116	-3.198128	-2.115393
61	1	0	-3.206648	-5.041993	-0.491175
62	7	0	-0.948653	-2.677000	-1.325251
63	8	0	-0.709668	-0.242965	-2.515161
64	1	0	-1.396118	-0.054474	-3.167144
65	1	0	-0.807198	-1.204853	-2.246587

2_{dp}-H_2O (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1567.34996093 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.824247	-0.696663	1.560925
2	6	0	1.938786	0.123932	2.095417
3	1	0	1.589707	1.163038	2.112411
4	1	0	2.200838	-0.158361	3.125012
5	6	0	1.160569	-2.144540	1.572467
6	1	0	2.251980	-2.226648	1.502382
7	1	0	0.868294	-2.613520	2.521183
8	6	0	-0.502583	-0.440268	2.174186
9	1	0	-1.083079	-1.362066	2.078302
10	1	0	-0.408551	-0.234891	3.249450
11	28	0	0.778415	-0.073892	-0.492701
12	6	0	3.134633	-0.018906	1.179556
13	6	0	4.443889	0.035964	1.638366
14	6	0	3.873915	-0.309439	-1.018564
15	6	0	5.505824	-0.066178	0.732387
16	1	0	4.631765	0.158409	2.701145
17	6	0	5.198697	-0.244786	-0.631157
18	1	0	3.609027	-0.465351	-2.060982
19	1	0	6.533887	-0.022376	1.072912
20	1	0	5.981849	-0.345636	-1.374809
21	6	0	0.529714	-2.857643	0.403599
22	6	0	0.154184	-4.200123	0.463176
23	6	0	-0.340946	-4.826028	-0.678502
24	1	0	0.258809	-4.746537	1.395610
25	6	0	-0.090298	-2.741014	-1.836533
26	6	0	-0.459671	-4.077979	-1.858806
27	1	0	-0.634180	-5.870259	-0.651568
28	1	0	-0.193532	-2.116183	-2.718432
29	1	0	-0.838907	-4.520444	-2.773077
30	7	0	2.835107	-0.190476	-0.149282
31	7	0	0.398246	-2.131980	-0.737218
32	6	0	-1.239589	0.709565	1.491468
33	1	0	-2.236529	0.822222	1.935587
34	1	0	-0.707826	1.647920	1.665999
35	7	0	-1.326470	0.516295	0.017066
36	6	0	-1.521727	1.827239	-0.659389
37	1	0	-1.656065	1.605952	-1.727505
38	1	0	-2.433309	2.330489	-0.315600
39	6	0	-2.384165	-0.469492	-0.389079

40	1	0	-2.275215	-0.597887	-1.469896
41	1	0	-2.126822	-1.426626	0.069505
42	6	0	-3.818106	-0.109050	-0.049937
43	6	0	-4.603420	0.637757	-0.940915
44	6	0	-4.399342	-0.539640	1.152340
45	6	0	-5.923079	0.965988	-0.628801
46	1	0	-4.186281	0.950128	-1.895096
47	6	0	-5.718466	-0.212047	1.469261
48	1	0	-3.822943	-1.155273	1.839489
49	6	0	-6.481675	0.546313	0.580161
50	1	0	-6.517726	1.539771	-1.333172
51	1	0	-6.152260	-0.557506	2.402793
52	1	0	-7.509813	0.797646	0.821692
53	6	0	-0.322062	2.712216	-0.457414
54	6	0	-0.429789	4.078595	-0.257015
55	6	0	0.726139	4.866076	-0.151501
56	1	0	-1.415874	4.529569	-0.193932
57	6	0	2.015564	2.846954	-0.411892
58	6	0	1.972122	4.215858	-0.237944
59	1	0	0.659928	5.937196	0.000044
60	1	0	2.960950	2.319785	-0.465957
61	1	0	2.900788	4.771790	-0.162519
62	7	0	0.893175	2.070230	-0.533276
63	8	0	0.715230	0.254222	-2.667024
64	1	0	1.418898	-0.148168	-3.195842
65	1	0	0.929862	1.201219	-2.600422

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1 (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1490.68856073 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.188657	-1.621250	-1.084288
2	6	0	-2.172341	-1.304474	-2.148760
3	1	0	-1.636223	-0.838438	-2.983265
4	1	0	-2.640641	-2.213870	-2.546062
5	6	0	-1.750430	-2.591762	-0.105885
6	1	0	-2.837715	-2.457832	-0.085805
7	1	0	-1.564634	-3.624696	-0.424179
8	6	0	0.140414	-2.050341	-1.617234
9	1	0	0.622839	-2.653419	-0.844481
10	1	0	0.021067	-2.693911	-2.497613
11	28	0	-0.847812	0.169608	-0.024747

12	6	0	-3.224402	-0.337629	-1.635893
13	6	0	-4.505537	-0.289402	-2.180160
14	6	0	-3.711155	1.428674	-0.202463
15	6	0	-5.407702	0.665607	-1.709863
16	1	0	-4.791016	-0.986782	-2.961173
17	6	0	-5.002719	1.542323	-0.702637
18	1	0	-3.356529	2.089898	0.580198
19	1	0	-6.410682	0.721154	-2.120889
20	1	0	-5.672463	2.297851	-0.307616
21	6	0	-1.223020	-2.354210	1.294625
22	6	0	-1.195854	-3.365229	2.253549
23	6	0	-0.786768	-3.059834	3.551605
24	1	0	-1.496173	-4.373706	1.987865
25	6	0	-0.441484	-0.798797	2.841907
26	6	0	-0.405841	-1.751158	3.853177
27	1	0	-0.762524	-3.831792	4.314135
28	1	0	-0.138588	0.227073	3.023066
29	1	0	-0.079987	-1.472277	4.848895
30	7	0	-2.834600	0.508796	-0.653161
31	7	0	-0.844006	-1.090369	1.589065
32	6	0	1.010369	-0.838653	-1.963091
33	1	0	1.990219	-1.169110	-2.323878
34	1	0	0.550545	-0.268151	-2.776072
35	7	0	1.138735	0.066285	-0.783151
36	6	0	1.403158	1.480474	-1.164524
37	1	0	2.462748	1.647791	-1.382875
38	1	0	0.850124	1.696651	-2.086811
39	6	0	2.158573	-0.428150	0.231513
40	1	0	2.063328	0.233647	1.096377
41	1	0	1.825376	-1.417687	0.551000
42	6	0	3.594679	-0.479865	-0.236238
43	6	0	4.450721	0.615284	-0.035982
44	6	0	4.112093	-1.635732	-0.843126
45	6	0	5.778891	0.569101	-0.460870
46	1	0	4.086708	1.498929	0.483953
47	6	0	5.439611	-1.683392	-1.269846
48	1	0	3.486121	-2.518265	-0.956908
49	6	0	6.272716	-0.578037	-1.085363
50	1	0	6.431286	1.419887	-0.291541
51	1	0	5.827319	-2.586128	-1.731099
52	1	0	7.307453	-0.617320	-1.410262
53	6	0	0.920631	2.423456	-0.078079
54	6	0	1.539190	3.645434	0.178711
55	6	0	1.009061	4.485114	1.158783

56	1	0	2.421963	3.933573	-0.382675
57	6	0	-0.683122	2.839898	1.560054
58	6	0	-0.121606	4.073739	1.866538
59	1	0	1.475645	5.441589	1.372111
60	1	0	-1.555901	2.474795	2.093094
61	1	0	-0.559227	4.691590	2.642610
62	7	0	-0.181534	2.031579	0.604410

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1 (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1490.66057049 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.129118	-1.391250	-1.216216
2	6	0	-2.128419	-0.992116	-2.254671
3	1	0	-1.614144	-0.410265	-3.026653
4	1	0	-2.555868	-1.875578	-2.743800
5	6	0	-1.701573	-2.495199	-0.372348
6	1	0	-2.771652	-2.295821	-0.258009
7	1	0	-1.604967	-3.445403	-0.910100
8	6	0	0.186080	-1.800791	-1.820828
9	1	0	0.678222	-2.461287	-1.104079
10	1	0	0.023963	-2.375469	-2.740055
11	28	0	-0.820051	0.229827	-0.169824
12	6	0	-3.188229	-0.145351	-1.596805
13	6	0	-4.492248	-0.052157	-2.071076
14	6	0	-3.640089	1.353940	0.119883
15	6	0	-5.392337	0.790620	-1.417600
16	1	0	-4.796773	-0.628464	-2.938520
17	6	0	-4.956472	1.504423	-0.302360
18	1	0	-3.273720	1.896133	0.981046
19	1	0	-6.414444	0.882667	-1.770370
20	1	0	-5.621019	2.167548	0.239882
21	6	0	-1.075748	-2.571516	1.002533
22	6	0	-0.923640	-3.788639	1.666571
23	6	0	-0.441646	-3.781520	2.976906
24	1	0	-1.184430	-4.721290	1.176183
25	6	0	-0.285588	-1.395840	2.824601
26	6	0	-0.120550	-2.561460	3.570705
27	1	0	-0.318431	-4.712374	3.521154
28	1	0	-0.031556	-0.427631	3.247986
29	1	0	0.255501	-2.510002	4.586561
30	7	0	-2.763563	0.547781	-0.509094

31	7	0	-0.755933	-1.391401	1.566895
32	6	0	1.029806	-0.560567	-2.077222
33	1	0	2.037695	-0.828378	-2.409253
34	1	0	0.581598	0.055422	-2.861103
35	7	0	1.068943	0.250692	-0.819146
36	6	0	1.295380	1.707878	-1.083434
37	1	0	2.353944	1.922279	-1.258320
38	1	0	0.744995	1.981294	-1.990088
39	6	0	2.085986	-0.289057	0.189568
40	1	0	1.950056	0.307350	1.093939
41	1	0	1.768684	-1.304260	0.429494
42	6	0	3.529107	-0.267797	-0.255329
43	6	0	4.347594	0.839366	0.022003
44	6	0	4.093156	-1.374562	-0.910611
45	6	0	5.684643	0.854256	-0.376037
46	1	0	3.948005	1.682298	0.581697
47	6	0	5.429826	-1.361172	-1.310062
48	1	0	3.496192	-2.267604	-1.083601
49	6	0	6.225016	-0.243115	-1.049838
50	1	0	6.307837	1.713000	-0.147529
51	1	0	5.853865	-2.226561	-1.809258
52	1	0	7.266668	-0.234661	-1.354221
53	6	0	0.749800	2.475087	0.093000
54	6	0	1.270107	3.676307	0.563308
55	6	0	0.693812	4.272300	1.686607
56	1	0	2.116830	4.132160	0.061118
57	6	0	-0.839628	2.432561	1.801972
58	6	0	-0.367340	3.630601	2.326194
59	1	0	1.081335	5.211340	2.068552
60	1	0	-1.643927	1.886532	2.282268
61	1	0	-0.821400	4.043125	3.220135
62	7	0	-0.313539	1.879874	0.691305

1(square pyramidal) (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1490.65417652 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.771933	-0.843001	1.787157
2	6	0	1.947245	-0.111352	2.270274
3	1	0	1.642739	0.915598	2.505920
4	1	0	2.366895	-0.535311	3.194558
5	6	0	0.997390	-2.269974	1.560251

6	1	0	2.031168	-2.525560	1.822841
7	1	0	0.368874	-2.886067	2.215169
8	6	0	-0.546107	-0.476548	2.335384
9	1	0	-1.171480	-1.372113	2.329136
10	1	0	-0.480689	-0.160236	3.385477
11	28	0	0.706180	0.196619	-0.314578
12	6	0	3.028935	-0.077401	1.198524
13	6	0	4.384708	-0.174185	1.508107
14	6	0	3.535316	0.065395	-1.085688
15	6	0	5.332426	-0.139731	0.484265
16	1	0	4.690785	-0.281819	2.543594
17	6	0	4.900068	-0.024358	-0.837487
18	1	0	3.149111	0.157474	-2.095249
19	1	0	6.390495	-0.213542	0.714743
20	1	0	5.600842	-0.007324	-1.664618
21	6	0	0.768609	-2.689186	0.111948
22	6	0	0.736238	-4.040790	-0.240853
23	6	0	0.582174	-4.400016	-1.576480
24	1	0	0.835092	-4.798614	0.530354
25	6	0	0.490171	-2.071139	-2.118512
26	6	0	0.460906	-3.392980	-2.537985
27	1	0	0.556854	-5.445961	-1.865199
28	1	0	0.391005	-1.256394	-2.828875
29	1	0	0.340855	-3.624118	-3.590441
30	7	0	2.623134	0.050331	-0.092679
31	7	0	0.635118	-1.724585	-0.818717
32	6	0	-1.234436	0.647776	1.547036
33	1	0	-2.267413	0.762272	1.893632
34	1	0	-0.723368	1.595156	1.731632
35	7	0	-1.236922	0.428603	0.049956
36	6	0	-1.638756	1.695134	-0.633006
37	1	0	-1.842945	1.456559	-1.682548
38	1	0	-2.565687	2.094951	-0.210239
39	6	0	-2.185907	-0.694709	-0.358802
40	1	0	-2.018132	-0.847606	-1.427238
41	1	0	-1.844327	-1.593063	0.155099
42	6	0	-3.653886	-0.452307	-0.085852
43	6	0	-4.474855	0.125144	-1.067738
44	6	0	-4.235066	-0.849092	1.129419
45	6	0	-5.833970	0.329436	-0.829487
46	1	0	-4.059151	0.393888	-2.036290
47	6	0	-5.594002	-0.644758	1.369948
48	1	0	-3.633032	-1.348318	1.885432
49	6	0	-6.393903	-0.048977	0.392640

50	1	0	-6.457615	0.768576	-1.601635
51	1	0	-6.030441	-0.963496	2.311152
52	1	0	-7.452776	0.103033	0.575671
53	6	0	-0.517003	2.689557	-0.562050
54	6	0	-0.711127	4.063526	-0.668355
55	6	0	0.395597	4.910622	-0.641843
56	1	0	-1.716002	4.459106	-0.772228
57	6	0	1.787331	2.973691	-0.383557
58	6	0	1.666050	4.352414	-0.495848
59	1	0	0.268546	5.984999	-0.727186
60	1	0	2.757487	2.511253	-0.263509
61	1	0	2.555355	4.971717	-0.464280
62	7	0	0.718030	2.147006	-0.420319

1(square pyramidal) (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1490.65417652 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.822073	-0.806982	1.524576
2	6	0	1.949255	-0.118070	2.207606
3	1	0	1.626355	0.901432	2.447963
4	1	0	2.203444	-0.609149	3.155613
5	6	0	1.114620	-2.259714	1.335560
6	1	0	2.197288	-2.404393	1.408050
7	1	0	0.667941	-2.852665	2.141233
8	6	0	-0.509032	-0.571973	2.167656
9	1	0	-1.100961	-1.480578	2.043023
10	1	0	-0.395388	-0.413771	3.246522
11	28	0	0.779329	0.077626	-0.364751
12	6	0	3.154797	-0.080272	1.283635
13	6	0	4.464500	-0.110425	1.757852
14	6	0	3.895855	-0.014063	-0.921936
15	6	0	5.517335	-0.079146	0.841237
16	1	0	4.657154	-0.163674	2.824595
17	6	0	5.229064	-0.037629	-0.523557
18	1	0	3.625077	0.014708	-1.973319
19	1	0	6.545632	-0.100515	1.187919
20	1	0	6.017456	-0.028436	-1.267911
21	6	0	0.669859	-2.768729	-0.021301
22	6	0	0.443313	-4.124180	-0.256666
23	6	0	0.139681	-4.547945	-1.550365
24	1	0	0.511150	-4.836577	0.559339
25	6	0	0.282900	-2.266379	-2.262176

26	6	0	0.064160	-3.602505	-2.574835
27	1	0	-0.036137	-5.599182	-1.755190
28	1	0	0.220149	-1.495624	-3.024780
29	1	0	-0.166367	-3.889699	-3.594544
30	7	0	2.878642	-0.023734	-0.039635
31	7	0	0.579626	-1.855445	-1.012469
32	6	0	-1.236343	0.616420	1.539133
33	1	0	-2.237346	0.707282	1.977105
34	1	0	-0.701433	1.544638	1.761047
35	7	0	-1.320392	0.482622	0.052299
36	6	0	-1.647393	1.792926	-0.560045
37	1	0	-1.955873	1.608320	-1.595519
38	1	0	-2.501320	2.268202	-0.063872
39	6	0	-2.327500	-0.565194	-0.383230
40	1	0	-2.222005	-0.642748	-1.468942
41	1	0	-1.995880	-1.517064	0.035531
42	6	0	-3.771429	-0.302922	-0.012499
43	6	0	-4.619783	0.391454	-0.888971
44	6	0	-4.300323	-0.780582	1.197327
45	6	0	-5.953081	0.627026	-0.552984
46	1	0	-4.247669	0.728431	-1.853755
47	6	0	-5.633114	-0.544722	1.536597
48	1	0	-3.678312	-1.367168	1.870391
49	6	0	-6.459818	0.165093	0.663600
50	1	0	-6.599139	1.156937	-1.245727
51	1	0	-6.029018	-0.926529	2.472320
52	1	0	-7.498878	0.342066	0.922208
53	6	0	-0.459984	2.726744	-0.580662
54	6	0	-0.628147	4.107547	-0.674280
55	6	0	0.494757	4.926133	-0.778262
56	1	0	-1.627474	4.530402	-0.670590
57	6	0	1.854289	2.958876	-0.660841
58	6	0	1.761629	4.338770	-0.774864
59	1	0	0.384131	6.003024	-0.856838
60	1	0	2.817460	2.464215	-0.642589
61	1	0	2.662528	4.936767	-0.853316
62	7	0	0.768024	2.159052	-0.566103

$\mathbf{1}_{\text{pt-A}}$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1490.82532347 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-1.799482	-1.147323	-1.194042
2	6	0	-2.661677	-0.450888	-2.195142
3	1	0	-2.017029	-0.024932	-2.971793
4	1	0	-3.328762	-1.161614	-2.696150
5	6	0	-2.584447	-2.115868	-0.368861
6	1	0	-3.629428	-1.787569	-0.370668
7	1	0	-2.562568	-3.112222	-0.824303
8	6	0	-0.545034	-1.733409	-1.755518
9	1	0	-0.221216	-2.528438	-1.080679
10	1	0	-0.732347	-2.197167	-2.731566
11	28	0	-1.168754	0.293432	0.072475
12	6	0	-3.451811	0.659752	-1.523334
13	6	0	-4.666725	1.114993	-2.023262
14	6	0	-3.522558	2.235322	0.209327
15	6	0	-5.313493	2.174850	-1.381388
16	1	0	-5.104000	0.649756	-2.901102
17	6	0	-4.731694	2.743429	-0.245703
18	1	0	-3.045494	2.636040	1.097936
19	1	0	-6.262577	2.543862	-1.758103
20	1	0	-5.208648	3.560382	0.284508
21	6	0	-2.106508	-2.158313	1.069036
22	6	0	-2.377195	-3.245044	1.897583
23	6	0	-2.023112	-3.180194	3.245853
24	1	0	-2.869886	-4.124759	1.495407
25	6	0	-1.140602	-0.989850	2.845448
26	6	0	-1.399586	-2.027328	3.730374
27	1	0	-2.233145	-4.014203	3.908382
28	1	0	-0.656246	-0.079276	3.184770
29	1	0	-1.117483	-1.933350	4.773242
30	7	0	-2.886193	1.218274	-0.417863
31	7	0	-1.481624	-1.049646	1.538714
32	6	0	0.536558	-0.665954	-1.904905
33	1	0	1.441352	-1.119967	-2.321697
34	1	0	0.205487	0.101536	-2.611159
35	7	0	0.884546	0.039114	-0.599898
36	6	0	1.657189	1.254697	-1.035706
37	1	0	2.473371	0.928454	-1.690306
38	1	0	0.984948	1.865896	-1.650826
39	6	0	1.736379	-0.889708	0.295709
40	1	0	1.925415	-0.335674	1.218906
41	1	0	1.080280	-1.719629	0.562277
42	6	0	3.032270	-1.396736	-0.287056
43	6	0	4.233196	-0.693120	-0.091987
44	6	0	3.074541	-2.620319	-0.979016

45	6	0	5.436246	-1.180629	-0.602315
46	1	0	4.241569	0.218862	0.500451
47	6	0	4.276468	-3.108366	-1.491429
48	1	0	2.173090	-3.219122	-1.089919
49	6	0	5.457902	-2.385291	-1.309646
50	1	0	6.359173	-0.636005	-0.430808
51	1	0	4.295575	-4.059111	-2.014179
52	1	0	6.395277	-2.770260	-1.697963
53	6	0	2.296118	2.194662	-0.026737
54	6	0	3.332426	3.032960	-0.433570
55	6	0	3.870293	3.974083	0.447475
56	1	0	3.717113	2.947508	-1.444443
57	6	0	2.360512	3.226185	2.142554
58	6	0	3.379319	4.072779	1.756244
59	1	0	4.675306	4.624035	0.116862
60	1	0	1.928210	3.218787	3.136495
61	1	0	3.784381	4.787083	2.464693
62	7	0	1.851641	2.333249	1.248739
63	1	0	1.121305	1.713153	1.578741

1$_{\text{pt-A}}$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1490.81050971 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.754528	0.039819	0.747178
2	6	0	1.756221	1.552664	0.875760
3	1	0	0.866889	1.878920	1.427736
4	1	0	2.634691	1.840771	1.461664
5	6	0	2.621681	-0.634079	1.796320
6	1	0	3.485301	0.011778	1.983575
7	1	0	2.066240	-0.730342	2.734715
8	6	0	0.350132	-0.534677	0.832029
9	1	0	0.442170	-1.622555	0.825222
10	1	0	-0.021192	-0.229343	1.815554
11	28	0	2.648438	-0.374499	-0.878517
12	6	0	1.839695	2.188110	-0.489263
13	6	0	1.567016	3.526544	-0.744856
14	6	0	2.466195	1.833316	-2.728847
15	6	0	1.773559	4.021606	-2.035603
16	1	0	1.202619	4.168949	0.049973
17	6	0	2.231079	3.165162	-3.041564
18	1	0	2.816684	1.126047	-3.475721

19	1	0	1.580135	5.067223	-2.254770
20	1	0	2.404520	3.519047	-4.051857
21	6	0	3.094442	-1.963299	1.261225
22	6	0	3.499221	-3.039108	2.038596
23	6	0	4.009598	-4.175279	1.399784
24	1	0	3.434376	-2.991033	3.120826
25	6	0	3.647917	-3.106018	-0.717981
26	6	0	4.085123	-4.209465	0.005341
27	1	0	4.344385	-5.024750	1.987312
28	1	0	3.681303	-3.087172	-1.803652
29	1	0	4.476350	-5.074308	-0.519161
30	7	0	2.278164	1.362908	-1.474320
31	7	0	3.171190	-2.005253	-0.095471
32	6	0	-0.627050	-0.074601	-0.262405
33	1	0	-0.553472	1.012018	-0.409035
34	1	0	-0.355739	-0.553906	-1.209561
35	7	0	-2.004588	-0.473187	0.076107
36	6	0	-2.889389	-0.450729	-1.098410
37	1	0	-3.269674	0.547176	-1.354165
38	1	0	-2.321768	-0.795275	-1.972149
39	6	0	-2.585622	0.252180	1.264148
40	1	0	-3.672114	0.142420	1.191726
41	1	0	-2.292589	-0.295350	2.166066
42	6	0	-2.227867	1.718151	1.451789
43	6	0	-2.650503	2.718438	0.560995
44	6	0	-1.500786	2.104158	2.591049
45	6	0	-2.339632	4.059945	0.793634
46	1	0	-3.263031	2.467816	-0.300370
47	6	0	-1.195068	3.448126	2.832167
48	1	0	-1.225650	1.356162	3.332957
49	6	0	-1.609575	4.428763	1.927815
50	1	0	-2.697902	4.821696	0.107934
51	1	0	-0.669401	3.730119	3.739563
52	1	0	-1.401104	5.475793	2.125136
53	6	0	-4.077635	-1.384788	-0.946036
54	6	0	-5.280828	-1.249753	-1.628140
55	6	0	-6.281164	-2.212468	-1.461555
56	1	0	-5.433877	-0.399327	-2.283916
57	6	0	-4.870573	-3.401201	0.065938
58	6	0	-6.075571	-3.301958	-0.605557
59	1	0	-7.222503	-2.110622	-1.993093
60	1	0	-4.628562	-4.201160	0.755868
61	1	0	-6.839112	-4.056766	-0.455634
62	7	0	-3.924416	-2.452385	-0.129138

63	1	0	-3.032086	-2.489823	0.367013

$1_{pt\text{-}B}$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1490.83805576 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.412890	-1.098730	-0.796328
2	6	0	-2.360828	-0.769025	-1.927331
3	1	0	-1.830147	-0.103608	-2.614425
4	1	0	-2.561772	-1.692511	-2.484315
5	6	0	-2.041552	-2.059550	0.165733
6	1	0	-3.056300	-1.709376	0.378950
7	1	0	-2.126835	-3.057020	-0.283321
8	6	0	-0.176800	-1.731663	-1.418816
9	1	0	0.261081	-2.387055	-0.663118
10	1	0	-0.467340	-2.366917	-2.263669
11	28	0	-0.427554	0.365878	0.413815
12	6	0	-3.713216	-0.163797	-1.594550
13	6	0	-4.865837	-0.916265	-1.398383
14	6	0	-5.033881	1.839041	-1.446849
15	6	0	-6.105117	-0.287033	-1.211029
16	1	0	-4.806915	-1.999093	-1.424418
17	6	0	-6.190464	1.107134	-1.229495
18	1	0	-5.011039	2.921488	-1.510200
19	1	0	-6.999624	-0.887208	-1.071071
20	1	0	-7.136417	1.622703	-1.102657
21	6	0	-1.289492	-2.129439	1.480013
22	6	0	-1.380303	-3.232911	2.322751
23	6	0	-0.745383	-3.190700	3.566958
24	1	0	-1.940921	-4.110779	2.017425
25	6	0	0.037092	-0.989736	3.033555
26	6	0	-0.029760	-2.047401	3.930828
27	1	0	-0.806605	-4.040165	4.240366
28	1	0	0.596883	-0.088837	3.261980
29	1	0	0.475609	-1.977683	4.887833
30	7	0	-3.854213	1.193792	-1.614934
31	7	0	-0.583130	-1.028231	1.831600
32	6	0	0.845838	-0.687751	-1.865929
33	1	0	1.703450	-1.183993	-2.332275
34	1	0	0.420777	-0.021646	-2.622557
35	7	0	1.278533	0.134566	-0.696432
36	6	0	1.670709	1.531729	-1.057774

37	1	0	2.724587	1.573225	-1.348507
38	1	0	1.090319	1.842454	-1.934535
39	6	0	2.384739	-0.548309	0.131700
40	1	0	2.520951	0.086402	1.011658
41	1	0	1.965892	-1.497591	0.472673
42	6	0	3.692899	-0.765239	-0.583316
43	6	0	4.713921	0.198363	-0.511630
44	6	0	3.931973	-1.955133	-1.292908
45	6	0	5.929698	-0.006703	-1.164091
46	1	0	4.576961	1.094031	0.090867
47	6	0	5.147576	-2.159606	-1.945857
48	1	0	3.184451	-2.746168	-1.304270
49	6	0	6.143783	-1.181713	-1.888970
50	1	0	6.715705	0.737996	-1.091484
51	1	0	5.325575	-3.086602	-2.481206
52	1	0	7.092918	-1.344967	-2.389139
53	6	0	1.378361	2.482775	0.087484
54	6	0	2.105720	3.649656	0.298350
55	6	0	1.730463	4.510199	1.333393
56	1	0	2.953261	3.883145	-0.337956
57	6	0	-0.044575	2.996909	1.881227
58	6	0	0.636230	4.178702	2.137556
59	1	0	2.288568	5.424001	1.513439
60	1	0	-0.892069	2.692156	2.487513
61	1	0	0.319977	4.819652	2.953190
62	7	0	0.314789	2.164028	0.874623
63	1	0	-3.041851	1.766222	-1.829015

$\mathbf{1}_{\text{pt-B}}$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1490.82557756 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.814253	-1.592008	-0.266621
2	6	0	-1.629976	-1.594921	-1.551840
3	1	0	-1.052302	-1.065298	-2.313647
4	1	0	-1.704572	-2.636972	-1.881455
5	6	0	-1.606653	-2.107815	0.891886
6	1	0	-2.364792	-2.830495	0.573873
7	1	0	-0.923533	-2.652175	1.552038
8	6	0	0.428642	-2.428002	-0.518173
9	1	0	0.820605	-2.719079	0.457359
10	1	0	0.179477	-3.347933	-1.058377

11	28	0	-0.140293	0.221996	0.175873
12	6	0	-3.046879	-1.053471	-1.537138
13	6	0	-4.167292	-1.873446	-1.476542
14	6	0	-4.482960	0.837037	-1.890502
15	6	0	-5.454051	-1.332257	-1.615282
16	1	0	-4.041156	-2.944363	-1.357287
17	6	0	-5.615036	0.039324	-1.822653
18	1	0	-4.512965	1.905680	-2.072506
19	1	0	-6.321233	-1.985642	-1.580885
20	1	0	-6.595290	0.485921	-1.950856
21	6	0	-2.200533	-0.964933	1.674991
22	6	0	-3.184284	-1.184657	2.634835
23	6	0	-3.571415	-0.138801	3.472557
24	1	0	-3.617210	-2.173920	2.747845
25	6	0	-1.984731	1.252230	2.334122
26	6	0	-2.943414	1.098414	3.326644
27	1	0	-4.327440	-0.293294	4.236285
28	1	0	-1.464589	2.192124	2.232768
29	1	0	-3.179102	1.934195	3.976429
30	7	0	-3.258765	0.277522	-1.747186
31	7	0	-1.621948	0.255156	1.492030
32	6	0	1.444304	-1.588427	-1.272740
33	1	0	2.409715	-2.100725	-1.333797
34	1	0	1.121254	-1.386298	-2.297085
35	7	0	1.583810	-0.282091	-0.552875
36	6	0	2.087233	0.806186	-1.434312
37	1	0	3.174530	0.746280	-1.540445
38	1	0	1.655616	0.676783	-2.433513
39	6	0	2.486677	-0.409501	0.714957
40	1	0	2.469295	0.578151	1.179856
41	1	0	1.973731	-1.100693	1.388348
42	6	0	3.899948	-0.860732	0.456774
43	6	0	4.918568	0.085346	0.246349
44	6	0	4.234580	-2.225943	0.486654
45	6	0	6.234678	-0.326848	0.038613
46	1	0	4.693679	1.148937	0.287606
47	6	0	5.550801	-2.637032	0.278203
48	1	0	3.476750	-2.973066	0.714871
49	6	0	6.550008	-1.688013	0.046379
50	1	0	7.016137	0.411513	-0.108738
51	1	0	5.800978	-3.692255	0.315911
52	1	0	7.575782	-2.007689	-0.106202
53	6	0	1.634691	2.121148	-0.867135
54	6	0	2.273017	3.321028	-1.163635

55	6	0	1.737408	4.518802	-0.690871
56	1	0	3.176134	3.313865	-1.765397
57	6	0	-0.018763	3.241597	0.326324
58	6	0	0.558448	4.474273	0.054623
59	1	0	2.223672	5.465081	-0.906863
60	1	0	-0.940481	3.194104	0.886478
61	1	0	0.089920	5.378221	0.428065
62	7	0	0.506772	2.068474	-0.099805
63	1	0	-2.451814	0.890249	-1.832453

$1_{pt\text{-}C}$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1490.83574347 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.082166	1.176239	-1.196490
2	6	0	2.145018	0.720119	-2.166511
3	1	0	1.683924	0.020506	-2.870637
4	1	0	2.525974	1.563841	-2.753341
5	6	0	1.624942	2.429580	-0.538386
6	1	0	2.619290	2.186838	-0.154710
7	1	0	1.764589	3.177586	-1.327540
8	6	0	-0.224698	1.450891	-1.901570
9	1	0	-0.795192	2.144924	-1.283680
10	1	0	-0.045597	1.936171	-2.867789
11	28	0	0.860683	-0.508281	-0.156047
12	6	0	3.241243	0.032698	-1.390448
13	6	0	4.562967	-0.004316	-1.816408
14	6	0	3.743171	-1.259059	0.481383
15	6	0	5.501200	-0.710086	-1.058197
16	1	0	4.854681	0.503169	-2.730516
17	6	0	5.080999	-1.342875	0.111452
18	1	0	3.394501	-1.751156	1.377799
19	1	0	6.538489	-0.760069	-1.374695
20	1	0	5.773707	-1.899366	0.733369
21	6	0	0.817305	3.092013	0.559913
22	6	0	-0.026472	4.176234	0.349145
23	6	0	-0.636142	4.824301	1.434134
24	1	0	-0.184118	4.542272	-0.659990
25	6	0	0.463278	3.309442	2.925452
26	6	0	-0.392153	4.384383	2.737053
27	1	0	-1.282070	5.679818	1.258407
28	1	0	0.730708	2.919466	3.901482

29	1	0	-0.836022	4.874336	3.597105
30	7	0	2.827032	-0.586277	-0.248930
31	7	0	1.027594	2.706915	1.852289
32	6	0	-0.989851	0.147692	-2.067782
33	1	0	-2.013896	0.332825	-2.407253
34	1	0	-0.513402	-0.493461	-2.813609
35	7	0	-0.989820	-0.584436	-0.757235
36	6	0	-1.233161	-2.056033	-0.961146
37	1	0	-2.301579	-2.255694	-1.081443
38	1	0	-0.730893	-2.365241	-1.884008
39	6	0	-1.995887	0.005869	0.252688
40	1	0	-1.829846	-0.543890	1.181541
41	1	0	-1.679487	1.038744	0.419875
42	6	0	-3.445486	-0.055786	-0.155546
43	6	0	-4.248193	-1.135613	0.250704
44	6	0	-4.031284	0.979422	-0.904647
45	6	0	-5.594528	-1.194023	-0.110346
46	1	0	-3.830235	-1.918975	0.879386
47	6	0	-5.376480	0.920029	-1.268207
48	1	0	-3.447370	1.855383	-1.182081
49	6	0	-6.157385	-0.170795	-0.877010
50	1	0	-6.207192	-2.027533	0.217550
51	1	0	-5.819749	1.727582	-1.841818
52	1	0	-7.205811	-0.213916	-1.153791
53	6	0	-0.642718	-2.779065	0.216049
54	6	0	-1.114857	-3.988510	0.712431
55	6	0	-0.501037	-4.548759	1.834534
56	1	0	-1.953802	-4.480278	0.230836
57	6	0	0.972664	-2.657072	1.896862
58	6	0	0.546036	-3.858266	2.448379
59	1	0	-0.848775	-5.495537	2.236089
60	1	0	1.764214	-2.086082	2.365625
61	1	0	1.026193	-4.238966	3.343114
62	7	0	0.415002	-2.136432	0.781580
63	1	0	1.684880	1.952012	2.031673

1$_{\text{pt-C}}$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1490.83088438 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.200252	1.278717	-1.104917
2	6	0	2.193783	0.735224	-2.108447

3	1	0	1.631208	0.221947	-2.893169
4	1	0	2.726282	1.554443	-2.602546
5	6	0	1.778010	2.589283	-0.621590
6	1	0	2.804838	2.379756	-0.304930
7	1	0	1.848260	3.271117	-1.478750
8	6	0	-0.132909	1.466619	-1.783913
9	1	0	-0.734811	2.125513	-1.157236
10	1	0	-0.002002	1.963230	-2.753433
11	28	0	0.867040	-0.458738	0.178506
12	6	0	3.160164	-0.256014	-1.506678
13	6	0	4.450213	-0.436938	-1.992736
14	6	0	3.400271	-2.061903	-0.040098
15	6	0	5.228255	-1.478661	-1.477759
16	1	0	4.838356	0.211633	-2.771729
17	6	0	4.691519	-2.307591	-0.490271
18	1	0	2.941385	-2.677731	0.724732
19	1	0	6.236153	-1.642023	-1.847058
20	1	0	5.261143	-3.131039	-0.073588
21	6	0	1.068506	3.348544	0.485016
22	6	0	0.040180	4.261166	0.277054
23	6	0	-0.466876	5.017723	1.343695
24	1	0	-0.340790	4.417764	-0.726198
25	6	0	1.106811	3.968289	2.808349
26	6	0	0.067582	4.866825	2.625643
27	1	0	-1.259604	5.738529	1.164963
28	1	0	1.606475	3.811496	3.758215
29	1	0	-0.291348	5.451208	3.466099
30	7	0	2.648577	-1.051240	-0.535064
31	7	0	1.560891	3.247785	1.754737
32	6	0	-0.866202	0.132454	-1.977020
33	1	0	-1.853688	0.321113	-2.411069
34	1	0	-0.331279	-0.519220	-2.673222
35	7	0	-0.979895	-0.576365	-0.673123
36	6	0	-1.180876	-2.051832	-0.781823
37	1	0	-2.221539	-2.290941	-1.020528
38	1	0	-0.561100	-2.423921	-1.606104
39	6	0	-2.044506	0.053370	0.246053
40	1	0	-1.969506	-0.475727	1.198680
41	1	0	-1.733161	1.087478	0.420862
42	6	0	-3.458783	0.005986	-0.278279
43	6	0	-4.301763	-1.067187	0.056346
44	6	0	-3.968929	1.046001	-1.073938
45	6	0	-5.612566	-1.113887	-0.418970
46	1	0	-3.946418	-1.853289	0.718737

47	6	0	-5.278847	0.998840	-1.550589
48	1	0	-3.355299	1.916515	-1.299278
49	6	0	-6.099413	-0.085524	-1.229346
50	1	0	-6.258125	-1.942148	-0.145337
51	1	0	-5.664774	1.811006	-2.158148
52	1	0	-7.120766	-0.119477	-1.594470
53	6	0	-0.755422	-2.708138	0.520731
54	6	0	-1.308442	-3.900493	0.977798
55	6	0	-0.849101	-4.449450	2.177517
56	1	0	-2.087235	-4.392330	0.403733
57	6	0	0.654660	-2.595213	2.386528
58	6	0	0.144152	-3.781505	2.897966
59	1	0	-1.267568	-5.379812	2.549051
60	1	0	1.425839	-2.043103	2.915249
61	1	0	0.515869	-4.169042	3.840177
62	7	0	0.222087	-2.070574	1.217362
63	1	0	2.365866	2.647537	1.917744

Ni^{I} HNPy **2$_A$** (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1491.22872786 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.577350	-1.550748	-1.097497
2	6	0	-2.549804	-1.061976	-2.085604
3	1	0	-1.996633	-0.661226	-2.943316
4	1	0	-3.185088	-1.866679	-2.482290
5	6	0	-2.164612	-2.447812	-0.090060
6	1	0	-3.243808	-2.256990	-0.058895
7	1	0	-2.048836	-3.506206	-0.361984
8	6	0	-0.282963	-2.000135	-1.642150
9	1	0	0.168962	-2.672836	-0.909120
10	1	0	-0.400843	-2.583488	-2.567101
11	28	0	-1.027470	0.289327	0.016510
12	6	0	-3.427310	0.049743	-1.520364
13	6	0	-4.727019	0.239849	-1.986834
14	6	0	-3.630795	1.885603	-0.101419
15	6	0	-5.487578	1.298890	-1.492065
16	1	0	-5.137205	-0.436872	-2.729535
17	6	0	-4.928326	2.138863	-0.529319
18	1	0	-3.163048	2.504539	0.656057
19	1	0	-6.500720	1.459702	-1.846523
20	1	0	-5.484717	2.969779	-0.110455

21	6	0	-1.624394	-2.213165	1.313706
22	6	0	-1.694249	-3.224412	2.273407
23	6	0	-1.297546	-2.959438	3.582306
24	1	0	-2.064348	-4.206030	1.994741
25	6	0	-0.773301	-0.731212	2.886341
26	6	0	-0.833243	-1.681963	3.897510
27	1	0	-1.350237	-3.733715	4.340946
28	1	0	-0.410000	0.270554	3.090269
29	1	0	-0.518699	-1.425731	4.902969
30	7	0	-2.885471	0.867503	-0.581264
31	7	0	-1.153388	-0.979548	1.615538
32	6	0	0.658341	-0.825616	-1.938239
33	1	0	1.592704	-1.203786	-2.368688
34	1	0	0.198690	-0.178183	-2.691835
35	7	0	0.951414	0.039886	-0.736750
36	6	0	1.578242	1.294017	-1.236427
37	1	0	2.557706	1.087304	-1.683070
38	1	0	0.938529	1.693717	-2.032903
39	6	0	1.871590	-0.666815	0.255198
40	1	0	1.971552	0.008563	1.109408
41	1	0	1.318803	-1.535774	0.612163
42	6	0	3.238738	-1.075464	-0.249815
43	6	0	4.346053	-0.227948	-0.084716
44	6	0	3.441063	-2.329941	-0.848038
45	6	0	5.612001	-0.607230	-0.532834
46	1	0	4.226379	0.722088	0.431384
47	6	0	4.704929	-2.711564	-1.298891
48	1	0	2.613896	-3.029835	-0.939225
49	6	0	5.791350	-1.847390	-1.148595
50	1	0	6.459903	0.054732	-0.387094
51	1	0	4.844678	-3.687458	-1.752890
52	1	0	6.776243	-2.146971	-1.492122
53	6	0	1.762016	2.396420	-0.212252
54	6	0	2.843519	3.273614	-0.240277
55	6	0	2.906685	4.329623	0.671578
56	1	0	3.627162	3.127441	-0.975634
57	6	0	0.835556	3.604389	1.621128
58	6	0	1.890990	4.499204	1.619292
59	1	0	3.747226	5.016149	0.646206
60	1	0	0.005544	3.655308	2.316994
61	1	0	1.917523	5.306778	2.341755
62	7	0	0.802969	2.601507	0.717329
63	1	0	-0.018972	1.914969	0.710618

Ni^{I} HNPy **2$_A$** (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1491.18994690 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.470259	-0.958902	-1.137180
2	6	0	-2.168579	-0.261335	-2.252780
3	1	0	-1.453633	0.415836	-2.730689
4	1	0	-2.499325	-0.974573	-3.019122
5	6	0	-2.331338	-2.069360	-0.614744
6	1	0	-3.377515	-1.804279	-0.797273
7	1	0	-2.137798	-2.996627	-1.166043
8	6	0	-0.146957	-1.524609	-1.555348
9	1	0	0.158427	-2.213224	-0.764429
10	1	0	-0.298139	-2.130936	-2.459361
11	28	0	-1.426200	0.473957	0.430168
12	6	0	-3.338847	0.546597	-1.727960
13	6	0	-4.441710	0.871627	-2.513418
14	6	0	-4.210591	1.727518	0.084032
15	6	0	-5.453830	1.660279	-1.963361
16	1	0	-4.508560	0.513115	-3.535567
17	6	0	-5.338043	2.094039	-0.641420
18	1	0	-4.070078	2.040134	1.114153
19	1	0	-6.322151	1.927186	-2.557174
20	1	0	-6.106202	2.702230	-0.177269
21	6	0	-2.155993	-2.273939	0.872864
22	6	0	-2.339421	-3.507170	1.493293
23	6	0	-2.260623	-3.581304	2.885224
24	1	0	-2.547972	-4.391235	0.899577
25	6	0	-1.801059	-1.230497	2.927543
26	6	0	-1.991931	-2.423124	3.616317
27	1	0	-2.404388	-4.530966	3.390663
28	1	0	-1.572772	-0.302853	3.443419
29	1	0	-1.923780	-2.440792	4.698163
30	7	0	-3.232661	0.970043	-0.448701
31	7	0	-1.886287	-1.159521	1.585905
32	6	0	0.974896	-0.524735	-1.846309
33	1	0	1.772975	-1.091631	-2.348916
34	1	0	0.630597	0.216892	-2.573610
35	7	0	1.486688	0.202315	-0.669485
36	6	0	2.282002	1.361356	-1.091993
37	1	0	3.285477	1.089086	-1.449203
38	1	0	1.770780	1.843679	-1.934924

39	6	0	2.228890	-0.661852	0.308118
40	1	0	2.436502	-0.035492	1.181908
41	1	0	1.530239	-1.430011	0.650886
42	6	0	3.514564	-1.299565	-0.181445
43	6	0	4.747937	-0.660347	0.019296
44	6	0	3.505567	-2.543449	-0.831890
45	6	0	5.935434	-1.233421	-0.437961
46	1	0	4.785434	0.279197	0.567050
47	6	0	4.690633	-3.119406	-1.291462
48	1	0	2.570470	-3.085155	-0.956676
49	6	0	5.907521	-2.461908	-1.100509
50	1	0	6.881818	-0.730595	-0.264639
51	1	0	4.666543	-4.085815	-1.785267
52	1	0	6.830449	-2.912479	-1.451244
53	6	0	2.433948	2.412774	-0.014463
54	6	0	3.547241	3.241152	0.103527
55	6	0	3.568856	4.241032	1.077799
56	1	0	4.387563	3.099105	-0.567083
57	6	0	1.392009	3.560223	1.794630
58	6	0	2.477221	4.405655	1.938400
59	1	0	4.435458	4.888377	1.169006
60	1	0	0.500970	3.605291	2.410865
61	1	0	2.469857	5.171305	2.705253
62	7	0	1.404300	2.607984	0.838460
63	1	0	0.563128	1.983622	0.743964

Ni^{I} HNPy **2_B** (doublet)E(B3LYP/ SDD-6-31G(d,p))= -1491.24714738 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.238806	-1.321970	-1.099506
2	6	0	-1.967341	-0.826885	-2.290231
3	1	0	-1.265179	-0.265715	-2.915392
4	1	0	-2.334207	-1.660140	-2.905691
5	6	0	-2.077023	-2.305788	-0.357649
6	1	0	-3.129746	-2.066035	-0.549036
7	1	0	-1.920666	-3.322142	-0.740572
8	6	0	0.073822	-1.909734	-1.528050
9	1	0	0.421341	-2.543664	-0.708152
10	1	0	-0.061936	-2.561139	-2.403489
11	28	0	-0.454585	0.085468	0.411107
12	6	0	-3.136942	0.089029	-1.996850

13	6	0	-4.307290	0.097637	-2.749509
14	6	0	-3.959927	1.914144	-0.700201
15	6	0	-5.304684	1.036783	-2.473348
16	1	0	-4.432598	-0.623992	-3.549462
17	6	0	-5.131216	1.959417	-1.435984
18	1	0	-3.741103	2.580294	0.126085
19	1	0	-6.216279	1.045487	-3.062770
20	1	0	-5.890138	2.695850	-1.198541
21	6	0	-1.869878	-2.269266	1.146207
22	6	0	-2.153336	-3.384812	1.931799
23	6	0	-2.046819	-3.286979	3.319379
24	1	0	-2.455107	-4.316554	1.463738
25	6	0	-1.368999	-1.008507	3.031732
26	6	0	-1.651630	-2.072499	3.880333
27	1	0	-2.264501	-4.143873	3.948687
28	1	0	-1.037183	-0.053657	3.425292
29	1	0	-1.553132	-1.950109	4.953144
30	7	0	-3.013810	0.999052	-1.002874
31	7	0	-1.474823	-1.093210	1.687505
32	6	0	1.121570	-0.831373	-1.835031
33	1	0	2.038802	-1.313307	-2.191760
34	1	0	0.782762	-0.187030	-2.651622
35	7	0	1.370932	0.012463	-0.641765
36	6	0	1.674938	1.429825	-0.940776
37	1	0	2.726226	1.584819	-1.208338
38	1	0	1.077379	1.729517	-1.810077
39	6	0	2.403284	-0.596565	0.292973
40	1	0	2.394447	0.017239	1.197831
41	1	0	2.024473	-1.582505	0.577211
42	6	0	3.810988	-0.714670	-0.248235
43	6	0	4.735311	0.327722	-0.072190
44	6	0	4.231967	-1.880318	-0.908075
45	6	0	6.033161	0.222529	-0.573376
46	1	0	4.449406	1.215187	0.488043
47	6	0	5.529339	-1.987594	-1.410671
48	1	0	3.554027	-2.725939	-1.002536
49	6	0	6.429454	-0.932496	-1.250677
50	1	0	6.738906	1.033303	-0.422027
51	1	0	5.841653	-2.898492	-1.911605
52	1	0	7.441025	-1.017761	-1.634560
53	6	0	1.290270	2.314668	0.232777
54	6	0	1.957482	3.507999	0.503384
55	6	0	1.526310	4.309806	1.560080
56	1	0	2.804889	3.802292	-0.107441

57	6	0	-0.173711	2.683374	2.002398
58	6	0	0.437914	3.889163	2.325137
59	1	0	2.034898	5.241485	1.786298
60	1	0	-1.017056	2.313904	2.577885
61	1	0	0.073453	4.475713	3.161117
62	7	0	0.233751	1.904949	0.978096
63	1	0	-2.139297	0.947204	-0.425523

Ni^{I} HNPy **2$_B$** (quartet)E(B3LYP/ SDD-6-31G(d,p))= -1491.21774673 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.175300	-1.611359	-1.156700
2	6	0	-2.144342	-1.303958	-2.272111
3	1	0	-1.557217	-0.887947	-3.101010
4	1	0	-2.615899	-2.220759	-2.642124
5	6	0	-1.755112	-2.595680	-0.206343
6	1	0	-2.841435	-2.452090	-0.206065
7	1	0	-1.565769	-3.624527	-0.536041
8	6	0	0.169688	-2.031766	-1.661092
9	1	0	0.638288	-2.647111	-0.889459
10	1	0	0.069467	-2.660528	-2.554309
11	28	0	-0.828012	0.156347	-0.053533
12	6	0	-3.161353	-0.325653	-1.787002
13	6	0	-4.495275	-0.567371	-1.591892
14	6	0	-3.460951	1.899387	-0.782426
15	6	0	-5.348260	0.395272	-1.007966
16	1	0	-4.894399	-1.530084	-1.899384
17	6	0	-4.783421	1.631229	-0.599534
18	1	0	-2.997657	2.846049	-0.535478
19	1	0	-6.405528	0.197773	-0.885565
20	1	0	-5.407763	2.395699	-0.148628
21	6	0	-1.259232	-2.382967	1.209746
22	6	0	-1.273437	-3.406247	2.155999
23	6	0	-0.898246	-3.124094	3.469291
24	1	0	-1.581158	-4.406424	1.868454
25	6	0	-0.501054	-0.858835	2.804164
26	6	0	-0.508855	-1.824783	3.801667
27	1	0	-0.907310	-3.906803	4.221195
28	1	0	-0.190438	0.160279	3.008489
29	1	0	-0.210142	-1.564556	4.810829
30	7	0	-2.567747	0.926055	-1.358879

31	7	0	-0.869077	-1.128544	1.534257
32	6	0	1.044889	-0.814307	-1.971959
33	1	0	2.036237	-1.134724	-2.308868
34	1	0	0.604720	-0.233480	-2.788299
35	7	0	1.138785	0.072521	-0.774871
36	6	0	1.426145	1.493262	-1.112538
37	1	0	2.494347	1.654818	-1.288370
38	1	0	0.911472	1.734145	-2.050927
39	6	0	2.124874	-0.446940	0.265948
40	1	0	2.005431	0.200884	1.138091
41	1	0	1.776689	-1.439667	0.556036
42	6	0	3.573899	-0.497501	-0.159183
43	6	0	4.429367	0.588074	0.090314
44	6	0	4.103527	-1.645511	-0.770627
45	6	0	5.770415	0.540859	-0.291787
46	1	0	4.054449	1.463855	0.615822
47	6	0	5.444016	-1.693900	-1.154373
48	1	0	3.476486	-2.521722	-0.921309
49	6	0	6.277219	-0.597657	-0.921728
50	1	0	6.422290	1.383582	-0.084558
51	1	0	5.841270	-2.590393	-1.619579
52	1	0	7.321806	-0.637787	-1.213250
53	6	0	0.911024	2.412343	-0.019244
54	6	0	1.512188	3.633323	0.277754
55	6	0	0.942701	4.452624	1.254166
56	1	0	2.410407	3.937894	-0.249484
57	6	0	-0.754350	2.791682	1.571064
58	6	0	-0.211134	4.025045	1.913223
59	1	0	1.395583	5.408085	1.499323
60	1	0	-1.650699	2.417139	2.056065
61	1	0	-0.681935	4.630560	2.679591
62	7	0	-0.208129	2.001046	0.624482
63	1	0	-2.046572	1.356536	-2.131477

Ni^{I} HNPy **2$_C$** (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1491.25013806 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.239316	1.276037	-1.207833
2	6	0	2.216815	0.712941	-2.183408
3	1	0	1.671085	0.048308	-2.860186
4	1	0	2.662635	1.501757	-2.804732

5	6	0	1.855141	2.461195	-0.566604
6	1	0	2.904951	2.219187	-0.360892
7	1	0	1.858013	3.323909	-1.246664
8	6	0	-0.068364	1.616770	-1.844312
9	1	0	-0.568321	2.340375	-1.194354
10	1	0	0.084308	2.114360	-2.811784
11	28	0	0.873611	-0.578889	-0.080594
12	6	0	3.294436	-0.084168	-1.471937
13	6	0	4.605162	-0.138811	-1.938213
14	6	0	3.783068	-1.560581	0.250217
15	6	0	5.527526	-0.950910	-1.275081
16	1	0	4.897884	0.437226	-2.810265
17	6	0	5.107920	-1.675475	-0.160548
18	1	0	3.417690	-2.111045	1.110100
19	1	0	6.553619	-1.013557	-1.622866
20	1	0	5.789509	-2.318824	0.384599
21	6	0	1.236905	2.894295	0.744722
22	6	0	1.114537	4.226297	1.128697
23	6	0	0.637084	4.542066	2.403588
24	1	0	1.399128	5.009413	0.434382
25	6	0	0.396484	2.208187	2.870011
26	6	0	0.274762	3.521366	3.289411
27	1	0	0.545307	5.581283	2.703781
28	1	0	0.130473	1.353328	3.480947
29	1	0	-0.099287	3.738369	4.283250
30	7	0	2.886711	-0.782285	-0.385663
31	7	0	0.870474	1.941288	1.633472
32	6	0	-0.962884	0.385371	-2.036381
33	1	0	-1.922154	0.705161	-2.461148
34	1	0	-0.510622	-0.294395	-2.764249
35	7	0	-1.134594	-0.362383	-0.766099
36	6	0	-1.490520	-1.789082	-0.977164
37	1	0	-2.560173	-1.922716	-1.170960
38	1	0	-0.957623	-2.143512	-1.866948
39	6	0	-2.097816	0.304498	0.190488
40	1	0	-2.035699	-0.264735	1.122606
41	1	0	-1.699027	1.302204	0.395533
42	6	0	-3.539586	0.411761	-0.258504
43	6	0	-4.467200	-0.586368	0.078847
44	6	0	-3.984728	1.520301	-0.996007
45	6	0	-5.796171	-0.495064	-0.336684
46	1	0	-4.154839	-1.428427	0.692441
47	6	0	-5.312717	1.613580	-1.413899
48	1	0	-3.297904	2.332432	-1.225973

49	6	0	-6.218826	0.601707	-1.090311
50	1	0	-6.503323	-1.271609	-0.062559
51	1	0	-5.642863	2.478971	-1.979889
52	1	0	-7.253260	0.675653	-1.410194
53	6	0	-1.052200	-2.625088	0.211592
54	6	0	-1.756183	-3.754826	0.623391
55	6	0	-1.269816	-4.509899	1.691076
56	1	0	-2.669473	-4.039163	0.110733
57	6	0	0.549239	-2.962092	1.859599
58	6	0	-0.095731	-4.102958	2.325032
59	1	0	-1.800848	-5.395450	2.025265
60	1	0	1.462542	-2.609906	2.328696
61	1	0	0.315001	-4.654708	3.163191
62	7	0	0.092236	-2.235577	0.821072
63	1	0	0.925140	0.945365	1.304433

Ni^{I} HNPy **2$_C$** (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1491.21618689 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.209012	-1.875584	-0.875647
2	6	0	-2.363673	-1.729403	-1.805518
3	1	0	-1.982876	-1.602401	-2.825011
4	1	0	-2.962509	-2.646773	-1.822090
5	6	0	-1.407147	-3.000199	0.111144
6	1	0	-2.470751	-2.988592	0.386604
7	1	0	-1.200547	-3.971026	-0.353328
8	6	0	0.082685	-2.003370	-1.621302
9	1	0	0.790491	-2.517458	-0.968907
10	1	0	-0.043339	-2.627289	-2.514087
11	28	0	-0.976918	-0.089955	0.274450
12	6	0	-3.242802	-0.536761	-1.489681
13	6	0	-4.522956	-0.422935	-2.031705
14	6	0	-3.428593	1.564153	-0.498976
15	6	0	-5.261742	0.734647	-1.796391
16	1	0	-4.929883	-1.228891	-2.634201
17	6	0	-4.700974	1.751316	-1.019152
18	1	0	-2.957127	2.319750	0.119034
19	1	0	-6.258693	0.842603	-2.211751
20	1	0	-5.240843	2.668806	-0.813830
21	6	0	-0.542563	-2.785108	1.309864
22	6	0	0.508657	-3.571122	1.702408

23	6	0	1.322020	-3.232263	2.806305
24	1	0	0.709881	-4.478487	1.139526
25	6	0	0.001680	-1.227747	3.136905
26	6	0	1.039866	-2.028684	3.502694
27	1	0	2.130946	-3.880475	3.118495
28	1	0	-0.276421	-0.326224	3.667575
29	1	0	1.643250	-1.734491	4.355293
30	7	0	-2.707481	0.442262	-0.726193
31	7	0	-0.837079	-1.544696	2.006401
32	6	0	0.619894	-0.623815	-2.010188
33	1	0	1.568919	-0.720533	-2.547589
34	1	0	-0.083199	-0.117077	-2.678406
35	7	0	0.772705	0.216052	-0.788818
36	6	0	0.742236	1.677730	-1.057342
37	1	0	1.701629	2.035295	-1.444444
38	1	0	-0.013385	1.865738	-1.828793
39	6	0	1.997947	-0.163417	0.039257
40	1	0	1.936994	0.428477	0.955395
41	1	0	1.871866	-1.208375	0.328511
42	6	0	3.336432	0.041970	-0.632619
43	6	0	4.035216	1.249647	-0.474919
44	6	0	3.925663	-0.983047	-1.390236
45	6	0	5.275775	1.439679	-1.084604
46	1	0	3.623622	2.035541	0.154536
47	6	0	5.165685	-0.794419	-2.001342
48	1	0	3.430429	-1.947379	-1.481371
49	6	0	5.838993	0.420111	-1.854682
50	1	0	5.809094	2.374900	-0.946607
51	1	0	5.612247	-1.598210	-2.577941
52	1	0	6.806928	0.564776	-2.323682
53	6	0	0.356224	2.423186	0.207065
54	6	0	0.810949	3.709896	0.487820
55	6	0	0.379515	4.345976	1.652756
56	1	0	1.492702	4.204088	-0.196683
57	6	0	-0.899759	2.388996	2.170820
58	6	0	-0.490501	3.673013	2.512396
59	1	0	0.722252	5.348406	1.888881
60	1	0	-1.578031	1.830752	2.809493
61	1	0	-0.844133	4.128762	3.430454
62	7	0	-0.491516	1.775231	1.042119
63	1	0	-1.821492	-1.536509	2.300624

Ni^{III}-H **2_D** (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1491.22976025 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.838886	-0.660225	1.501206
2	6	0	1.961062	0.106103	2.107537
3	1	0	1.633433	1.143412	2.236363
4	1	0	2.220073	-0.281560	3.101165
5	6	0	1.173942	-2.119215	1.451922
6	1	0	2.261805	-2.229054	1.485039
7	1	0	0.781188	-2.634540	2.335282
8	6	0	-0.490638	-0.439916	2.157875
9	1	0	-1.048410	-1.375759	2.084176
10	1	0	-0.363156	-0.228349	3.226138
11	28	0	0.746229	0.001253	-0.463075
12	6	0	3.156877	0.039864	1.173008
13	6	0	4.473605	0.102945	1.622784
14	6	0	3.859669	-0.182857	-1.036842
15	6	0	5.510282	0.028378	0.689156
16	1	0	4.685458	0.201492	2.682677
17	6	0	5.199773	-0.123377	-0.662685
18	1	0	3.567900	-0.298467	-2.075837
19	1	0	6.544280	0.075972	1.015777
20	1	0	5.976318	-0.197771	-1.415829
21	6	0	0.679803	-2.759334	0.178158
22	6	0	0.465567	-4.132164	0.071622
23	6	0	0.109773	-4.672480	-1.163732
24	1	0	0.583244	-4.767162	0.943767
25	6	0	0.182646	-2.459295	-2.082398
26	6	0	-0.027692	-3.820858	-2.260589
27	1	0	-0.057502	-5.739777	-1.267551
28	1	0	0.074833	-1.762132	-2.904215
29	1	0	-0.298793	-4.198527	-3.240076
30	7	0	2.859936	-0.094370	-0.141124
31	7	0	0.528732	-1.935272	-0.886087
32	6	0	-1.267609	0.681742	1.481986
33	1	0	-2.273192	0.751931	1.912797
34	1	0	-0.773893	1.639250	1.663524
35	7	0	-1.340145	0.470424	0.002770
36	6	0	-1.608550	1.757477	-0.675661
37	1	0	-1.825602	1.543841	-1.728653
38	1	0	-2.493418	2.256056	-0.263617
39	6	0	-2.365528	-0.571758	-0.392680
40	1	0	-2.252280	-0.702202	-1.472395

41	1	0	-2.059955	-1.509063	0.077060
42	6	0	-3.804957	-0.258849	-0.045743
43	6	0	-4.623121	0.440416	-0.946742
44	6	0	-4.358648	-0.692886	1.169215
45	6	0	-5.952142	0.722047	-0.629686
46	1	0	-4.231046	0.744713	-1.914463
47	6	0	-5.687258	-0.410833	1.489265
48	1	0	-3.758825	-1.280957	1.861045
49	6	0	-6.484064	0.302405	0.591633
50	1	0	-6.575776	1.254812	-1.340559
51	1	0	-6.103352	-0.759227	2.429248
52	1	0	-7.520006	0.515376	0.835190
53	6	0	-0.407530	2.666938	-0.602767
54	6	0	-0.533501	4.051956	-0.699141
55	6	0	0.611773	4.844990	-0.701110
56	1	0	-1.520610	4.495627	-0.778355
57	6	0	1.909578	2.841071	-0.491264
58	6	0	1.857471	4.224923	-0.597133
59	1	0	0.534137	5.924389	-0.783118
60	1	0	2.857385	2.325916	-0.416321
61	1	0	2.777652	4.798304	-0.597833
62	7	0	0.800020	2.072157	-0.481702
63	1	0	0.708205	0.284778	-1.865696

Ni^{III}-H **2_D** (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1491.18472695 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.819538	-0.812964	1.537700
2	6	0	1.945937	-0.123900	2.221538
3	1	0	1.622696	0.895524	2.461756
4	1	0	2.199766	-0.615023	3.169637
5	6	0	1.113029	-2.265288	1.347889
6	1	0	2.195935	-2.409104	1.418465
7	1	0	0.668135	-2.858884	2.154094
8	6	0	-0.512072	-0.580097	2.180203
9	1	0	-1.103566	-1.488570	2.052403
10	1	0	-0.399513	-0.424914	3.259644
11	28	0	0.777248	0.073616	-0.351699
12	6	0	3.152033	-0.085952	1.298241
13	6	0	4.461393	-0.115754	1.773420
14	6	0	3.894644	-0.020688	-0.906799

15	6	0	5.514905	-0.084735	0.857560
16	1	0	4.653281	-0.168627	2.840320
17	6	0	5.227598	-0.043899	-0.507441
18	1	0	3.624522	0.007519	-1.958335
19	1	0	6.542946	-0.105854	1.205019
20	1	0	6.016522	-0.034963	-1.251229
21	6	0	0.666274	-2.773766	-0.008398
22	6	0	0.437921	-4.128847	-0.243826
23	6	0	0.132515	-4.551918	-1.537387
24	1	0	0.505748	-4.841532	0.571926
25	6	0	0.277930	-2.270340	-2.248653
26	6	0	0.057262	-3.606142	-2.561511
27	1	0	-0.044790	-5.602892	-1.742305
28	1	0	0.216306	-1.497991	-3.010238
29	1	0	-0.174443	-3.892834	-3.581102
30	7	0	2.876823	-0.030026	-0.025286
31	7	0	0.576114	-1.860114	-0.999274
32	6	0	-1.239248	0.609677	1.554355
33	1	0	-2.240706	0.698882	1.991616
34	1	0	-0.704980	1.537415	1.779592
35	7	0	-1.321915	0.480261	0.067053
36	6	0	-1.646091	1.793066	-0.541283
37	1	0	-1.950846	1.612738	-1.578591
38	1	0	-2.501372	2.266964	-0.046112
39	6	0	-2.330032	-0.564703	-0.372596
40	1	0	-2.223343	-0.639378	-1.458388
41	1	0	-2.000252	-1.518215	0.043901
42	6	0	-3.774027	-0.301544	-0.002746
43	6	0	-4.620306	0.397278	-0.877664
44	6	0	-4.305092	-0.782914	1.204649
45	6	0	-5.953709	0.633408	-0.542500
46	1	0	-4.246432	0.737355	-1.840676
47	6	0	-5.637997	-0.546523	1.543111
48	1	0	-3.684643	-1.372755	1.876311
49	6	0	-6.462641	0.167615	0.671698
50	1	0	-6.598160	1.166808	-1.234067
51	1	0	-6.035598	-0.931245	2.476920
52	1	0	-7.501793	0.345036	0.929627
53	6	0	-0.457758	2.725815	-0.553502
54	6	0	-0.624116	4.107215	-0.641092
55	6	0	0.500032	4.925128	-0.736825
56	1	0	-1.623006	4.531123	-0.638951
57	6	0	1.856903	2.955714	-0.624304
58	6	0	1.766222	4.336334	-0.731698

59	1	0	0.390839	6.002522	-0.810350
60	1	0	2.819464	2.459897	-0.605526
61	1	0	2.668092	4.933685	-0.803727
62	7	0	0.769544	2.156666	-0.537327
63	1	0	0.456456	0.783860	-4.210748

Ni^{III}-H **2_E** (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1491.23380263 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.321913	1.600460	-1.320840
2	6	0	2.610651	1.229666	-1.955114
3	1	0	2.584299	1.400440	-3.038114
4	1	0	3.391442	1.884317	-1.553532
5	6	0	1.291943	3.003129	-0.835132
6	1	0	2.308460	3.285896	-0.542511
7	1	0	0.981309	3.698655	-1.624225
8	6	0	0.138786	1.292836	-2.194334
9	1	0	-0.660425	1.983714	-1.917495
10	1	0	0.381029	1.491194	-3.245451
11	28	0	1.062872	0.364519	0.391081
12	6	0	3.026363	-0.196597	-1.655543
13	6	0	3.985383	-0.845942	-2.432977
14	6	0	2.951015	-1.985445	-0.170472
15	6	0	4.438615	-2.104984	-2.044386
16	1	0	4.378399	-0.361957	-3.321489
17	6	0	3.917533	-2.681575	-0.884335
18	1	0	2.519202	-2.394116	0.735032
19	1	0	5.189782	-2.623657	-2.631405
20	1	0	4.250215	-3.652987	-0.536200
21	6	0	0.402861	3.152188	0.384931
22	6	0	-0.153418	4.380376	0.739222
23	6	0	-0.866616	4.487010	1.932859
24	1	0	-0.017721	5.241612	0.092812
25	6	0	-0.449845	2.159062	2.313298
26	6	0	-1.012855	3.356108	2.737887
27	1	0	-1.299446	5.436908	2.229860
28	1	0	-0.548651	1.250937	2.896894
29	1	0	-1.556414	3.394806	3.675190
30	7	0	2.501050	-0.773326	-0.555338
31	7	0	0.236835	2.057489	1.158700
32	6	0	-0.338087	-0.149780	-2.027360

33	1	0	-1.226555	-0.324211	-2.643422
34	1	0	0.431150	-0.848609	-2.363233
35	7	0	-0.615084	-0.418213	-0.587243
36	6	0	-0.574966	-1.864386	-0.235655
37	1	0	-1.509938	-2.366762	-0.501168
38	1	0	0.222080	-2.334948	-0.820296
39	6	0	-1.935513	0.194091	-0.129502
40	1	0	-1.973770	0.044238	0.951727
41	1	0	-1.862222	1.268513	-0.299082
42	6	0	-3.186955	-0.353169	-0.778523
43	6	0	-3.895289	-1.410545	-0.185235
44	6	0	-3.694392	0.217727	-1.957145
45	6	0	-5.059470	-1.907459	-0.772157
46	1	0	-3.552994	-1.828825	0.758855
47	6	0	-4.857510	-0.278522	-2.546531
48	1	0	-3.198523	1.076375	-2.404680
49	6	0	-5.537419	-1.347088	-1.958459
50	1	0	-5.600999	-2.719465	-0.297333
51	1	0	-5.240881	0.177670	-3.453686
52	1	0	-6.446207	-1.728619	-2.412672
53	6	0	-0.265141	-2.026434	1.238718
54	6	0	-0.728707	-3.101453	1.994392
55	6	0	-0.338607	-3.213438	3.330233
56	1	0	-1.382912	-3.839592	1.541875
57	6	0	0.924847	-1.194173	3.066180
58	6	0	0.504011	-2.244229	3.876201
59	1	0	-0.689278	-4.043670	3.935129
60	1	0	1.583861	-0.419204	3.444347
61	1	0	0.831404	-2.295706	4.908596
62	7	0	0.548475	-1.084190	1.776473
63	1	0	2.218241	0.863129	1.076776

Ni^{III}-H **2_E** (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1491.18882130 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.251124	-1.585357	-1.198761
2	6	0	-2.251605	-1.171942	-2.218587
3	1	0	-1.713751	-0.817804	-3.104545
4	1	0	-2.852945	-2.026570	-2.549545
5	6	0	-1.744880	-2.711784	-0.365653
6	1	0	-2.823107	-2.569980	-0.223886
7	1	0	-1.614431	-3.674308	-0.876500

8	6	0	0.089129	-1.856859	-1.806262
9	1	0	0.639168	-2.504431	-1.119552
10	1	0	-0.013311	-2.404352	-2.751261
11	28	0	-0.896143	0.012575	0.152594
12	6	0	-3.140338	-0.044390	-1.732879
13	6	0	-4.401141	0.179647	-2.281822
14	6	0	-3.323893	1.861310	-0.408489
15	6	0	-5.131120	1.295991	-1.873205
16	1	0	-4.801952	-0.505528	-3.021944
17	6	0	-4.579887	2.157044	-0.922516
18	1	0	-2.858165	2.494747	0.338547
19	1	0	-6.114428	1.489824	-2.289901
20	1	0	-5.113092	3.036750	-0.580148
21	6	0	-1.084009	-2.735440	0.999665
22	6	0	-0.972910	-3.910591	1.740267
23	6	0	-0.435408	-3.855034	3.026415
24	1	0	-1.307249	-4.852716	1.317934
25	6	0	-0.141272	-1.496946	2.732885
26	6	0	-0.015068	-2.624660	3.534510
27	1	0	-0.343698	-4.758469	3.620914
28	1	0	0.184449	-0.521471	3.078555
29	1	0	0.408400	-2.538605	4.528860
30	7	0	-2.613178	0.782603	-0.800790
31	7	0	-0.664683	-1.546103	1.491155
32	6	0	0.851283	-0.546613	-2.029317
33	1	0	1.826119	-0.746740	-2.485671
34	1	0	0.300895	0.097293	-2.722069
35	7	0	0.995629	0.182717	-0.737708
36	6	0	1.122554	1.657049	-0.892640
37	1	0	2.136096	1.947164	-1.187212
38	1	0	0.446926	1.974120	-1.695855
39	6	0	2.123931	-0.376696	0.118566
40	1	0	2.051096	0.133685	1.081936
41	1	0	1.888695	-1.427611	0.296320
42	6	0	3.519034	-0.237630	-0.447275
43	6	0	4.302777	0.888629	-0.148770
44	6	0	4.073379	-1.249603	-1.247667
45	6	0	5.592309	1.017086	-0.665618
46	1	0	3.915556	1.656487	0.517404
47	6	0	5.362454	-1.122552	-1.766326
48	1	0	3.509811	-2.159261	-1.444008
49	6	0	6.120580	0.015005	-1.482113
50	1	0	6.189697	1.889291	-0.419557
51	1	0	5.779807	-1.916167	-2.377851

52	1	0	7.125928	0.111287	-1.879342
53	6	0	0.714921	2.349137	0.395985
54	6	0	1.281998	3.550646	0.815685
55	6	0	0.823888	4.145272	1.992520
56	1	0	2.069577	4.011709	0.228619
57	6	0	-0.701716	2.316396	2.247861
58	6	0	-0.184323	3.516224	2.724541
59	1	0	1.252398	5.081540	2.335876
60	1	0	-1.487205	1.790228	2.783601
61	1	0	-0.562593	3.941466	3.647455
62	7	0	-0.267216	1.745286	1.106668
63	1	0	-3.646674	0.310128	3.417672

Ni^{III}-H **2_F** (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1491.23142826 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.056375	-1.991441	0.182578
2	6	0	1.932243	-2.015917	1.391797
3	1	0	1.633435	-2.832738	2.058932
4	1	0	2.956063	-2.240692	1.073929
5	6	0	1.765211	-2.545259	-0.999326
6	1	0	2.232937	-3.513337	-0.781721
7	1	0	1.028387	-2.709171	-1.792598
8	6	0	-0.287962	-2.582799	0.443551
9	1	0	-0.699001	-2.916296	-0.511233
10	1	0	-0.209974	-3.466922	1.087198
11	28	0	0.691391	0.021882	-0.342591
12	6	0	1.964122	-0.705270	2.145859
13	6	0	2.532685	-0.624266	3.418026
14	6	0	1.592114	1.589475	2.116040
15	6	0	2.632974	0.617093	4.041337
16	1	0	2.897671	-1.522400	3.906167
17	6	0	2.159913	1.748544	3.372735
18	1	0	1.205894	2.438773	1.564262
19	1	0	3.074522	0.701643	5.029179
20	1	0	2.224375	2.735869	3.816010
21	6	0	2.804966	-1.547586	-1.476528
22	6	0	3.984270	-1.941725	-2.104195
23	6	0	4.881908	-0.967121	-2.541604
24	1	0	4.193774	-2.996739	-2.248762
25	6	0	3.392983	0.697081	-1.674051
26	6	0	4.584299	0.376867	-2.315817

27	1	0	5.802677	-1.253531	-3.039554
28	1	0	3.133053	1.727769	-1.461011
29	1	0	5.260943	1.166088	-2.623737
30	7	0	1.486294	0.386377	1.511724
31	7	0	2.516926	-0.241640	-1.270931
32	6	0	-1.216513	-1.546403	1.089111
33	1	0	-2.199909	-1.989506	1.276036
34	1	0	-0.816648	-1.226338	2.054804
35	7	0	-1.322928	-0.352798	0.207657
36	6	0	-1.692507	0.899706	0.910291
37	1	0	-2.770017	0.955796	1.093697
38	1	0	-1.194044	0.909291	1.884746
39	6	0	-2.259421	-0.595207	-0.979385
40	1	0	-2.152913	0.277266	-1.627523
41	1	0	-1.854279	-1.447658	-1.527674
42	6	0	-3.712059	-0.829217	-0.638818
43	6	0	-4.619221	0.242516	-0.605031
44	6	0	-4.195313	-2.126203	-0.399117
45	6	0	-5.964700	0.029113	-0.304400
46	1	0	-4.278971	1.246588	-0.848630
47	6	0	-5.540192	-2.341823	-0.097649
48	1	0	-3.526870	-2.980692	-0.480392
49	6	0	-6.425099	-1.262942	-0.042344
50	1	0	-6.655896	0.865879	-0.291138
51	1	0	-5.900214	-3.350646	0.077323
52	1	0	-7.473025	-1.430984	0.184437
53	6	0	-1.232828	2.088696	0.084298
54	6	0	-1.929080	3.295447	0.060045
55	6	0	-1.450960	4.344049	-0.727220
56	1	0	-2.837312	3.405462	0.643781
57	6	0	0.347497	2.918408	-1.413342
58	6	0	-0.296352	4.148977	-1.485768
59	1	0	-1.981051	5.290545	-0.761375
60	1	0	1.235024	2.717452	-2.002568
61	1	0	0.096788	4.927706	-2.129657
62	7	0	-0.096424	1.916033	-0.631176
63	1	0	0.216063	-0.302295	-1.640335

Ni^{III}-H **2_F** (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1491.18681144 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	1.049155	-1.857090	0.574887
2	6	0	2.084150	-1.708084	1.637917
3	1	0	1.960887	-2.479431	2.407022
4	1	0	3.065381	-1.877441	1.180699
5	6	0	1.568683	-2.658743	-0.563692
6	1	0	2.029254	-3.597151	-0.230140
7	1	0	0.720529	-2.930108	-1.203404
8	6	0	-0.263767	-2.340056	1.108651
9	1	0	-0.745751	-2.933605	0.329735
10	1	0	-0.115667	-3.007340	1.965276
11	28	0	0.720321	0.090386	-0.226391
12	6	0	2.110533	-0.330147	2.266442
13	6	0	2.685337	-0.111206	3.518167
14	6	0	1.727887	1.948849	1.989682
15	6	0	2.784812	1.192744	4.001231
16	1	0	3.055072	-0.949285	4.100286
17	6	0	2.303922	2.244569	3.218764
18	1	0	1.332667	2.730109	1.349568
19	1	0	3.231408	1.385148	4.971554
20	1	0	2.367801	3.273752	3.553672
21	6	0	2.557538	-1.841707	-1.376037
22	6	0	3.604364	-2.440124	-2.073089
23	6	0	4.461311	-1.642772	-2.832668
24	1	0	3.746485	-3.514701	-2.020220
25	6	0	3.197669	0.263989	-2.126965
26	6	0	4.257655	-0.262995	-2.855309
27	1	0	5.280757	-2.090448	-3.385892
28	1	0	3.022151	1.333459	-2.099691
29	1	0	4.908697	0.396189	-3.418382
30	7	0	1.627989	0.687400	1.522574
31	7	0	2.351429	-0.502166	-1.409992
32	6	0	-1.167221	-1.169375	1.516996
33	1	0	-2.152502	-1.546900	1.811824
34	1	0	-0.743353	-0.648691	2.379386
35	7	0	-1.267540	-0.191068	0.400883
36	6	0	-1.703620	1.159810	0.827478
37	1	0	-2.787371	1.210311	0.974450
38	1	0	-1.233714	1.378523	1.792723
39	6	0	-2.116698	-0.699331	-0.759177
40	1	0	-2.024010	0.046126	-1.553277
41	1	0	-1.641492	-1.613165	-1.127021
42	6	0	-3.575517	-0.954485	-0.453266
43	6	0	-4.531191	0.052048	-0.665245
44	6	0	-4.007955	-2.206704	0.011527

45	6	0	-5.879831	-0.176933	-0.390150
46	1	0	-4.225289	1.010809	-1.077966
47	6	0	-5.355918	-2.437219	0.287644
48	1	0	-3.296380	-3.020688	0.131846
49	6	0	-6.292656	-1.419950	0.093487
50	1	0	-6.608897	0.607279	-0.567798
51	1	0	-5.676666	-3.412813	0.638827
52	1	0	-7.342350	-1.601294	0.300930
53	6	0	-1.253890	2.187414	-0.194881
54	6	0	-1.968888	3.359467	-0.431135
55	6	0	-1.492578	4.272878	-1.372397
56	1	0	-2.888645	3.549134	0.112663
57	6	0	0.341944	2.789919	-1.779399
58	6	0	-0.317762	3.979588	-2.065166
59	1	0	-2.036596	5.190971	-1.570467
60	1	0	1.250079	2.520602	-2.306390
61	1	0	0.079833	4.652198	-2.816808
62	7	0	-0.102555	1.912236	-0.857534
63	1	0	-0.860553	-3.246209	-3.136253

2_{dp} (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1490.95436955 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.258897	-1.558146	-1.131226
2	6	0	-2.221362	-1.158060	-2.175558
3	1	0	-1.658936	-0.672887	-2.980833
4	1	0	-2.726568	-2.026282	-2.623899
5	6	0	-1.820186	-2.591959	-0.238259
6	1	0	-2.890167	-2.378683	-0.127152
7	1	0	-1.738551	-3.599410	-0.672850
8	6	0	0.069554	-1.927154	-1.675770
9	1	0	0.569582	-2.544485	-0.924398
10	1	0	-0.026695	-2.546875	-2.580090
11	28	0	-0.971164	0.185966	0.114868
12	6	0	-3.237042	-0.162005	-1.650617
13	6	0	-4.528990	-0.090844	-2.166379
14	6	0	-3.628199	1.656802	-0.273645
15	6	0	-5.391637	0.908576	-1.714885
16	1	0	-4.850184	-0.806088	-2.917476
17	6	0	-4.925394	1.804478	-0.752761
18	1	0	-3.231882	2.330346	0.479614

19	1	0	-6.401430	0.984565	-2.104761
20	1	0	-5.554178	2.601743	-0.371414
21	6	0	-1.193602	-2.555779	1.142611
22	6	0	-1.040497	-3.711025	1.908629
23	6	0	-0.536491	-3.606415	3.205246
24	1	0	-1.317121	-4.676136	1.495430
25	6	0	-0.364600	-1.242701	2.857279
26	6	0	-0.194620	-2.344735	3.690845
27	1	0	-0.411455	-4.491540	3.820777
28	1	0	-0.101121	-0.243278	3.191849
29	1	0	0.201964	-2.212472	4.691686
30	7	0	-2.788146	0.692453	-0.700671
31	7	0	-0.852795	-1.333856	1.607353
32	6	0	0.931174	-0.693787	-1.988790
33	1	0	1.878946	-1.025448	-2.435269
34	1	0	0.431133	-0.078942	-2.742782
35	7	0	1.133002	0.138368	-0.788353
36	6	0	1.293720	1.576622	-1.051769
37	1	0	2.316046	1.848964	-1.348557
38	1	0	0.633531	1.838138	-1.886951
39	6	0	2.174693	-0.391715	0.144583
40	1	0	2.100961	0.201426	1.060950
41	1	0	1.879675	-1.409671	0.411851
42	6	0	3.604869	-0.383738	-0.361718
43	6	0	4.439162	0.722272	-0.137627
44	6	0	4.132293	-1.486577	-1.050785
45	6	0	5.751194	0.738927	-0.612746
46	1	0	4.065694	1.568116	0.435016
47	6	0	5.443642	-1.473888	-1.528264
48	1	0	3.520995	-2.374578	-1.195189
49	6	0	6.254248	-0.357510	-1.315367
50	1	0	6.383758	1.601334	-0.424492
51	1	0	5.835576	-2.338807	-2.054996
52	1	0	7.276255	-0.348131	-1.681493
53	6	0	0.871726	2.401857	0.152208
54	6	0	1.524351	3.583849	0.499310
55	6	0	1.061113	4.332899	1.581821
56	1	0	2.383388	3.911849	-0.077455
57	6	0	-0.634410	2.671986	1.896084
58	6	0	-0.040327	3.865871	2.296820
59	1	0	1.554419	5.257805	1.863318
60	1	0	-1.490114	2.266518	2.428628
61	1	0	-0.433228	4.407604	3.150282
62	7	0	-0.200875	1.951289	0.844522

2_{dp} (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1490.91221472 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.209009	-1.669643	-1.015491
2	6	0	-2.237062	-1.405252	-2.051416
3	1	0	-1.730306	-0.907454	-2.889763
4	1	0	-2.668960	-2.336239	-2.442741
5	6	0	-1.729163	-2.575248	0.048469
6	1	0	-2.808890	-2.378139	0.114590
7	1	0	-1.608974	-3.630350	-0.228770
8	6	0	0.100830	-2.111300	-1.563718
9	1	0	0.599559	-2.693895	-0.785478
10	1	0	-0.036287	-2.777861	-2.425990
11	28	0	-0.906114	0.201131	-0.055656
12	6	0	-3.310681	-0.496339	-1.501876
13	6	0	-4.623463	-0.535169	-1.954420
14	6	0	-3.782837	1.358649	-0.158056
15	6	0	-5.542452	0.412178	-1.495863
16	1	0	-4.921990	-1.299537	-2.665763
17	6	0	-5.099025	1.382053	-0.578342
18	1	0	-3.408139	2.091404	0.548155
19	1	0	-6.571544	0.396169	-1.836746
20	1	0	-5.772743	2.138164	-0.190638
21	6	0	-1.078609	-2.280183	1.372651
22	6	0	-0.801803	-3.264636	2.318281
23	6	0	-0.302002	-2.901706	3.568202
24	1	0	-0.991656	-4.306321	2.076997
25	6	0	-0.350921	-0.611340	2.840798
26	6	0	-0.079624	-1.537014	3.832552
27	1	0	-0.087362	-3.655219	4.318002
28	1	0	-0.175021	0.448629	2.995425
29	1	0	0.300557	-1.203300	4.791484
30	7	0	-2.881050	0.442399	-0.599663
31	7	0	-0.843153	-0.956807	1.628050
32	6	0	0.974316	-0.915289	-1.965655
33	1	0	1.950692	-1.268080	-2.318538
34	1	0	0.508477	-0.384454	-2.801176
35	7	0	1.108078	0.045356	-0.840488
36	6	0	1.328052	1.450229	-1.284882
37	1	0	2.365904	1.630267	-1.584945

38	1	0	0.699873	1.605286	-2.173680
39	6	0	2.116007	-0.382723	0.195487
40	1	0	2.015299	0.323744	1.022742
41	1	0	1.793113	-1.356438	0.570486
42	6	0	3.558488	-0.448948	-0.261132
43	6	0	4.397241	0.670324	-0.143653
44	6	0	4.096213	-1.636004	-0.781885
45	6	0	5.727179	0.613775	-0.561935
46	1	0	4.011319	1.585258	0.299450
47	6	0	5.425595	-1.695445	-1.202211
48	1	0	3.479642	-2.530459	-0.836631
49	6	0	6.242033	-0.567891	-1.098460
50	1	0	6.363744	1.487291	-0.458420
51	1	0	5.826440	-2.623647	-1.598003
52	1	0	7.277896	-0.614296	-1.419923
53	6	0	0.892878	2.415796	-0.207092
54	6	0	1.537735	3.617460	0.035584
55	6	0	1.020987	4.505243	0.991910
56	1	0	2.433230	3.865921	-0.526012
57	6	0	-0.729361	2.908504	1.408162
58	6	0	-0.138195	4.127540	1.687775
59	1	0	1.508084	5.453120	1.189997
60	1	0	-1.616220	2.579271	1.940727
61	1	0	-0.573767	4.771925	2.443879
62	7	0	-0.241281	2.049265	0.469591

3$_A$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1491.83263048 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.784795	-1.215089	-1.192855
2	6	0	-2.566992	-0.485542	-2.234400
3	1	0	-2.143850	-0.645753	-3.232692
4	1	0	-3.583189	-0.893216	-2.260090
5	6	0	-2.424149	-2.498833	-0.766438
6	1	0	-3.509279	-2.352801	-0.758771
7	1	0	-2.205817	-3.314859	-1.466294
8	6	0	-0.379243	-1.498353	-1.647239
9	1	0	0.035580	-2.235033	-0.957579
10	1	0	-0.434977	-1.982532	-2.631524
11	28	0	-1.850385	-0.105300	0.476887
12	6	0	-2.663384	0.989791	-1.916052

13	6	0	-3.095278	1.920653	-2.858501
14	6	0	-2.577572	2.632340	-0.262781
15	6	0	-3.274417	3.247739	-2.472987
16	1	0	-3.302218	1.603255	-3.875515
17	6	0	-3.018190	3.606410	-1.148280
18	1	0	-2.382270	2.856655	0.777625
19	1	0	-3.617924	3.986051	-3.190406
20	1	0	-3.164350	4.622840	-0.800529
21	6	0	-1.974719	-2.833192	0.637634
22	6	0	-1.934036	-4.129564	1.138989
23	6	0	-1.597201	-4.328112	2.479059
24	1	0	-2.172263	-4.968390	0.493328
25	6	0	-1.355239	-1.952620	2.708128
26	6	0	-1.306796	-3.220721	3.275386
27	1	0	-1.565961	-5.330656	2.893334
28	1	0	-1.149667	-1.062048	3.287371
29	1	0	-1.049745	-3.330826	4.322804
30	7	0	-2.388308	1.345926	-0.635478
31	7	0	-1.676718	-1.756818	1.412622
32	6	0	0.556986	-0.292421	-1.755854
33	1	0	1.388816	-0.589636	-2.410987
34	1	0	0.042680	0.527350	-2.266908
35	7	0	1.049886	0.213346	-0.459150
36	6	0	1.620222	1.555554	-0.598892
37	1	0	2.632986	1.561951	-1.026711
38	1	0	0.987839	2.136293	-1.282604
39	6	0	2.003594	-0.722722	0.231022
40	1	0	2.214940	-0.285043	1.212432
41	1	0	1.458349	-1.648991	0.428339
42	6	0	3.307384	-1.021430	-0.482605
43	6	0	4.453561	-0.252016	-0.228640
44	6	0	3.403508	-2.080321	-1.399053
45	6	0	5.654300	-0.514650	-0.889899
46	1	0	4.418606	0.538445	0.518556
47	6	0	4.601751	-2.345444	-2.063130
48	1	0	2.545305	-2.725082	-1.576045
49	6	0	5.727862	-1.558268	-1.814078
50	1	0	6.534388	0.082870	-0.673426
51	1	0	4.661223	-3.173708	-2.762252
52	1	0	6.662381	-1.768689	-2.324201
53	6	0	1.653139	2.301414	0.718326
54	6	0	2.597821	3.268861	1.050531
55	6	0	2.503971	3.939783	2.271231
56	1	0	3.399843	3.487490	0.354031

57	6	0	0.547041	2.669420	2.800095
58	6	0	1.465473	3.637764	3.161390
59	1	0	3.240797	4.693048	2.532431
60	1	0	-0.289760	2.365752	3.418474
61	1	0	1.373525	4.140812	4.116810
62	7	0	0.668424	2.043783	1.608263
63	1	0	-0.024515	1.319398	1.348984
64	1	0	-1.846483	0.702300	1.707596

3_A (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1491.837405 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.690056	-1.190789	-1.119443
2	6	0	-2.590667	-0.627430	-2.156314
3	1	0	-1.975162	-0.131536	-2.915090
4	1	0	-3.150740	-1.417399	-2.673654
5	6	0	-2.418133	-2.176545	-0.274697
6	1	0	-3.474290	-1.886503	-0.255027
7	1	0	-2.374241	-3.180822	-0.714168
8	6	0	-0.436077	-1.762335	-1.676763
9	1	0	-0.057530	-2.487972	-0.953403
10	1	0	-0.632653	-2.314537	-2.605606
11	28	0	-1.156043	0.442443	0.174030
12	6	0	-3.535084	0.388647	-1.539259
13	6	0	-4.788583	0.670537	-2.076374
14	6	0	-3.826460	1.984727	0.131519
15	6	0	-5.573856	1.655665	-1.474364
16	1	0	-5.143962	0.130561	-2.948128
17	6	0	-5.085960	2.324541	-0.351041
18	1	0	-3.395675	2.470141	1.001075
19	1	0	-6.554303	1.892963	-1.874941
20	1	0	-5.668312	3.092327	0.145780
21	6	0	-1.915433	-2.183637	1.153280
22	6	0	-2.063329	-3.289261	1.988912
23	6	0	-1.681715	-3.181632	3.326481
24	1	0	-2.478790	-4.213764	1.600912
25	6	0	-1.028304	-0.917945	2.893156
26	6	0	-1.160941	-1.972234	3.789841
27	1	0	-1.791816	-4.028208	3.996689
28	1	0	-0.628831	0.044080	3.196275
29	1	0	-0.860453	-1.846254	4.823886
30	7	0	-3.068539	1.036300	-0.449313

31	7	0	-1.392854	-1.022919	1.601557
32	6	0	0.609078	-0.683757	-1.945403
33	1	0	1.492154	-1.142534	-2.406468
34	1	0	0.213261	0.034702	-2.670819
35	7	0	0.988898	0.086724	-0.719455
36	6	0	1.727597	1.291233	-1.200719
37	1	0	2.595607	0.985297	-1.797294
38	1	0	1.055578	1.837514	-1.874254
39	6	0	1.825188	-0.739629	0.241382
40	1	0	2.005404	-0.101876	1.110747
41	1	0	1.180659	-1.550315	0.586215
42	6	0	3.135147	-1.297246	-0.279445
43	6	0	4.341868	-0.614362	-0.062563
44	6	0	3.180186	-2.533089	-0.945888
45	6	0	5.552478	-1.131504	-0.525862
46	1	0	4.342484	0.312192	0.505383
47	6	0	4.387903	-3.051857	-1.413493
48	1	0	2.271222	-3.115153	-1.077975
49	6	0	5.576407	-2.347756	-1.210655
50	1	0	6.477821	-0.595887	-0.337751
51	1	0	4.403527	-4.011174	-1.921023
52	1	0	6.517514	-2.754302	-1.566744
53	6	0	2.229925	2.283301	-0.171129
54	6	0	3.478855	2.890645	-0.289508
55	6	0	3.858646	3.887803	0.612187
56	1	0	4.146541	2.584007	-1.086618
57	6	0	1.760608	3.636806	1.725929
58	6	0	2.990445	4.267757	1.639562
59	1	0	4.829221	4.363918	0.513980
60	1	0	1.020440	3.865129	2.484925
61	1	0	3.258428	5.035514	2.355951
62	7	0	1.420254	2.685512	0.833332
63	1	0	0.446239	2.233796	0.922090
64	1	0	-0.802804	1.715242	1.082819

3_B (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1491.83468660 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.510931	-1.257133	-0.524710
2	6	0	-2.498671	-1.262712	-1.639690
3	1	0	-2.020835	-0.789174	-2.505289

4	1	0	-2.716978	-2.298033	-1.935411
5	6	0	-2.081549	-1.863857	0.706960
6	1	0	-3.087021	-1.455414	0.853569
7	1	0	-2.193939	-2.951459	0.598263
8	6	0	-0.296030	-2.020260	-0.973947
9	1	0	0.164239	-2.452888	-0.083642
10	1	0	-0.588306	-2.860331	-1.617562
11	28	0	-0.590402	0.681225	0.183461
12	6	0	-3.837172	-0.582816	-1.419314
13	6	0	-5.008018	-1.108162	-1.961464
14	6	0	-5.054583	1.287136	-0.608559
15	6	0	-6.211131	-0.408720	-1.830928
16	1	0	-4.977713	-2.055908	-2.487879
17	6	0	-6.238993	0.808380	-1.145728
18	1	0	-4.979913	2.213746	-0.049689
19	1	0	-7.121843	-0.816546	-2.258203
20	1	0	-7.156902	1.371646	-1.024132
21	6	0	-1.265786	-1.543917	1.944939
22	6	0	-1.296298	-2.375964	3.063466
23	6	0	-0.611284	-1.992038	4.216231
24	1	0	-1.853126	-3.307075	3.033501
25	6	0	0.095244	-0.020784	3.055797
26	6	0	0.093857	-0.788216	4.215084
27	1	0	-0.626877	-2.623437	5.098810
28	1	0	0.640325	0.915766	3.000613
29	1	0	0.638867	-0.450531	5.089358
30	7	0	-3.907942	0.596750	-0.762668
31	7	0	-0.568257	-0.388340	1.943015
32	6	0	0.714421	-1.131490	-1.697698
33	1	0	1.537234	-1.746006	-2.080665
34	1	0	0.248205	-0.652764	-2.564841
35	7	0	1.203090	-0.065444	-0.787788
36	6	0	1.703222	1.132231	-1.512572
37	1	0	2.714747	0.979745	-1.903190
38	1	0	1.050440	1.304504	-2.377296
39	6	0	2.244098	-0.569862	0.198242
40	1	0	2.438572	0.262696	0.879187
41	1	0	1.765431	-1.353373	0.788386
42	6	0	3.540054	-1.076999	-0.393820
43	6	0	4.632106	-0.212834	-0.573390
44	6	0	3.691296	-2.429882	-0.738423
45	6	0	5.830607	-0.680311	-1.113743
46	1	0	4.556298	0.826155	-0.260529
47	6	0	4.888529	-2.899607	-1.279571

48	1	0	2.880366	-3.131915	-0.555356
49	6	0	5.957746	-2.023121	-1.474725
50	1	0	6.668601	-0.001836	-1.238845
51	1	0	4.991998	-3.949663	-1.534216
52	1	0	6.891853	-2.388811	-1.888945
53	6	0	1.643789	2.353978	-0.615484
54	6	0	2.528516	3.423209	-0.737253
55	6	0	2.353765	4.541875	0.079207
56	1	0	3.335584	3.381412	-1.461436
57	6	0	0.455128	3.456561	1.057080
58	6	0	1.298373	4.560527	0.992508
59	1	0	3.031032	5.386547	0.002218
60	1	0	-0.390506	3.424372	1.736948
61	1	0	1.127700	5.412603	1.640841
62	7	0	0.629481	2.373859	0.276705
63	1	0	-3.007887	0.996597	-0.296426
64	1	0	-1.973887	1.483180	0.373830

3_B (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1491.81984928 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.372358	-0.982230	-0.883467
2	6	0	-2.311754	-0.498103	-1.943625
3	1	0	-1.786175	0.258370	-2.534902
4	1	0	-2.539490	-1.328662	-2.624435
5	6	0	-2.034919	-2.058495	-0.081839
6	1	0	-3.004874	-1.674961	0.250577
7	1	0	-2.235103	-2.927416	-0.723580
8	6	0	-0.162425	-1.553817	-1.592041
9	1	0	0.304675	-2.256678	-0.901473
10	1	0	-0.473901	-2.122872	-2.477147
11	28	0	-0.526857	0.472681	0.309990
12	6	0	-3.645111	0.092263	-1.526877
13	6	0	-4.793633	-0.102904	-2.289968
14	6	0	-4.860287	1.531523	-0.072089
15	6	0	-5.981064	0.544671	-1.938306
16	1	0	-4.757004	-0.753679	-3.156791
17	6	0	-6.018599	1.375687	-0.814638
18	1	0	-4.797401	2.140179	0.822819
19	1	0	-6.874628	0.395229	-2.536305
20	1	0	-6.926782	1.885532	-0.514890
21	6	0	-1.241197	-2.478886	1.141094

22	6	0	-1.449110	-3.732907	1.719316
23	6	0	-0.772991	-4.045630	2.898411
24	1	0	-2.127192	-4.447396	1.262380
25	6	0	0.254060	-1.884891	2.790615
26	6	0	0.092826	-3.101085	3.450160
27	1	0	-0.917525	-5.010113	3.374623
28	1	0	0.931056	-1.128548	3.178797
29	1	0	0.638757	-3.302630	4.365251
30	7	0	-3.727255	0.904247	-0.449903
31	7	0	-0.397251	-1.573244	1.657779
32	6	0	0.822198	-0.454853	-1.967328
33	1	0	1.701417	-0.882945	-2.460249
34	1	0	0.374875	0.249147	-2.674419
35	7	0	1.192696	0.292670	-0.734581
36	6	0	1.569051	1.713292	-0.997511
37	1	0	2.603586	1.804348	-1.342139
38	1	0	0.920839	2.095950	-1.793868
39	6	0	2.281607	-0.416959	0.068172
40	1	0	2.375233	0.144826	1.000343
41	1	0	1.879616	-1.395620	0.330570
42	6	0	3.626154	-0.551117	-0.608698
43	6	0	4.616320	0.429885	-0.436777
44	6	0	3.929392	-1.681635	-1.384737
45	6	0	5.861821	0.302306	-1.052423
46	1	0	4.424993	1.284835	0.207999
47	6	0	5.173891	-1.810775	-2.002447
48	1	0	3.201929	-2.484684	-1.483047
49	6	0	6.139261	-0.814710	-1.843067
50	1	0	6.619740	1.064826	-0.903028
51	1	0	5.395353	-2.694008	-2.593180
52	1	0	7.110181	-0.917852	-2.316911
53	6	0	1.321332	2.505562	0.261512
54	6	0	2.051096	3.628993	0.634655
55	6	0	1.712024	4.299337	1.811335
56	1	0	2.872210	3.970918	0.013441
57	6	0	-0.033697	2.689142	2.155762
58	6	0	0.656344	3.817389	2.585154
59	1	0	2.267816	5.178407	2.121254
60	1	0	-0.860440	2.276111	2.720092
61	1	0	0.366500	4.303300	3.509959
62	7	0	0.287693	2.046816	1.013638
63	1	0	-2.855427	0.991106	0.147530
64	1	0	-1.781044	0.772399	1.043866

3_C (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1491.83582128 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.324376	1.129202	-1.117285
2	6	0	2.204445	0.419707	-2.091757
3	1	0	1.575510	-0.229886	-2.708744
4	1	0	2.690222	1.127231	-2.777149
5	6	0	2.097295	2.285754	-0.584007
6	1	0	3.040791	1.890163	-0.191178
7	1	0	2.355697	2.970114	-1.403622
8	6	0	0.037230	1.559364	-1.736182
9	1	0	-0.414307	2.297464	-1.068592
10	1	0	0.208748	2.062429	-2.698501
11	28	0	0.818475	-0.609972	0.215732
12	6	0	3.238835	-0.431721	-1.381648
13	6	0	4.536293	-0.585770	-1.862927
14	6	0	3.658042	-1.881865	0.383964
15	6	0	5.412973	-1.435199	-1.184545
16	1	0	4.854799	-0.054754	-2.754114
17	6	0	4.966569	-2.093859	-0.039635
18	1	0	3.272775	-2.367629	1.273384
19	1	0	6.428195	-1.574056	-1.542241
20	1	0	5.616059	-2.757322	0.520237
21	6	0	1.448783	3.113855	0.505451
22	6	0	1.408058	4.504612	0.458351
23	6	0	0.905037	5.223682	1.547626
24	1	0	1.777654	5.022608	-0.419781
25	6	0	0.482893	3.158553	2.674892
26	6	0	0.437010	4.544643	2.674734
27	1	0	0.879743	6.308370	1.513579
28	1	0	0.136182	2.546869	3.500824
29	1	0	0.043367	5.074021	3.534666
30	7	0	2.806668	-1.073071	-0.272426
31	7	0	0.981259	2.495681	1.614314
32	6	0	-0.927174	0.387663	-1.942734
33	1	0	-1.876863	0.769348	-2.334704
34	1	0	-0.533618	-0.292471	-2.702985
35	7	0	-1.127340	-0.394892	-0.692407
36	6	0	-1.541878	-1.796817	-0.981601
37	1	0	-2.610912	-1.862085	-1.208489
38	1	0	-1.005600	-2.129696	-1.878108

39	6	0	-2.082686	0.278202	0.277850
40	1	0	-2.036362	-0.309692	1.197803
41	1	0	-1.649662	1.255632	0.506014
42	6	0	-3.514446	0.432806	-0.183857
43	6	0	-4.470254	-0.549490	0.121060
44	6	0	-3.925524	1.570658	-0.896564
45	6	0	-5.792859	-0.413750	-0.302398
46	1	0	-4.184790	-1.413321	0.717160
47	6	0	-5.247113	1.708110	-1.322529
48	1	0	-3.217162	2.371702	-1.098344
49	6	0	-6.181180	0.711871	-1.031728
50	1	0	-6.522092	-1.177897	-0.052370
51	1	0	-5.550716	2.595903	-1.868317
52	1	0	-7.210796	0.820425	-1.357236
53	6	0	-1.176871	-2.716439	0.165249
54	6	0	-1.941677	-3.831504	0.502067
55	6	0	-1.515194	-4.657068	1.542845
56	1	0	-2.854499	-4.048232	-0.043194
57	6	0	0.359637	-3.197876	1.841824
58	6	0	-0.345213	-4.331945	2.229832
59	1	0	-2.093300	-5.532719	1.820324
60	1	0	1.259411	-2.890513	2.364414
61	1	0	0.012816	-4.937322	3.054907
62	7	0	-0.035835	-2.413965	0.822039
63	1	0	0.974204	1.409920	1.631416
64	1	0	0.887116	0.076853	1.650995

3_C (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1491.81270919 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.223295	1.077647	-1.168827
2	6	0	2.095178	0.361766	-2.198975
3	1	0	1.423158	-0.176576	-2.866229
4	1	0	2.608669	1.121703	-2.798287
5	6	0	2.004343	2.278746	-0.728719
6	1	0	2.999941	1.917846	-0.451671
7	1	0	2.126166	2.961875	-1.577336
8	6	0	-0.060103	1.487058	-1.847628
9	1	0	-0.535743	2.252662	-1.229133
10	1	0	0.151783	1.938720	-2.825156
11	28	0	0.660999	-0.235029	0.240864

12	6	0	3.066506	-0.638329	-1.623738
13	6	0	4.448172	-0.474543	-1.710411
14	6	0	3.286479	-2.691067	-0.613008
15	6	0	5.273403	-1.490037	-1.215551
16	1	0	4.875592	0.410125	-2.172864
17	6	0	4.682659	-2.619929	-0.657992
18	1	0	2.792573	-3.562142	-0.189785
19	1	0	6.353269	-1.399618	-1.275831
20	1	0	5.282912	-3.437379	-0.273354
21	6	0	1.449147	3.079664	0.428939
22	6	0	1.175032	4.441047	0.360279
23	6	0	0.773429	5.129062	1.511284
24	1	0	1.289168	4.963629	-0.583167
25	6	0	0.921144	3.089271	2.753429
26	6	0	0.645758	4.448037	2.724420
27	1	0	0.564996	6.193181	1.459200
28	1	0	0.848127	2.481164	3.647873
29	1	0	0.341672	4.956585	3.631995
30	7	0	2.488429	-1.728050	-1.086062
31	7	0	1.309901	2.460892	1.626625
32	6	0	-0.980623	0.274674	-1.994877
33	1	0	-1.950043	0.577479	-2.402970
34	1	0	-0.558744	-0.456177	-2.687516
35	7	0	-1.122395	-0.374234	-0.663486
36	6	0	-1.348638	-1.846562	-0.709483
37	1	0	-2.386873	-2.098468	-0.946719
38	1	0	-0.709056	-2.259792	-1.496939
39	6	0	-2.174375	0.322821	0.196729
40	1	0	-2.093876	-0.117041	1.192692
41	1	0	-1.861216	1.366934	0.281273
42	6	0	-3.599519	0.242682	-0.302260
43	6	0	-4.437060	-0.809120	0.103056
44	6	0	-4.125910	1.234786	-1.144908
45	6	0	-5.754457	-0.885650	-0.349491
46	1	0	-4.066986	-1.558946	0.798544
47	6	0	-5.442984	1.159523	-1.599388
48	1	0	-3.515319	2.090044	-1.427291
49	6	0	-6.256806	0.094755	-1.207683
50	1	0	-6.392108	-1.700772	-0.022249
51	1	0	-5.837427	1.936930	-2.245987
52	1	0	-7.283245	0.038601	-1.555607
53	6	0	-0.919762	-2.424815	0.620227
54	6	0	-1.431066	-3.606430	1.146798
55	6	0	-0.929399	-4.084150	2.358517

56	1	0	-2.206989	-4.144449	0.612329
57	6	0	0.533126	-2.184485	2.435725
58	6	0	0.067597	-3.360365	3.012728
59	1	0	-1.313544	-5.004979	2.785572
60	1	0	1.312751	-1.592323	2.897405
61	1	0	0.483198	-3.696726	3.955859
62	7	0	0.049928	-1.722661	1.264067
63	1	0	1.483364	1.423019	1.620338
64	1	0	1.854122	-0.009934	1.106508

$3_{dp\text{-}A}$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1491.53246982 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.876363	-0.774450	1.492747
2	6	0	1.984682	0.017700	2.050161
3	1	0	1.638204	1.050693	2.164652
4	1	0	2.292494	-0.333534	3.047428
5	6	0	1.203344	-2.215914	1.465899
6	1	0	2.292508	-2.320730	1.423483
7	1	0	0.879659	-2.720490	2.387057
8	6	0	-0.444216	-0.527093	2.117209
9	1	0	-1.033146	-1.439877	1.994486
10	1	0	-0.350919	-0.360543	3.200693
11	28	0	0.767601	-0.015247	-0.674064
12	6	0	3.174208	-0.005191	1.100596
13	6	0	4.491211	0.069664	1.554583
14	6	0	3.880588	-0.094192	-1.110534
15	6	0	5.528819	0.068030	0.620945
16	1	0	4.698702	0.124257	2.618718
17	6	0	5.220963	-0.018254	-0.736574
18	1	0	3.574874	-0.155342	-2.150769
19	1	0	6.561511	0.125103	0.950818
20	1	0	5.998155	-0.029493	-1.492746
21	6	0	0.632404	-2.910662	0.245792
22	6	0	0.342077	-4.275624	0.238634
23	6	0	-0.078589	-4.868239	-0.951856
24	1	0	0.449920	-4.861554	1.146292
25	6	0	0.094051	-2.720822	-2.000808
26	6	0	-0.197759	-4.079151	-2.096023
27	1	0	-0.308952	-5.928637	-0.984426
28	1	0	0.013942	-2.045687	-2.847539

29	1	0	-0.516399	-4.501530	-3.042656
30	7	0	2.882869	-0.085485	-0.213698
31	7	0	0.494932	-2.149878	-0.853800
32	6	0	-1.191578	0.650427	1.486954
33	1	0	-2.176782	0.746289	1.962919
34	1	0	-0.650679	1.576764	1.692217
35	7	0	-1.310534	0.515336	0.013510
36	6	0	-1.557167	1.823705	-0.624118
37	1	0	-1.715298	1.631753	-1.692242
38	1	0	-2.464155	2.307078	-0.237174
39	6	0	-2.340460	-0.487638	-0.413568
40	1	0	-2.223123	-0.589249	-1.496126
41	1	0	-2.057210	-1.446867	0.025118
42	6	0	-3.783922	-0.171975	-0.067473
43	6	0	-4.593521	0.550580	-0.956736
44	6	0	-4.348976	-0.615837	1.137742
45	6	0	-5.920928	0.842132	-0.640930
46	1	0	-4.188271	0.871721	-1.913166
47	6	0	-5.675801	-0.324884	1.458693
48	1	0	-3.753779	-1.214492	1.823906
49	6	0	-6.463410	0.409656	0.570820
50	1	0	-6.534092	1.396616	-1.344979
51	1	0	-6.096689	-0.680818	2.394278
52	1	0	-7.497599	0.631850	0.815259
53	6	0	-0.378518	2.760843	-0.499503
54	6	0	-0.550695	4.143755	-0.591459
55	6	0	0.568660	4.971409	-0.566096
56	1	0	-1.549465	4.557790	-0.687618
57	6	0	1.912751	3.004409	-0.335156
58	6	0	1.829642	4.388938	-0.437883
59	1	0	0.459478	6.048641	-0.642890
60	1	0	2.874892	2.513749	-0.235413
61	1	0	2.731549	4.990689	-0.413367
62	7	0	0.836751	2.199242	-0.362920
63	1	0	0.668031	0.234794	-2.239175

$3_{dp\text{-}A}$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1491.51565940 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.974732	0.538995	1.045152
2	6	0	-1.805161	-0.483732	1.752143

3	1	0	-1.370861	-1.461755	1.524214
4	1	0	-1.712942	-0.336593	2.837455
5	6	0	-1.625254	1.876330	1.071624
6	1	0	-2.693450	1.739985	0.890951
7	1	0	-1.515235	2.360858	2.052015
8	6	0	0.357007	0.642028	1.723665
9	1	0	0.787961	1.606614	1.443224
10	1	0	0.212112	0.661332	2.814215
11	28	0	-0.585859	0.207980	-1.043002
12	6	0	-3.284677	-0.508742	1.407023
13	6	0	-4.226538	-0.667386	2.429894
14	6	0	-4.942520	-0.459197	-0.189634
15	6	0	-5.579830	-0.738465	2.099091
16	1	0	-3.906666	-0.734200	3.465324
17	6	0	-5.950143	-0.628917	0.760520
18	1	0	-5.189267	-0.361473	-1.244640
19	1	0	-6.328694	-0.866576	2.874605
20	1	0	-6.990402	-0.668400	0.455516
21	6	0	-1.087078	2.754481	-0.027601
22	6	0	-1.079006	4.144936	0.060658
23	6	0	-0.653918	4.895420	-1.033879
24	1	0	-1.407959	4.627108	0.975396
25	6	0	-0.264479	2.837941	-2.203660
26	6	0	-0.243157	4.227321	-2.186808
27	1	0	-0.643688	5.979658	-0.986913
28	1	0	0.045539	2.272529	-3.072177
29	1	0	0.092675	4.767595	-3.064691
30	7	0	-3.638999	-0.408637	0.115735
31	7	0	-0.675062	2.106835	-1.143856
32	6	0	1.341353	-0.465211	1.345887
33	1	0	2.199604	-0.421875	2.032505
34	1	0	0.881657	-1.445872	1.499848
35	7	0	1.746319	-0.344968	-0.058051
36	6	0	1.936831	-1.618711	-0.737797
37	1	0	2.322678	-1.397912	-1.741621
38	1	0	2.682373	-2.270314	-0.254723
39	6	0	2.841897	0.623369	-0.303578
40	1	0	2.909092	0.749107	-1.389532
41	1	0	2.523801	1.589436	0.102496
42	6	0	4.203290	0.260269	0.266084
43	6	0	5.086471	-0.562306	-0.449554
44	6	0	4.605749	0.735992	1.522832
45	6	0	6.325120	-0.917911	0.084678
46	1	0	4.812760	-0.911834	-1.442178

47	6	0	5.844189	0.382094	2.061696
48	1	0	3.954325	1.408797	2.076650
49	6	0	6.704596	-0.450545	1.344879
50	1	0	6.998998	-1.549216	-0.486901
51	1	0	6.140512	0.764822	3.033816
52	1	0	7.670722	-0.722542	1.758838
53	6	0	0.652872	-2.402812	-0.919567
54	6	0	0.693219	-3.797561	-0.987147
55	6	0	-0.466360	-4.513980	-1.267757
56	1	0	1.637905	-4.307157	-0.827716
57	6	0	-1.632234	-2.424686	-1.364330
58	6	0	-1.653283	-3.809962	-1.465108
59	1	0	-0.443487	-5.597362	-1.331207
60	1	0	-2.526892	-1.828709	-1.486701
61	1	0	-2.584337	-4.317362	-1.691614
62	7	0	-0.507830	-1.728972	-1.087754
63	1	0	-0.396394	0.124762	-2.476493

3$_{\mathbf{dp\text{-}B}}$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1491.52817657 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.439134	1.538345	-1.250574
2	6	0	2.737154	1.139443	-1.831003
3	1	0	2.789341	1.372347	-2.904566
4	1	0	3.513008	1.731923	-1.334358
5	6	0	1.431854	2.955946	-0.827906
6	1	0	2.413049	3.168560	-0.390508
7	1	0	1.289239	3.640374	-1.676727
8	6	0	0.280137	1.218333	-2.129744
9	1	0	-0.514109	1.930950	-1.894027
10	1	0	0.542814	1.378878	-3.185390
11	28	0	1.228881	0.419472	0.608825
12	6	0	3.098453	-0.314316	-1.592255
13	6	0	4.046995	-0.954733	-2.393022
14	6	0	2.965748	-2.148532	-0.190518
15	6	0	4.465200	-2.239363	-2.053539
16	1	0	4.456390	-0.446289	-3.260512
17	6	0	3.921152	-2.846839	-0.921189
18	1	0	2.513101	-2.579916	0.697080
19	1	0	5.205421	-2.754380	-2.657680
20	1	0	4.224572	-3.840664	-0.610996

21	6	0	0.402199	3.233325	0.250722
22	6	0	-0.138170	4.508917	0.423931
23	6	0	-0.978854	4.748277	1.509454
24	1	0	0.106767	5.301185	-0.276590
25	6	0	-0.699156	2.453732	2.130717
26	6	0	-1.260181	3.700910	2.386918
27	1	0	-1.405010	5.733873	1.667946
28	1	0	-0.896804	1.605941	2.779990
29	1	0	-1.904913	3.841325	3.247514
30	7	0	2.551546	-0.913499	-0.519973
31	7	0	0.109977	2.218293	1.085906
32	6	0	-0.250774	-0.211324	-1.953637
33	1	0	-1.081057	-0.368415	-2.655149
34	1	0	0.526833	-0.929573	-2.219256
35	7	0	-0.645570	-0.459412	-0.552761
36	6	0	-0.589037	-1.873109	-0.143740
37	1	0	-1.486237	-2.435685	-0.430590
38	1	0	0.255340	-2.339682	-0.660685
39	6	0	-1.960745	0.160836	-0.186782
40	1	0	-2.057568	0.062616	0.898052
41	1	0	-1.885699	1.229446	-0.393169
42	6	0	-3.193431	-0.407482	-0.865075
43	6	0	-3.925569	-1.445753	-0.268975
44	6	0	-3.646695	0.108440	-2.089165
45	6	0	-5.057576	-1.974682	-0.890583
46	1	0	-3.619948	-1.827523	0.702488
47	6	0	-4.777554	-0.418144	-2.714861
48	1	0	-3.126644	0.946531	-2.547347
49	6	0	-5.481923	-1.466001	-2.119373
50	1	0	-5.614272	-2.774264	-0.411054
51	1	0	-5.115305	-0.002493	-3.659442
52	1	0	-6.364958	-1.872854	-2.602365
53	6	0	-0.353390	-1.995681	1.353165
54	6	0	-0.901929	-3.031200	2.110821
55	6	0	-0.589211	-3.120354	3.467880
56	1	0	-1.561457	-3.754388	1.641396
57	6	0	0.771866	-1.166186	3.211671
58	6	0	0.263981	-2.171740	4.030938
59	1	0	-1.006896	-3.917614	4.074997
60	1	0	1.452202	-0.405280	3.582753
61	1	0	0.534253	-2.205974	5.080572
62	7	0	0.467022	-1.078244	1.906538
63	1	0	2.471852	0.971148	1.437466

$3_{dp\text{-}B}$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1491.50072715 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.674420	1.802157	-1.120438
2	6	0	2.916081	1.262016	-1.652871
3	1	0	3.030900	1.485038	-2.725856
4	1	0	3.753717	1.755537	-1.146959
5	6	0	1.749804	2.989867	-0.277782
6	1	0	2.773404	3.067897	0.104726
7	1	0	1.550347	3.919661	-0.833524
8	6	0	0.510552	1.707919	-1.998617
9	1	0	-0.229906	2.439214	-1.662531
10	1	0	0.763675	1.977734	-3.037529
11	28	0	1.344111	0.216088	0.669241
12	6	0	3.122565	-0.242160	-1.456475
13	6	0	3.992007	-0.936276	-2.300804
14	6	0	2.797163	-2.159674	-0.174313
15	6	0	4.270855	-2.278549	-2.056917
16	1	0	4.449430	-0.417296	-3.137497
17	6	0	3.664586	-2.901727	-0.966148
18	1	0	2.296643	-2.590517	0.684833
19	1	0	4.949028	-2.826260	-2.703607
20	1	0	3.854909	-3.942439	-0.728845
21	6	0	0.831091	2.950651	0.941550
22	6	0	0.304526	4.130751	1.468167
23	6	0	-0.440673	4.092626	2.645457
24	1	0	0.488366	5.070943	0.957860
25	6	0	-0.111805	1.721843	2.682036
26	6	0	-0.647987	2.862875	3.268136
27	1	0	-0.850517	5.004985	3.066933
28	1	0	-0.249172	0.739354	3.118550
29	1	0	-1.216774	2.780927	4.187575
30	7	0	2.521315	-0.861574	-0.414888
31	7	0	0.604692	1.758402	1.542803
32	6	0	-0.104551	0.301092	-2.012949
33	1	0	-0.964201	0.287748	-2.695838
34	1	0	0.627974	-0.401912	-2.418147
35	7	0	-0.480036	-0.181519	-0.659547
36	6	0	-0.693585	-1.649944	-0.706184
37	1	0	-1.560504	-1.900953	-1.330718
38	1	0	0.184523	-2.087133	-1.193764

39	6	0	-1.710047	0.515802	-0.134728
40	1	0	-1.840593	0.167416	0.891618
41	1	0	-1.475008	1.579298	-0.077035
42	6	0	-3.002002	0.330733	-0.911545
43	6	0	-3.904771	-0.689124	-0.573880
44	6	0	-3.347752	1.204712	-1.954151
45	6	0	-5.101694	-0.848870	-1.273548
46	1	0	-3.677590	-1.352905	0.256083
47	6	0	-4.542370	1.047360	-2.658115
48	1	0	-2.689017	2.032710	-2.205384
49	6	0	-5.420315	0.015331	-2.322402
50	1	0	-5.790020	-1.640504	-0.992711
51	1	0	-4.792651	1.736717	-3.458878
52	1	0	-6.352850	-0.105376	-2.865027
53	6	0	-0.847233	-2.299800	0.657475
54	6	0	-1.708554	-3.387937	0.836326
55	6	0	-1.761260	-4.011401	2.082843
56	1	0	-2.322879	-3.738543	0.012623
57	6	0	-0.133661	-2.432975	2.846038
58	6	0	-0.957627	-3.525676	3.113645
59	1	0	-2.420030	-4.858890	2.245881
60	1	0	0.514766	-2.023211	3.617713
61	1	0	-0.966461	-3.977935	4.099635
62	7	0	-0.073786	-1.831313	1.649369
63	1	0	2.459097	0.348376	1.588546

3$_{\mathbf{dp\text{-}C}}$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1491.52403113 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.158646	-1.924253	0.296735
2	6	0	1.941718	-1.815559	1.546263
3	1	0	1.607307	-2.563843	2.277857
4	1	0	2.987046	-2.059342	1.326096
5	6	0	1.949859	-2.535692	-0.792784
6	1	0	2.375704	-3.508410	-0.506062
7	1	0	1.270442	-2.689052	-1.637763
8	6	0	-0.175352	-2.534392	0.507996
9	1	0	-0.537943	-2.877923	-0.462841
10	1	0	-0.111702	-3.415055	1.164232
11	28	0	0.677737	0.021571	-0.575506
12	6	0	1.932089	-0.439777	2.189083
13	6	0	2.459566	-0.266782	3.473668

14	6	0	1.535476	1.827411	1.994136
15	6	0	2.526348	1.013435	4.013713
16	1	0	2.816574	-1.126181	4.033355
17	6	0	2.061455	2.088653	3.253788
18	1	0	1.151868	2.628962	1.371121
19	1	0	2.934799	1.171386	5.006996
20	1	0	2.099570	3.105549	3.628622
21	6	0	3.049726	-1.594303	-1.249396
22	6	0	4.248162	-2.073084	-1.779297
23	6	0	5.192166	-1.163981	-2.255436
24	1	0	4.433526	-3.141896	-1.821574
25	6	0	3.703697	0.596021	-1.611593
26	6	0	4.915919	0.199961	-2.170272
27	1	0	6.128084	-1.514681	-2.678789
28	1	0	3.451760	1.648596	-1.516262
29	1	0	5.623002	0.943695	-2.521026
30	7	0	1.463002	0.590533	1.468005
31	7	0	2.785724	-0.274188	-1.165732
32	6	0	-1.167198	-1.524356	1.106732
33	1	0	-2.109344	-2.034329	1.343350
34	1	0	-0.773195	-1.136149	2.050481
35	7	0	-1.370530	-0.382643	0.186515
36	6	0	-1.748196	0.880474	0.848039
37	1	0	-2.811195	0.915940	1.116945
38	1	0	-1.176129	0.956845	1.778110
39	6	0	-2.291472	-0.707120	-0.958840
40	1	0	-2.221943	0.131290	-1.654968
41	1	0	-1.854336	-1.555940	-1.485279
42	6	0	-3.736440	-0.984395	-0.594812
43	6	0	-4.685617	0.049585	-0.580441
44	6	0	-4.169035	-2.286079	-0.296268
45	6	0	-6.017085	-0.201638	-0.246059
46	1	0	-4.384447	1.056209	-0.860765
47	6	0	-5.499088	-2.541955	0.040158
48	1	0	-3.466057	-3.113934	-0.354282
49	6	0	-6.425113	-1.497942	0.073029
50	1	0	-6.737827	0.610715	-0.247608
51	1	0	-5.814679	-3.556893	0.262612
52	1	0	-7.461498	-1.696237	0.328523
53	6	0	-1.398656	2.063388	-0.041064
54	6	0	-2.211775	3.194872	-0.121859
55	6	0	-1.829730	4.252158	-0.947681
56	1	0	-3.132604	3.239946	0.450924
57	6	0	0.103195	2.977832	-1.555126

58	6	0	-0.651340	4.140810	-1.684623
59	1	0	-2.449090	5.140283	-1.025096
60	1	0	1.016825	2.834254	-2.124240
61	1	0	-0.324422	4.929743	-2.352940
62	7	0	-0.248766	1.968473	-0.743489
63	1	0	0.297062	-0.478250	-2.036114

$3_{dp\text{-}C}$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1491.50743211 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.055344	-1.990882	0.358015
2	6	0	1.769836	-1.762266	1.610462
3	1	0	1.382772	-2.408999	2.411729
4	1	0	2.821576	-2.053368	1.487926
5	6	0	1.865533	-2.629905	-0.672467
6	1	0	2.236447	-3.628804	-0.382589
7	1	0	1.230364	-2.770700	-1.555199
8	6	0	-0.263324	-2.607730	0.530533
9	1	0	-0.593605	-2.969747	-0.447063
10	1	0	-0.214055	-3.490839	1.192465
11	28	0	1.173597	0.464228	-0.736017
12	6	0	1.778124	-0.327783	2.126632
13	6	0	2.032802	-0.109202	3.486008
14	6	0	1.723398	1.960142	1.753142
15	6	0	2.144338	1.187437	3.974685
16	1	0	2.144138	-0.961565	4.149197
17	6	0	1.992455	2.250363	3.083930
18	1	0	1.581076	2.757189	1.031327
19	1	0	2.343163	1.365941	5.026798
20	1	0	2.072462	3.281742	3.408797
21	6	0	3.045673	-1.775970	-1.077975
22	6	0	4.271551	-2.355054	-1.414966
23	6	0	5.331469	-1.548814	-1.818471
24	1	0	4.382519	-3.432899	-1.356232
25	6	0	3.896474	0.340761	-1.511410
26	6	0	5.139901	-0.168295	-1.862891
27	1	0	6.287539	-1.986959	-2.086668
28	1	0	3.701029	1.406450	-1.543051
29	1	0	5.932430	0.506870	-2.165294
30	7	0	1.612884	0.703423	1.271064
31	7	0	2.865313	-0.439458	-1.125148

32	6	0	-1.306437	-1.631834	1.085489
33	1	0	-2.223667	-2.192336	1.323290
34	1	0	-0.949414	-1.228271	2.038835
35	7	0	-1.540640	-0.520566	0.169129
36	6	0	-1.765082	0.765817	0.798899
37	1	0	-2.804909	0.925844	1.127971
38	1	0	-1.144947	0.814524	1.700937
39	6	0	-2.444422	-0.817843	-0.964730
40	1	0	-2.340222	0.000388	-1.685092
41	1	0	-2.058095	-1.710868	-1.465661
42	6	0	-3.911079	-1.020195	-0.620769
43	6	0	-4.803376	0.062391	-0.613097
44	6	0	-4.407739	-2.292661	-0.299853
45	6	0	-6.144932	-0.114530	-0.270718
46	1	0	-4.450192	1.048662	-0.905547
47	6	0	-5.748152	-2.474686	0.044033
48	1	0	-3.746438	-3.154986	-0.343929
49	6	0	-6.618985	-1.383847	0.065264
50	1	0	-6.822439	0.734400	-0.278654
51	1	0	-6.114896	-3.468642	0.282745
52	1	0	-7.663359	-1.524587	0.326637
53	6	0	-1.373599	1.926649	-0.096811
54	6	0	-2.204232	3.049080	-0.179762
55	6	0	-1.847284	4.132874	-0.975193
56	1	0	-3.131855	3.055233	0.383045
57	6	0	0.118115	2.913593	-1.580674
58	6	0	-0.657632	4.059302	-1.697249
59	1	0	-2.489198	5.005567	-1.043017
60	1	0	1.035040	2.803547	-2.146496
61	1	0	-0.335453	4.862147	-2.350878
62	7	0	-0.209435	1.867879	-0.785711
63	1	0	0.906866	0.307140	-2.151513

TS_A (triplet)E(B3LYP/ SDD-6-31G(d,p))= -1491.82788406 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.620128	-1.245658	-1.207638
2	6	0	-2.487567	-0.558987	-2.197295
3	1	0	-1.846386	-0.060760	-2.931872
4	1	0	-3.102698	-1.277621	-2.752817
5	6	0	-2.376774	-2.285967	-0.459457

6	1	0	-3.412428	-1.942855	-0.357096
7	1	0	-2.404248	-3.226800	-1.022517
8	6	0	-0.345918	-1.775596	-1.772798
9	1	0	0.023268	-2.539147	-1.083821
10	1	0	-0.518565	-2.267673	-2.738344
11	28	0	-1.052458	0.180423	0.204101
12	6	0	-3.357686	0.481287	-1.514196
13	6	0	-4.570181	0.898305	-2.055529
14	6	0	-3.568309	1.993502	0.249742
15	6	0	-5.289384	1.907775	-1.413202
16	1	0	-4.944482	0.442788	-2.966667
17	6	0	-4.778839	2.466754	-0.240672
18	1	0	-3.137322	2.392879	1.161560
19	1	0	-6.236094	2.248297	-1.820503
20	1	0	-5.307901	3.250632	0.289348
21	6	0	-1.799630	-2.496194	0.923675
22	6	0	-1.950443	-3.692690	1.620483
23	6	0	-1.460842	-3.784762	2.923732
24	1	0	-2.447384	-4.535695	1.151394
25	6	0	-0.699758	-1.521166	2.732082
26	6	0	-0.825921	-2.678433	3.490708
27	1	0	-1.570889	-4.706432	3.486209
28	1	0	-0.205379	-0.640739	3.128967
29	1	0	-0.430577	-2.708295	4.499760
30	7	0	-2.867350	1.020958	-0.370921
31	7	0	-1.177150	-1.429499	1.473911
32	6	0	0.673532	-0.655376	-1.933506
33	1	0	1.613699	-1.062011	-2.319139
34	1	0	0.314575	0.063141	-2.675565
35	7	0	0.916982	0.101325	-0.656134
36	6	0	1.470902	1.441486	-1.068670
37	1	0	2.377566	1.276251	-1.660571
38	1	0	0.728647	1.893156	-1.737995
39	6	0	1.883644	-0.641752	0.265943
40	1	0	2.003268	0.001996	1.140301
41	1	0	1.357979	-1.540988	0.592689
42	6	0	3.231816	-1.020525	-0.307360
43	6	0	4.336006	-0.162108	-0.189411
44	6	0	3.417637	-2.272451	-0.917295
45	6	0	5.582373	-0.531542	-0.696590
46	1	0	4.229255	0.787634	0.326535
47	6	0	4.662152	-2.643145	-1.426909
48	1	0	2.591970	-2.979556	-0.970277
49	6	0	5.745700	-1.768681	-1.323083

50	1	0	6.429279	0.138961	-0.589610
51	1	0	4.790024	-3.616809	-1.889196
52	1	0	6.716819	-2.057745	-1.711956
53	6	0	1.768798	2.434344	0.034169
54	6	0	2.914311	3.232167	-0.032207
55	6	0	3.106801	4.222877	0.932176
56	1	0	3.637632	3.086889	-0.828181
57	6	0	1.047966	3.531511	1.933452
58	6	0	2.155721	4.377072	1.939041
59	1	0	3.985242	4.859352	0.896839
60	1	0	0.284401	3.616938	2.704023
61	1	0	2.264617	5.131209	2.710613
62	7	0	0.849395	2.587623	1.000366
63	1	0	-0.672100	1.538344	1.648483
64	1	0	-1.271859	1.153321	1.945355

TS_B (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1491.83050778 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.449767	-1.237016	-0.640785
2	6	0	-2.416284	-1.113000	-1.777667
3	1	0	-1.911841	-0.550950	-2.571676
4	1	0	-2.618186	-2.112346	-2.184905
5	6	0	-2.057627	-1.972378	0.503178
6	1	0	-3.072261	-1.589747	0.650482
7	1	0	-2.149562	-3.043010	0.277684
8	6	0	-0.228513	-1.965772	-1.134170
9	1	0	0.223997	-2.465849	-0.275437
10	1	0	-0.515906	-2.750064	-1.845367
11	28	0	-0.572839	0.555644	0.234572
12	6	0	-3.754510	-0.452183	-1.497675
13	6	0	-4.907028	-0.913184	-2.135283
14	6	0	-4.963606	1.278863	-0.494571
15	6	0	-6.112122	-0.232132	-1.947826
16	1	0	-4.863535	-1.788431	-2.775260
17	6	0	-6.144839	0.886063	-1.114619
18	1	0	-4.922498	2.130175	0.179229
19	1	0	-7.014251	-0.576938	-2.443050
20	1	0	-7.061839	1.437786	-0.941429
21	6	0	-1.283541	-1.767673	1.790458
22	6	0	-1.350892	-2.685978	2.837349

23	6	0	-0.694989	-2.401441	4.034934
24	1	0	-1.914044	-3.605827	2.717129
25	6	0	0.057788	-0.348029	3.060644
26	6	0	0.018904	-1.207554	4.151644
27	1	0	-0.739659	-3.101332	4.863232
28	1	0	0.608576	0.586253	3.097345
29	1	0	0.541017	-0.947265	5.065439
30	7	0	-3.807238	0.626797	-0.694018
31	7	0	-0.577645	-0.621602	1.904125
32	6	0	0.783894	-1.018178	-1.773435
33	1	0	1.632080	-1.587747	-2.168156
34	1	0	0.333692	-0.493182	-2.621176
35	7	0	1.224166	-0.003776	-0.777949
36	6	0	1.679435	1.267434	-1.402794
37	1	0	2.710832	1.194247	-1.762071
38	1	0	1.050160	1.463353	-2.279413
39	6	0	2.277252	-0.541415	0.182052
40	1	0	2.430316	0.244689	0.926085
41	1	0	1.823859	-1.386941	0.702758
42	6	0	3.597744	-0.947438	-0.431196
43	6	0	4.655726	-0.028759	-0.525467
44	6	0	3.807121	-2.262141	-0.878243
45	6	0	5.878346	-0.404539	-1.082945
46	1	0	4.535275	0.978120	-0.131738
47	6	0	5.028617	-2.639604	-1.436904
48	1	0	3.023730	-3.008071	-0.761722
49	6	0	6.063476	-1.708578	-1.546616
50	1	0	6.689920	0.313829	-1.141377
51	1	0	5.177740	-3.661309	-1.771433
52	1	0	7.016439	-2.003223	-1.974230
53	6	0	1.521120	2.419492	-0.429843
54	6	0	2.340707	3.545097	-0.454038
55	6	0	2.077940	4.594160	0.428421
56	1	0	3.166676	3.600114	-1.155616
57	6	0	0.227556	3.335304	1.281989
58	6	0	1.002382	4.488803	1.312190
59	1	0	2.703977	5.480845	0.425767
60	1	0	-0.625691	3.207370	1.940668
61	1	0	0.764993	5.283258	2.010675
62	7	0	0.484279	2.319728	0.433674
63	1	0	-2.695602	1.035420	0.056132
64	1	0	-2.029819	1.338391	0.630684

TS_C (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1491.82563055 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.790073	-1.245790	1.199161
2	6	0	1.975729	-0.867527	2.031512
3	1	0	1.765302	0.088621	2.526783
4	1	0	2.149139	-1.603218	2.826819
5	6	0	0.946682	-2.684318	0.798501
6	1	0	1.955047	-2.791820	0.389034
7	1	0	0.894719	-3.304900	1.702252
8	6	0	-0.496060	-1.017675	1.924887
9	1	0	-1.233910	-1.698413	1.497185
10	1	0	-0.399336	-1.277939	2.986684
11	28	0	0.953941	0.352024	-0.234862
12	6	0	3.197194	-0.735326	1.143065
13	6	0	4.472123	-1.138521	1.528580
14	6	0	3.967954	-0.104524	-0.961589
15	6	0	5.526195	-1.002073	0.622524
16	1	0	4.635746	-1.560878	2.514618
17	6	0	5.267908	-0.488826	-0.649063
18	1	0	3.718809	0.283625	-1.944453
19	1	0	6.529306	-1.310069	0.899821
20	1	0	6.053693	-0.392465	-1.389859
21	6	0	-0.039581	-3.203996	-0.226077
22	6	0	-0.755795	-4.379107	0.010254
23	6	0	-1.561255	-4.899132	-1.006553
24	1	0	-0.674184	-4.889394	0.964839
25	6	0	-0.896425	-3.045775	-2.368143
26	6	0	-1.630009	-4.223923	-2.222595
27	1	0	-2.119832	-5.816165	-0.848446
28	1	0	-0.928577	-2.483649	-3.298442
29	1	0	-2.235593	-4.594236	-3.042422
30	7	0	2.956161	-0.206497	-0.078759
31	7	0	-0.117392	-2.546191	-1.398200
32	6	0	-0.971761	0.430384	1.793527
33	1	0	-1.958233	0.536576	2.259549
34	1	0	-0.294263	1.106000	2.328561
35	7	0	-1.008851	0.880522	0.365772
36	6	0	-1.172979	2.362203	0.289677
37	1	0	-1.974606	2.596011	-0.414935
38	1	0	-1.513619	2.759565	1.252131
39	6	0	-2.088276	0.180314	-0.454242

40	1	0	-1.913000	0.492068	-1.487539
41	1	0	-1.874780	-0.887354	-0.406159
42	6	0	-3.520349	0.467001	-0.062944
43	6	0	-4.263350	1.430853	-0.763484
44	6	0	-4.151201	-0.244585	0.971196
45	6	0	-5.587878	1.702157	-0.418825
46	1	0	-3.817425	1.952141	-1.608184
47	6	0	-5.474497	0.027023	1.319412
48	1	0	-3.621703	-1.039005	1.492181
49	6	0	-6.192552	1.006363	0.629365
50	1	0	-6.150261	2.444012	-0.976811
51	1	0	-5.949677	-0.534815	2.117327
52	1	0	-7.224377	1.212220	0.895371
53	6	0	0.074584	3.097404	-0.151693
54	6	0	0.092079	4.493771	-0.178289
55	6	0	1.226406	5.154395	-0.638582
56	1	0	-0.778895	5.049646	0.154429
57	6	0	2.245750	3.018813	-0.991013
58	6	0	2.326460	4.400088	-1.057753
59	1	0	1.255239	6.238892	-0.670778
60	1	0	3.080051	2.397005	-1.289905
61	1	0	3.230341	4.872904	-1.424672
62	7	0	1.141448	2.372316	-0.549759
63	1	0	0.533255	-0.814983	-1.708383
64	1	0	0.718624	-0.079953	-1.957902

Co

1'-H_2O (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1542.03365992 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.806867	-0.843152	1.539301
2	6	0	1.897366	-0.094585	2.205289
3	1	0	1.552004	0.930555	2.379037
4	1	0	2.143505	-0.521812	3.186957
5	6	0	1.128382	-2.291239	1.472591
6	1	0	2.216702	-2.400085	1.421473
7	1	0	0.804826	-2.811590	2.382823
8	6	0	-0.527705	-0.605133	2.155905
9	1	0	-1.136532	-1.493590	1.973753

10	1	0	-0.445083	-0.498559	3.245448
11	27	0	0.760983	-0.065702	-0.534720
12	6	0	3.124282	-0.073787	1.314313
13	6	0	4.420378	-0.046882	1.827580
14	6	0	3.931576	-0.077996	-0.864136
15	6	0	5.500417	-0.029137	0.944215
16	1	0	4.579870	-0.047240	2.901091
17	6	0	5.252574	-0.052060	-0.429295
18	1	0	3.691458	-0.094807	-1.922850
19	1	0	6.517764	-0.009854	1.321932
20	1	0	6.062583	-0.054213	-1.150140
21	6	0	0.536632	-2.948343	0.244554
22	6	0	0.223045	-4.307288	0.226156
23	6	0	-0.247076	-4.883150	-0.953354
24	1	0	0.348988	-4.904396	1.123650
25	6	0	-0.085598	-2.728294	-1.980332
26	6	0	-0.404722	-4.076795	-2.081516
27	1	0	-0.493338	-5.939590	-0.988946
28	1	0	-0.226380	-2.062337	-2.825544
29	1	0	-0.776084	-4.478693	-3.017537
30	7	0	2.885540	-0.081456	-0.015726
31	7	0	0.383704	-2.167026	-0.847094
32	6	0	-1.209528	0.626126	1.565854
33	1	0	-2.202638	0.748939	2.013910
34	1	0	-0.634806	1.523732	1.809912
35	7	0	-1.306589	0.542958	0.078932
36	6	0	-1.570903	1.887883	-0.485637
37	1	0	-1.848191	1.756476	-1.538406
38	1	0	-2.426825	2.368243	0.002065
39	6	0	-2.377954	-0.430127	-0.378340
40	1	0	-2.279702	-0.488951	-1.466551
41	1	0	-2.107333	-1.409576	0.018959
42	6	0	-3.805208	-0.092770	-0.001045
43	6	0	-4.614098	0.665781	-0.861184
44	6	0	-4.359564	-0.565463	1.199193
45	6	0	-5.932446	0.967442	-0.518890
46	1	0	-4.222602	1.003024	-1.818190
47	6	0	-5.677072	-0.263131	1.545332
48	1	0	-3.769406	-1.197995	1.858979
49	6	0	-6.463781	0.508928	0.688466
50	1	0	-6.548231	1.547079	-1.199351
51	1	0	-6.092862	-0.641163	2.473979
52	1	0	-7.491353	0.737839	0.952269
53	6	0	-0.354402	2.780282	-0.414256

54	6	0	-0.477646	4.167443	-0.324204
55	6	0	0.671145	4.956238	-0.336004
56	1	0	-1.461904	4.618137	-0.247980
57	6	0	1.956621	2.942095	-0.497569
58	6	0	1.914884	4.329880	-0.427671
59	1	0	0.597560	6.037115	-0.269915
60	1	0	2.904372	2.419513	-0.556955
61	1	0	2.836481	4.901172	-0.438486
62	7	0	0.848655	2.170959	-0.494109
63	8	0	0.887267	0.295114	-2.703862
64	1	0	1.206485	-0.283121	-3.410292
65	1	0	1.031187	1.207300	-2.991969

1'-H_2O (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1542.01484898 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.778712	-0.772140	-1.733638
2	6	0	-1.931109	-0.024198	-2.273836
3	1	0	-1.622478	1.014289	-2.439177
4	1	0	-2.277223	-0.416481	-3.240310
5	6	0	-1.064752	-2.220328	-1.632022
6	1	0	-2.143002	-2.378626	-1.741110
7	1	0	-0.593283	-2.780806	-2.448165
8	6	0	0.551683	-0.487100	-2.328897
9	1	0	1.137392	-1.407855	-2.277269
10	1	0	0.474269	-0.226079	-3.392345
11	27	0	-0.708622	0.064267	0.294496
12	6	0	-3.058268	-0.075043	-1.252199
13	6	0	-4.402806	-0.116161	-1.612615
14	6	0	-3.619230	-0.156444	1.014855
15	6	0	-5.377675	-0.172312	-0.613883
16	1	0	-4.681653	-0.112158	-2.661423
17	6	0	-4.979327	-0.198508	0.722434
18	1	0	-3.247674	-0.160784	2.033277
19	1	0	-6.429928	-0.205897	-0.877819
20	1	0	-5.703700	-0.253465	1.527366
21	6	0	-0.645515	-2.785108	-0.290164
22	6	0	-0.467599	-4.156611	-0.103849
23	6	0	-0.158225	-4.639595	1.165361
24	1	0	-0.575326	-4.833365	-0.945663
25	6	0	-0.203877	-2.379092	1.952559
26	6	0	-0.026607	-3.730676	2.216887

27	1	0	-0.018280	-5.703014	1.330828
28	1	0	-0.089683	-1.635705	2.731759
29	1	0	0.217327	-4.058571	3.221150
30	7	0	-2.680058	-0.089593	0.052829
31	7	0	-0.507869	-1.907078	0.725613
32	6	0	1.281066	0.632908	-1.586253
33	1	0	2.311213	0.711652	-1.950006
34	1	0	0.794173	1.588144	-1.791357
35	7	0	1.280415	0.432995	-0.091678
36	6	0	1.587053	1.732177	0.568724
37	1	0	1.740403	1.532359	1.635055
38	1	0	2.515579	2.167529	0.184381
39	6	0	2.291377	-0.617853	0.341643
40	1	0	2.138988	-0.745282	1.416229
41	1	0	1.994917	-1.550736	-0.139480
42	6	0	3.744887	-0.315525	0.048761
43	6	0	4.538779	0.362618	0.987050
44	6	0	4.340166	-0.750465	-1.146215
45	6	0	5.883570	0.625443	0.725218
46	1	0	4.113088	0.665752	1.940895
47	6	0	5.684667	-0.487725	-1.411095
48	1	0	3.759292	-1.323440	-1.865959
49	6	0	6.456654	0.206306	-0.477430
50	1	0	6.486950	1.142951	1.464311
51	1	0	6.131991	-0.836445	-2.336487
52	1	0	7.504647	0.404347	-0.678329
53	6	0	0.430441	2.680298	0.403857
54	6	0	0.583762	4.064463	0.453938
55	6	0	-0.541121	4.879120	0.335746
56	1	0	1.572466	4.492749	0.581855
57	6	0	-1.866023	2.892772	0.112267
58	6	0	-1.789243	4.279373	0.161946
59	1	0	-0.445023	5.959566	0.372112
60	1	0	-2.817925	2.395974	-0.023558
61	1	0	-2.691816	4.871600	0.060557
62	7	0	-0.780694	2.096279	0.231003
63	8	0	-0.945074	0.679259	2.815514
64	1	0	-0.948855	0.307740	3.708692
65	1	0	-1.101403	1.625151	2.938869

2'$_{dp}$-H_2O (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1542.28099021 hartree

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Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	7	0	-0.809548	-0.866173	-1.549124
2	6	0	-1.908632	-0.151692	-2.211122
3	1	0	-1.587149	0.884760	-2.366728
4	1	0	-2.143278	-0.566998	-3.205620
5	6	0	-1.086974	-2.309772	-1.416090
6	1	0	-2.169940	-2.438145	-1.319417
7	1	0	-0.780809	-2.872396	-2.310601
8	6	0	0.521479	-0.607849	-2.137517
9	1	0	1.136231	-1.494112	-1.957870
10	1	0	0.461046	-0.491242	-3.230610
11	27	0	-0.893425	-0.056531	0.554506
12	6	0	-3.161834	-0.158009	-1.350294
13	6	0	-4.431793	-0.140393	-1.925117
14	6	0	-4.073860	-0.176561	0.775139
15	6	0	-5.559529	-0.123338	-1.102847
16	1	0	-4.533054	-0.143148	-3.006193
17	6	0	-5.373855	-0.146063	0.279418
18	1	0	-3.891203	-0.206516	1.845898
19	1	0	-6.556229	-0.104898	-1.531576
20	1	0	-6.215699	-0.148521	0.963598
21	6	0	-0.441997	-2.894860	-0.176120
22	6	0	0.035175	-4.204096	-0.147869
23	6	0	0.546866	-4.721654	1.043133
24	1	0	-0.000005	-4.809779	-1.048360
25	6	0	0.091548	-2.596517	2.055282
26	6	0	0.571286	-3.898152	2.168155
27	1	0	0.920099	-5.739695	1.088297
28	1	0	0.114945	-1.915907	2.900242
29	1	0	0.962222	-4.249410	3.117116
30	7	0	-2.976100	-0.172444	-0.007639
31	7	0	-0.411630	-2.089061	0.911546
32	6	0	1.210723	0.622986	-1.542336
33	1	0	2.174856	0.771684	-2.050975
34	1	0	0.605906	1.509263	-1.752913
35	7	0	1.373635	0.533194	-0.075165
36	6	0	1.572044	1.860655	0.518919
37	1	0	1.816527	1.709809	1.578591
38	1	0	2.423165	2.401787	0.078496
39	6	0	2.438903	-0.419956	0.354601
40	1	0	2.361705	-0.492055	1.443944
41	1	0	2.173573	-1.403530	-0.039695
42	6	0	3.865730	-0.078218	-0.040522
43	6	0	4.678036	0.698299	0.799183

44	6	0	4.409564	-0.542203	-1.247833
45	6	0	5.985767	1.021038	0.434913
46	1	0	4.291281	1.037757	1.757209
47	6	0	5.716375	-0.220571	-1.617811
48	1	0	3.813216	-1.179121	-1.897325
49	6	0	6.506311	0.566487	-0.778262
50	1	0	6.601139	1.617123	1.102266
51	1	0	6.120480	-0.593000	-2.554465
52	1	0	7.525204	0.812728	-1.061070
53	6	0	0.334195	2.729464	0.437999
54	6	0	0.447846	4.119909	0.378279
55	6	0	-0.701998	4.906769	0.380349
56	1	0	1.432872	4.574075	0.333044
57	6	0	-1.974092	2.879101	0.467532
58	6	0	-1.941826	4.268554	0.428889
59	1	0	-0.632162	5.989073	0.339395
60	1	0	-2.918923	2.346759	0.488877
61	1	0	-2.869145	4.831449	0.428345
62	7	0	-0.866126	2.105682	0.473507
63	8	0	-0.946176	0.309151	2.908005
64	1	0	-1.664020	-0.121171	3.391004
65	1	0	-1.105322	1.257969	3.001199

2'$_{dp}$-H_2O (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1542.24523559 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.686904	-0.892892	-1.848242
2	6	0	-1.842711	-0.168051	-2.378895
3	1	0	-1.538080	0.868275	-2.564855
4	1	0	-2.202551	-0.575839	-3.338319
5	6	0	-0.912624	-2.318743	-1.628923
6	1	0	-1.971010	-2.542636	-1.808383
7	1	0	-0.352557	-2.939115	-2.342617
8	6	0	0.641649	-0.538751	-2.365954
9	1	0	1.272296	-1.428444	-2.286456
10	1	0	0.610869	-0.282753	-3.436105
11	27	0	-0.710297	0.182774	0.234550
12	6	0	-2.983768	-0.177263	-1.371142
13	6	0	-4.311955	-0.333773	-1.762416
14	6	0	-3.613975	-0.059138	0.871929
15	6	0	-5.317615	-0.340242	-0.794458
16	1	0	-4.550964	-0.453728	-2.814263

17	6	0	-4.960188	-0.207368	0.545557
18	1	0	-3.278303	0.056123	1.898824
19	1	0	-6.357281	-0.457674	-1.083334
20	1	0	-5.704912	-0.219356	1.333759
21	6	0	-0.588305	-2.758301	-0.207270
22	6	0	-0.394536	-4.110614	0.081875
23	6	0	-0.185044	-4.506199	1.399951
24	1	0	-0.413761	-4.840029	-0.722493
25	6	0	-0.372371	-2.200158	2.032295
26	6	0	-0.184261	-3.529760	2.395369
27	1	0	-0.031423	-5.552552	1.644718
28	1	0	-0.398902	-1.415332	2.780596
29	1	0	-0.039755	-3.784550	3.439466
30	7	0	-2.643994	-0.033159	-0.064515
31	7	0	-0.557442	-1.808559	0.751487
32	6	0	1.301051	0.629898	-1.618663
33	1	0	2.327361	0.759009	-1.987348
34	1	0	0.763537	1.554808	-1.839870
35	7	0	1.295748	0.468746	-0.128945
36	6	0	1.614248	1.771940	0.516479
37	1	0	1.771250	1.565602	1.582079
38	1	0	2.540875	2.210247	0.126462
39	6	0	2.259596	-0.591636	0.339729
40	1	0	2.085647	-0.696152	1.413374
41	1	0	1.950202	-1.529998	-0.122243
42	6	0	3.731640	-0.342833	0.070754
43	6	0	4.530748	0.319266	1.015056
44	6	0	4.337182	-0.802502	-1.108778
45	6	0	5.887464	0.540455	0.776397
46	1	0	4.093486	0.648586	1.954446
47	6	0	5.693555	-0.582648	-1.352215
48	1	0	3.749607	-1.357053	-1.836859
49	6	0	6.470657	0.094933	-0.411289
50	1	0	6.490700	1.049693	1.521872
51	1	0	6.144762	-0.949706	-2.269094
52	1	0	7.527362	0.261933	-0.595828
53	6	0	0.456048	2.712649	0.364785
54	6	0	0.606416	4.093246	0.335506
55	6	0	-0.521835	4.911984	0.269261
56	1	0	1.604507	4.518743	0.371195
57	6	0	-1.852982	2.908193	0.231353
58	6	0	-1.772225	4.293096	0.218501
59	1	0	-0.427600	5.992245	0.253668
60	1	0	-2.813542	2.412686	0.188712

61	1	0	-2.686301	4.874685	0.162266
62	7	0	-0.762896	2.095233	0.310694
63	8	0	-1.422740	0.528304	3.261615
64	1	0	-1.328817	1.395214	3.677775
65	1	0	-1.083510	0.644075	2.340962

1' (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1465.59413739 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.248353	-1.536295	-1.210114
2	6	0	-2.168074	-1.060767	-2.269168
3	1	0	-1.572789	-0.601626	-3.065463
4	1	0	-2.715015	-1.891302	-2.733260
5	6	0	-1.881325	-2.599674	-0.393679
6	1	0	-2.963369	-2.422623	-0.392737
7	1	0	-1.726505	-3.592397	-0.835501
8	6	0	0.081077	-1.934395	-1.750267
9	1	0	0.555207	-2.586958	-1.012623
10	1	0	-0.022495	-2.520219	-2.673246
11	27	0	-0.847553	0.173515	0.165967
12	6	0	-3.126941	-0.017388	-1.735336
13	6	0	-4.381925	0.194521	-2.301243
14	6	0	-3.445201	1.749194	-0.253068
15	6	0	-5.182096	1.229133	-1.815611
16	1	0	-4.724981	-0.439164	-3.112690
17	6	0	-4.703466	2.024690	-0.773649
18	1	0	-3.033134	2.342124	0.556630
19	1	0	-6.163090	1.410164	-2.243298
20	1	0	-5.291619	2.840071	-0.368007
21	6	0	-1.411404	-2.577554	1.045932
22	6	0	-1.445181	-3.717087	1.847281
23	6	0	-1.093199	-3.615474	3.193343
24	1	0	-1.749123	-4.668734	1.423395
25	6	0	-0.679971	-1.284915	2.841925
26	6	0	-0.706085	-2.374620	3.702586
27	1	0	-1.117760	-4.491717	3.833412
28	1	0	-0.370171	-0.304123	3.189089
29	1	0	-0.423506	-2.252202	4.742044
30	7	0	-2.669250	0.746858	-0.717277
31	7	0	-1.026366	-1.378299	1.539921
32	6	0	0.954335	-0.703113	-2.008949

33	1	0	1.934443	-1.009115	-2.389605
34	1	0	0.499730	-0.072867	-2.778725
35	7	0	1.083107	0.111453	-0.768581
36	6	0	1.358977	1.548025	-1.037048
37	1	0	2.406582	1.713493	-1.309762
38	1	0	0.750887	1.856275	-1.896105
39	6	0	2.107501	-0.470653	0.201220
40	1	0	2.032041	0.123907	1.115772
41	1	0	1.765239	-1.478374	0.446185
42	6	0	3.538935	-0.505860	-0.283370
43	6	0	4.406649	0.568794	-0.029853
44	6	0	4.039226	-1.629802	-0.960338
45	6	0	5.729921	0.535143	-0.470762
46	1	0	4.056093	1.424619	0.542928
47	6	0	5.362033	-1.664812	-1.402594
48	1	0	3.403231	-2.498125	-1.118266
49	6	0	6.206931	-0.578897	-1.164546
50	1	0	6.391946	1.369157	-0.260314
51	1	0	5.736604	-2.543179	-1.918480
52	1	0	7.237935	-0.608391	-1.502111
53	6	0	0.982467	2.405183	0.160230
54	6	0	1.643772	3.598236	0.447163
55	6	0	1.224409	4.368196	1.532219
56	1	0	2.475438	3.917623	-0.172372
57	6	0	-0.453315	2.719172	1.971476
58	6	0	0.157386	3.919224	2.312860
59	1	0	1.727372	5.300309	1.769548
60	1	0	-1.283358	2.328601	2.553341
61	1	0	-0.193485	4.482739	3.170102
62	7	0	-0.057861	1.976299	0.915837

1' (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1465.57837194 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.137158	-1.547519	-1.109797
2	6	0	-2.131073	-1.243337	-2.180626
3	1	0	-1.609660	-0.737596	-3.000934
4	1	0	-2.562227	-2.163293	-2.593845
5	6	0	-1.706876	-2.546129	-0.148224
6	1	0	-2.790878	-2.395988	-0.115817
7	1	0	-1.534214	-3.564892	-0.513517

8	6	0	0.184369	-2.008372	-1.659517
9	1	0	0.660830	-2.615937	-0.887340
10	1	0	0.036940	-2.651049	-2.535382
11	27	0	-0.818773	0.171398	-0.168167
12	6	0	-3.198176	-0.333745	-1.614283
13	6	0	-4.490920	-0.282426	-2.126139
14	6	0	-3.687298	1.316772	-0.053267
15	6	0	-5.403374	0.617450	-1.573858
16	1	0	-4.777716	-0.934989	-2.944317
17	6	0	-4.992764	1.430465	-0.517859
18	1	0	-3.337042	1.932692	0.765162
19	1	0	-6.416513	0.677594	-1.958142
20	1	0	-5.668882	2.140604	-0.055266
21	6	0	-1.156177	-2.352202	1.246482
22	6	0	-1.107400	-3.390927	2.174421
23	6	0	-0.681102	-3.114007	3.473859
24	1	0	-1.404185	-4.394977	1.888410
25	6	0	-0.367646	-0.833408	2.809195
26	6	0	-0.308497	-1.809388	3.799139
27	1	0	-0.638522	-3.903571	4.217215
28	1	0	-0.069797	0.189735	3.015907
29	1	0	0.028977	-1.550832	4.796621
30	7	0	-2.797525	0.454784	-0.583653
31	7	0	-0.784592	-1.091723	1.556090
32	6	0	1.053046	-0.802397	-2.000073
33	1	0	2.051682	-1.117215	-2.319283
34	1	0	0.614438	-0.238955	-2.828821
35	7	0	1.117109	0.103237	-0.808635
36	6	0	1.369967	1.528870	-1.185170
37	1	0	2.432883	1.716038	-1.365253
38	1	0	0.840970	1.735093	-2.123174
39	6	0	2.129145	-0.372708	0.230966
40	1	0	1.999967	0.287234	1.091602
41	1	0	1.805743	-1.367022	0.542514
42	6	0	3.574035	-0.396714	-0.208930
43	6	0	4.404604	0.715737	0.003913
44	6	0	4.127261	-1.546600	-0.795614
45	6	0	5.742668	0.692259	-0.390437
46	1	0	4.012859	1.595075	0.510759
47	6	0	5.464823	-1.571608	-1.191646
48	1	0	3.521325	-2.442156	-0.916490
49	6	0	6.272186	-0.449151	-0.996063
50	1	0	6.374855	1.556241	-0.211720
51	1	0	5.880181	-2.469854	-1.637276

52	1	0	7.314599	-0.470631	-1.297195
53	6	0	0.822049	2.420676	-0.095926
54	6	0	1.370451	3.655004	0.240497
55	6	0	0.782434	4.405921	1.259473
56	1	0	2.246044	4.018917	-0.286771
57	6	0	-0.821024	2.647302	1.542094
58	6	0	-0.326455	3.887401	1.929330
59	1	0	1.192193	5.372249	1.535421
60	1	0	-1.667050	2.198068	2.050923
61	1	0	-0.800151	4.427777	2.741203
62	7	0	-0.275024	1.932000	0.538125

1'(square pyramidal) (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1465.57346714 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.811614	-0.744582	1.646117
2	6	0	1.979095	-0.019948	2.197011
3	1	0	1.676912	1.014522	2.397194
4	1	0	2.328374	-0.445186	3.147660
5	6	0	1.075178	-2.199473	1.515606
6	1	0	2.144730	-2.381256	1.666876
7	1	0	0.559273	-2.768312	2.297491
8	6	0	-0.506130	-0.439116	2.269444
9	1	0	-1.102523	-1.353659	2.249060
10	1	0	-0.397268	-0.161354	3.325126
11	27	0	0.734646	0.117537	-0.322625
12	6	0	3.095151	-0.043149	1.164489
13	6	0	4.444119	-0.088798	1.506675
14	6	0	3.627662	-0.070504	-1.111392
15	6	0	5.406136	-0.115389	0.494584
16	1	0	4.736304	-0.109685	2.551610
17	6	0	4.991060	-0.112672	-0.837268
18	1	0	3.257143	-0.066660	-2.131391
19	1	0	6.461905	-0.149786	0.743883
20	1	0	5.704609	-0.146045	-1.652919
21	6	0	0.704579	-2.726240	0.141884
22	6	0	0.564922	-4.092480	-0.104431
23	6	0	0.313600	-4.528965	-1.403728
24	1	0	0.658978	-4.801890	0.711779
25	6	0	0.339159	-2.239668	-2.104469
26	6	0	0.205100	-3.583831	-2.426461
27	1	0	0.204434	-5.587747	-1.615709

28	1	0	0.249047	-1.470468	-2.865854
29	1	0	0.013767	-3.878309	-3.452199
30	7	0	2.699749	-0.026213	-0.135665
31	7	0	0.579489	-1.815446	-0.845318
32	6	0	-1.236166	0.677739	1.521497
33	1	0	-2.262851	0.768116	1.892487
34	1	0	-0.739935	1.633638	1.702124
35	7	0	-1.248315	0.448525	0.030984
36	6	0	-1.597564	1.724552	-0.657192
37	1	0	-1.804681	1.490479	-1.707690
38	1	0	-2.512975	2.161467	-0.244761
39	6	0	-2.239236	-0.638017	-0.369370
40	1	0	-2.092265	-0.788703	-1.441623
41	1	0	-1.917805	-1.552094	0.131069
42	6	0	-3.695780	-0.358407	-0.071785
43	6	0	-4.512676	0.270367	-1.024879
44	6	0	-4.271005	-0.768138	1.141946
45	6	0	-5.860820	0.511041	-0.759429
46	1	0	-4.103346	0.551188	-1.992646
47	6	0	-5.618915	-0.527436	1.410048
48	1	0	-3.672483	-1.305609	1.874510
49	6	0	-6.414088	0.118478	0.461313
50	1	0	-6.481924	0.989904	-1.509733
51	1	0	-6.050764	-0.856484	2.349844
52	1	0	-7.464703	0.298925	0.664965
53	6	0	-0.446192	2.690543	-0.586017
54	6	0	-0.615310	4.065686	-0.725721
55	6	0	0.505203	4.894280	-0.705099
56	1	0	-1.611525	4.476820	-0.851113
57	6	0	1.858980	2.941148	-0.390230
58	6	0	1.765227	4.318747	-0.534135
59	1	0	0.397022	5.968508	-0.815601
60	1	0	2.819711	2.463034	-0.251499
61	1	0	2.664248	4.924143	-0.508431
62	7	0	0.776807	2.130131	-0.414830

1’(square pyramidal) (q) E(B3LYP/ SDD-6-31G(d,p))= -1465.582229 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.805607	-0.916510	1.491459
2	6	0	1.900442	-0.258910	2.250614
3	1	0	1.554760	0.738741	2.544822

4	1	0	2.131748	-0.803696	3.175223
5	6	0	1.105287	-2.354486	1.248375
6	1	0	2.189646	-2.494598	1.312871
7	1	0	0.665439	-2.987083	2.028178
8	6	0	-0.530503	-0.706942	2.124841
9	1	0	-1.141275	-1.586365	1.913563
10	1	0	-0.439015	-0.643996	3.216176
11	27	0	0.791196	0.088104	-0.436803
12	6	0	3.135600	-0.135591	1.381157
13	6	0	4.426972	-0.217220	1.898786
14	6	0	3.960494	0.150909	-0.773689
15	6	0	5.514372	-0.099898	1.031802
16	1	0	4.577955	-0.376350	2.961653
17	6	0	5.277488	0.078238	-0.331844
18	1	0	3.733570	0.283541	-1.827912
19	1	0	6.528656	-0.160323	1.413342
20	1	0	6.092825	0.155657	-1.042414
21	6	0	0.666682	-2.817199	-0.126944
22	6	0	0.419965	-4.161850	-0.398734
23	6	0	0.125752	-4.551202	-1.705746
24	1	0	0.465152	-4.894269	0.400898
25	6	0	0.318657	-2.258510	-2.363132
26	6	0	0.080419	-3.582347	-2.709785
27	1	0	-0.065508	-5.594476	-1.936193
28	1	0	0.280885	-1.470523	-3.109707
29	1	0	-0.140961	-3.842354	-3.738739
30	7	0	2.907484	0.058170	0.063007
31	7	0	0.604934	-1.878252	-1.099189
32	6	0	-1.217921	0.549555	1.589919
33	1	0	-2.211726	0.645166	2.043533
34	1	0	-0.648630	1.442494	1.868751
35	7	0	-1.317517	0.523702	0.100631
36	6	0	-1.656675	1.869375	-0.422930
37	1	0	-2.065303	1.741538	-1.431432
38	1	0	-2.447276	2.344933	0.168290
39	6	0	-2.327306	-0.497583	-0.397753
40	1	0	-2.234498	-0.497896	-1.487699
41	1	0	-1.988225	-1.475448	-0.052278
42	6	0	-3.768164	-0.266259	0.004569
43	6	0	-4.631841	0.468138	-0.822908
44	6	0	-4.279676	-0.811794	1.193254
45	6	0	-5.962158	0.676938	-0.458767
46	1	0	-4.274933	0.857721	-1.773441
47	6	0	-5.609428	-0.602921	1.560623

48	1	0	-3.647212	-1.429771	1.827103
49	6	0	-6.451091	0.147629	0.737363
50	1	0	-6.619624	1.238895	-1.114533
51	1	0	-5.991342	-1.036892	2.479264
52	1	0	-7.487745	0.304174	1.017853
53	6	0	-0.453734	2.777145	-0.529736
54	6	0	-0.603733	4.163573	-0.542683
55	6	0	0.512104	4.970269	-0.754635
56	1	0	-1.586230	4.600194	-0.395705
57	6	0	1.835338	2.980321	-0.886442
58	6	0	1.756861	4.364651	-0.936268
59	1	0	0.413535	6.050997	-0.774521
60	1	0	2.786494	2.475557	-0.998238
61	1	0	2.652746	4.951334	-1.105225
62	7	0	0.755004	2.190052	-0.691004

1'$_{pt\text{-}A}$ (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1465.74302710 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.897783	-1.084239	-1.302355
2	6	0	-2.752269	-0.197845	-2.141021
3	1	0	-2.133761	0.249439	-2.926286
4	1	0	-3.531801	-0.770562	-2.656385
5	6	0	-2.703039	-2.146725	-0.635505
6	1	0	-3.728098	-1.773922	-0.528569
7	1	0	-2.759895	-3.047147	-1.258486
8	6	0	-0.714115	-1.623308	-2.028342
9	1	0	-0.353988	-2.495690	-1.477075
10	1	0	-0.985155	-1.973846	-3.032604
11	27	0	-1.085585	0.118490	0.248275
12	6	0	-3.364763	0.912115	-1.308274
13	6	0	-4.561490	1.529111	-1.659766
14	6	0	-3.142667	2.318488	0.552342
15	6	0	-5.046798	2.578643	-0.875857
16	1	0	-5.109985	1.191539	-2.533486
17	6	0	-4.324770	2.979233	0.251657
18	1	0	-2.562956	2.582773	1.431742
19	1	0	-5.980215	3.068683	-1.135660
20	1	0	-4.676436	3.780202	0.892593
21	6	0	-2.185228	-2.477496	0.750058
22	6	0	-2.487622	-3.683539	1.376263

23	6	0	-2.089667	-3.885470	2.699274
24	1	0	-3.038026	-4.450500	0.840500
25	6	0	-1.104199	-1.703490	2.677810
26	6	0	-1.390751	-2.873861	3.364439
27	1	0	-2.324129	-4.817443	3.204526
28	1	0	-0.558597	-0.894962	3.154942
29	1	0	-1.072443	-2.989903	4.394539
30	7	0	-2.660787	1.308568	-0.214048
31	7	0	-1.488681	-1.504567	1.392740
32	6	0	0.371241	-0.555809	-2.149472
33	1	0	1.232947	-0.952137	-2.691009
34	1	0	-0.005357	0.282393	-2.741679
35	7	0	0.800738	0.011176	-0.810926
36	6	0	1.557942	1.277941	-1.127254
37	1	0	2.448949	1.010890	-1.707456
38	1	0	0.918461	1.874949	-1.781140
39	6	0	1.650311	-0.991472	-0.011347
40	1	0	1.636714	-0.642198	1.026078
41	1	0	1.090771	-1.929043	-0.029435
42	6	0	3.094231	-1.220751	-0.423734
43	6	0	4.116061	-0.879497	0.487519
44	6	0	3.463456	-1.855249	-1.621933
45	6	0	5.461528	-1.115150	0.187235
46	1	0	3.852545	-0.513146	1.479245
47	6	0	4.808665	-2.077004	-1.927973
48	1	0	2.714839	-2.229845	-2.312388
49	6	0	5.811152	-1.696466	-1.033684
50	1	0	6.230213	-0.875594	0.915627
51	1	0	5.071197	-2.571049	-2.857979
52	1	0	6.853314	-1.884142	-1.270643
53	6	0	1.971523	2.190582	0.012268
54	6	0	1.194606	3.247441	0.474192
55	6	0	1.711845	4.150219	1.414707
56	1	0	0.203164	3.399560	0.059827
57	6	0	3.771054	2.933497	1.407033
58	6	0	3.016812	3.995382	1.885504
59	1	0	1.107093	4.985087	1.756153
60	1	0	4.794383	2.739408	1.709804
61	1	0	3.452334	4.687562	2.597876
62	7	0	3.234759	2.082544	0.506437
63	1	0	3.808691	1.287916	0.193621

1'$_{pt\text{-}A}$ (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1465.71066440 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.807352	-1.305697	-1.188767
2	6	0	-2.882381	-0.757605	-2.077382
3	1	0	-2.407843	-0.291100	-2.948428
4	1	0	-3.528182	-1.559020	-2.454976
5	6	0	-2.384054	-2.238543	-0.162695
6	1	0	-3.454817	-2.026698	-0.081142
7	1	0	-2.292913	-3.273491	-0.508297
8	6	0	-0.642374	-1.897960	-1.924162
9	1	0	-0.234149	-2.705917	-1.314959
10	1	0	-0.965417	-2.344824	-2.871276
11	27	0	-1.130516	0.277258	-0.183994
12	6	0	-3.669657	0.270245	-1.290751
13	6	0	-4.986426	0.615517	-1.570508
14	6	0	-3.603629	1.775882	0.507347
15	6	0	-5.614055	1.588059	-0.786480
16	1	0	-5.516353	0.132243	-2.385193
17	6	0	-4.913056	2.173979	0.270731
18	1	0	-3.027683	2.184802	1.331735
19	1	0	-6.641465	1.873605	-0.990593
20	1	0	-5.374363	2.919468	0.909058
21	6	0	-1.769575	-2.071011	1.218198
22	6	0	-1.878541	-3.080234	2.173845
23	6	0	-1.425854	-2.839105	3.471635
24	1	0	-2.324626	-4.034540	1.911028
25	6	0	-0.770157	-0.645025	2.765678
26	6	0	-0.868985	-1.594615	3.775260
27	1	0	-1.510517	-3.608046	4.233216
28	1	0	-0.335365	0.331138	2.958249
29	1	0	-0.515157	-1.363045	4.773906
30	7	0	-2.986313	0.854275	-0.266138
31	7	0	-1.207549	-0.876171	1.509173
32	6	0	0.397210	-0.816346	-2.186025
33	1	0	1.272277	-1.230289	-2.692135
34	1	0	-0.024052	-0.063775	-2.860980
35	7	0	0.794418	-0.094074	-0.909263
36	6	0	1.548960	1.138040	-1.362388
37	1	0	2.457549	0.810937	-1.881350
38	1	0	0.925108	1.642451	-2.104465
39	6	0	1.638724	-0.970460	0.022631
40	1	0	1.582678	-0.495357	1.004602
41	1	0	1.098482	-1.914009	0.115955

42	6	0	3.097623	-1.219942	-0.321868
43	6	0	4.079167	-0.811376	0.606663
44	6	0	3.520971	-1.934498	-1.455511
45	6	0	5.436858	-1.066075	0.385355
46	1	0	3.771848	-0.375036	1.556809
47	6	0	4.878301	-2.174647	-1.684173
48	1	0	2.805548	-2.357835	-2.152549
49	6	0	5.840239	-1.732045	-0.773742
50	1	0	6.172077	-0.771895	1.128100
51	1	0	5.182067	-2.731184	-2.565060
52	1	0	6.891633	-1.934685	-0.949708
53	6	0	1.924586	2.189303	-0.334778
54	6	0	1.164826	3.327888	-0.088977
55	6	0	1.652581	4.339388	0.752031
56	1	0	0.215276	3.457870	-0.598818
57	6	0	3.650819	3.064534	1.073788
58	6	0	2.912092	4.209265	1.339238
59	1	0	1.061768	5.234374	0.923380
60	1	0	4.641265	2.882744	1.477080
61	1	0	3.326498	4.981818	1.977787
62	7	0	3.143840	2.110880	0.264196
63	1	0	3.708184	1.263176	0.104703

1'$_{pt\text{-}B}$ (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1465.74091980 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.367313	-0.982006	-0.951406
2	6	0	-2.203131	-0.439763	-2.084371
3	1	0	-1.597387	0.299812	-2.615482
4	1	0	-2.393151	-1.254225	-2.794670
5	6	0	-2.111579	-2.046375	-0.204787
6	1	0	-3.127178	-1.680180	-0.024689
7	1	0	-2.197019	-2.954862	-0.814598
8	6	0	-0.098870	-1.567469	-1.562055
9	1	0	0.281481	-2.309808	-0.855330
10	1	0	-0.345759	-2.105298	-2.485486
11	27	0	-0.320648	0.159519	0.585127
12	6	0	-3.553498	0.171220	-1.756024
13	6	0	-4.752210	-0.527561	-1.842652
14	6	0	-4.790652	2.176111	-1.284867
15	6	0	-5.975213	0.127602	-1.637690

16	1	0	-4.737469	-1.581117	-2.100746
17	6	0	-5.995549	1.494774	-1.351296
18	1	0	-4.713008	3.241345	-1.097065
19	1	0	-6.905497	-0.427169	-1.719677
20	1	0	-6.925643	2.032699	-1.202228
21	6	0	-1.498063	-2.381126	1.144200
22	6	0	-1.736243	-3.607981	1.756800
23	6	0	-1.242278	-3.835122	3.043836
24	1	0	-2.304115	-4.375629	1.240594
25	6	0	-0.291574	-1.637324	3.007700
26	6	0	-0.513002	-2.829512	3.683016
27	1	0	-1.422135	-4.784965	3.538079
28	1	0	0.285383	-0.835082	3.456503
29	1	0	-0.114073	-2.967801	4.681944
30	7	0	-3.629874	1.505622	-1.481482
31	7	0	-0.777081	-1.412197	1.762793
32	6	0	0.974258	-0.509265	-1.840092
33	1	0	1.835023	-0.981467	-2.324524
34	1	0	0.604191	0.245101	-2.539399
35	7	0	1.386775	0.172214	-0.571858
36	6	0	1.705453	1.624266	-0.745743
37	1	0	2.768291	1.760712	-0.965582
38	1	0	1.158022	1.999313	-1.618078
39	6	0	2.530240	-0.568388	0.154987
40	1	0	2.648942	-0.049639	1.111508
41	1	0	2.150297	-1.571636	0.368882
42	6	0	3.841128	-0.639781	-0.582135
43	6	0	4.822785	0.348347	-0.391083
44	6	0	4.123977	-1.720335	-1.435915
45	6	0	6.040760	0.277916	-1.067505
46	1	0	4.656144	1.153028	0.322211
47	6	0	5.341635	-1.789698	-2.112906
48	1	0	3.411145	-2.535772	-1.542472
49	6	0	6.297159	-0.785954	-1.935909
50	1	0	6.796520	1.038970	-0.902333
51	1	0	5.553519	-2.634276	-2.760526
52	1	0	7.248603	-0.845580	-2.454421
53	6	0	1.293470	2.442487	0.466909
54	6	0	1.965124	3.604561	0.834264
55	6	0	1.492655	4.358466	1.911443
56	1	0	2.847701	3.916524	0.285097
57	6	0	-0.266276	2.756983	2.194522
58	6	0	0.356349	3.928080	2.602315
59	1	0	2.008598	5.265478	2.211634

60	1	0	-1.141728	2.375003	2.710425
61	1	0	-0.034995	4.483152	3.447801
62	7	0	0.186656	2.026941	1.145863
63	1	0	-2.772464	2.051393	-1.472937

1'$_{pt\text{-}B}$ (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1465.72273867 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.285712	-1.243632	-0.686659
2	6	0	-2.195997	-0.997540	-1.876912
3	1	0	-1.639661	-0.387755	-2.594350
4	1	0	-2.375703	-1.962493	-2.365089
5	6	0	-1.983077	-2.059708	0.365439
6	1	0	-3.043185	-1.791533	0.359457
7	1	0	-1.920756	-3.127942	0.129375
8	6	0	-0.065488	-1.983372	-1.215602
9	1	0	0.375339	-2.510671	-0.367393
10	1	0	-0.366789	-2.741026	-1.948173
11	27	0	-0.385428	0.358295	0.227814
12	6	0	-3.561732	-0.374482	-1.648627
13	6	0	-4.728760	-1.120508	-1.527083
14	6	0	-4.880492	1.634263	-1.616144
15	6	0	-5.975969	-0.484902	-1.436422
16	1	0	-4.672161	-2.203949	-1.532632
17	6	0	-6.053315	0.909108	-1.475689
18	1	0	-4.848472	2.716037	-1.686262
19	1	0	-6.880572	-1.080528	-1.353190
20	1	0	-7.003408	1.429833	-1.421444
21	6	0	-1.450503	-1.769408	1.750906
22	6	0	-1.591727	-2.675221	2.797207
23	6	0	-1.174805	-2.304085	4.078131
24	1	0	-2.023788	-3.654793	2.618456
25	6	0	-0.484700	-0.192990	3.178352
26	6	0	-0.616479	-1.038683	4.271775
27	1	0	-1.279248	-2.994882	4.909186
28	1	0	-0.026829	0.783979	3.279179
29	1	0	-0.276048	-0.714771	5.249184
30	7	0	-3.694767	0.983261	-1.693837
31	7	0	-0.899097	-0.542280	1.937933
32	6	0	0.943794	-1.008531	-1.818516
33	1	0	1.837519	-1.543494	-2.155234

34	1	0	0.534910	-0.492698	-2.691959
35	7	0	1.288997	0.009493	-0.779505
36	6	0	1.722691	1.334269	-1.318426
37	1	0	2.780697	1.315223	-1.597521
38	1	0	1.154328	1.546921	-2.231784
39	6	0	2.345055	-0.530037	0.226268
40	1	0	2.440960	0.245180	0.988861
41	1	0	1.894680	-1.404517	0.700565
42	6	0	3.684191	-0.870904	-0.371214
43	6	0	4.710011	0.090274	-0.413042
44	6	0	3.950562	-2.168705	-0.842463
45	6	0	5.959342	-0.229671	-0.943910
46	1	0	4.548741	1.079636	0.009832
47	6	0	5.199896	-2.487777	-1.373878
48	1	0	3.196476	-2.948799	-0.757777
49	6	0	6.202263	-1.515945	-1.432638
50	1	0	6.748231	0.515350	-0.958734
51	1	0	5.398407	-3.495722	-1.723409
52	1	0	7.177269	-1.766766	-1.837787
53	6	0	1.433906	2.394078	-0.276052
54	6	0	2.103119	3.612343	-0.219536
55	6	0	1.728643	4.552176	0.743654
56	1	0	2.905429	3.823257	-0.919352
57	6	0	0.068556	3.010765	1.527880
58	6	0	0.691109	4.247356	1.629060
59	1	0	2.241520	5.507186	0.804471
60	1	0	-0.738881	2.730486	2.196810
61	1	0	0.372608	4.951796	2.389618
62	7	0	0.430671	2.095940	0.597821
63	1	0	-2.866253	1.551042	-1.849272

1'$_{pt\text{-}C}$ (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1465.73211305 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.252333	1.222478	-1.081885
2	6	0	2.233601	0.653972	-2.076998
3	1	0	1.668572	0.065684	-2.806092
4	1	0	2.721293	1.456365	-2.642179
5	6	0	1.884716	2.492630	-0.566930
6	1	0	2.892732	2.227258	-0.231955
7	1	0	2.008617	3.184164	-1.410655

8	6	0	-0.062480	1.487684	-1.763454
9	1	0	-0.630744	2.169947	-1.130505
10	1	0	0.097080	1.990429	-2.726104
11	27	0	0.858377	-0.667473	0.145545
12	6	0	3.255069	-0.252341	-1.429610
13	6	0	4.565702	-0.357557	-1.881105
14	6	0	3.588350	-1.985454	0.104275
15	6	0	5.404925	-1.320890	-1.311185
16	1	0	4.924455	0.288596	-2.675975
17	6	0	4.906262	-2.150648	-0.305381
18	1	0	3.156515	-2.613090	0.876443
19	1	0	6.430198	-1.423872	-1.653372
20	1	0	5.522984	-2.915737	0.153364
21	6	0	1.190049	3.272275	0.534570
22	6	0	0.226295	4.250343	0.314100
23	6	0	-0.269913	5.014396	1.380108
24	1	0	-0.111025	4.449093	-0.697285
25	6	0	1.186820	3.841198	2.871223
26	6	0	0.210294	4.804571	2.675264
27	1	0	-1.011437	5.785521	1.191929
28	1	0	1.643659	3.634841	3.833043
29	1	0	-0.141528	5.391921	3.516605
30	7	0	2.777857	-1.049403	-0.441224
31	7	0	1.632383	3.116225	1.816765
32	6	0	-0.873788	0.204530	-1.983835
33	1	0	-1.848636	0.465391	-2.409767
34	1	0	-0.381958	-0.455746	-2.703725
35	7	0	-1.028442	-0.542072	-0.703803
36	6	0	-1.365392	-1.986507	-0.885840
37	1	0	-2.428146	-2.116106	-1.112529
38	1	0	-0.803749	-2.367120	-1.747727
39	6	0	-2.029293	0.130908	0.253398
40	1	0	-1.978825	-0.436295	1.186141
41	1	0	-1.634895	1.130810	0.457337
42	6	0	-3.452746	0.207653	-0.239781
43	6	0	-4.371544	-0.801555	0.094727
44	6	0	-3.895309	1.298914	-1.006900
45	6	0	-5.691134	-0.736884	-0.353584
46	1	0	-4.065651	-1.624849	0.736481
47	6	0	-5.213925	1.363338	-1.456741
48	1	0	-3.218964	2.121715	-1.231684
49	6	0	-6.111048	0.341121	-1.136304
50	1	0	-6.394540	-1.516775	-0.080385
51	1	0	-5.546498	2.213590	-2.043404

52	1	0	-7.138874	0.394188	-1.480396
53	6	0	-0.983678	-2.773071	0.360061
54	6	0	-1.637886	-3.946858	0.721490
55	6	0	-1.218728	-4.641367	1.858646
56	1	0	-2.464593	-4.313173	0.121187
57	6	0	0.450250	-2.958652	2.205420
58	6	0	-0.160390	-4.134473	2.617977
59	1	0	-1.717548	-5.559555	2.153460
60	1	0	1.270501	-2.525361	2.769426
61	1	0	0.183615	-4.637898	3.514787
62	7	0	0.056709	-2.291809	1.094454
63	1	0	2.394870	2.466246	1.992007

1'$_{pt\text{-}C}$ (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1465.73258932 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.082199	1.172305	-1.197880
2	6	0	2.140174	0.689274	-2.159602
3	1	0	1.672928	-0.027349	-2.843742
4	1	0	2.517547	1.513431	-2.776077
5	6	0	1.629328	2.446904	-0.587474
6	1	0	2.642416	2.226431	-0.240493
7	1	0	1.725374	3.184268	-1.393270
8	6	0	-0.229267	1.426372	-1.901771
9	1	0	-0.800141	2.125500	-1.290041
10	1	0	-0.059396	1.901098	-2.875232
11	27	0	0.853459	-0.552305	-0.133539
12	6	0	3.252351	0.021077	-1.380957
13	6	0	4.569885	-0.000072	-1.822409
14	6	0	3.796979	-1.249179	0.494553
15	6	0	5.527354	-0.685649	-1.069394
16	1	0	4.844759	0.504167	-2.743516
17	6	0	5.131702	-1.315344	0.110960
18	1	0	3.464025	-1.733971	1.402164
19	1	0	6.561559	-0.721792	-1.397737
20	1	0	5.841472	-1.854314	0.729084
21	6	0	0.858795	3.112685	0.535560
22	6	0	-0.062788	4.136144	0.346648
23	6	0	-0.635650	4.789909	1.447960
24	1	0	-0.309360	4.454102	-0.660847
25	6	0	0.658118	3.408194	2.912102
26	6	0	-0.276042	4.418980	2.745793

27	1	0	-1.343002	5.598585	1.287614
28	1	0	1.020050	3.078398	3.879892
29	1	0	-0.689308	4.916693	3.616577
30	7	0	2.861032	-0.597137	-0.230581
31	7	0	1.182561	2.796015	1.823713
32	6	0	-1.004709	0.123710	-2.057852
33	1	0	-2.023327	0.322210	-2.406973
34	1	0	-0.532911	-0.524473	-2.801620
35	7	0	-1.020256	-0.609513	-0.749650
36	6	0	-1.304569	-2.072150	-0.946466
37	1	0	-2.379044	-2.248208	-1.048859
38	1	0	-0.830197	-2.393453	-1.880753
39	6	0	-2.000533	0.005387	0.266755
40	1	0	-1.851215	-0.559520	1.190480
41	1	0	-1.649442	1.026578	0.443513
42	6	0	-3.454818	-0.000828	-0.130285
43	6	0	-4.292911	-1.052953	0.276616
44	6	0	-4.007279	1.056682	-0.873366
45	6	0	-5.642013	-1.063292	-0.078986
46	1	0	-3.899581	-1.852435	0.900819
47	6	0	-5.355210	1.045406	-1.231404
48	1	0	-3.393865	1.912108	-1.151380
49	6	0	-6.172049	-0.018721	-0.840002
50	1	0	-6.281826	-1.876214	0.248734
51	1	0	-5.772452	1.869326	-1.801274
52	1	0	-7.222507	-0.024335	-1.112333
53	6	0	-0.710785	-2.826734	0.213052
54	6	0	-1.211752	-4.033489	0.687754
55	6	0	-0.583925	-4.652603	1.770549
56	1	0	-2.081605	-4.480612	0.217609
57	6	0	0.964400	-2.823130	1.837328
58	6	0	0.513277	-4.026163	2.364496
59	1	0	-0.955043	-5.598030	2.153876
60	1	0	1.800630	-2.304073	2.288794
61	1	0	1.013866	-4.458371	3.223878
62	7	0	0.384600	-2.236847	0.766075
63	1	0	1.906877	2.100226	1.983989

Co^{I} HNPy **2'$_D$** (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1466.12714691 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-1.656410	-1.351374	-1.170373
2	6	0	-2.577825	-0.678431	-2.112284
3	1	0	-1.994204	-0.303529	-2.960091
4	1	0	-3.306236	-1.380815	-2.536466
5	6	0	-2.290951	-2.474465	-0.440947
6	1	0	-3.333986	-2.194393	-0.247684
7	1	0	-2.316470	-3.393158	-1.043559
8	6	0	-0.357055	-1.728401	-1.776050
9	1	0	0.106423	-2.474644	-1.126453
10	1	0	-0.492884	-2.206247	-2.757059
11	27	0	-1.253681	0.011891	0.392899
12	6	0	-3.300022	0.503404	-1.484200
13	6	0	-4.534877	0.922257	-1.977299
14	6	0	-3.280233	2.254912	0.045263
15	6	0	-5.148123	2.051044	-1.436207
16	1	0	-5.010356	0.365118	-2.778303
17	6	0	-4.504663	2.732097	-0.402797
18	1	0	-2.759053	2.756005	0.854365
19	1	0	-6.109891	2.387656	-1.809383
20	1	0	-4.943054	3.611719	0.055058
21	6	0	-1.612635	-2.738242	0.894147
22	6	0	-1.640451	-4.002542	1.479660
23	6	0	-1.092052	-4.182285	2.749345
24	1	0	-2.094218	-4.833437	0.948958
25	6	0	-0.510354	-1.859391	2.743986
26	6	0	-0.519551	-3.086498	3.395850
27	1	0	-1.110810	-5.158296	3.223316
28	1	0	-0.064048	-0.986671	3.209885
29	1	0	-0.082767	-3.177587	4.384048
30	7	0	-2.669812	1.164072	-0.474874
31	7	0	-1.039977	-1.674539	1.515438
32	6	0	0.556503	-0.516469	-1.942440
33	1	0	1.474840	-0.822746	-2.457912
34	1	0	0.063933	0.215734	-2.588697
35	7	0	0.878661	0.177181	-0.653944
36	6	0	1.406351	1.517962	-1.010235
37	1	0	2.366641	1.448619	-1.535886
38	1	0	0.691255	1.984505	-1.698694
39	6	0	1.890726	-0.601851	0.169042
40	1	0	1.994781	-0.061503	1.115315
41	1	0	1.414915	-1.553033	0.410145
42	6	0	3.257302	-0.835973	-0.442004
43	6	0	4.322581	0.037395	-0.171481
44	6	0	3.503172	-1.955232	-1.253828

45	6	0	5.587168	-0.180521	-0.719890
46	1	0	4.173430	0.876370	0.504754
47	6	0	4.765217	-2.174998	-1.806787
48	1	0	2.712482	-2.679468	-1.434958
49	6	0	5.808150	-1.283910	-1.546171
50	1	0	6.402799	0.498053	-0.489986
51	1	0	4.938535	-3.048716	-2.427015
52	1	0	6.792179	-1.459102	-1.968982
53	6	0	1.583383	2.471255	0.148539
54	6	0	2.643465	3.366635	0.264392
55	6	0	2.672615	4.276287	1.323762
56	1	0	3.436017	3.345926	-0.475204
57	6	0	0.608282	3.377942	2.133678
58	6	0	1.644709	4.281816	2.275226
59	1	0	3.496922	4.977228	1.411698
60	1	0	-0.227477	3.307711	2.820240
61	1	0	1.647738	4.973324	3.109750
62	7	0	0.610825	2.521562	1.086786
63	1	0	-0.166053	1.843203	0.957670

Co^{I} HNPy **2'$_{D}$** (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1466.08305435 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.651587	-1.668768	-0.780799
2	6	0	-2.694778	-1.462750	-1.818213
3	1	0	-2.195016	-1.250949	-2.771134
4	1	0	-3.304110	-2.361778	-1.974423
5	6	0	-2.213858	-2.272931	0.458999
6	1	0	-3.303519	-2.164279	0.436830
7	1	0	-2.008626	-3.348322	0.505975
8	6	0	-0.398072	-2.320933	-1.262027
9	1	0	0.029782	-2.880667	-0.428856
10	1	0	-0.600965	-3.041210	-2.063194
11	27	0	-1.084282	0.263460	-0.274650
12	6	0	-3.559897	-0.278742	-1.420704
13	6	0	-4.869651	-0.115038	-1.856930
14	6	0	-3.647427	1.749392	-0.245771
15	6	0	-5.576687	1.026918	-1.472542
16	1	0	-5.330422	-0.868839	-2.487011
17	6	0	-4.956644	1.971826	-0.653649
18	1	0	-3.117782	2.449588	0.388767

19	1	0	-6.599936	1.172090	-1.804218
20	1	0	-5.474614	2.868684	-0.333177
21	6	0	-1.690459	-1.568329	1.692054
22	6	0	-1.772619	-2.117988	2.968743
23	6	0	-1.328455	-1.374596	4.062625
24	1	0	-2.182058	-3.114440	3.100241
25	6	0	-0.721895	0.392024	2.554459
26	6	0	-0.795657	-0.102065	3.850952
27	1	0	-1.390597	-1.787139	5.064555
28	1	0	-0.278467	1.350260	2.310786
29	1	0	-0.431355	0.502301	4.674018
30	7	0	-2.960477	0.648436	-0.622697
31	7	0	-1.171688	-0.330232	1.506727
32	6	0	0.581204	-1.253393	-1.747140
33	1	0	1.529954	-1.709594	-2.048351
34	1	0	0.175621	-0.747625	-2.631639
35	7	0	0.826010	-0.198418	-0.691413
36	6	0	1.425604	0.994393	-1.392509
37	1	0	2.259951	0.639780	-2.008046
38	1	0	0.659188	1.361092	-2.092566
39	6	0	1.734662	-0.723831	0.420345
40	1	0	1.855837	0.112214	1.107540
41	1	0	1.168492	-1.499395	0.938318
42	6	0	3.070740	-1.279670	-0.023545
43	6	0	4.193299	-0.448807	-0.168377
44	6	0	3.224949	-2.659179	-0.241383
45	6	0	5.425704	-0.979793	-0.550542
46	1	0	4.113677	0.613661	0.040228
47	6	0	4.456427	-3.191733	-0.623096
48	1	0	2.385604	-3.333233	-0.081451
49	6	0	5.558488	-2.349905	-0.784893
50	1	0	6.286308	-0.325920	-0.650566
51	1	0	4.559212	-4.260942	-0.778918
52	1	0	6.519603	-2.762046	-1.075136
53	6	0	1.911183	2.169763	-0.554126
54	6	0	2.917571	2.977059	-1.097661
55	6	0	3.322531	4.114510	-0.400140
56	1	0	3.374362	2.722847	-2.049494
57	6	0	1.739945	3.530764	1.295193
58	6	0	2.721659	4.400228	0.824815
59	1	0	4.095889	4.759798	-0.804465
60	1	0	1.255928	3.716253	2.251106
61	1	0	3.007512	5.269738	1.406516
62	7	0	1.333111	2.439952	0.625328

63	1	0	-0.758612	1.604714	0.123674

Co^{I} HNPy **2'$_E$** (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1466.13856350 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.348366	1.104907	-1.146802
2	6	0	2.115463	0.482368	-2.248445
3	1	0	1.440267	-0.171487	-2.810628
4	1	0	2.480665	1.237435	-2.959458
5	6	0	2.135035	2.223409	-0.569584
6	1	0	3.163775	1.872009	-0.420632
7	1	0	2.191790	3.069689	-1.269853
8	6	0	0.039082	1.608040	-1.676748
9	1	0	-0.333422	2.347983	-0.965046
10	1	0	0.189775	2.131686	-2.632597
11	27	0	0.511373	-0.054741	0.683891
12	6	0	3.293883	-0.358228	-1.808928
13	6	0	4.496211	-0.423713	-2.506544
14	6	0	4.095358	-1.996432	-0.273263
15	6	0	5.499689	-1.297270	-2.079442
16	1	0	4.640892	0.202909	-3.379894
17	6	0	5.298794	-2.096966	-0.948637
18	1	0	3.854074	-2.568505	0.614893
19	1	0	6.437067	-1.351152	-2.624315
20	1	0	6.061219	-2.781479	-0.595351
21	6	0	1.595152	2.690650	0.765163
22	6	0	1.846991	3.979043	1.233138
23	6	0	1.394531	4.343117	2.501126
24	1	0	2.391023	4.685453	0.614234
25	6	0	0.465763	2.147348	2.720265
26	6	0	0.692119	3.407146	3.261189
27	1	0	1.583248	5.340160	2.885968
28	1	0	-0.088467	1.394208	3.271249
29	1	0	0.318898	3.646378	4.250586
30	7	0	3.144216	-1.148316	-0.721109
31	7	0	0.905468	1.786157	1.494052
32	6	0	-0.992229	0.494940	-1.854837
33	1	0	-1.896618	0.913894	-2.309923
34	1	0	-0.622011	-0.251303	-2.563245
35	7	0	-1.288603	-0.184474	-0.567699
36	6	0	-1.525014	-1.639285	-0.733773

37	1	0	-2.564158	-1.863949	-0.997829
38	1	0	-0.906254	-1.990837	-1.567492
39	6	0	-2.412125	0.483933	0.200595
40	1	0	-2.449691	-0.013854	1.174946
41	1	0	-2.090016	1.513217	0.382586
42	6	0	-3.783054	0.472476	-0.439986
43	6	0	-4.683971	-0.574174	-0.185662
44	6	0	-4.196080	1.524812	-1.272680
45	6	0	-5.948125	-0.587808	-0.776107
46	1	0	-4.408362	-1.368069	0.505258
47	6	0	-5.459593	1.513396	-1.864925
48	1	0	-3.540093	2.377318	-1.435737
49	6	0	-6.334539	0.452602	-1.623471
50	1	0	-6.636480	-1.399612	-0.562784
51	1	0	-5.766540	2.338256	-2.500253
52	1	0	-7.320328	0.446540	-2.077452
53	6	0	-1.109487	-2.412956	0.499230
54	6	0	-1.785005	-3.555424	0.922806
55	6	0	-1.319678	-4.255259	2.036842
56	1	0	-2.667733	-3.887981	0.386534
57	6	0	0.439765	-2.643178	2.224594
58	6	0	-0.186274	-3.787986	2.703062
59	1	0	-1.837114	-5.144517	2.382501
60	1	0	1.320290	-2.241899	2.717224
61	1	0	0.204907	-4.293958	3.578606
62	7	0	-0.001059	-1.964033	1.141280
63	1	0	2.247644	-1.037809	-0.185082

Co^{I} HNPy **2'$_E$** (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1466.11879973 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.816658	-1.838897	0.212729
2	6	0	-1.691003	-2.312638	-0.912430
3	1	0	-1.035887	-2.539027	-1.759830
4	1	0	-2.168727	-3.257897	-0.630330
5	6	0	-1.479138	-2.052135	1.535898
6	1	0	-2.015957	-3.008636	1.579046
7	1	0	-0.693122	-2.087596	2.297195
8	6	0	0.505350	-2.552566	0.084876
9	1	0	0.953505	-2.606784	1.077904
10	1	0	0.371092	-3.584000	-0.262633

11	27	0	-0.299481	0.128312	0.323530
12	6	0	-2.752551	-1.378511	-1.449856
13	6	0	-4.012312	-1.811588	-1.849668
14	6	0	-3.220309	0.794027	-2.289556
15	6	0	-4.878840	-0.919438	-2.488945
16	1	0	-4.308468	-2.840299	-1.674585
17	6	0	-4.478262	0.400412	-2.718349
18	1	0	-2.833085	1.799605	-2.411382
19	1	0	-5.861597	-1.254008	-2.806006
20	1	0	-5.127937	1.111598	-3.215453
21	6	0	-2.399474	-0.890653	1.830457
22	6	0	-3.535615	-1.017646	2.623664
23	6	0	-4.311664	0.111130	2.889744
24	1	0	-3.803417	-1.986578	3.032807
25	6	0	-2.793405	1.374804	1.529096
26	6	0	-3.935713	1.327418	2.320956
27	1	0	-5.194730	0.038623	3.516134
28	1	0	-2.489475	2.299985	1.055196
29	1	0	-4.515761	2.229428	2.481825
30	7	0	-2.404368	-0.095468	-1.690846
31	7	0	-2.010329	0.298695	1.297630
32	6	0	1.400245	-1.757367	-0.864356
33	1	0	2.380534	-2.234094	-0.966135
34	1	0	0.958256	-1.710472	-1.864375
35	7	0	1.509172	-0.367452	-0.341423
36	6	0	1.798306	0.658827	-1.380274
37	1	0	2.849525	0.653453	-1.688394
38	1	0	1.194009	0.428340	-2.264763
39	6	0	2.525048	-0.280984	0.803557
40	1	0	2.475228	0.742781	1.175988
41	1	0	2.148247	-0.921905	1.603749
42	6	0	3.950009	-0.652267	0.459316
43	6	0	4.855977	0.323102	0.012213
44	6	0	4.409003	-1.968815	0.625823
45	6	0	6.174707	-0.015583	-0.292803
46	1	0	4.539543	1.360617	-0.066273
47	6	0	5.727452	-2.309636	0.322030
48	1	0	3.742959	-2.730521	1.026004
49	6	0	6.610132	-1.334069	-0.145402
50	1	0	6.865772	0.750909	-0.629144
51	1	0	6.069008	-3.329987	0.464501
52	1	0	7.637908	-1.596111	-0.375334
53	6	0	1.404333	1.999307	-0.801240
54	6	0	2.032876	3.190575	-1.148045

55	6	0	1.652785	4.374902	-0.514159
56	1	0	2.820020	3.185983	-1.895073
57	6	0	0.088802	3.091234	0.773049
58	6	0	0.676247	4.317292	0.478813
59	1	0	2.130183	5.315105	-0.770335
60	1	0	-0.646563	3.007836	1.563265
61	1	0	0.378399	5.201754	1.030806
62	7	0	0.409353	1.948893	0.128638
63	1	0	-1.481582	0.222274	-1.213240

Co^{I} HNPy **2'$_F$** (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1466.13390023 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.370007	1.228515	-1.173389
2	6	0	2.268037	0.557267	-2.154949
3	1	0	1.646666	-0.051644	-2.817716
4	1	0	2.782337	1.288958	-2.792823
5	6	0	2.078724	2.410728	-0.635444
6	1	0	3.114899	2.111625	-0.432535
7	1	0	2.125513	3.224174	-1.373568
8	6	0	0.071373	1.614304	-1.796599
9	1	0	-0.402796	2.347039	-1.137310
10	1	0	0.233991	2.118675	-2.760252
11	27	0	0.838123	-0.674249	0.118467
12	6	0	3.264819	-0.353773	-1.472665
13	6	0	4.584417	-0.473513	-1.898420
14	6	0	3.575097	-2.002776	0.135023
15	6	0	5.419757	-1.400551	-1.269641
16	1	0	4.951797	0.141023	-2.713994
17	6	0	4.905441	-2.179876	-0.234987
18	1	0	3.128927	-2.600728	0.922818
19	1	0	6.451828	-1.511901	-1.586343
20	1	0	5.515912	-2.916370	0.275352
21	6	0	1.519088	2.974294	0.651752
22	6	0	1.468149	4.335091	0.938141
23	6	0	1.036630	4.765261	2.195927
24	1	0	1.772376	5.050426	0.181795
25	6	0	0.699631	2.485794	2.838861
26	6	0	0.648797	3.830359	3.162298
27	1	0	1.000612	5.826734	2.420634
28	1	0	0.411307	1.691187	3.517551

29	1	0	0.310095	4.136984	4.145147
30	7	0	2.766813	-1.105641	-0.463471
31	7	0	1.130119	2.107779	1.615536
32	6	0	-0.871267	0.422017	-2.011893
33	1	0	-1.807016	0.791087	-2.449599
34	1	0	-0.442059	-0.272201	-2.739432
35	7	0	-1.106631	-0.331124	-0.757499
36	6	0	-1.549540	-1.728981	-0.992448
37	1	0	-2.609025	-1.785015	-1.266375
38	1	0	-0.976395	-2.124337	-1.839208
39	6	0	-2.044562	0.388253	0.190127
40	1	0	-2.032771	-0.183481	1.122325
41	1	0	-1.591505	1.360574	0.404880
42	6	0	-3.470751	0.578702	-0.281404
43	6	0	-4.457427	-0.368001	0.036042
44	6	0	-3.842685	1.714231	-1.018225
45	6	0	-5.773202	-0.199670	-0.396904
46	1	0	-4.201250	-1.230754	0.646714
47	6	0	-5.157373	1.884226	-1.453710
48	1	0	-3.108568	2.487654	-1.234810
49	6	0	-6.123483	0.923475	-1.148806
50	1	0	-6.526352	-0.937087	-0.137567
51	1	0	-5.430141	2.769871	-2.018944
52	1	0	-7.147609	1.057343	-1.482095
53	6	0	-1.273758	-2.592082	0.227547
54	6	0	-2.082587	-3.678717	0.555505
55	6	0	-1.753732	-4.466062	1.659295
56	1	0	-2.955339	-3.904197	-0.048922
57	6	0	0.127673	-3.032697	2.029031
58	6	0	-0.628283	-4.134342	2.413949
59	1	0	-2.368823	-5.318713	1.928637
60	1	0	1.009378	-2.738807	2.590777
61	1	0	-0.339693	-4.713509	3.283969
62	7	0	-0.176128	-2.276142	0.954658
63	1	0	1.131214	1.088631	1.357022

Co^{I} HNPy **2'$_F$** (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1466.12399484 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.154618	1.245356	-1.260378
2	6	0	2.159208	0.733756	-2.246622

3	1	0	1.642356	0.066715	-2.942614
4	1	0	2.591673	1.550654	-2.839699
5	6	0	1.752534	2.434017	-0.581048
6	1	0	2.802682	2.201317	-0.374617
7	1	0	1.743780	3.297908	-1.256986
8	6	0	-0.151948	1.604366	-1.905092
9	1	0	-0.648381	2.329763	-1.255111
10	1	0	0.009601	2.096778	-2.872246
11	27	0	0.840911	-0.443121	-0.184691
12	6	0	3.227330	-0.030228	-1.496773
13	6	0	4.537709	-0.126324	-1.951625
14	6	0	3.700563	-1.366093	0.338082
15	6	0	5.454878	-0.890004	-1.227295
16	1	0	4.833681	0.383407	-2.862874
17	6	0	5.024713	-1.518424	-0.060517
18	1	0	3.342194	-1.844543	1.239307
19	1	0	6.481299	-0.986301	-1.565674
20	1	0	5.699460	-2.118414	0.539770
21	6	0	1.115046	2.837225	0.730118
22	6	0	0.961336	4.161876	1.127302
23	6	0	0.468378	4.447224	2.404343
24	1	0	1.233324	4.962317	0.447559
25	6	0	0.282693	2.099466	2.828767
26	6	0	0.125803	3.404086	3.270104
27	1	0	0.349711	5.479043	2.719857
28	1	0	0.032405	1.230423	3.427266
29	1	0	-0.259031	3.596603	4.265041
30	7	0	2.800837	-0.641266	-0.358034
31	7	0	0.771050	1.858816	1.596331
32	6	0	-1.021143	0.360898	-2.067779
33	1	0	-2.017724	0.637406	-2.428550
34	1	0	-0.585812	-0.307723	-2.814917
35	7	0	-1.085384	-0.381180	-0.773112
36	6	0	-1.381008	-1.833164	-0.982377
37	1	0	-2.449979	-2.013447	-1.131642
38	1	0	-0.864016	-2.157008	-1.891706
39	6	0	-2.077359	0.235213	0.203970
40	1	0	-1.963896	-0.330198	1.132402
41	1	0	-1.726818	1.251552	0.398251
42	6	0	-3.528482	0.262177	-0.222000
43	6	0	-4.393950	-0.788668	0.121652
44	6	0	-4.048998	1.355883	-0.932335
45	6	0	-5.734741	-0.763067	-0.263723
46	1	0	-4.024831	-1.620403	0.717579

47	6	0	-5.389015	1.383368	-1.319851
48	1	0	-3.412363	2.207783	-1.163111
49	6	0	-6.232058	0.319626	-0.991872
50	1	0	-6.393271	-1.579715	0.014735
51	1	0	-5.777673	2.237908	-1.864670
52	1	0	-7.275945	0.342326	-1.287838
53	6	0	-0.842131	-2.602679	0.197229
54	6	0	-1.430544	-3.764040	0.688449
55	6	0	-0.857014	-4.406844	1.785963
56	1	0	-2.325283	-4.156005	0.216060
57	6	0	0.808307	-2.682656	1.827034
58	6	0	0.276620	-3.845667	2.372797
59	1	0	-1.295014	-5.316763	2.183066
60	1	0	1.676348	-2.212403	2.273557
61	1	0	0.744701	-4.295468	3.241231
62	7	0	0.282734	-2.072358	0.744397
63	1	0	0.824868	0.837222	1.197394

Co^{III}-H **2'$_A$** (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1466.14666319 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.838549	-0.614224	1.611475
2	6	0	2.019980	0.134441	2.107919
3	1	0	1.734821	1.183567	2.240868
4	1	0	2.371139	-0.236406	3.079557
5	6	0	1.122437	-2.080159	1.596737
6	1	0	2.202729	-2.232927	1.685947
7	1	0	0.671181	-2.575010	2.463495
8	6	0	-0.473288	-0.316520	2.265057
9	1	0	-1.039532	-1.249666	2.301656
10	1	0	-0.336386	0.010035	3.302741
11	27	0	0.714716	0.048111	-0.376087
12	6	0	3.109979	0.010555	1.055136
13	6	0	4.469049	0.003802	1.353435
14	6	0	3.560328	-0.222955	-1.230134
15	6	0	5.394484	-0.111768	0.312342
16	1	0	4.798446	0.082084	2.384507
17	6	0	4.933097	-0.231489	-0.998178
18	1	0	3.149410	-0.306944	-2.229507
19	1	0	6.458672	-0.117601	0.525623
20	1	0	5.618660	-0.331040	-1.832249

21	6	0	0.668011	-2.711333	0.304140
22	6	0	0.487551	-4.086962	0.170935
23	6	0	0.170320	-4.613660	-1.079842
24	1	0	0.602797	-4.733133	1.035256
25	6	0	0.218179	-2.382661	-1.958731
26	6	0	0.042063	-3.744887	-2.164687
27	1	0	0.028036	-5.682150	-1.205958
28	1	0	0.116357	-1.671128	-2.768296
29	1	0	-0.196916	-4.110275	-3.157111
30	7	0	2.670447	-0.099022	-0.228198
31	7	0	0.518803	-1.869918	-0.744154
32	6	0	-1.251614	0.734449	1.482536
33	1	0	-2.284190	0.789313	1.842112
34	1	0	-0.804459	1.717699	1.633497
35	7	0	-1.241050	0.445758	-0.000222
36	6	0	-1.530947	1.710079	-0.736490
37	1	0	-1.658045	1.457818	-1.794569
38	1	0	-2.465176	2.163092	-0.389662
39	6	0	-2.256333	-0.624966	-0.379206
40	1	0	-2.101608	-0.807739	-1.444664
41	1	0	-1.964316	-1.531115	0.153557
42	6	0	-3.706515	-0.298903	-0.100828
43	6	0	-4.493954	0.349272	-1.065732
44	6	0	-4.305951	-0.686140	1.108586
45	6	0	-5.837074	0.630503	-0.815033
46	1	0	-4.065963	0.613715	-2.029837
47	6	0	-5.648986	-0.404962	1.361539
48	1	0	-3.730137	-1.237645	1.849203
49	6	0	-6.414485	0.259745	0.401496
50	1	0	-6.436028	1.124283	-1.573626
51	1	0	-6.100240	-0.716930	2.298024
52	1	0	-7.461377	0.472192	0.593120
53	6	0	-0.370831	2.650721	-0.584568
54	6	0	-0.496865	4.029488	-0.728845
55	6	0	0.637661	4.831944	-0.624710
56	1	0	-1.472411	4.462213	-0.924354
57	6	0	1.915379	2.841313	-0.224830
58	6	0	1.865148	4.222605	-0.366646
59	1	0	0.564719	5.908508	-0.739893
60	1	0	2.856861	2.345950	-0.032027
61	1	0	2.776620	4.802530	-0.275295
62	7	0	0.819950	2.058591	-0.325597
63	1	0	0.661168	0.310112	-1.799289

Co^{III}-H **2'$_A$** (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1466.12547935 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.830068	-0.718497	1.477495
2	6	0	1.924478	0.056983	2.121750
3	1	0	1.572507	1.084372	2.264541
4	1	0	2.169134	-0.345251	3.113348
5	6	0	1.182091	-2.169566	1.424727
6	1	0	2.272260	-2.263692	1.449071
7	1	0	0.803509	-2.695782	2.308406
8	6	0	-0.501558	-0.511183	2.129199
9	1	0	-1.075570	-1.431259	2.000928
10	1	0	-0.384185	-0.358514	3.209038
11	27	0	0.742843	-0.027640	-0.543222
12	6	0	3.141528	0.044002	1.218141
13	6	0	4.447137	0.089291	1.702008
14	6	0	3.897666	-0.055821	-0.982333
15	6	0	5.505777	0.067109	0.791229
16	1	0	4.632922	0.134221	2.770322
17	6	0	5.227742	-0.014324	-0.574149
18	1	0	3.631738	-0.113936	-2.033315
19	1	0	6.531625	0.101278	1.144192
20	1	0	6.022071	-0.047292	-1.311522
21	6	0	0.692332	-2.817733	0.152459
22	6	0	0.480706	-4.190622	0.052911
23	6	0	0.132350	-4.739519	-1.181719
24	1	0	0.594620	-4.820781	0.928994
25	6	0	0.209320	-2.535153	-2.117568
26	6	0	0.000686	-3.897490	-2.287041
27	1	0	-0.033173	-5.807867	-1.278350
28	1	0	0.108394	-1.842321	-2.944106
29	1	0	-0.263774	-4.283863	-3.264900
30	7	0	2.875210	-0.019241	-0.106322
31	7	0	0.546054	-2.001270	-0.920644
32	6	0	-1.249180	0.659828	1.505299
33	1	0	-2.249262	0.743330	1.946698
34	1	0	-0.725314	1.596124	1.714894
35	7	0	-1.334828	0.504390	0.022960
36	6	0	-1.621048	1.808259	-0.615242
37	1	0	-1.879424	1.617800	-1.663240
38	1	0	-2.487021	2.301555	-0.159625
39	6	0	-2.360262	-0.531576	-0.401229

40	1	0	-2.251784	-0.627476	-1.485336
41	1	0	-2.051311	-1.482494	0.037297
42	6	0	-3.799112	-0.232231	-0.040203
43	6	0	-4.625862	0.476769	-0.925518
44	6	0	-4.343556	-0.688308	1.170982
45	6	0	-5.954506	0.746291	-0.596842
46	1	0	-4.240680	0.798826	-1.890188
47	6	0	-5.671720	-0.418123	1.502627
48	1	0	-3.737350	-1.283899	1.850587
49	6	0	-6.477272	0.304940	0.620737
50	1	0	-6.584728	1.286931	-1.295842
51	1	0	-6.080689	-0.783198	2.439400
52	1	0	-7.512840	0.508793	0.873514
53	6	0	-0.413367	2.709182	-0.576782
54	6	0	-0.539891	4.096996	-0.623383
55	6	0	0.606074	4.887096	-0.674533
56	1	0	-1.528267	4.544876	-0.626786
57	6	0	1.902844	2.872791	-0.605854
58	6	0	1.851999	4.259444	-0.669376
59	1	0	0.528655	5.968691	-0.718888
60	1	0	2.851558	2.354330	-0.603904
61	1	0	2.773604	4.828883	-0.713298
62	7	0	0.794229	2.104675	-0.549906
63	1	0	0.688496	0.309512	-1.981832

Co^{III}-H **2'$_A$** (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1466.09032648 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.842530	-0.834231	1.484348
2	6	0	1.938100	-0.079116	2.145323
3	1	0	1.583580	0.938262	2.346537
4	1	0	2.206872	-0.523116	3.112566
5	6	0	1.182443	-2.278437	1.391323
6	1	0	2.273046	-2.374831	1.389698
7	1	0	0.823182	-2.822422	2.273113
8	6	0	-0.486343	-0.616549	2.124320
9	1	0	-1.086222	-1.511215	1.946870
10	1	0	-0.385491	-0.514149	3.212281
11	27	0	0.766932	0.079922	-0.568962
12	6	0	3.139940	-0.034570	1.222498
13	6	0	4.455639	-0.045840	1.679036
14	6	0	3.853099	0.024577	-0.997802

15	6	0	5.495611	-0.014604	0.747376
16	1	0	4.662347	-0.086994	2.743589
17	6	0	5.190558	0.013140	-0.614569
18	1	0	3.564191	0.046899	-2.044469
19	1	0	6.528534	-0.024783	1.080701
20	1	0	5.969609	0.022222	-1.368646
21	6	0	0.660511	-2.905162	0.118579
22	6	0	0.411591	-4.274107	0.032550
23	6	0	0.041099	-4.822364	-1.195512
24	1	0	0.515188	-4.900799	0.912665
25	6	0	0.169459	-2.622578	-2.134595
26	6	0	-0.074767	-3.980970	-2.301989
27	1	0	-0.153410	-5.886367	-1.285178
28	1	0	0.077530	-1.928796	-2.963478
29	1	0	-0.355769	-4.362773	-3.277136
30	7	0	2.850811	0.009662	-0.097017
31	7	0	0.528251	-2.088680	-0.949140
32	6	0	-1.193294	0.609456	1.552006
33	1	0	-2.192540	0.701085	1.993337
34	1	0	-0.644274	1.520826	1.806701
35	7	0	-1.289894	0.537612	0.063066
36	6	0	-1.608449	1.873498	-0.501120
37	1	0	-1.917729	1.727909	-1.541826
38	1	0	-2.457413	2.330612	0.018541
39	6	0	-2.307767	-0.488755	-0.414282
40	1	0	-2.187757	-0.536460	-1.499594
41	1	0	-1.994456	-1.454072	-0.015317
42	6	0	-3.749082	-0.207082	-0.050525
43	6	0	-4.580132	0.505115	-0.929460
44	6	0	-4.294132	-0.687334	1.151394
45	6	0	-5.913270	0.754729	-0.603546
46	1	0	-4.194803	0.843916	-1.888322
47	6	0	-5.626676	-0.436651	1.480356
48	1	0	-3.686286	-1.288298	1.824582
49	6	0	-6.436355	0.290307	0.605233
50	1	0	-6.546455	1.297513	-1.298174
51	1	0	-6.036150	-0.820689	2.409274
52	1	0	-7.475344	0.478612	0.856015
53	6	0	-0.416325	2.798915	-0.491568
54	6	0	-0.573241	4.183853	-0.504872
55	6	0	0.555411	4.996117	-0.600683
56	1	0	-1.567342	4.615210	-0.449005
57	6	0	1.897695	3.013544	-0.634005
58	6	0	1.815782	4.398059	-0.671125

59	1	0	0.454116	6.076624	-0.619682
60	1	0	2.855515	2.510345	-0.678487
61	1	0	2.719662	4.991594	-0.749473
62	7	0	0.805815	2.221736	-0.541930
63	1	0	0.495660	0.050394	-2.227022

Co^{III}-H **2'$_B$** (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1466.15003768 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.214747	1.409926	-1.495221
2	6	0	2.501375	1.028905	-2.151481
3	1	0	2.438198	1.139414	-3.239580
4	1	0	3.276036	1.717506	-1.798783
5	6	0	1.148630	2.876228	-1.209777
6	1	0	2.159789	3.219503	-0.970351
7	1	0	0.807720	3.438659	-2.086229
8	6	0	0.013811	0.968304	-2.310763
9	1	0	-0.789960	1.677413	-2.104312
10	1	0	0.244380	1.045642	-3.378725
11	27	0	1.103596	0.464938	0.239151
12	6	0	2.914725	-0.361707	-1.752118
13	6	0	3.849330	-1.095403	-2.478390
14	6	0	2.852201	-1.981429	-0.088545
15	6	0	4.299043	-2.313694	-1.972697
16	1	0	4.228742	-0.706786	-3.417869
17	6	0	3.797591	-2.756447	-0.748399
18	1	0	2.446751	-2.295927	0.863858
19	1	0	5.032037	-2.899636	-2.517644
20	1	0	4.129240	-3.688568	-0.305025
21	6	0	0.273441	3.121627	-0.007571
22	6	0	-0.335105	4.348501	0.242483
23	6	0	-1.028103	4.532479	1.438847
24	1	0	-0.254248	5.150105	-0.484455
25	6	0	-0.484931	2.270269	2.021658
26	6	0	-1.096228	3.475501	2.346326
27	1	0	-1.502658	5.483374	1.658445
28	1	0	-0.528377	1.423742	2.695022
29	1	0	-1.618598	3.574458	3.291199
30	7	0	2.398651	-0.809642	-0.582568
31	7	0	0.184063	2.087996	0.865822
32	6	0	-0.437769	-0.446541	-1.949256
33	1	0	-1.341147	-0.702214	-2.513425

34	1	0	0.326987	-1.178192	-2.215451
35	7	0	-0.662794	-0.505304	-0.480695
36	6	0	-0.538179	-1.855674	0.123630
37	1	0	-1.478399	-2.413582	0.080674
38	1	0	0.196745	-2.428319	-0.450906
39	6	0	-1.989425	0.120769	-0.075070
40	1	0	-1.998125	0.119960	1.017428
41	1	0	-1.961805	1.164705	-0.389707
42	6	0	-3.236381	-0.550531	-0.606199
43	6	0	-3.895518	-1.537056	0.145072
44	6	0	-3.788920	-0.165698	-1.838739
45	6	0	-5.052339	-2.149302	-0.338944
46	1	0	-3.523756	-1.806348	1.131465
47	6	0	-4.944673	-0.777159	-2.325405
48	1	0	-3.335319	0.640142	-2.411971
49	6	0	-5.573293	-1.776265	-1.579381
50	1	0	-5.554699	-2.904333	0.257402
51	1	0	-5.362689	-0.463747	-3.276753
52	1	0	-6.476191	-2.247635	-1.953994
53	6	0	-0.048906	-1.718793	1.552382
54	6	0	-0.367431	-2.631176	2.555595
55	6	0	0.190872	-2.476513	3.825978
56	1	0	-1.042161	-3.453392	2.340682
57	6	0	1.330315	-0.525474	3.023129
58	6	0	1.056287	-1.407711	4.062898
59	1	0	-0.047171	-3.179754	4.617750
60	1	0	1.997920	0.319070	3.151513
61	1	0	1.514712	-1.254572	5.033474
62	7	0	0.787763	-0.674018	1.796604
63	1	0	2.299431	1.097207	0.760028

Co^{III}-H **2'$_B$** (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1466.12835902 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.323903	1.654920	-1.262113
2	6	0	2.537056	1.271876	-2.022679
3	1	0	2.384962	1.398981	-3.101548
4	1	0	3.353498	1.948623	-1.749198
5	6	0	1.416378	3.017058	-0.684542
6	1	0	2.463656	3.210837	-0.429410
7	1	0	1.115447	3.789896	-1.403396
8	6	0	0.073357	1.482864	-2.064305

9	1	0	-0.680535	2.157781	-1.652971
10	1	0	0.237317	1.790301	-3.105117
11	27	0	1.060697	0.243079	0.468543
12	6	0	3.009475	-0.136823	-1.729794
13	6	0	3.945208	-0.763989	-2.554210
14	6	0	3.058104	-1.928630	-0.243681
15	6	0	4.446909	-2.011511	-2.192248
16	1	0	4.281393	-0.270203	-3.460552
17	6	0	3.999231	-2.602559	-1.008024
18	1	0	2.683419	-2.343945	0.684183
19	1	0	5.179807	-2.511167	-2.817671
20	1	0	4.372494	-3.566082	-0.679809
21	6	0	0.609073	3.137883	0.590092
22	6	0	0.124006	4.363955	1.042903
23	6	0	-0.517274	4.431158	2.279263
24	1	0	0.257325	5.253641	0.435909
25	6	0	-0.167147	2.074257	2.515160
26	6	0	-0.662302	3.264195	3.031772
27	1	0	-0.895511	5.378466	2.649992
28	1	0	-0.261623	1.141127	3.059398
29	1	0	-1.150040	3.271326	4.000007
30	7	0	2.559650	-0.724584	-0.603276
31	7	0	0.447895	2.010068	1.315912
32	6	0	-0.435250	0.043623	-2.022489
33	1	0	-1.344708	-0.052057	-2.625156
34	1	0	0.309025	-0.633017	-2.450719
35	7	0	-0.674884	-0.367664	-0.611079
36	6	0	-0.673461	-1.846255	-0.432055
37	1	0	-1.617309	-2.291583	-0.762247
38	1	0	0.119316	-2.262632	-1.063535
39	6	0	-1.958202	0.231204	-0.040331
40	1	0	-1.982959	-0.061629	1.012394
41	1	0	-1.838510	1.315034	-0.065189
42	6	0	-3.245335	-0.170240	-0.724548
43	6	0	-3.983815	-1.274500	-0.269389
44	6	0	-3.751377	0.580962	-1.797691
45	6	0	-5.178955	-1.637997	-0.891060
46	1	0	-3.640345	-1.835103	0.597296
47	6	0	-4.945696	0.218870	-2.421131
48	1	0	-3.227032	1.473102	-2.133143
49	6	0	-5.657377	-0.895840	-1.972775
50	1	0	-5.743704	-2.488600	-0.522773
51	1	0	-5.327711	0.813301	-3.244966
52	1	0	-6.590135	-1.174059	-2.452710

53	6	0	-0.382801	-2.200415	1.013048
54	6	0	-0.900245	-3.340595	1.624311
55	6	0	-0.536332	-3.633519	2.939704
56	1	0	-1.576527	-3.988529	1.076404
57	6	0	0.812959	-1.653711	2.944107
58	6	0	0.335672	-2.775302	3.612181
59	1	0	-0.929688	-4.516903	3.432786
60	1	0	1.498377	-0.961396	3.421855
61	1	0	0.642571	-2.967728	4.634164
62	7	0	0.462457	-1.367698	1.672043
63	1	0	2.204600	0.507678	1.355122

Co^{III}-H **2'$_B$** (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1466.08466714 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.403131	1.590129	-1.221664
2	6	0	2.658642	1.192857	-1.923014
3	1	0	2.565759	1.354005	-3.003336
4	1	0	3.463905	1.851564	-1.581134
5	6	0	1.456040	3.000389	-0.736114
6	1	0	2.479328	3.204938	-0.402978
7	1	0	1.236522	3.706239	-1.546373
8	6	0	0.178534	1.360029	-2.064711
9	1	0	-0.590740	2.051576	-1.714987
10	1	0	0.392024	1.619681	-3.108445
11	27	0	1.159288	0.345307	0.528434
12	6	0	3.091702	-0.233089	-1.638504
13	6	0	4.034018	-0.868477	-2.446960
14	6	0	3.050033	-2.047591	-0.178148
15	6	0	4.495834	-2.132884	-2.084768
16	1	0	4.406926	-0.374784	-3.338812
17	6	0	4.000313	-2.731279	-0.923314
18	1	0	2.634137	-2.468252	0.730631
19	1	0	5.234001	-2.641792	-2.696498
20	1	0	4.341916	-3.708614	-0.601517
21	6	0	0.527693	3.231262	0.441150
22	6	0	0.021713	4.495541	0.736766
23	6	0	-0.735116	4.668477	1.896392
24	1	0	0.224904	5.331884	0.075642
25	6	0	-0.452032	2.335976	2.358042
26	6	0	-0.973237	3.570087	2.725303
27	1	0	-1.132569	5.646410	2.148856

28	1	0	-0.613768	1.450149	2.963108
29	1	0	-1.553557	3.664888	3.636188
30	7	0	2.596681	-0.825006	-0.530947
31	7	0	0.278686	2.167886	1.237936
32	6	0	-0.333012	-0.077793	-1.977546
33	1	0	-1.210504	-0.192157	-2.623765
34	1	0	0.426017	-0.773763	-2.343187
35	7	0	-0.648885	-0.432269	-0.566577
36	6	0	-0.631960	-1.894524	-0.322328
37	1	0	-1.555900	-2.372262	-0.664176
38	1	0	0.190160	-2.328397	-0.901677
39	6	0	-1.960855	0.176076	-0.090680
40	1	0	-2.026638	-0.053860	0.975459
41	1	0	-1.857534	1.258666	-0.174780
42	6	0	-3.210853	-0.285934	-0.805712
43	6	0	-3.954972	-1.372008	-0.317393
44	6	0	-3.677070	0.390306	-1.944690
45	6	0	-5.115825	-1.790933	-0.968458
46	1	0	-3.643342	-1.874124	0.595818
47	6	0	-4.836563	-0.027783	-2.598312
48	1	0	-3.151226	1.270660	-2.308247
49	6	0	-5.553662	-1.124037	-2.114525
50	1	0	-5.685906	-2.626188	-0.574133
51	1	0	-5.188387	0.509691	-3.473172
52	1	0	-6.459856	-1.445531	-2.617756
53	6	0	-0.394870	-2.164237	1.147854
54	6	0	-0.929430	-3.271424	1.803675
55	6	0	-0.628548	-3.475800	3.151354
56	1	0	-1.571599	-3.960388	1.264607
57	6	0	0.695268	-1.479197	3.089521
58	6	0	0.196777	-2.561724	3.806761
59	1	0	-1.035345	-4.331734	3.680535
60	1	0	1.350167	-0.748540	3.552359
61	1	0	0.454438	-2.680453	4.853319
62	7	0	0.407107	-1.281705	1.786858
63	1	0	2.207473	0.510251	1.861649

Co^{III}-H **2'$_C$** (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1466.14742538 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.994308	-1.964252	-0.094651
2	6	0	1.896117	-2.159872	1.095788

3	1	0	1.620213	-3.079484	1.622251
4	1	0	2.916178	-2.309841	0.728504
5	6	0	1.705874	-2.390521	-1.340849
6	1	0	2.156876	-3.383582	-1.230284
7	1	0	0.973557	-2.437201	-2.151587
8	6	0	-0.341687	-2.615971	0.120125
9	1	0	-0.771854	-2.828725	-0.859855
10	1	0	-0.231476	-3.572102	0.642880
11	27	0	0.620181	-0.040914	-0.385891
12	6	0	1.915401	-0.980516	2.036513
13	6	0	2.494011	-1.074957	3.303078
14	6	0	1.530471	1.287463	2.316579
15	6	0	2.591499	0.071974	4.087607
16	1	0	2.869032	-2.028139	3.662214
17	6	0	2.109561	1.280176	3.579344
18	1	0	1.134192	2.203158	1.891099
19	1	0	3.039220	0.025647	5.075165
20	1	0	2.174592	2.199328	4.150775
21	6	0	2.750126	-1.337098	-1.637287
22	6	0	3.946362	-1.602793	-2.295447
23	6	0	4.855070	-0.562813	-2.499958
24	1	0	4.164293	-2.608826	-2.638877
25	6	0	3.340129	0.897441	-1.349854
26	6	0	4.552183	0.705228	-2.005445
27	1	0	5.790538	-0.745834	-3.018661
28	1	0	3.077842	1.861535	-0.930461
29	1	0	5.241289	1.534892	-2.116245
30	7	0	1.421857	0.177901	1.556677
31	7	0	2.443436	-0.092421	-1.188604
32	6	0	-1.233776	-1.657225	0.908156
33	1	0	-2.236376	-2.072920	1.043695
34	1	0	-0.816994	-1.469311	1.900580
35	7	0	-1.280489	-0.361133	0.163150
36	6	0	-1.610155	0.826796	1.001359
37	1	0	-2.685235	0.900764	1.187540
38	1	0	-1.111843	0.720349	1.968623
39	6	0	-2.256518	-0.440789	-1.027364
40	1	0	-2.123788	0.489342	-1.580992
41	1	0	-1.893809	-1.242373	-1.670355
42	6	0	-3.709255	-0.654746	-0.674410
43	6	0	-4.572247	0.440323	-0.502265
44	6	0	-4.241546	-1.950902	-0.573740
45	6	0	-5.920156	0.246109	-0.199698
46	1	0	-4.196961	1.452033	-0.639572

47	6	0	-5.589014	-2.147426	-0.270531
48	1	0	-3.610612	-2.815723	-0.767318
49	6	0	-6.428208	-1.048633	-0.074941
50	1	0	-6.576474	1.102025	-0.078436
51	1	0	-5.986926	-3.154987	-0.204161
52	1	0	-7.478241	-1.200844	0.153222
53	6	0	-1.095511	2.044086	0.264521
54	6	0	-1.690807	3.299868	0.342157
55	6	0	-1.171761	4.349558	-0.417990
56	1	0	-2.557331	3.446969	0.978516
57	6	0	0.462295	2.824704	-1.286882
58	6	0	-0.086597	4.102388	-1.258450
59	1	0	-1.623031	5.335553	-0.372871
60	1	0	1.286764	2.583984	-1.946512
61	1	0	0.326270	4.878755	-1.892690
62	7	0	-0.008139	1.821612	-0.521221
63	1	0	0.177215	-0.262827	-1.735278

Co^{III}-H **2'$_c$** (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1466.12612230 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.079933	-1.932092	0.398654
2	6	0	2.003962	-1.839830	1.561575
3	1	0	1.783956	-2.626147	2.293858
4	1	0	3.022979	-2.029531	1.206113
5	6	0	1.722954	-2.643933	-0.732215
6	1	0	2.178947	-3.592593	-0.421156
7	1	0	0.947979	-2.883552	-1.468037
8	6	0	-0.256833	-2.480584	0.763920
9	1	0	-0.679697	-2.956348	-0.123156
10	1	0	-0.168176	-3.260577	1.529922
11	27	0	0.755558	0.129149	-0.351299
12	6	0	2.010533	-0.484884	2.235930
13	6	0	2.529406	-0.327401	3.521551
14	6	0	1.658444	1.807895	2.052114
15	6	0	2.619217	0.950530	4.069756
16	1	0	2.864969	-1.195520	4.079923
17	6	0	2.181646	2.041964	3.316407
18	1	0	1.294468	2.623261	1.436850
19	1	0	3.023838	1.092726	5.066819
20	1	0	2.237321	3.054098	3.701010
21	6	0	2.753687	-1.747953	-1.385115

22	6	0	3.892179	-2.246586	-2.013992
23	6	0	4.771001	-1.360619	-2.637648
24	1	0	4.083626	-3.314751	-2.015532
25	6	0	3.340843	0.433886	-1.952790
26	6	0	4.492135	0.006060	-2.602823
27	1	0	5.660766	-1.730575	-3.136896
28	1	0	3.091873	1.487966	-1.897463
29	1	0	5.151081	0.731148	-3.066963
30	7	0	1.568216	0.570150	1.516661
31	7	0	2.488845	-0.422660	-1.355800
32	6	0	-1.187717	-1.372936	1.258903
33	1	0	-2.171015	-1.790598	1.499458
34	1	0	-0.790924	-0.928319	2.175008
35	7	0	-1.296255	-0.300409	0.233729
36	6	0	-1.724657	0.998833	0.815154
37	1	0	-2.806441	1.021133	0.980601
38	1	0	-1.245033	1.111136	1.793599
39	6	0	-2.207327	-0.692410	-0.930319
40	1	0	-2.134188	0.124408	-1.651978
41	1	0	-1.754151	-1.568491	-1.398168
42	6	0	-3.652557	-0.965325	-0.585400
43	6	0	-4.610278	0.059363	-0.659086
44	6	0	-4.077490	-2.257217	-0.234285
45	6	0	-5.948862	-0.191567	-0.355896
46	1	0	-4.314580	1.052874	-0.989007
47	6	0	-5.415037	-2.510320	0.070356
48	1	0	-3.367701	-3.081711	-0.228944
49	6	0	-6.351296	-1.475514	0.017210
50	1	0	-6.679216	0.608223	-0.426815
51	1	0	-5.729167	-3.515647	0.332348
52	1	0	-7.393484	-1.673583	0.246173
53	6	0	-1.300977	2.147929	-0.078450
54	6	0	-2.065091	3.305260	-0.216365
55	6	0	-1.599319	4.339156	-1.029335
56	1	0	-3.012847	3.389529	0.305323
57	6	0	0.323178	2.996937	-1.517178
58	6	0	-0.383804	4.180284	-1.695924
59	1	0	-2.181199	5.247320	-1.150194
60	1	0	1.262108	2.826954	-2.032476
61	1	0	0.008654	4.950634	-2.350182
62	7	0	-0.115215	2.006633	-0.714709
63	1	0	0.228884	-0.137950	-1.691048

Co^{III}-H **2'$_C$** (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1466.08239764 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.048468	-1.821496	0.568213
2	6	0	1.964057	-1.572702	1.721989
3	1	0	1.632520	-2.145687	2.595195
4	1	0	2.957522	-1.957153	1.467258
5	6	0	1.713078	-2.684156	-0.450930
6	1	0	2.080722	-3.617419	-0.006274
7	1	0	0.960972	-2.956392	-1.200208
8	6	0	-0.265762	-2.382811	1.002447
9	1	0	-0.693803	-2.928359	0.159077
10	1	0	-0.137434	-3.107529	1.815449
11	27	0	0.615754	0.099905	-0.456698
12	6	0	2.127193	-0.115544	2.102331
13	6	0	2.763600	0.231249	3.295841
14	6	0	1.919948	2.124161	1.512277
15	6	0	2.985584	1.575388	3.583872
16	1	0	3.086821	-0.544288	3.983224
17	6	0	2.560597	2.542754	2.669607
18	1	0	1.560334	2.838672	0.780619
19	1	0	3.482574	1.864556	4.504446
20	1	0	2.716993	3.600155	2.851040
21	6	0	2.834116	-1.932045	-1.131967
22	6	0	3.998947	-2.554860	-1.576947
23	6	0	4.956958	-1.794703	-2.249996
24	1	0	4.150565	-3.615386	-1.403354
25	6	0	3.540035	0.117184	-1.973431
26	6	0	4.725682	-0.433440	-2.450025
27	1	0	5.869384	-2.258586	-2.610709
28	1	0	3.314083	1.169559	-2.114274
29	1	0	5.444661	0.192438	-2.966774
30	7	0	1.702654	0.819921	1.229888
31	7	0	2.619995	-0.615433	-1.323977
32	6	0	-1.205013	-1.263382	1.440442
33	1	0	-2.178988	-1.673049	1.728416
34	1	0	-0.794918	-0.749354	2.314638
35	7	0	-1.346591	-0.262302	0.345896
36	6	0	-1.830677	1.050169	0.854834
37	1	0	-2.904500	1.018548	1.065291
38	1	0	-1.318600	1.254096	1.801958
39	6	0	-2.226044	-0.761101	-0.803656
40	1	0	-2.190308	0.017342	-1.569177

41	1	0	-1.728387	-1.638015	-1.224731
42	6	0	-3.658087	-1.088140	-0.446824
43	6	0	-4.660957	-0.112088	-0.561968
44	6	0	-4.019472	-2.380883	-0.034627
45	6	0	-5.985732	-0.411886	-0.242806
46	1	0	-4.411914	0.878904	-0.934649
47	6	0	-5.343586	-2.681962	0.285172
48	1	0	-3.271175	-3.169342	0.008145
49	6	0	-6.327113	-1.695379	0.188280
50	1	0	-6.752611	0.349234	-0.345978
51	1	0	-5.609888	-3.687794	0.593959
52	1	0	-7.358539	-1.931261	0.429729
53	6	0	-1.506152	2.152948	-0.129592
54	6	0	-2.305859	3.284140	-0.282547
55	6	0	-1.916892	4.273289	-1.187082
56	1	0	-3.218176	3.385103	0.296279
57	6	0	-0.002696	2.939451	-1.728712
58	6	0	-0.745605	4.097194	-1.926584
59	1	0	-2.525796	5.161560	-1.322409
60	1	0	0.901795	2.746549	-2.296703
61	1	0	-0.417721	4.834427	-2.650852
62	7	0	-0.366183	1.995210	-0.837970
63	1	0	0.579166	0.022671	-2.168534

2'$_{dp}$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1465.85041792 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.275565	-1.621796	-1.024056
2	6	0	-2.252875	-1.322284	-2.080731
3	1	0	-1.715387	-0.859313	-2.916534
4	1	0	-2.726975	-2.231785	-2.482213
5	6	0	-1.826377	-2.540519	-0.008213
6	1	0	-2.901956	-2.341731	0.063881
7	1	0	-1.718164	-3.595147	-0.302885
8	6	0	0.043958	-2.052787	-1.537658
9	1	0	0.530631	-2.624916	-0.743068
10	1	0	-0.058236	-2.733658	-2.396636
11	27	0	-0.948633	0.291314	0.050247
12	6	0	-3.320250	-0.350635	-1.600525
13	6	0	-4.597583	-0.346901	-2.160315
14	6	0	-3.859344	1.439500	-0.234692
15	6	0	-5.527175	0.601268	-1.734255

16	1	0	-4.856960	-1.078196	-2.919683
17	6	0	-5.148980	1.515168	-0.751337
18	1	0	-3.524815	2.129614	0.533458
19	1	0	-6.525989	0.622660	-2.158393
20	1	0	-5.836431	2.270136	-0.385770
21	6	0	-1.223365	-2.309509	1.364040
22	6	0	-1.076291	-3.348921	2.280902
23	6	0	-0.607251	-3.068477	3.564736
24	1	0	-1.332991	-4.363510	1.991839
25	6	0	-0.451773	-0.768301	2.909446
26	6	0	-0.293421	-1.747600	3.884823
27	1	0	-0.488350	-3.862296	4.295046
28	1	0	-0.206424	0.269406	3.114238
29	1	0	0.074342	-1.476400	4.868546
30	7	0	-2.955126	0.527863	-0.640031
31	7	0	-0.905450	-1.028197	1.666830
32	6	0	0.932967	-0.864660	-1.936964
33	1	0	1.875320	-1.245701	-2.353584
34	1	0	0.445718	-0.300000	-2.738134
35	7	0	1.150752	0.060440	-0.804879
36	6	0	1.400265	1.456296	-1.215571
37	1	0	2.437382	1.631028	-1.530141
38	1	0	0.765448	1.663283	-2.086124
39	6	0	2.161638	-0.427105	0.187090
40	1	0	2.111056	0.257780	1.038290
41	1	0	1.813877	-1.397502	0.549833
42	6	0	3.593040	-0.539834	-0.302420
43	6	0	4.482517	0.537863	-0.172075
44	6	0	4.066514	-1.727532	-0.881039
45	6	0	5.796825	0.442510	-0.631459
46	1	0	4.149563	1.451584	0.314807
47	6	0	5.379793	-1.826840	-1.342529
48	1	0	3.410441	-2.592234	-0.951136
49	6	0	6.246433	-0.738881	-1.223953
50	1	0	6.472391	1.284951	-0.516604
51	1	0	5.729240	-2.755853	-1.782974
52	1	0	7.269894	-0.816259	-1.577750
53	6	0	1.017565	2.426319	-0.111577
54	6	0	1.756795	3.579721	0.143963
55	6	0	1.332408	4.462514	1.137986
56	1	0	2.654016	3.780770	-0.433150
57	6	0	-0.509703	2.984234	1.540608
58	6	0	0.175290	4.154534	1.852442
59	1	0	1.894355	5.366171	1.350876

60	1	0	-1.416715	2.711654	2.072261
61	1	0	-0.195349	4.805457	2.636926
62	7	0	-0.109691	2.125930	0.579819

2'$_{dp}$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1465.81441560 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.187595	-1.532990	-1.122109
2	6	0	-2.177748	-1.195365	-2.180405
3	1	0	-1.636398	-0.684308	-2.984341
4	1	0	-2.633553	-2.097730	-2.610763
5	6	0	-1.734014	-2.574324	-0.210245
6	1	0	-2.804672	-2.369569	-0.096033
7	1	0	-1.639575	-3.576821	-0.649406
8	6	0	0.136443	-1.930821	-1.686991
9	1	0	0.639870	-2.543155	-0.934295
10	1	0	0.009486	-2.558108	-2.580067
11	27	0	-0.919176	0.153416	-0.081641
12	6	0	-3.207860	-0.255355	-1.614832
13	6	0	-4.515500	-0.197200	-2.076620
14	6	0	-3.567756	1.536920	-0.189685
15	6	0	-5.378976	0.783284	-1.582249
16	1	0	-4.848499	-0.905338	-2.829371
17	6	0	-4.878755	1.669497	-0.627186
18	1	0	-3.165605	2.212057	0.555612
19	1	0	-6.402737	0.852910	-1.932916
20	1	0	-5.498548	2.457103	-0.211800
21	6	0	-1.091002	-2.506420	1.156411
22	6	0	-0.969374	-3.626139	1.977551
23	6	0	-0.451820	-3.469560	3.264239
24	1	0	-1.282272	-4.601780	1.618416
25	6	0	-0.211106	-1.132118	2.792338
26	6	0	-0.069538	-2.194736	3.681048
27	1	0	-0.349921	-4.324470	3.924899
28	1	0	0.082536	-0.124790	3.075619
29	1	0	0.337485	-2.023207	4.671820
30	7	0	-2.716391	0.587951	-0.655863
31	7	0	-0.707823	-1.272286	1.550562
32	6	0	0.984389	-0.697990	-2.009483
33	1	0	1.962461	-1.010981	-2.397568
34	1	0	0.502856	-0.106842	-2.792238

35	7	0	1.100593	0.154949	-0.802499
36	6	0	1.240938	1.602881	-1.085364
37	1	0	2.271576	1.892816	-1.326521
38	1	0	0.611801	1.831192	-1.952706
39	6	0	2.148991	-0.329782	0.162264
40	1	0	2.035420	0.276037	1.065006
41	1	0	1.878235	-1.350842	0.438340
42	6	0	3.587017	-0.285485	-0.315286
43	6	0	4.384186	0.847654	-0.091208
44	6	0	4.163621	-1.387324	-0.965752
45	6	0	5.707481	0.891529	-0.531758
46	1	0	3.972857	1.693422	0.454739
47	6	0	5.486464	-1.347406	-1.408434
48	1	0	3.581847	-2.295568	-1.106596
49	6	0	6.259405	-0.204216	-1.197914
50	1	0	6.310671	1.774853	-0.344594
51	1	0	5.916374	-2.211653	-1.905682
52	1	0	7.290229	-0.173313	-1.537010
53	6	0	0.724125	2.385169	0.099525
54	6	0	1.292232	3.575300	0.539717
55	6	0	0.733367	4.242421	1.633505
56	1	0	2.160564	3.975214	0.026054
57	6	0	-0.882057	2.474810	1.779058
58	6	0	-0.368690	3.673314	2.267686
59	1	0	1.157183	5.177208	1.985405
60	1	0	-1.729308	1.991404	2.254109
61	1	0	-0.827992	4.141565	3.131433
62	7	0	-0.367559	1.840838	0.703507

3'$_A$ (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1466.74194080 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.768366	-1.038317	-1.230052
2	6	0	-2.528509	-0.241398	-2.219933
3	1	0	-1.823004	0.212569	-2.923110
4	1	0	-3.196722	-0.872925	-2.819939
5	6	0	-2.639794	-2.064701	-0.610038
6	1	0	-3.654533	-1.653066	-0.557660
7	1	0	-2.697741	-2.969255	-1.230148
8	6	0	-0.529699	-1.628439	-1.790532
9	1	0	-0.208118	-2.424056	-1.113471
10	1	0	-0.714294	-2.100108	-2.766479

11	27	0	-1.100489	0.344584	0.432987
12	6	0	-3.304619	0.867325	-1.538888
13	6	0	-4.477496	1.396860	-2.071280
14	6	0	-3.364306	2.377229	0.232885
15	6	0	-5.098368	2.461846	-1.416481
16	1	0	-4.897829	0.983375	-2.982440
17	6	0	-4.532081	2.962704	-0.243728
18	1	0	-2.886224	2.717693	1.146039
19	1	0	-6.013456	2.889301	-1.813974
20	1	0	-4.986884	3.784790	0.297287
21	6	0	-2.206587	-2.403081	0.799318
22	6	0	-2.505787	-3.625668	1.396695
23	6	0	-2.172048	-3.824194	2.737010
24	1	0	-2.999721	-4.404590	0.824773
25	6	0	-1.265621	-1.608040	2.774748
26	6	0	-1.545540	-2.795078	3.441817
27	1	0	-2.399921	-4.767336	3.223462
28	1	0	-0.779500	-0.774657	3.272061
29	1	0	-1.276523	-2.907383	4.486022
30	7	0	-2.760990	1.351907	-0.401344
31	7	0	-1.584273	-1.416712	1.478707
32	6	0	0.567960	-0.580779	-1.947026
33	1	0	1.454714	-1.044950	-2.393624
34	1	0	0.237406	0.195368	-2.642868
35	7	0	0.921957	0.098459	-0.659361
36	6	0	1.647263	1.349248	-1.039616
37	1	0	2.485163	1.102837	-1.702906
38	1	0	0.948569	1.960117	-1.624768
39	6	0	1.766585	-0.800822	0.234617
40	1	0	1.947578	-0.236696	1.153233
41	1	0	1.125075	-1.640447	0.510640
42	6	0	3.074679	-1.315904	-0.331140
43	6	0	4.277939	-0.630463	-0.103602
44	6	0	3.119580	-2.522342	-1.049315
45	6	0	5.485305	-1.116241	-0.607138
46	1	0	4.279918	0.271472	0.502412
47	6	0	4.324503	-3.009916	-1.555983
48	1	0	2.212440	-3.105117	-1.191692
49	6	0	5.509402	-2.303163	-1.341778
50	1	0	6.408653	-0.579971	-0.411351
51	1	0	4.340935	-3.947199	-2.103035
52	1	0	6.448708	-2.685582	-1.728087
53	6	0	2.210331	2.238925	0.052345
54	6	0	3.420594	2.909235	-0.122991

55	6	0	3.866660	3.812714	0.844093
56	1	0	4.008469	2.722998	-1.014691
57	6	0	1.914501	3.343975	2.136450
58	6	0	3.106346	4.034360	1.995847
59	1	0	4.806332	4.336950	0.700866
60	1	0	1.258152	3.445992	2.993814
61	1	0	3.428932	4.724189	2.766931
62	7	0	1.504433	2.489311	1.177096
63	1	0	0.563236	1.983127	1.332360
64	1	0	-0.623097	1.381117	1.626236

3'$_A$ (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1466.73453364 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.021581	-1.168421	-1.040375
2	6	0	-2.992076	-0.391586	-1.869241
3	1	0	-2.814484	-0.557037	-2.938188
4	1	0	-4.001774	-0.763352	-1.665692
5	6	0	-2.609624	-2.421346	-0.478101
6	1	0	-3.652758	-2.216901	-0.213915
7	1	0	-2.614404	-3.234277	-1.214708
8	6	0	-0.765329	-1.482233	-1.793701
9	1	0	-0.277911	-2.314141	-1.281739
10	1	0	-1.014379	-1.830003	-2.804473
11	27	0	-1.510080	-0.046965	0.577606
12	6	0	-2.966389	1.087484	-1.545142
13	6	0	-3.629738	2.015273	-2.347362
14	6	0	-2.394364	2.746680	-0.016981
15	6	0	-3.670336	3.350881	-1.953456
16	1	0	-4.118472	1.689561	-3.260159
17	6	0	-3.046806	3.720864	-0.760043
18	1	0	-1.911668	2.982959	0.922949
19	1	0	-4.187171	4.087192	-2.560467
20	1	0	-3.069853	4.745059	-0.405134
21	6	0	-1.869737	-2.817794	0.780975
22	6	0	-1.839150	-4.126586	1.253136
23	6	0	-1.228219	-4.390888	2.479628
24	1	0	-2.295905	-4.923252	0.675064
25	6	0	-0.718014	-2.054624	2.656144
26	6	0	-0.663506	-3.334743	3.194927
27	1	0	-1.198073	-5.402850	2.870437

28	1	0	-0.298384	-1.202322	3.175726
29	1	0	-0.188389	-3.494749	4.156201
30	7	0	-2.337060	1.451148	-0.400678
31	7	0	-1.300766	-1.793546	1.467653
32	6	0	0.177672	-0.288826	-1.881111
33	1	0	1.014433	-0.543445	-2.544085
34	1	0	-0.342835	0.556777	-2.340382
35	7	0	0.661164	0.143762	-0.540405
36	6	0	1.225998	1.505474	-0.682252
37	1	0	2.087474	1.513454	-1.362869
38	1	0	0.452915	2.137960	-1.135254
39	6	0	1.679145	-0.819722	0.034547
40	1	0	1.925062	-0.448444	1.033307
41	1	0	1.158278	-1.766592	0.184764
42	6	0	2.948368	-1.045700	-0.763581
43	6	0	4.099260	-0.280442	-0.519273
44	6	0	3.013662	-2.053640	-1.739364
45	6	0	5.270508	-0.493587	-1.247614
46	1	0	4.093682	0.465755	0.271570
47	6	0	4.181885	-2.268553	-2.471415
48	1	0	2.155335	-2.699033	-1.912657
49	6	0	5.311137	-1.483420	-2.231240
50	1	0	6.155128	0.099486	-1.037245
51	1	0	4.215757	-3.057043	-3.216604
52	1	0	6.222994	-1.654704	-2.794229
53	6	0	1.659203	2.179740	0.601993
54	6	0	2.775309	3.011786	0.668891
55	6	0	3.079566	3.677852	1.857994
56	1	0	3.399585	3.132857	-0.209323
57	6	0	1.172601	2.664839	2.880762
58	6	0	2.270144	3.501230	2.985178
59	1	0	3.947527	4.328001	1.906903
60	1	0	0.486616	2.467575	3.697301
61	1	0	2.484858	3.999943	3.923088
62	7	0	0.900933	2.043769	1.713003
63	1	0	0.033401	1.423917	1.672077
64	1	0	-1.220265	0.758243	1.852181

3'$_B$ (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1466.73730445 hartree

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Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	7	0	-1.608752	-1.258530	-0.510594
2	6	0	-2.561499	-1.296336	-1.649966
3	1	0	-2.046093	-0.890034	-2.527190
4	1	0	-2.823113	-2.336142	-1.894985
5	6	0	-2.228949	-1.795242	0.718214
6	1	0	-3.242650	-1.384742	0.794255
7	1	0	-2.340458	-2.889014	0.675883
8	6	0	-0.396361	-2.040786	-0.896254
9	1	0	0.047789	-2.441308	0.017606
10	1	0	-0.673388	-2.909602	-1.510468
11	27	0	-0.478205	0.831281	0.236294
12	6	0	-3.862680	-0.539013	-1.486796
13	6	0	-5.095165	-1.087594	-1.831087
14	6	0	-4.922676	1.523553	-0.972644
15	6	0	-6.251297	-0.304929	-1.750757
16	1	0	-5.148556	-2.117250	-2.167132
17	6	0	-6.168018	1.020022	-1.316185
18	1	0	-4.760673	2.537007	-0.622070
19	1	0	-7.211653	-0.730254	-2.024838
20	1	0	-7.046605	1.650352	-1.243149
21	6	0	-1.491293	-1.409785	1.985806
22	6	0	-1.586242	-2.206436	3.126919
23	6	0	-0.988332	-1.783377	4.313385
24	1	0	-2.128415	-3.145659	3.085750
25	6	0	-0.226013	0.160314	3.148459
26	6	0	-0.297792	-0.571321	4.326878
27	1	0	-1.058319	-2.391146	5.209896
28	1	0	0.318015	1.098720	3.107201
29	1	0	0.183066	-0.201771	5.225494
30	7	0	-3.827573	0.746451	-1.069307
31	7	0	-0.808544	-0.241997	1.997532
32	6	0	0.631250	-1.192930	-1.646642
33	1	0	1.434350	-1.834978	-2.025774
34	1	0	0.168252	-0.715580	-2.515444
35	7	0	1.169281	-0.121996	-0.769149
36	6	0	1.745347	1.014573	-1.537548
37	1	0	2.713959	0.754296	-1.977301
38	1	0	1.062741	1.239481	-2.366046
39	6	0	2.180467	-0.657118	0.238768
40	1	0	2.424522	0.179782	0.897494
41	1	0	1.656861	-1.396319	0.848311
42	6	0	3.446474	-1.255859	-0.333554
43	6	0	4.583826	-0.459246	-0.541748

44	6	0	3.522945	-2.626209	-0.629803
45	6	0	5.755174	-1.010789	-1.061871
46	1	0	4.564083	0.593547	-0.269425
47	6	0	4.693163	-3.179771	-1.150379
48	1	0	2.673547	-3.275002	-0.426800
49	6	0	5.808988	-2.370741	-1.373646
50	1	0	6.628914	-0.383936	-1.209738
51	1	0	4.738858	-4.242230	-1.367707
52	1	0	6.721898	-2.801588	-1.772190
53	6	0	1.869948	2.252784	-0.666152
54	6	0	2.836160	3.228503	-0.904488
55	6	0	2.849288	4.378916	-0.115248
56	1	0	3.562175	3.089744	-1.698990
57	6	0	0.965033	3.506355	1.075642
58	6	0	1.895677	4.522408	0.893804
59	1	0	3.592662	5.151224	-0.285453
60	1	0	0.197229	3.578906	1.840176
61	1	0	1.870554	5.401709	1.527518
62	7	0	0.953433	2.391730	0.318882
63	1	0	-2.868986	1.160348	-0.791330
64	1	0	-1.688482	1.677566	-0.463702

3'$_B$ (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1466.73043159 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.420416	-1.188025	-0.687588
2	6	0	-2.400310	-1.017005	-1.801962
3	1	0	-1.910739	-0.426906	-2.584793
4	1	0	-2.622891	-1.997171	-2.244077
5	6	0	-2.006735	-2.034380	0.395317
6	1	0	-3.011329	-1.657936	0.612866
7	1	0	-2.119516	-3.072347	0.054437
8	6	0	-0.202011	-1.878476	-1.260144
9	1	0	0.266755	-2.428939	-0.443147
10	1	0	-0.500652	-2.616815	-2.014975
11	27	0	-0.573500	0.526059	0.208296
12	6	0	-3.736350	-0.364269	-1.499234
13	6	0	-4.890359	-0.732281	-2.187119
14	6	0	-4.957148	1.320884	-0.352906
15	6	0	-6.085149	-0.045595	-1.956416
16	1	0	-4.853144	-1.547523	-2.901544
17	6	0	-6.123274	0.997803	-1.026923

18	1	0	-4.892988	2.102661	0.395801
19	1	0	-6.983466	-0.329387	-2.495692
20	1	0	-7.036894	1.543958	-0.822960
21	6	0	-1.189152	-1.973544	1.669977
22	6	0	-1.256918	-2.989602	2.622974
23	6	0	-0.562464	-2.834751	3.822778
24	1	0	-1.846456	-3.881148	2.433207
25	6	0	0.213585	-0.717320	3.014448
26	6	0	0.182434	-1.672699	4.025805
27	1	0	-0.602003	-3.607570	4.583652
28	1	0	0.790103	0.195962	3.125137
29	1	0	0.735263	-1.509569	4.944245
30	7	0	-3.816901	0.648807	-0.610183
31	7	0	-0.454784	-0.860120	1.856051
32	6	0	0.783151	-0.874874	-1.844725
33	1	0	1.645170	-1.395138	-2.276371
34	1	0	0.318922	-0.305353	-2.655446
35	7	0	1.191049	0.080481	-0.777662
36	6	0	1.604427	1.410933	-1.313368
37	1	0	2.636386	1.401725	-1.677500
38	1	0	0.962747	1.648886	-2.170107
39	6	0	2.276294	-0.489267	0.127947
40	1	0	2.403239	0.241258	0.930374
41	1	0	1.860915	-1.388747	0.583796
42	6	0	3.606062	-0.793356	-0.523805
43	6	0	4.629148	0.168400	-0.547674
44	6	0	3.861938	-2.058720	-1.076624
45	6	0	5.860786	-0.114385	-1.139176
46	1	0	4.474239	1.134807	-0.072936
47	6	0	5.092186	-2.343338	-1.670182
48	1	0	3.108381	-2.841095	-1.015739
49	6	0	6.090846	-1.368277	-1.708870
50	1	0	6.644580	0.636513	-1.142148
51	1	0	5.276792	-3.328477	-2.086777
52	1	0	7.050818	-1.591084	-2.163474
53	6	0	1.397046	2.456478	-0.241959
54	6	0	2.170822	3.607216	-0.125790
55	6	0	1.861282	4.534745	0.870546
56	1	0	3.000137	3.773541	-0.805312
57	6	0	0.054580	3.111622	1.551375
58	6	0	0.787068	4.280771	1.723996
59	1	0	2.451372	5.439029	0.979688
60	1	0	-0.793127	2.869311	2.181416
61	1	0	0.515667	4.974934	2.511349

62	7	0	0.352670	2.213865	0.590218
63	1	0	-2.928605	0.889595	-0.047840
64	1	0	-1.887216	1.084077	0.775326

3'$_C$ (quarete) E(B3LYP/ SDD-6-31G(d,p))= -1466.73919491 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.546675	1.050299	-1.087986
2	6	0	2.302643	0.212771	-2.055838
3	1	0	1.588286	-0.272254	-2.726486
4	1	0	2.952239	0.826266	-2.695148
5	6	0	2.461109	2.122962	-0.624196
6	1	0	3.365127	1.633518	-0.241562
7	1	0	2.776187	2.750887	-1.470543
8	6	0	0.304215	1.594412	-1.692180
9	1	0	-0.083534	2.361725	-1.016737
10	1	0	0.505329	2.093570	-2.652860
11	27	0	0.724628	-0.738692	0.449164
12	6	0	3.107459	-0.873593	-1.379073
13	6	0	4.373973	-1.245546	-1.823357
14	6	0	3.119809	-2.562029	0.218741
15	6	0	5.021419	-2.322609	-1.214918
16	1	0	4.843522	-0.704228	-2.638251
17	6	0	4.380704	-2.996136	-0.175985
18	1	0	2.587462	-3.056781	1.024517
19	1	0	6.008189	-2.628469	-1.547576
20	1	0	4.844114	-3.839298	0.323648
21	6	0	1.948258	3.053674	0.453702
22	6	0	2.072653	4.437722	0.366536
23	6	0	1.687934	5.241350	1.444279
24	1	0	2.478590	4.882681	-0.535196
25	6	0	1.051772	3.274319	2.643369
26	6	0	1.171943	4.654798	2.602327
27	1	0	1.791871	6.319857	1.378156
28	1	0	0.657986	2.730294	3.495045
29	1	0	0.868115	5.251112	3.454779
30	7	0	2.491847	-1.522225	-0.365715
31	7	0	1.438176	2.527940	1.590942
32	6	0	-0.755781	0.512497	-1.919192
33	1	0	-1.663373	0.979694	-2.317552

34	1	0	-0.417593	-0.194229	-2.680971
35	7	0	-1.053614	-0.263066	-0.684736
36	6	0	-1.622936	-1.601767	-1.013661
37	1	0	-2.658600	-1.520852	-1.360529
38	1	0	-1.037020	-2.017427	-1.842122
39	6	0	-1.963488	0.505917	0.266787
40	1	0	-2.012765	-0.083367	1.185974
41	1	0	-1.435201	1.430475	0.512467
42	6	0	-3.357911	0.816768	-0.230934
43	6	0	-4.421189	-0.061222	0.033547
44	6	0	-3.626630	2.005966	-0.927458
45	6	0	-5.711607	0.227048	-0.412091
46	1	0	-4.245480	-0.963134	0.615300
47	6	0	-4.915831	2.295441	-1.375784
48	1	0	-2.830753	2.727874	-1.098639
49	6	0	-5.959290	1.402612	-1.123672
50	1	0	-6.525182	-0.457117	-0.192430
51	1	0	-5.108612	3.221484	-1.908178
52	1	0	-6.963892	1.630048	-1.465560
53	6	0	-1.532682	-2.550704	0.166279
54	6	0	-2.470389	-3.559419	0.379307
55	6	0	-2.303212	-4.424494	1.461568
56	1	0	-3.316567	-3.664525	-0.291833
57	6	0	-0.322565	-3.212038	2.043599
58	6	0	-1.212570	-4.245124	2.313836
59	1	0	-3.020164	-5.218870	1.643289
60	1	0	0.529005	-3.018272	2.688876
61	1	0	-1.056067	-4.885340	3.174666
62	7	0	-0.469109	-2.390698	0.985445
63	1	0	1.306200	1.459113	1.651151
64	1	0	1.062928	0.133052	1.788019

3'$_C$ (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1466.72158512 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.296890	1.221494	-1.177500
2	6	0	2.232467	0.566976	-2.175949
3	1	0	1.630942	0.216309	-3.019100
4	1	0	2.915234	1.315823	-2.589550
5	6	0	1.950703	2.504070	-0.759105
6	1	0	2.974340	2.251811	-0.465857
7	1	0	2.011762	3.184106	-1.617371

8	6	0	-0.021110	1.480344	-1.858243
9	1	0	-0.575157	2.198496	-1.248382
10	1	0	0.134574	1.942563	-2.841779
11	27	0	0.826367	-0.174739	0.316527
12	6	0	2.998245	-0.611681	-1.627834
13	6	0	4.250850	-0.966014	-2.125892
14	6	0	2.941147	-2.464452	-0.250502
15	6	0	4.850825	-2.136738	-1.660327
16	1	0	4.744228	-0.345412	-2.867282
17	6	0	4.179741	-2.904551	-0.709294
18	1	0	2.399732	-3.017918	0.509674
19	1	0	5.824557	-2.439819	-2.031394
20	1	0	4.608309	-3.821384	-0.320095
21	6	0	1.313476	3.262706	0.385394
22	6	0	0.880433	4.580396	0.287285
23	6	0	0.419921	5.246683	1.429177
24	1	0	0.918723	5.088192	-0.670318
25	6	0	0.827926	3.269317	2.713585
26	6	0	0.394656	4.586582	2.659676
27	1	0	0.087973	6.277667	1.356326
28	1	0	0.842723	2.680684	3.624145
29	1	0	0.050035	5.079654	3.561313
30	7	0	2.354319	-1.342569	-0.701353
31	7	0	1.268876	2.659979	1.597439
32	6	0	-0.813252	0.176899	-1.996158
33	1	0	-1.780683	0.372629	-2.470950
34	1	0	-0.281796	-0.534648	-2.632913
35	7	0	-0.967076	-0.434752	-0.652664
36	6	0	-1.130588	-1.912397	-0.641254
37	1	0	-2.143453	-2.222221	-0.919095
38	1	0	-0.436719	-2.331204	-1.378404
39	6	0	-2.072019	0.242316	0.153589
40	1	0	-2.013158	-0.170842	1.162625
41	1	0	-1.805432	1.300405	0.226185
42	6	0	-3.476250	0.097311	-0.390127
43	6	0	-4.288812	-0.973997	0.014356
44	6	0	-4.007356	1.045767	-1.278593
45	6	0	-5.585463	-1.111514	-0.481847
46	1	0	-3.916581	-1.691363	0.742094
47	6	0	-5.303702	0.909715	-1.776498
48	1	0	-3.417287	1.913808	-1.565382
49	6	0	-6.092143	-0.173573	-1.383723
50	1	0	-6.204339	-1.941050	-0.154725
51	1	0	-5.702240	1.654143	-2.458470

52	1	0	-7.102744	-0.277084	-1.765503
53	6	0	-0.758302	-2.415395	0.739150
54	6	0	-1.281046	-3.579210	1.294910
55	6	0	-0.851796	-3.981578	2.561158
56	1	0	-2.011661	-4.161171	0.742645
57	6	0	0.562491	-2.045308	2.629597
58	6	0	0.083253	-3.200019	3.239839
59	1	0	-1.246051	-4.886949	3.011424
60	1	0	1.295292	-1.406947	3.108137
61	1	0	0.438891	-3.474295	4.226653
62	7	0	0.155512	-1.659184	1.403274
63	1	0	1.558220	1.625309	1.612678
64	1	0	1.904461	0.267951	1.347858

3'$_{dp\text{-}A}$ (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1466.41352706 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.887498	-0.791195	1.468652
2	6	0	1.986163	0.010102	2.030298
3	1	0	1.630317	1.040189	2.141968
4	1	0	2.290227	-0.336592	3.030616
5	6	0	1.219442	-2.230893	1.454317
6	1	0	2.308892	-2.330433	1.399510
7	1	0	0.909877	-2.727833	2.384833
8	6	0	-0.437427	-0.545624	2.084429
9	1	0	-1.028092	-1.455029	1.945007
10	1	0	-0.352209	-0.394842	3.171247
11	27	0	0.776476	-0.031195	-0.739695
12	6	0	3.189078	0.003226	1.096202
13	6	0	4.497717	0.068866	1.575300
14	6	0	3.939613	-0.038224	-1.104524
15	6	0	5.552824	0.087798	0.661421
16	1	0	4.685795	0.100666	2.643925
17	6	0	5.272255	0.030553	-0.703611
18	1	0	3.651990	-0.078709	-2.151084
19	1	0	6.578885	0.138354	1.012524
20	1	0	6.064178	0.036026	-1.444376
21	6	0	0.637866	-2.946788	0.250095
22	6	0	0.336202	-4.308838	0.272938

23	6	0	-0.092832	-4.923080	-0.904037
24	1	0	0.441541	-4.876758	1.192227
25	6	0	0.095164	-2.802697	-2.002928
26	6	0	-0.208840	-4.160044	-2.066272
27	1	0	-0.332117	-5.982040	-0.912207
28	1	0	0.020806	-2.142355	-2.862255
29	1	0	-0.533340	-4.602048	-3.001863
30	7	0	2.924908	-0.048303	-0.225810
31	7	0	0.502936	-2.211485	-0.868072
32	6	0	-1.182018	0.644144	1.471233
33	1	0	-2.162735	0.737520	1.956982
34	1	0	-0.635902	1.565531	1.684451
35	7	0	-1.316573	0.532250	-0.002697
36	6	0	-1.568309	1.848612	-0.622626
37	1	0	-1.729002	1.668689	-1.692674
38	1	0	-2.475473	2.323712	-0.226022
39	6	0	-2.349506	-0.465970	-0.437376
40	1	0	-2.241431	-0.548789	-1.522630
41	1	0	-2.060920	-1.431869	-0.016778
42	6	0	-3.789640	-0.157571	-0.072187
43	6	0	-4.608646	0.576713	-0.943021
44	6	0	-4.342013	-0.619421	1.132163
45	6	0	-5.933182	0.861981	-0.609844
46	1	0	-4.213200	0.911940	-1.898684
47	6	0	-5.665904	-0.334788	1.470305
48	1	0	-3.739394	-1.226943	1.803901
49	6	0	-6.463088	0.411452	0.600879
50	1	0	-6.553908	1.425697	-1.299777
51	1	0	-6.077127	-0.704649	2.404787
52	1	0	-7.495056	0.628748	0.858730
53	6	0	-0.392629	2.788532	-0.491697
54	6	0	-0.572699	4.171783	-0.560953
55	6	0	0.542339	5.005131	-0.534048
56	1	0	-1.574572	4.581650	-0.641160
57	6	0	1.898913	3.042085	-0.346018
58	6	0	1.807492	4.427347	-0.426942
59	1	0	0.426757	6.082762	-0.593602
60	1	0	2.864769	2.555394	-0.263490
61	1	0	2.706516	5.033379	-0.402128
62	7	0	0.826985	2.230917	-0.375419
63	1	0	0.668787	0.199266	-2.347778

3'$_{dp\text{-}A}$ (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1466.42701655 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.875516	-0.667966	1.404774
2	6	0	1.932481	0.136031	2.053479
3	1	0	1.569376	1.167061	2.128133
4	1	0	2.135807	-0.210328	3.078769
5	6	0	1.256837	-2.105031	1.369220
6	1	0	2.347861	-2.173885	1.338162
7	1	0	0.934625	-2.628117	2.279557
8	6	0	-0.457211	-0.506842	2.050213
9	1	0	-0.996641	-1.447658	1.914225
10	1	0	-0.349555	-0.361368	3.134664
11	27	0	0.791661	-0.044160	-0.683648
12	6	0	3.212679	0.104579	1.233237
13	6	0	4.468770	0.253180	1.823704
14	6	0	4.155490	-0.115678	-0.867966
15	6	0	5.602444	0.224495	1.010759
16	1	0	4.557181	0.383431	2.898017
17	6	0	5.446259	0.031711	-0.361755
18	1	0	3.977187	-0.266173	-1.929187
19	1	0	6.590862	0.340007	1.444537
20	1	0	6.301525	-0.008392	-1.027561
21	6	0	0.720153	-2.784060	0.132983
22	6	0	0.456404	-4.151985	0.091263
23	6	0	0.061581	-4.732823	-1.113018
24	1	0	0.566670	-4.750454	0.990047
25	6	0	0.204811	-2.559419	-2.119504
26	6	0	-0.059022	-3.920005	-2.239345
27	1	0	-0.146265	-5.796552	-1.169520
28	1	0	0.119414	-1.882320	-2.959787
29	1	0	-0.357843	-4.325485	-3.199598
30	7	0	3.061145	-0.072392	-0.092871
31	7	0	0.583661	-1.990937	-0.955435
32	6	0	-1.276348	0.633305	1.449423
33	1	0	-2.236080	0.706132	1.980845
34	1	0	-0.756548	1.581256	1.612073
35	7	0	-1.455886	0.452801	-0.004206
36	6	0	-1.662890	1.727673	-0.697509
37	1	0	-1.860936	1.495419	-1.751511
38	1	0	-2.533440	2.285143	-0.321290
39	6	0	-2.489375	-0.557340	-0.369547
40	1	0	-2.413315	-0.691333	-1.453002
41	1	0	-2.192729	-1.507436	0.083889

42	6	0	-3.921701	-0.233115	0.017606
43	6	0	-4.750314	0.501915	-0.843427
44	6	0	-4.450886	-0.666691	1.242409
45	6	0	-6.061239	0.814417	-0.481947
46	1	0	-4.374077	0.816500	-1.813932
47	6	0	-5.761309	-0.355305	1.608895
48	1	0	-3.840271	-1.272606	1.908488
49	6	0	-6.567963	0.390897	0.748351
50	1	0	-6.689960	1.378177	-1.164666
51	1	0	-6.154726	-0.703845	2.559155
52	1	0	-7.589400	0.629392	1.028507
53	6	0	-0.437645	2.609500	-0.643952
54	6	0	-0.564570	3.998397	-0.703778
55	6	0	0.576021	4.794661	-0.746841
56	1	0	-1.555294	4.441029	-0.722643
57	6	0	1.868420	2.780722	-0.643688
58	6	0	1.820357	4.167703	-0.720484
59	1	0	0.495388	5.875697	-0.800076
60	1	0	2.817083	2.261752	-0.630640
61	1	0	2.743377	4.735743	-0.757847
62	7	0	0.769124	2.000813	-0.598691
63	1	0	0.747545	0.179946	-2.166989

3'$_{dp\text{-}B}$ (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1466.42283783 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.381877	1.736962	-1.211836
2	6	0	2.678184	1.386670	-1.803499
3	1	0	2.720245	1.628997	-2.876594
4	1	0	3.447769	1.993273	-1.313938
5	6	0	1.330064	3.066406	-0.585724
6	1	0	2.331538	3.293140	-0.205219
7	1	0	1.067296	3.862312	-1.299059
8	6	0	0.226135	1.458674	-2.093010
9	1	0	-0.587888	2.124992	-1.795012
10	1	0	0.460351	1.700273	-3.141112
11	27	0	1.169800	0.347330	0.551932
12	6	0	3.079067	-0.065626	-1.594572
13	6	0	4.037794	-0.657884	-2.418915
14	6	0	2.999276	-1.953421	-0.257156
15	6	0	4.489908	-1.943248	-2.130853

16	1	0	4.428764	-0.107653	-3.269350
17	6	0	3.965175	-2.601437	-1.018654
18	1	0	2.564253	-2.424926	0.617136
19	1	0	5.238479	-2.418200	-2.757000
20	1	0	4.291995	-3.598193	-0.743487
21	6	0	0.386246	3.114290	0.605338
22	6	0	-0.216814	4.311483	0.993034
23	6	0	-0.976340	4.350552	2.160881
24	1	0	-0.080530	5.202327	0.387725
25	6	0	-0.503313	2.020432	2.444470
26	6	0	-1.115686	3.180693	2.906517
27	1	0	-1.447508	5.274210	2.481484
28	1	0	-0.593514	1.084950	2.986334
29	1	0	-1.691565	3.159495	3.825190
30	7	0	2.549375	-0.715319	-0.537502
31	7	0	0.228283	1.976211	1.316381
32	6	0	-0.243330	0.000458	-2.011438
33	1	0	-1.097361	-0.145620	-2.685158
34	1	0	0.552743	-0.661657	-2.359195
35	7	0	-0.566662	-0.375799	-0.614099
36	6	0	-0.537795	-1.839417	-0.392475
37	1	0	-1.435045	-2.336371	-0.780531
38	1	0	0.316328	-2.241075	-0.947345
39	6	0	-1.878342	0.201997	-0.148820
40	1	0	-1.956564	-0.040801	0.913488
41	1	0	-1.793536	1.287244	-0.213070
42	6	0	-3.128266	-0.258187	-0.874819
43	6	0	-3.868426	-1.355216	-0.407516
44	6	0	-3.597175	0.427144	-2.006261
45	6	0	-5.024528	-1.773949	-1.067690
46	1	0	-3.549459	-1.871671	0.494820
47	6	0	-4.751773	0.011170	-2.670345
48	1	0	-3.069011	1.309731	-2.359497
49	6	0	-5.464847	-1.095249	-2.205357
50	1	0	-5.587180	-2.621420	-0.687737
51	1	0	-5.100701	0.557112	-3.541672
52	1	0	-6.366351	-1.417135	-2.717450
53	6	0	-0.345990	-2.160066	1.078705
54	6	0	-0.920652	-3.282416	1.676870
55	6	0	-0.643872	-3.553390	3.017632
56	1	0	-1.569998	-3.932861	1.099093
57	6	0	0.729241	-1.589879	3.051611
58	6	0	0.198810	-2.691961	3.719414
59	1	0	-1.079399	-4.420533	3.504237

60	1	0	1.397641	-0.892282	3.548096
61	1	0	0.442869	-2.865104	4.761933
62	7	0	0.464374	-1.322763	1.761485
63	1	0	2.343506	0.792770	1.365523

3'$_{dp\text{-}B}$ (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1466.42098757 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.444419	1.590710	-1.186747
2	6	0	2.729251	1.207105	-1.802840
3	1	0	2.757068	1.465534	-2.871716
4	1	0	3.515482	1.791725	-1.312867
5	6	0	1.454149	2.999357	-0.734183
6	1	0	2.427095	3.184013	-0.265618
7	1	0	1.349485	3.702698	-1.573456
8	6	0	0.268179	1.306305	-2.051682
9	1	0	-0.521317	2.007658	-1.770577
10	1	0	0.509081	1.510353	-3.105474
11	27	0	1.263306	0.457656	0.769481
12	6	0	3.103423	-0.251900	-1.611819
13	6	0	4.021673	-0.864569	-2.468794
14	6	0	3.026183	-2.127725	-0.266110
15	6	0	4.453889	-2.158141	-2.186143
16	1	0	4.396053	-0.329132	-3.335958
17	6	0	3.953436	-2.802215	-1.053958
18	1	0	2.606887	-2.589532	0.622985
19	1	0	5.170487	-2.652597	-2.834430
20	1	0	4.268781	-3.805035	-0.787476
21	6	0	0.396785	3.282282	0.315587
22	6	0	-0.149938	4.557912	0.466380
23	6	0	-1.026287	4.801491	1.522472
24	1	0	0.117367	5.347225	-0.229160
25	6	0	-0.767579	2.510014	2.162251
26	6	0	-1.337974	3.757553	2.393593
27	1	0	-1.457135	5.787789	1.662838
28	1	0	-0.988238	1.665727	2.809030
29	1	0	-2.012127	3.900697	3.230807
30	7	0	2.599931	-0.883144	-0.538431
31	7	0	0.077636	2.270374	1.145961
32	6	0	-0.258125	-0.128001	-1.926445
33	1	0	-1.087962	-0.261764	-2.633731
34	1	0	0.521741	-0.831690	-2.223334

35	7	0	-0.652574	-0.439087	-0.537813
36	6	0	-0.577507	-1.872838	-0.212488
37	1	0	-1.466961	-2.429547	-0.533595
38	1	0	0.273335	-2.295682	-0.755898
39	6	0	-1.977019	0.143982	-0.149393
40	1	0	-2.073175	0.000619	0.931027
41	1	0	-1.917206	1.221114	-0.313331
42	6	0	-3.203233	-0.413352	-0.848955
43	6	0	-3.920423	-1.484181	-0.293668
44	6	0	-3.664633	0.143566	-2.051796
45	6	0	-5.045682	-2.004003	-0.934900
46	1	0	-3.608433	-1.899708	0.661860
47	6	0	-4.788645	-0.373910	-2.697229
48	1	0	-3.156453	1.006061	-2.476730
49	6	0	-5.478035	-1.453791	-2.142838
50	1	0	-5.590893	-2.829307	-0.486755
51	1	0	-5.132910	0.073537	-3.624786
52	1	0	-6.355757	-1.853699	-2.641079
53	6	0	-0.334369	-2.091145	1.269239
54	6	0	-0.882012	-3.171437	1.962276
55	6	0	-0.555352	-3.355575	3.306261
56	1	0	-1.551512	-3.856354	1.451590
57	6	0	0.817674	-1.398700	3.167312
58	6	0	0.312383	-2.454034	3.922006
59	1	0	-0.972723	-4.189136	3.862677
60	1	0	1.507275	-0.670042	3.584468
61	1	0	0.595511	-2.561379	4.963221
62	7	0	0.498955	-1.219106	1.873360
63	1	0	2.568076	0.970598	1.600336

3'$_{dp\text{-}C}$ (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1466.40619378 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.203935	-1.826709	0.444782
2	6	0	1.984571	-1.564808	1.674494
3	1	0	1.698646	-2.264754	2.471641
4	1	0	3.040366	-1.766076	1.462524
5	6	0	1.997851	-2.571326	-0.556773
6	1	0	2.383344	-3.521679	-0.158746
7	1	0	1.329169	-2.792733	-1.395814
8	6	0	-0.109094	-2.450753	0.727782
9	1	0	-0.469282	-2.894392	-0.202515

10	1	0	-0.013245	-3.265393	1.461256
11	27	0	0.747779	0.093130	-0.648565
12	6	0	1.905592	-0.141709	2.199814
13	6	0	2.340088	0.142547	3.499029
14	6	0	1.500866	2.097804	1.797028
15	6	0	2.359439	1.462990	3.937454
16	1	0	2.663415	-0.664100	4.150083
17	6	0	1.938018	2.467006	3.063962
18	1	0	1.147978	2.841324	1.089237
19	1	0	2.697013	1.705083	4.940349
20	1	0	1.940435	3.511106	3.356979
21	6	0	3.134307	-1.720476	-1.084578
22	6	0	4.316087	-2.285658	-1.564092
23	6	0	5.293021	-1.453644	-2.109483
24	1	0	4.463358	-3.360038	-1.514160
25	6	0	3.866239	0.406430	-1.626774
26	6	0	5.065009	-0.078203	-2.141937
27	1	0	6.217266	-1.871372	-2.495970
28	1	0	3.650619	1.471618	-1.626562
29	1	0	5.799203	0.607665	-2.550109
30	7	0	1.477953	0.822239	1.366807
31	7	0	2.917054	-0.391203	-1.113715
32	6	0	-1.120724	-1.418707	1.236496
33	1	0	-2.054503	-1.925154	1.512162
34	1	0	-0.739528	-0.944414	2.145732
35	7	0	-1.339533	-0.365458	0.222068
36	6	0	-1.790880	0.916566	0.795813
37	1	0	-2.851355	0.899250	1.077903
38	1	0	-1.216100	1.096321	1.710585
39	6	0	-2.230062	-0.813737	-0.907571
40	1	0	-2.199776	-0.019025	-1.655171
41	1	0	-1.740281	-1.666978	-1.377784
42	6	0	-3.661109	-1.148703	-0.536553
43	6	0	-4.664785	-0.168456	-0.583366
44	6	0	-4.025085	-2.453621	-0.168969
45	6	0	-5.983465	-0.473345	-0.243053
46	1	0	-4.415884	0.836715	-0.915353
47	6	0	-5.342214	-2.763086	0.173247
48	1	0	-3.277171	-3.243249	-0.176050
49	6	0	-6.323612	-1.770856	0.143621
50	1	0	-6.746987	0.297355	-0.292513
51	1	0	-5.604317	-3.780091	0.449286
52	1	0	-7.349908	-2.011175	0.403724
53	6	0	-1.532485	2.055046	-0.174008

54	6	0	-2.411262	3.131487	-0.306170
55	6	0	-2.107499	4.153180	-1.205697
56	1	0	-3.320966	3.161816	0.285064
57	6	0	-0.122180	2.948898	-1.785554
58	6	0	-0.941667	4.059574	-1.965283
59	1	0	-2.777563	4.999155	-1.322699
60	1	0	0.780788	2.814836	-2.374429
61	1	0	-0.675199	4.820532	-2.690403
62	7	0	-0.397684	1.977755	-0.899936
63	1	0	0.408575	-0.489668	-2.130311

3'$_{dp\text{-}C}$ (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1466.40963436 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.101442	-1.809936	0.028081
2	6	0	1.659049	-1.821068	1.401488
3	1	0	1.168415	-2.584398	2.019568
4	1	0	2.714797	-2.113211	1.354328
5	6	0	2.033194	-2.441870	-0.929666
6	1	0	2.277154	-3.479821	-0.653230
7	1	0	1.530171	-2.467371	-1.902555
8	6	0	-0.218314	-2.481425	-0.034192
9	1	0	-0.475004	-2.594437	-1.090621
10	1	0	-0.146476	-3.494457	0.396883
11	27	0	1.309421	0.411836	-0.676518
12	6	0	1.603794	-0.484916	2.118161
13	6	0	1.686847	-0.429016	3.512473
14	6	0	1.574820	1.830375	1.992708
15	6	0	1.724676	0.807917	4.150013
16	1	0	1.723137	-1.350175	4.085757
17	6	0	1.673640	1.965157	3.372069
18	1	0	1.513052	2.702772	1.349747
19	1	0	1.790296	0.868175	5.231761
20	1	0	1.702274	2.952113	3.820190
21	6	0	3.299366	-1.633543	-1.070996
22	6	0	4.536539	-2.213759	-1.349680
23	6	0	5.653207	-1.395829	-1.510099
24	1	0	4.616144	-3.292301	-1.440431
25	6	0	4.237648	0.488036	-1.081611
26	6	0	5.500692	-0.016438	-1.369527
27	1	0	6.623957	-1.826591	-1.733430
28	1	0	4.073126	1.554470	-0.964815

29	1	0	6.340510	0.660600	-1.478505
30	7	0	1.538204	0.635515	1.369256
31	7	0	3.155049	-0.299234	-0.939247
32	6	0	-1.340467	-1.705332	0.662471
33	1	0	-2.198890	-2.380682	0.791138
34	1	0	-1.032134	-1.430618	1.676481
35	7	0	-1.688313	-0.502915	-0.079030
36	6	0	-1.797334	0.733901	0.667452
37	1	0	-2.814559	0.941498	1.037223
38	1	0	-1.156334	0.660172	1.551362
39	6	0	-2.683803	-0.681695	-1.154624
40	1	0	-2.641603	0.208777	-1.791280
41	1	0	-2.348416	-1.516394	-1.779310
42	6	0	-4.113708	-0.925312	-0.700170
43	6	0	-4.987714	0.148229	-0.470662
44	6	0	-4.591998	-2.227503	-0.489540
45	6	0	-6.289441	-0.069074	-0.016552
46	1	0	-4.655250	1.162890	-0.677624
47	6	0	-5.892919	-2.449980	-0.035043
48	1	0	-3.950456	-3.078028	-0.708338
49	6	0	-6.742897	-1.369984	0.209171
50	1	0	-6.953368	0.774587	0.148254
51	1	0	-6.246592	-3.465718	0.115575
52	1	0	-7.756998	-1.541559	0.557048
53	6	0	-1.336620	1.922104	-0.159166
54	6	0	-2.125208	3.072321	-0.249865
55	6	0	-1.706043	4.152075	-1.023210
56	1	0	-3.068982	3.105851	0.284758
57	6	0	0.230294	2.868233	-1.587568
58	6	0	-0.501245	4.043546	-1.714102
59	1	0	-2.315003	5.047351	-1.100437
60	1	0	1.155164	2.728752	-2.137434
61	1	0	-0.135535	4.840091	-2.352460
62	7	0	-0.154736	1.830217	-0.812604
63	1	0	1.135182	0.201641	-2.147220

TS'$_A$ (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1466.73527484 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.744049	-1.085369	-1.259977
2	6	0	-2.488822	-0.258103	-2.237532
3	1	0	-1.780407	0.155844	-2.961921

4	1	0	-3.200485	-0.860591	-2.815826
5	6	0	-2.626232	-2.108049	-0.648763
6	1	0	-3.638741	-1.690370	-0.598934
7	1	0	-2.686090	-3.009541	-1.272326
8	6	0	-0.497793	-1.671895	-1.815343
9	1	0	-0.182005	-2.471442	-1.139903
10	1	0	-0.672423	-2.133548	-2.797072
11	27	0	-1.051336	0.234269	0.375351
12	6	0	-3.195748	0.893150	-1.550517
13	6	0	-4.333828	1.491986	-2.084307
14	6	0	-3.171465	2.410524	0.220903
15	6	0	-4.891518	2.593820	-1.434002
16	1	0	-4.776070	1.102673	-2.995700
17	6	0	-4.299280	3.063462	-0.260600
18	1	0	-2.681877	2.728236	1.136077
19	1	0	-5.778262	3.074415	-1.835038
20	1	0	-4.704521	3.913096	0.277129
21	6	0	-2.198688	-2.454881	0.760720
22	6	0	-2.515639	-3.674293	1.354222
23	6	0	-2.181458	-3.885481	2.692544
24	1	0	-3.022718	-4.442620	0.779574
25	6	0	-1.238306	-1.685427	2.740857
26	6	0	-1.535345	-2.870952	3.401283
27	1	0	-2.422863	-4.827613	3.174421
28	1	0	-0.733698	-0.867972	3.246094
29	1	0	-1.263088	-2.993669	4.443441
30	7	0	-2.626633	1.348173	-0.410270
31	7	0	-1.558818	-1.480599	1.445337
32	6	0	0.591455	-0.611993	-1.941005
33	1	0	1.502961	-1.064563	-2.344805
34	1	0	0.279606	0.155795	-2.653953
35	7	0	0.885712	0.079767	-0.641180
36	6	0	1.553217	1.379473	-0.998256
37	1	0	2.405179	1.168877	-1.654584
38	1	0	0.827853	1.949658	-1.591420
39	6	0	1.770439	-0.785368	0.259629
40	1	0	1.939515	-0.199960	1.166230
41	1	0	1.162994	-1.648918	0.542281
42	6	0	3.087613	-1.261039	-0.316987
43	6	0	4.260592	-0.506436	-0.161118
44	6	0	3.170012	-2.500669	-0.972624
45	6	0	5.475231	-0.963470	-0.673696
46	1	0	4.233114	0.430189	0.388039
47	6	0	4.382909	-2.958967	-1.487181

48	1	0	2.286596	-3.129732	-1.059819
49	6	0	5.537346	-2.186876	-1.343719
50	1	0	6.375749	-0.373088	-0.536478
51	1	0	4.429990	-3.922271	-1.985042
52	1	0	6.483552	-2.545058	-1.736415
53	6	0	2.045703	2.274095	0.125309
54	6	0	3.213577	3.021449	-0.049540
55	6	0	3.606754	3.922868	0.941178
56	1	0	3.805772	2.900861	-0.950602
57	6	0	1.689923	3.267048	2.207015
58	6	0	2.833755	4.049302	2.095661
59	1	0	4.508527	4.513298	0.813755
60	1	0	1.048932	3.315359	3.083543
61	1	0	3.108513	4.732990	2.890909
62	7	0	1.309039	2.414137	1.242022
63	1	0	0.078484	1.648067	1.505104
64	1	0	-0.671186	1.233914	1.772462

TS'$_B$ (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1466.72898904 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.463206	-1.241055	-0.605623
2	6	0	-2.378869	-1.176195	-1.797933
3	1	0	-1.844591	-0.639360	-2.588987
4	1	0	-2.551741	-2.194960	-2.167423
5	6	0	-2.166576	-1.845975	0.556030
6	1	0	-3.208470	-1.513887	0.533144
7	1	0	-2.183974	-2.941338	0.484749
8	6	0	-0.262222	-2.065631	-0.964823
9	1	0	0.139196	-2.489821	-0.040939
10	1	0	-0.555096	-2.912578	-1.598670
11	27	0	-0.453139	0.660696	0.138670
12	6	0	-3.726631	-0.518677	-1.562152
13	6	0	-4.900534	-1.134595	-2.000422
14	6	0	-4.905291	1.317087	-0.792133
15	6	0	-6.117195	-0.469868	-1.826948
16	1	0	-4.866928	-2.110030	-2.475443
17	6	0	-6.122614	0.779191	-1.209801
18	1	0	-4.862765	2.289806	-0.308984
19	1	0	-7.042400	-0.924151	-2.166952
20	1	0	-7.044295	1.329004	-1.054315

21	6	0	-1.586629	-1.416160	1.884306
22	6	0	-1.793650	-2.162422	3.044099
23	6	0	-1.332219	-1.673344	4.265071
24	1	0	-2.317291	-3.111309	2.988639
25	6	0	-0.474815	0.234784	3.106219
26	6	0	-0.663314	-0.447227	4.299070
27	1	0	-1.490206	-2.240702	5.176831
28	1	0	0.054847	1.181857	3.078979
29	1	0	-0.289087	-0.031007	5.227453
30	7	0	-3.735002	0.686240	-0.964095
31	7	0	-0.927056	-0.235660	1.920591
32	6	0	0.816268	-1.243333	-1.667467
33	1	0	1.649291	-1.888938	-1.965043
34	1	0	0.418641	-0.791055	-2.579998
35	7	0	1.276869	-0.147293	-0.771148
36	6	0	1.852038	1.013790	-1.504943
37	1	0	2.880981	0.814097	-1.820891
38	1	0	1.261317	1.168622	-2.415872
39	6	0	2.241893	-0.633897	0.310422
40	1	0	2.409328	0.221310	0.971083
41	1	0	1.707054	-1.388493	0.891260
42	6	0	3.562249	-1.184939	-0.175858
43	6	0	4.679876	-0.345697	-0.312531
44	6	0	3.706985	-2.552307	-0.460935
45	6	0	5.901579	-0.853772	-0.754982
46	1	0	4.605138	0.705290	-0.041792
47	6	0	4.928069	-3.061675	-0.903690
48	1	0	2.871723	-3.232462	-0.308511
49	6	0	6.024863	-2.211300	-1.058156
50	1	0	6.759569	-0.195546	-0.847957
51	1	0	5.027433	-4.121890	-1.113427
52	1	0	6.976778	-2.608339	-1.395769
53	6	0	1.784618	2.276114	-0.662343
54	6	0	2.696211	3.318100	-0.817418
55	6	0	2.532091	4.484297	-0.068807
56	1	0	3.517952	3.218307	-1.519043
57	6	0	0.591760	3.499831	0.929865
58	6	0	1.460228	4.578137	0.821112
59	1	0	3.231022	5.307504	-0.178011
60	1	0	-0.259643	3.531033	1.603205
61	1	0	1.297711	5.467463	1.419490
62	7	0	0.749826	2.369683	0.208614
63	1	0	-2.080154	1.440849	-0.978446
64	1	0	-1.375619	1.772626	-1.119938

TS'$_B$ (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1466.72295049 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.383445	-1.180646	-0.790121
2	6	0	-2.356060	-0.893463	-1.898878
3	1	0	-1.836810	-0.262168	-2.627682
4	1	0	-2.589419	-1.836354	-2.408691
5	6	0	-2.000561	-2.095136	0.217920
6	1	0	-3.007201	-1.723127	0.433162
7	1	0	-2.113162	-3.104026	-0.199289
8	6	0	-0.168123	-1.836856	-1.400381
9	1	0	0.301696	-2.443459	-0.624096
10	1	0	-0.466348	-2.517794	-2.206416
11	27	0	-0.571863	0.438659	0.214262
12	6	0	-3.666765	-0.222379	-1.528916
13	6	0	-4.839432	-0.557093	-2.207323
14	6	0	-4.785882	1.420767	-0.314746
15	6	0	-6.011785	0.148129	-1.926663
16	1	0	-4.836799	-1.350671	-2.947660
17	6	0	-5.987773	1.158487	-0.965227
18	1	0	-4.710400	2.181777	0.457125
19	1	0	-6.931820	-0.094904	-2.448599
20	1	0	-6.878021	1.725207	-0.716722
21	6	0	-1.207798	-2.130302	1.508439
22	6	0	-1.292516	-3.209569	2.387651
23	6	0	-0.614667	-3.142995	3.604815
24	1	0	-1.883390	-4.082088	2.127438
25	6	0	0.183031	-0.977970	2.962408
26	6	0	0.133756	-2.002962	3.901233
27	1	0	-0.669107	-3.967382	4.308571
28	1	0	0.762815	-0.078567	3.146057
29	1	0	0.674237	-1.909319	4.836525
30	7	0	-3.658781	0.751207	-0.602981
31	7	0	-0.470818	-1.035790	1.787206
32	6	0	0.805667	-0.784630	-1.910815
33	1	0	1.698946	-1.251693	-2.336990
34	1	0	0.348916	-0.184529	-2.702297
35	7	0	1.157090	0.124672	-0.778430
36	6	0	1.543008	1.496709	-1.233154
37	1	0	2.574618	1.523055	-1.596263

38	1	0	0.895106	1.774516	-2.072804
39	6	0	2.249698	-0.468401	0.115634
40	1	0	2.342638	0.216612	0.961004
41	1	0	1.849628	-1.404140	0.505483
42	6	0	3.593172	-0.693991	-0.536761
43	6	0	4.582746	0.302277	-0.502961
44	6	0	3.896697	-1.923002	-1.145296
45	6	0	5.828326	0.089838	-1.094330
46	1	0	4.391610	1.238493	0.016974
47	6	0	5.141424	-2.136825	-1.738100
48	1	0	3.169929	-2.732468	-1.129739
49	6	0	6.105896	-1.127211	-1.720357
50	1	0	6.586198	0.865717	-1.053296
51	1	0	5.363772	-3.094151	-2.198563
52	1	0	7.076865	-1.295358	-2.175036
53	6	0	1.318867	2.460936	-0.092868
54	6	0	2.044292	3.633906	0.088708
55	6	0	1.718080	4.473945	1.155120
56	1	0	2.848304	3.885183	-0.595010
57	6	0	-0.004134	2.925109	1.776321
58	6	0	0.679194	4.111771	2.013815
59	1	0	2.269355	5.395115	1.314623
60	1	0	-0.819690	2.602482	2.413846
61	1	0	0.398224	4.735564	2.854841
62	7	0	0.307163	2.114152	0.743676
63	1	0	-2.454704	0.880201	0.288992
64	1	0	-1.904278	0.934771	0.982268

TS'$_C$ (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1466.73134930 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.292577	1.333444	-1.002984
2	6	0	2.299651	0.830129	-1.979716
3	1	0	1.783382	0.225989	-2.733019
4	1	0	2.773540	1.658733	-2.520931
5	6	0	1.858396	2.570972	-0.373053
6	1	0	2.796854	2.277933	0.111297
7	1	0	2.116808	3.289359	-1.162355
8	6	0	-0.004795	1.607455	-1.685131
9	1	0	-0.586999	2.261835	-1.034254
10	1	0	0.148593	2.151793	-2.627319

11	27	0	0.937727	-0.562931	0.301798
12	6	0	3.343152	-0.041438	-1.321924
13	6	0	4.673402	-0.066763	-1.731282
14	6	0	3.735531	-1.741676	0.222835
15	6	0	5.552118	-0.971251	-1.132585
16	1	0	5.014723	0.608191	-2.509163
17	6	0	5.074156	-1.827313	-0.139675
18	1	0	3.320733	-2.387613	0.989580
19	1	0	6.593347	-1.006182	-1.436975
20	1	0	5.722466	-2.546224	0.348254
21	6	0	0.977656	3.277098	0.638156
22	6	0	0.724313	4.645892	0.537223
23	6	0	-0.012960	5.277734	1.542342
24	1	0	1.106417	5.212637	-0.305720
25	6	0	-0.202292	3.158739	2.637749
26	6	0	-0.485214	4.523319	2.614806
27	1	0	-0.211858	6.343229	1.485909
28	1	0	-0.545227	2.525202	3.451711
29	1	0	-1.056894	4.975727	3.417446
30	7	0	2.885578	-0.865060	-0.352135
31	7	0	0.510588	2.557034	1.674746
32	6	0	-0.777260	0.317915	-1.966585
33	1	0	-1.754740	0.559955	-2.397677
34	1	0	-0.251598	-0.292944	-2.705979
35	7	0	-0.924585	-0.500566	-0.730462
36	6	0	-1.191988	-1.935319	-1.036131
37	1	0	-2.232489	-2.088762	-1.340406
38	1	0	-0.562575	-2.224189	-1.886431
39	6	0	-1.979556	0.063770	0.221974
40	1	0	-1.923661	-0.543647	1.129566
41	1	0	-1.646229	1.068870	0.488537
42	6	0	-3.398213	0.092575	-0.298577
43	6	0	-4.266553	-0.985404	-0.061483
44	6	0	-3.887577	1.211649	-0.991528
45	6	0	-5.579824	-0.958979	-0.531788
46	1	0	-3.924460	-1.838271	0.520682
47	6	0	-5.200155	1.239078	-1.463652
48	1	0	-3.251608	2.081627	-1.139732
49	6	0	-6.045846	0.150594	-1.239975
50	1	0	-6.242690	-1.795222	-0.333264
51	1	0	-5.566753	2.113307	-1.992174
52	1	0	-7.069123	0.174458	-1.600701
53	6	0	-0.849066	-2.817133	0.150671
54	6	0	-1.508922	-4.018511	0.399721

55	6	0	-1.117298	-4.796890	1.489809
56	1	0	-2.317115	-4.337444	-0.250287
57	6	0	0.523514	-3.133974	2.011726
58	6	0	-0.085922	-4.344661	2.315206
59	1	0	-1.617874	-5.737038	1.698775
60	1	0	1.317256	-2.732675	2.634677
61	1	0	0.236568	-4.912328	3.180737
62	7	0	0.160903	-2.390419	0.945412
63	1	0	0.896275	1.002037	1.752743
64	1	0	1.130173	0.204111	1.901090

TS'$_C$ (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1466.71671232 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.183730	1.338680	-1.182680
2	6	0	2.195712	0.803885	-2.173094
3	1	0	1.650853	0.398844	-3.030808
4	1	0	2.798312	1.629244	-2.564365
5	6	0	1.689617	2.671551	-0.702662
6	1	0	2.736543	2.524031	-0.420770
7	1	0	1.670183	3.384680	-1.534863
8	6	0	-0.141943	1.485426	-1.880091
9	1	0	-0.761951	2.153508	-1.277736
10	1	0	-0.012679	1.960248	-2.860677
11	27	0	0.837048	-0.099686	0.270781
12	6	0	3.075605	-0.290587	-1.621466
13	6	0	4.352207	-0.529565	-2.127397
14	6	0	3.210909	-2.129573	-0.224454
15	6	0	5.066099	-1.631892	-1.656612
16	1	0	4.776844	0.128214	-2.879062
17	6	0	4.481229	-2.452125	-0.691711
18	1	0	2.731100	-2.726076	0.544414
19	1	0	6.061257	-1.843389	-2.034324
20	1	0	4.999960	-3.319295	-0.298559
21	6	0	0.957656	3.274107	0.479102
22	6	0	0.377604	4.539622	0.440089
23	6	0	-0.182331	5.069568	1.607899
24	1	0	0.378459	5.111362	-0.482201
25	6	0	0.435477	3.059886	2.754119
26	6	0	-0.152834	4.321813	2.784870
27	1	0	-0.630362	6.058124	1.596151
28	1	0	0.495108	2.429205	3.636213

29	1	0	-0.569667	4.705086	3.709465
30	7	0	2.514868	-1.072532	-0.680421
31	7	0	0.972319	2.567866	1.628152
32	6	0	-0.807235	0.116342	-2.023436
33	1	0	-1.792145	0.212327	-2.491228
34	1	0	-0.208867	-0.543384	-2.656878
35	7	0	-0.898115	-0.506382	-0.673828
36	6	0	-0.956518	-1.994540	-0.673077
37	1	0	-1.949985	-2.366365	-0.943343
38	1	0	-0.244978	-2.360082	-1.421648
39	6	0	-2.054318	0.082334	0.144060
40	1	0	-1.973643	-0.352337	1.142165
41	1	0	-1.854476	1.151945	0.243499
42	6	0	-3.440202	-0.142729	-0.415735
43	6	0	-4.185410	-1.271991	-0.039598
44	6	0	-4.025187	0.790980	-1.286220
45	6	0	-5.468019	-1.479638	-0.547745
46	1	0	-3.774334	-1.978713	0.677695
47	6	0	-5.307457	0.584517	-1.795687
48	1	0	-3.490501	1.701520	-1.548178
49	6	0	-6.027457	-0.555449	-1.432570
50	1	0	-6.035771	-2.352837	-0.242439
51	1	0	-5.749085	1.317932	-2.462793
52	1	0	-7.027468	-0.713800	-1.823294
53	6	0	-0.536463	-2.472994	0.700078
54	6	0	-0.958027	-3.674846	1.259673
55	6	0	-0.492027	-4.036545	2.525335
56	1	0	-1.640483	-4.316417	0.711908
57	6	0	0.755682	-1.988857	2.586224
58	6	0	0.376130	-3.177740	3.200284
59	1	0	-0.808176	-4.970346	2.979167
60	1	0	1.431705	-1.291092	3.066669
61	1	0	0.754906	-3.418038	4.187325
62	7	0	0.314241	-1.642813	1.359431
63	1	0	1.484837	1.315254	1.508413
64	1	0	1.913910	0.442668	1.363330

Fe

1''-H_2O (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1520.11531775 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.821787	-0.862477	1.531620
2	6	0	1.909640	-0.126894	2.210195
3	1	0	1.566099	0.896685	2.397032
4	1	0	2.154763	-0.565740	3.187585
5	6	0	1.126897	-2.312850	1.458639
6	1	0	2.213929	-2.431379	1.397595
7	1	0	0.807555	-2.832544	2.371187
8	6	0	-0.522126	-0.616529	2.124343
9	1	0	-1.131214	-1.503023	1.933314
10	1	0	-0.457051	-0.511333	3.215482
11	26	0	0.791063	-0.052976	-0.577492
12	6	0	3.144799	-0.093039	1.327680
13	6	0	4.433001	-0.044969	1.858668
14	6	0	3.987061	-0.096131	-0.841040
15	6	0	5.525671	-0.013280	0.991463
16	1	0	4.577010	-0.040053	2.934365
17	6	0	5.299944	-0.045536	-0.385806
18	1	0	3.762026	-0.125590	-1.902667
19	1	0	6.536654	0.022959	1.384853
20	1	0	6.121216	-0.038225	-1.093715
21	6	0	0.518181	-2.970316	0.236379
22	6	0	0.184378	-4.325164	0.238812
23	6	0	-0.294755	-4.912590	-0.931067
24	1	0	0.302464	-4.910463	1.145160
25	6	0	-0.098826	-2.777984	-1.991625
26	6	0	-0.438763	-4.122548	-2.072732
27	1	0	-0.556667	-5.965712	-0.949854
28	1	0	-0.223146	-2.125935	-2.850810
29	1	0	-0.813396	-4.534569	-3.003051
30	7	0	2.927559	-0.110727	-0.007348
31	7	0	0.374647	-2.202891	-0.867173
32	6	0	-1.198994	0.618663	1.533709
33	1	0	-2.187621	0.746321	1.990686
34	1	0	-0.617289	1.512202	1.775415
35	7	0	-1.316193	0.545974	0.045639
36	6	0	-1.588665	1.899512	-0.500356
37	1	0	-1.865560	1.780742	-1.554932
38	1	0	-2.448913	2.364441	-0.005389
39	6	0	-2.394731	-0.421058	-0.406915
40	1	0	-2.311910	-0.467583	-1.497293
41	1	0	-2.117141	-1.404868	-0.025351

42	6	0	-3.816895	-0.089295	-0.006578
43	6	0	-4.637472	0.679075	-0.846735
44	6	0	-4.354865	-0.575824	1.195563
45	6	0	-5.951070	0.976567	-0.483209
46	1	0	-4.258877	1.027740	-1.804840
47	6	0	-5.667592	-0.277763	1.562938
48	1	0	-3.755639	-1.215330	1.840266
49	6	0	-6.465956	0.503948	0.725807
50	1	0	-6.575972	1.564018	-1.148494
51	1	0	-6.070712	-0.666465	2.492768
52	1	0	-7.489868	0.729559	1.006163
53	6	0	-0.381175	2.805251	-0.416510
54	6	0	-0.519164	4.189290	-0.302848
55	6	0	0.621603	4.990078	-0.303861
56	1	0	-1.507695	4.628802	-0.216900
57	6	0	1.928801	2.993662	-0.503160
58	6	0	1.872360	4.379478	-0.408606
59	1	0	0.536528	6.068829	-0.219585
60	1	0	2.881755	2.480273	-0.573459
61	1	0	2.787280	4.961499	-0.411280
62	7	0	0.828412	2.211984	-0.509370
63	8	0	1.058480	0.326135	-2.745045
64	1	0	1.149307	-0.263870	-3.505767
65	1	0	1.175417	1.231326	-3.065767

1''-H_2O (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1520.09169535 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.857866	-0.651794	1.566203
2	6	0	1.991748	0.135355	2.118486
3	1	0	1.666641	1.173844	2.233457
4	1	0	2.299708	-0.227578	3.107779
5	6	0	1.213149	-2.108876	1.585306
6	1	0	2.302461	-2.206335	1.577530
7	1	0	0.865115	-2.578130	2.512098
8	6	0	-0.462509	-0.439200	2.242227
9	1	0	-1.004146	-1.386379	2.191483
10	1	0	-0.327060	-0.204461	3.304688
11	26	0	0.729839	-0.027922	-0.364067
12	6	0	3.135621	0.035873	1.125113
13	6	0	4.474732	0.103100	1.499876
14	6	0	3.719582	-0.277632	-1.102916

15	6	0	5.463152	-0.014774	0.519913
16	1	0	4.739948	0.238023	2.543617
17	6	0	5.078017	-0.216384	-0.805062
18	1	0	3.383471	-0.439357	-2.121806
19	1	0	6.513021	0.035814	0.790053
20	1	0	5.810921	-0.330119	-1.596026
21	6	0	0.662699	-2.804738	0.369549
22	6	0	0.440709	-4.180162	0.329835
23	6	0	-0.001243	-4.763189	-0.856484
24	1	0	0.615664	-4.782765	1.215358
25	6	0	0.000891	-2.577434	-1.838854
26	6	0	-0.224366	-3.942924	-1.963206
27	1	0	-0.176469	-5.832579	-0.913453
28	1	0	-0.209026	-1.909934	-2.667241
29	1	0	-0.579907	-4.347253	-2.904329
30	7	0	2.759747	-0.143562	-0.169336
31	7	0	0.447598	-2.006035	-0.700322
32	6	0	-1.263865	0.651227	1.547865
33	1	0	-2.281983	0.685552	1.950354
34	1	0	-0.812252	1.625376	1.742795
35	7	0	-1.289462	0.435382	0.061319
36	6	0	-1.558535	1.735788	-0.603450
37	1	0	-1.720053	1.536994	-1.668755
38	1	0	-2.475106	2.201021	-0.223968
39	6	0	-2.340339	-0.581638	-0.347502
40	1	0	-2.202949	-0.726583	-1.422078
41	1	0	-2.073059	-1.519999	0.141654
42	6	0	-3.781922	-0.232833	-0.045336
43	6	0	-4.561403	0.470503	-0.977109
44	6	0	-4.381018	-0.646425	1.155258
45	6	0	-5.894208	0.778492	-0.703410
46	1	0	-4.134587	0.758366	-1.935142
47	6	0	-5.713525	-0.338253	1.432379
48	1	0	-3.812999	-1.239024	1.869588
49	6	0	-6.470244	0.380325	0.505002
50	1	0	-6.486576	1.315195	-1.437761
51	1	0	-6.163762	-0.670771	2.362336
52	1	0	-7.509089	0.613906	0.715076
53	6	0	-0.381500	2.662958	-0.438231
54	6	0	-0.523017	4.048168	-0.517482
55	6	0	0.604825	4.858503	-0.406091
56	1	0	-1.507695	4.479975	-0.664269
57	6	0	1.908851	2.865763	-0.131982
58	6	0	1.845989	4.251803	-0.210687

59	1	0	0.516884	5.938541	-0.466263
60	1	0	2.858762	2.369356	0.020877
61	1	0	2.753450	4.837772	-0.116214
62	7	0	0.821711	2.068255	-0.239254
63	8	0	0.635992	0.397001	-2.436037
64	1	0	1.091422	-0.190205	-3.055445
65	1	0	0.919647	1.295599	-2.660290

1''-H_2O (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1520.08822652 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.808900	-0.782315	1.658516
2	6	0	1.908796	0.001111	2.246378
3	1	0	1.562909	1.031844	2.384599
4	1	0	2.211988	-0.371728	3.235391
5	6	0	1.145413	-2.217903	1.567232
6	1	0	2.233895	-2.330193	1.603553
7	1	0	0.752587	-2.783296	2.421991
8	6	0	-0.528763	-0.549443	2.251262
9	1	0	-1.106110	-1.469750	2.134017
10	1	0	-0.466543	-0.356103	3.330746
11	26	0	0.723776	0.030401	-0.487134
12	6	0	3.094383	-0.022049	1.296180
13	6	0	4.411881	-0.001174	1.751054
14	6	0	3.812729	-0.138022	-0.913627
15	6	0	5.456036	-0.044689	0.826227
16	1	0	4.614424	0.039071	2.816547
17	6	0	5.150744	-0.123193	-0.532855
18	1	0	3.528384	-0.190817	-1.959336
19	1	0	6.487983	-0.031106	1.162187
20	1	0	5.929259	-0.175800	-1.285767
21	6	0	0.658173	-2.821481	0.268941
22	6	0	0.446559	-4.194987	0.145372
23	6	0	0.055924	-4.724383	-1.082272
24	1	0	0.589489	-4.838742	1.007445
25	6	0	0.086186	-2.497474	-1.956904
26	6	0	-0.129905	-3.854222	-2.157245
27	1	0	-0.109499	-5.790938	-1.195606
28	1	0	-0.083539	-1.789198	-2.759675
29	1	0	-0.446089	-4.213653	-3.130050
30	7	0	2.801126	-0.080333	-0.025401
31	7	0	0.481917	-1.976941	-0.774243

32	6	0	-1.257734	0.608875	1.573408
33	1	0	-2.270027	0.700469	1.983112
34	1	0	-0.739796	1.546633	1.788233
35	7	0	-1.319254	0.454041	0.082534
36	6	0	-1.619807	1.774321	-0.531198
37	1	0	-1.847978	1.605782	-1.590309
38	1	0	-2.510135	2.233412	-0.087332
39	6	0	-2.358524	-0.568366	-0.345848
40	1	0	-2.239507	-0.675662	-1.427856
41	1	0	-2.066786	-1.518028	0.104975
42	6	0	-3.799573	-0.249393	-0.010199
43	6	0	-4.606724	0.454208	-0.917722
44	6	0	-4.369407	-0.689213	1.195268
45	6	0	-5.939304	0.736159	-0.616472
46	1	0	-4.202009	0.762510	-1.879096
47	6	0	-5.701591	-0.407041	1.499792
48	1	0	-3.779030	-1.280784	1.891750
49	6	0	-6.486749	0.311414	0.596075
50	1	0	-6.553375	1.273064	-1.332592
51	1	0	-6.129548	-0.759559	2.432887
52	1	0	-7.525421	0.524314	0.827847
53	6	0	-0.429929	2.691359	-0.421322
54	6	0	-0.567046	4.078449	-0.399796
55	6	0	0.573296	4.878161	-0.353920
56	1	0	-1.557834	4.520324	-0.419455
57	6	0	1.884758	2.870972	-0.333650
58	6	0	1.823317	4.259036	-0.322559
59	1	0	0.488102	5.959986	-0.338186
60	1	0	2.838292	2.360231	-0.304467
61	1	0	2.739982	4.836967	-0.284433
62	7	0	0.783872	2.086095	-0.382359
63	8	0	0.930741	0.474161	-2.727219
64	1	0	1.150165	-0.067380	-3.498147
65	1	0	1.066899	1.394397	-2.992666

2''$_{dp}$-H_2O (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1520.32205281 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.798426	-0.822967	-1.752349
2	6	0	-1.944689	-0.071708	-2.284659
3	1	0	-1.625609	0.965401	-2.438504
4	1	0	-2.296415	-0.454772	-3.256819

5	6	0	-1.071380	-2.261444	-1.596681
6	1	0	-2.150339	-2.424373	-1.694978
7	1	0	-0.603080	-2.854407	-2.394235
8	6	0	0.528502	-0.528735	-2.329080
9	1	0	1.125670	-1.441748	-2.253380
10	1	0	0.464543	-0.289901	-3.401126
11	26	0	-0.764999	0.098760	0.309707
12	6	0	-3.085291	-0.107998	-1.278806
13	6	0	-4.418848	-0.179756	-1.670332
14	6	0	-3.699300	-0.141083	0.965882
15	6	0	-5.423074	-0.216978	-0.699839
16	1	0	-4.665973	-0.209732	-2.726926
17	6	0	-5.051611	-0.205750	0.643784
18	1	0	-3.363210	-0.132118	1.997768
19	1	0	-6.467777	-0.265980	-0.988798
20	1	0	-5.791848	-0.248974	1.435305
21	6	0	-0.647771	-2.788683	-0.235397
22	6	0	-0.435042	-4.150354	-0.019941
23	6	0	-0.133651	-4.600921	1.264050
24	1	0	-0.510282	-4.845716	-0.850634
25	6	0	-0.259525	-2.323772	2.006910
26	6	0	-0.051685	-3.667453	2.298075
27	1	0	0.034091	-5.656531	1.452523
28	1	0	-0.196579	-1.552859	2.769169
29	1	0	0.177592	-3.969056	3.314284
30	7	0	-2.723625	-0.077907	0.034283
31	7	0	-0.547897	-1.883109	0.762653
32	6	0	1.250643	0.617277	-1.611835
33	1	0	2.265665	0.715556	-2.019382
34	1	0	0.735567	1.559399	-1.813824
35	7	0	1.288528	0.447073	-0.126041
36	6	0	1.588837	1.753932	0.517361
37	1	0	1.742771	1.550006	1.583990
38	1	0	2.510966	2.204915	0.129678
39	6	0	2.281827	-0.594272	0.314378
40	1	0	2.143814	-0.697233	1.393688
41	1	0	1.973965	-1.540118	-0.135438
42	6	0	3.741714	-0.325298	0.000999
43	6	0	4.554270	0.366994	0.911554
44	6	0	4.321747	-0.791108	-1.188703
45	6	0	5.899104	0.609754	0.630555
46	1	0	4.136187	0.703960	1.856890
47	6	0	5.666314	-0.549809	-1.474518
48	1	0	3.722959	-1.366641	-1.891174

49	6	0	6.456862	0.156441	-0.566480
50	1	0	6.513371	1.142602	1.350161
51	1	0	6.098069	-0.921943	-2.398744
52	1	0	7.504473	0.340535	-0.783909
53	6	0	0.422261	2.686984	0.353566
54	6	0	0.570064	4.066101	0.314693
55	6	0	-0.557142	4.889861	0.246707
56	1	0	1.568921	4.490632	0.346708
57	6	0	-1.894215	2.887552	0.228707
58	6	0	-1.810452	4.269729	0.208185
59	1	0	-0.460883	5.969513	0.222954
60	1	0	-2.856682	2.394223	0.187560
61	1	0	-2.724218	4.852529	0.154294
62	7	0	-0.802466	2.062787	0.296768
63	8	0	-0.410623	0.762361	3.241996
64	1	0	-0.789330	1.052181	4.082298
65	1	0	-0.745027	1.385844	2.580243

2''$_{dp}$-H_2O (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1520.35117895 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.797748	-0.892530	-1.537669
2	6	0	-1.885270	-0.167657	-2.223092
3	1	0	-1.545583	0.864850	-2.369005
4	1	0	-2.097970	-0.582852	-3.221254
5	6	0	-1.083801	-2.333346	-1.403354
6	1	0	-2.166618	-2.449476	-1.290511
7	1	0	-0.794515	-2.898404	-2.302052
8	6	0	0.535248	-0.635373	-2.118065
9	1	0	1.161199	-1.506885	-1.908376
10	1	0	0.485235	-0.548050	-3.214394
11	26	0	-0.926342	-0.054721	0.612744
12	6	0	-3.141706	-0.173934	-1.378817
13	6	0	-4.407565	-0.252357	-1.943415
14	6	0	-4.052806	-0.125419	0.759640
15	6	0	-5.541156	-0.255581	-1.121202
16	1	0	-4.506365	-0.315728	-3.023105
17	6	0	-5.345485	-0.196810	0.262773
18	1	0	-3.873680	-0.078956	1.830455
19	1	0	-6.537223	-0.312001	-1.545947
20	1	0	-6.184421	-0.207237	0.950866
21	6	0	-0.423683	-2.924564	-0.174133

22	6	0	0.062281	-4.228055	-0.161739
23	6	0	0.595484	-4.755416	1.019343
24	1	0	0.018212	-4.825891	-1.066902
25	6	0	0.132132	-2.645364	2.057932
26	6	0	0.627087	-3.942837	2.150979
27	1	0	0.975934	-5.771088	1.049398
28	1	0	0.157130	-1.979178	2.914947
29	1	0	1.031454	-4.299776	3.092215
30	7	0	-2.943028	-0.108676	-0.027735
31	7	0	-0.387776	-2.126480	0.923336
32	6	0	1.192850	0.623378	-1.547729
33	1	0	2.161458	0.779594	-2.044586
34	1	0	0.574101	1.494282	-1.781854
35	7	0	1.339700	0.570085	-0.075361
36	6	0	1.561372	1.916280	0.478790
37	1	0	1.823343	1.791995	1.537787
38	1	0	2.410468	2.430490	0.006388
39	6	0	2.402996	-0.378476	0.383063
40	1	0	2.326311	-0.417164	1.474301
41	1	0	2.131213	-1.371042	0.019247
42	6	0	3.831363	-0.056362	-0.021004
43	6	0	4.650595	0.733451	0.799341
44	6	0	4.371557	-0.557384	-1.215213
45	6	0	5.961676	1.033697	0.428134
46	1	0	4.267014	1.101747	1.747880
47	6	0	5.681749	-0.258325	-1.591872
48	1	0	3.770168	-1.205137	-1.848962
49	6	0	6.478605	0.542613	-0.772254
50	1	0	6.582263	1.640917	1.080362
51	1	0	6.082846	-0.659086	-2.518003
52	1	0	7.500068	0.771395	-1.060288
53	6	0	0.328917	2.789903	0.399570
54	6	0	0.437523	4.170255	0.229162
55	6	0	-0.712010	4.959203	0.256668
56	1	0	1.416085	4.617125	0.083192
57	6	0	-1.973147	2.947065	0.579598
58	6	0	-1.944002	4.330423	0.442558
59	1	0	-0.647704	6.035261	0.131273
60	1	0	-2.914527	2.418851	0.691984
61	1	0	-2.869552	4.895574	0.468878
62	7	0	-0.864812	2.173883	0.560676
63	8	0	-1.038444	0.333519	2.903312
64	1	0	-1.588832	-0.189330	3.501491
65	1	0	-1.224220	1.261789	3.100034

1'' (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1443.67201787 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.268385	-1.494617	-1.209822
2	6	0	-2.194724	-1.007067	-2.257202
3	1	0	-1.605587	-0.509988	-3.035232
4	1	0	-2.720102	-1.835292	-2.750203
5	6	0	-1.893150	-2.573412	-0.403966
6	1	0	-2.975209	-2.396721	-0.390822
7	1	0	-1.742407	-3.557247	-0.866408
8	6	0	0.061712	-1.884816	-1.755507
9	1	0	0.533487	-2.548326	-1.026267
10	1	0	-0.044445	-2.459553	-2.685336
11	26	0	-0.880358	0.223247	0.192317
12	6	0	-3.189119	-0.004252	-1.702685
13	6	0	-4.443251	0.178935	-2.281636
14	6	0	-3.597735	1.705908	-0.174308
15	6	0	-5.287365	1.170525	-1.781462
16	1	0	-4.751878	-0.443862	-3.115078
17	6	0	-4.855740	1.952171	-0.708380
18	1	0	-3.222990	2.287352	0.662113
19	1	0	-6.267334	1.328293	-2.220643
20	1	0	-5.480544	2.732621	-0.289067
21	6	0	-1.410847	-2.582969	1.033722
22	6	0	-1.405363	-3.752361	1.791751
23	6	0	-1.048208	-3.690994	3.138970
24	1	0	-1.682227	-4.696455	1.333743
25	6	0	-0.714326	-1.336231	2.874501
26	6	0	-0.698752	-2.458376	3.693099
27	1	0	-1.041013	-4.591265	3.745249
28	1	0	-0.438839	-0.359604	3.260301
29	1	0	-0.415469	-2.366056	4.735501
30	7	0	-2.775325	0.748516	-0.655906
31	7	0	-1.060649	-1.389905	1.570063
32	6	0	0.943866	-0.658135	-2.005525
33	1	0	1.914477	-0.973018	-2.403950
34	1	0	0.486883	-0.015388	-2.763595
35	7	0	1.106515	0.148694	-0.762777
36	6	0	1.432977	1.571166	-1.045061
37	1	0	2.488023	1.698376	-1.309646
38	1	0	0.844367	1.890478	-1.913524

39	6	0	2.117461	-0.464791	0.199948
40	1	0	2.062764	0.130341	1.115779
41	1	0	1.746927	-1.462676	0.445312
42	6	0	3.546240	-0.540640	-0.288388
43	6	0	4.446655	0.504538	-0.025872
44	6	0	4.010586	-1.671287	-0.979565
45	6	0	5.767129	0.436146	-0.471192
46	1	0	4.122828	1.364579	0.556313
47	6	0	5.330501	-1.741021	-1.426442
48	1	0	3.348433	-2.518309	-1.145388
49	6	0	6.208413	-0.683800	-1.178912
50	1	0	6.454403	1.247633	-0.253706
51	1	0	5.677036	-2.624255	-1.953519
52	1	0	7.237066	-0.740438	-1.520180
53	6	0	1.071208	2.451961	0.137083
54	6	0	1.750478	3.638041	0.410814
55	6	0	1.336158	4.430167	1.481388
56	1	0	2.590811	3.934746	-0.208332
57	6	0	-0.368094	2.812382	1.934661
58	6	0	0.256908	4.008938	2.260956
59	1	0	1.851818	5.357774	1.708786
60	1	0	-1.205406	2.442914	2.520243
61	1	0	-0.091058	4.590325	3.107356
62	7	0	0.022525	2.047917	0.892046

1'' (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1443.63378047 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.130858	-1.706883	-0.954434
2	6	0	-2.138756	-1.530831	-2.035014
3	1	0	-1.634846	-1.097593	-2.907169
4	1	0	-2.560347	-2.491115	-2.357792
5	6	0	-1.673202	-2.567997	0.140181
6	1	0	-2.764404	-2.480348	0.135426
7	1	0	-1.436764	-3.623775	-0.034072
8	6	0	0.195185	-2.208491	-1.448133
9	1	0	0.665995	-2.749817	-0.624420
10	1	0	0.064992	-2.921553	-2.270868
11	26	0	-0.833367	0.140051	-0.206102
12	6	0	-3.224356	-0.592697	-1.542306
13	6	0	-4.516806	-0.616720	-2.057175

14	6	0	-3.769406	1.150699	-0.104975
15	6	0	-5.458412	0.291953	-1.572038
16	1	0	-4.782354	-1.337219	-2.824035
17	6	0	-5.077137	1.188970	-0.574522
18	1	0	-3.441332	1.830691	0.670922
19	1	0	-6.471859	0.292387	-1.960248
20	1	0	-5.777496	1.906271	-0.161659
21	6	0	-1.161286	-2.092049	1.477206
22	6	0	-1.128544	-2.908376	2.604957
23	6	0	-0.723452	-2.367844	3.825017
24	1	0	-1.422048	-3.950266	2.526915
25	6	0	-0.395293	-0.271402	2.707232
26	6	0	-0.354872	-1.023090	3.875338
27	1	0	-0.693946	-2.984745	4.717263
28	1	0	-0.100374	0.770697	2.701206
29	1	0	-0.033033	-0.559683	4.801220
30	7	0	-2.847248	0.284985	-0.573657
31	7	0	-0.791488	-0.788670	1.525156
32	6	0	1.071106	-1.035441	-1.878665
33	1	0	2.069041	-1.380403	-2.168176
34	1	0	0.639494	-0.547691	-2.758733
35	7	0	1.138149	-0.022837	-0.774511
36	6	0	1.424011	1.348267	-1.301075
37	1	0	2.493656	1.497893	-1.475987
38	1	0	0.929488	1.452802	-2.274933
39	6	0	2.143819	-0.407315	0.305957
40	1	0	2.024954	0.336859	1.096737
41	1	0	1.807770	-1.362855	0.712493
42	6	0	3.590648	-0.493617	-0.120446
43	6	0	4.437641	0.620340	0.000077
44	6	0	4.129465	-1.698743	-0.599919
45	6	0	5.777502	0.542220	-0.381098
46	1	0	4.056683	1.546646	0.424983
47	6	0	5.468636	-1.778514	-0.983049
48	1	0	3.510737	-2.592465	-0.645548
49	6	0	6.292451	-0.655606	-0.880989
50	1	0	6.422082	1.408899	-0.274004
51	1	0	5.872419	-2.718633	-1.345147
52	1	0	7.336103	-0.719226	-1.171693
53	6	0	0.863810	2.385248	-0.354122
54	6	0	1.439562	3.641591	-0.183122
55	6	0	0.831892	4.558490	0.674908
56	1	0	2.350347	3.895505	-0.715382
57	6	0	-0.846921	2.910834	1.130844

58	6	0	-0.330715	4.182654	1.348843
59	1	0	1.262720	5.543737	0.821451
60	1	0	-1.738032	2.578114	1.651538
61	1	0	-0.830384	4.858100	2.034194
62	7	0	-0.275860	2.022297	0.290401

1'' (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1443.65534806 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.165692	-1.500134	-1.172998
2	6	0	-2.110764	-1.093663	-2.256805
3	1	0	-1.534533	-0.604491	-3.048954
4	1	0	-2.589814	-1.969521	-2.710240
5	6	0	-1.773905	-2.592693	-0.352650
6	1	0	-2.857174	-2.427864	-0.334096
7	1	0	-1.606947	-3.569939	-0.821026
8	6	0	0.166889	-1.903844	-1.737592
9	1	0	0.655949	-2.538578	-0.995015
10	1	0	0.037915	-2.506868	-2.644853
11	26	0	-0.822721	0.132507	0.014048
12	6	0	-3.127943	-0.115060	-1.722414
13	6	0	-4.400233	0.027359	-2.267440
14	6	0	-3.512216	1.622250	-0.223660
15	6	0	-5.246789	1.015293	-1.761329
16	1	0	-4.722014	-0.619947	-3.076693
17	6	0	-4.793121	1.828845	-0.722948
18	1	0	-3.121740	2.233266	0.581889
19	1	0	-6.243176	1.145879	-2.171271
20	1	0	-5.417482	2.609121	-0.302568
21	6	0	-1.267589	-2.564604	1.070573
22	6	0	-1.243755	-3.700177	1.876754
23	6	0	-0.853416	-3.573675	3.210852
24	1	0	-1.531747	-4.664664	1.471132
25	6	0	-0.523798	-1.233172	2.824031
26	6	0	-0.489545	-2.316492	3.695033
27	1	0	-0.831241	-4.443381	3.859780
28	1	0	-0.233812	-0.240767	3.154008
29	1	0	-0.179208	-2.175705	4.724299
30	7	0	-2.689794	0.667868	-0.705712
31	7	0	-0.906509	-1.346714	1.536327
32	6	0	1.016620	-0.665368	-2.022320
33	1	0	2.009483	-0.954970	-2.381824

34	1	0	0.558462	-0.056117	-2.806529
35	7	0	1.098004	0.162370	-0.782470
36	6	0	1.305337	1.618486	-1.034306
37	1	0	2.352463	1.848980	-1.255832
38	1	0	0.717648	1.899243	-1.916432
39	6	0	2.137051	-0.372639	0.203009
40	1	0	2.031521	0.230348	1.108027
41	1	0	1.827789	-1.387951	0.458450
42	6	0	3.569952	-0.360671	-0.275563
43	6	0	4.396700	0.748039	-0.031585
44	6	0	4.114906	-1.474869	-0.934163
45	6	0	5.722774	0.756728	-0.465103
46	1	0	4.013016	1.597101	0.529892
47	6	0	5.440648	-1.467751	-1.368694
48	1	0	3.512072	-2.368306	-1.082642
49	6	0	6.243946	-0.348446	-1.141114
50	1	0	6.352849	1.616895	-0.262155
51	1	0	5.850156	-2.338982	-1.869903
52	1	0	7.277372	-0.345017	-1.472463
53	6	0	0.813499	2.404130	0.166043
54	6	0	1.362162	3.626108	0.547147
55	6	0	0.834962	4.297338	1.651253
56	1	0	2.191817	4.043245	-0.014080
57	6	0	-0.720642	2.495660	1.923037
58	6	0	-0.221596	3.718280	2.355970
59	1	0	1.249076	5.251123	1.962182
60	1	0	-1.537352	2.005953	2.444868
61	1	0	-0.651316	4.199698	3.227271
62	7	0	-0.226024	1.850134	0.845345

1''(square pyramidal) (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1443.632646 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.842667	-0.674384	1.523899
2	6	0	1.994125	0.069248	2.115135
3	1	0	1.680151	1.105629	2.277868
4	1	0	2.286038	-0.346270	3.087676
5	6	0	1.153554	-2.145681	1.482797
6	1	0	2.237656	-2.273630	1.555541
7	1	0	0.719744	-2.654057	2.349964
8	6	0	-0.477334	-0.425491	2.197794
9	1	0	-1.043012	-1.358359	2.158357

10	1	0	-0.332432	-0.182109	3.256344
11	26	0	0.752190	0.041364	-0.335867
12	6	0	3.139331	0.004694	1.121452
13	6	0	4.481181	0.018717	1.488402
14	6	0	3.697726	-0.168864	-1.135344
15	6	0	5.457147	-0.052526	0.490483
16	1	0	4.759479	0.079221	2.535654
17	6	0	5.058903	-0.153985	-0.842255
18	1	0	3.343151	-0.247547	-2.158423
19	1	0	6.510103	-0.040559	0.753087
20	1	0	5.784340	-0.223970	-1.645035
21	6	0	0.691483	-2.752636	0.182059
22	6	0	0.501982	-4.121415	0.004855
23	6	0	0.176572	-4.600064	-1.264363
24	1	0	0.615961	-4.800406	0.843799
25	6	0	0.231289	-2.340098	-2.059599
26	6	0	0.046746	-3.693036	-2.317929
27	1	0	0.027774	-5.662407	-1.428507
28	1	0	0.123746	-1.599690	-2.847715
29	1	0	-0.200220	-4.022946	-3.320717
30	7	0	2.754343	-0.081282	-0.178613
31	7	0	0.544335	-1.873232	-0.833341
32	6	0	-1.249501	0.681275	1.490673
33	1	0	-2.269732	0.737563	1.885735
34	1	0	-0.776544	1.647711	1.674720
35	7	0	-1.269171	0.448174	0.006691
36	6	0	-1.572304	1.730160	-0.685107
37	1	0	-1.773426	1.502134	-1.738658
38	1	0	-2.480777	2.196401	-0.287981
39	6	0	-2.292189	-0.606532	-0.389442
40	1	0	-2.161300	-0.753406	-1.464834
41	1	0	-1.988611	-1.533975	0.098991
42	6	0	-3.739038	-0.297660	-0.073407
43	6	0	-4.548731	0.375931	-1.001500
44	6	0	-4.312099	-0.719947	1.137012
45	6	0	-5.886713	0.647038	-0.714480
46	1	0	-4.142583	0.668227	-1.967141
47	6	0	-5.649744	-0.448729	1.427024
48	1	0	-3.719787	-1.291028	1.849178
49	6	0	-6.437187	0.241013	0.503172
50	1	0	-6.502702	1.160561	-1.445865
51	1	0	-6.079887	-0.787758	2.364078
52	1	0	-7.480024	0.445559	0.723370
53	6	0	-0.398347	2.672288	-0.599070

54	6	0	-0.545573	4.045158	-0.785689
55	6	0	0.582024	4.862640	-0.749273
56	1	0	-1.531963	4.463032	-0.958407
57	6	0	1.899079	2.904981	-0.331728
58	6	0	1.828633	4.278371	-0.517596
59	1	0	0.490026	5.934292	-0.894288
60	1	0	2.849881	2.422066	-0.146681
61	1	0	2.733415	4.874405	-0.477843
62	7	0	0.810472	2.100260	-0.367807

1''(square pyramidal) (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1443.644055 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.803053	-0.875684	1.610056
2	6	0	1.949737	-0.205803	2.271588
3	1	0	1.635297	0.804545	2.559086
4	1	0	2.258433	-0.720240	3.191329
5	6	0	1.062016	-2.319522	1.380785
6	1	0	2.129735	-2.511703	1.531352
7	1	0	0.536597	-2.936470	2.118891
8	6	0	-0.527463	-0.595077	2.222972
9	1	0	-1.143120	-1.488865	2.107672
10	1	0	-0.439293	-0.412888	3.301112
11	26	0	0.758764	0.167803	-0.300252
12	6	0	3.102797	-0.125803	1.288209
13	6	0	4.437458	-0.217354	1.674130
14	6	0	3.717687	0.082129	-0.952984
15	6	0	5.436687	-0.145639	0.701419
16	1	0	4.689700	-0.349186	2.721283
17	6	0	5.069778	-0.001517	-0.636754
18	1	0	3.387658	0.195847	-1.981077
19	1	0	6.482395	-0.213985	0.983676
20	1	0	5.812120	0.042839	-1.425780
21	6	0	0.707030	-2.761979	-0.028363
22	6	0	0.546827	-4.111995	-0.341360
23	6	0	0.315060	-4.482486	-1.665051
24	1	0	0.610463	-4.861306	0.441535
25	6	0	0.385567	-2.163097	-2.252524
26	6	0	0.239843	-3.488353	-2.642659
27	1	0	0.193044	-5.528156	-1.928848
28	1	0	0.313502	-1.357412	-2.977278
29	1	0	0.062071	-3.730337	-3.684451

30	7	0	2.750797	0.033897	-0.013838
31	7	0	0.615444	-1.801494	-0.971993
32	6	0	-1.213459	0.603992	1.560263
33	1	0	-2.229712	0.715935	1.954522
34	1	0	-0.672376	1.525832	1.795336
35	7	0	-1.257071	0.475240	0.058111
36	6	0	-1.638309	1.785047	-0.544944
37	1	0	-1.935293	1.595232	-1.582173
38	1	0	-2.511456	2.216224	-0.043884
39	6	0	-2.240826	-0.598844	-0.392953
40	1	0	-2.114328	-0.672770	-1.475742
41	1	0	-1.894411	-1.540395	0.033518
42	6	0	-3.694066	-0.360697	-0.045972
43	6	0	-4.543550	0.298835	-0.948373
44	6	0	-4.233976	-0.835335	1.160586
45	6	0	-5.888308	0.505365	-0.640537
46	1	0	-4.162588	0.630276	-1.911629
47	6	0	-5.578291	-0.628403	1.471505
48	1	0	-3.612007	-1.398132	1.853376
49	6	0	-6.405896	0.048254	0.573274
50	1	0	-6.534383	1.008322	-1.353024
51	1	0	-5.982192	-1.007648	2.404816
52	1	0	-7.453743	0.202383	0.810107
53	6	0	-0.480514	2.747891	-0.549362
54	6	0	-0.669368	4.125354	-0.639411
55	6	0	0.442628	4.961149	-0.722520
56	1	0	-1.674968	4.532611	-0.649200
57	6	0	1.832842	3.013773	-0.595719
58	6	0	1.717711	4.392309	-0.702324
59	1	0	0.317317	6.036626	-0.797659
60	1	0	2.804297	2.537437	-0.566136
61	1	0	2.610551	5.004277	-0.763024
62	7	0	0.757915	2.194480	-0.522147

1''(square pyramidal) (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1443.662767 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.817539	-0.960450	1.473444
2	6	0	1.915208	-0.341168	2.256364
3	1	0	1.577836	0.648501	2.585548
4	1	0	2.140273	-0.918003	3.163491
5	6	0	1.093923	-2.396403	1.193839

6	1	0	2.177670	-2.549504	1.239744
7	1	0	0.658060	-3.040706	1.966563
8	6	0	-0.521922	-0.743827	2.095852
9	1	0	-1.142910	-1.609066	1.857941
10	1	0	-0.441327	-0.708723	3.189522
11	26	0	0.845276	0.106228	-0.467693
12	6	0	3.163092	-0.193342	1.405197
13	6	0	4.443228	-0.264206	1.952109
14	6	0	4.040579	0.135636	-0.725590
15	6	0	5.549939	-0.115326	1.115402
16	1	0	4.570853	-0.438700	3.015625
17	6	0	5.346082	0.080991	-0.251518
18	1	0	3.838391	0.273729	-1.784216
19	1	0	6.554930	-0.166319	1.522217
20	1	0	6.178294	0.182737	-0.939028
21	6	0	0.630409	-2.832826	-0.184243
22	6	0	0.320792	-4.165339	-0.452494
23	6	0	0.005891	-4.544119	-1.757798
24	1	0	0.332539	-4.896967	0.349054
25	6	0	0.307022	-2.265061	-2.421635
26	6	0	0.004740	-3.576952	-2.764219
27	1	0	-0.235030	-5.577825	-1.984851
28	1	0	0.306971	-1.478845	-3.170805
29	1	0	-0.230320	-3.829058	-3.792135
30	7	0	2.966464	0.015263	0.082570
31	7	0	0.611298	-1.893147	-1.159314
32	6	0	-1.191941	0.535908	1.591411
33	1	0	-2.177468	0.637893	2.062226
34	1	0	-0.603824	1.412509	1.884447
35	7	0	-1.315240	0.552026	0.103548
36	6	0	-1.669957	1.912378	-0.370777
37	1	0	-2.123356	1.812169	-1.362809
38	1	0	-2.430990	2.377643	0.265956
39	6	0	-2.328691	-0.456718	-0.410015
40	1	0	-2.252731	-0.422182	-1.500723
41	1	0	-1.981114	-1.443910	-0.101263
42	6	0	-3.764603	-0.245211	0.021208
43	6	0	-4.645826	0.505904	-0.772051
44	6	0	-4.254018	-0.824344	1.203269
45	6	0	-5.970867	0.698300	-0.380458
46	1	0	-4.307123	0.921674	-1.718164
47	6	0	-5.578412	-0.632285	1.598132
48	1	0	-3.608325	-1.455507	1.810201
49	6	0	-6.437332	0.135369	0.809203

50	1	0	-6.641808	1.273895	-1.010254
51	1	0	-5.942764	-1.092250	2.511259
52	1	0	-7.469836	0.279295	1.110961
53	6	0	-0.469870	2.819773	-0.513409
54	6	0	-0.610776	4.207388	-0.493839
55	6	0	0.499211	5.010684	-0.745556
56	1	0	-1.581800	4.647670	-0.291747
57	6	0	1.801680	3.017482	-0.981874
58	6	0	1.730378	4.402650	-1.000858
59	1	0	0.406987	6.092154	-0.740617
60	1	0	2.742835	2.507835	-1.152042
61	1	0	2.619881	4.988305	-1.203580
62	7	0	0.725691	2.231683	-0.745448

1''$_{pt\text{-}A}$ (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1443.82407786 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.907375	-1.076183	-1.301580
2	6	0	-2.775330	-0.208346	-2.145842
3	1	0	-2.156718	0.255804	-2.921495
4	1	0	-3.534207	-0.798491	-2.672272
5	6	0	-2.687279	-2.148630	-0.616768
6	1	0	-3.725545	-1.806392	-0.539960
7	1	0	-2.704384	-3.064522	-1.218913
8	6	0	-0.698697	-1.591570	-2.008785
9	1	0	-0.336079	-2.461055	-1.454741
10	1	0	-0.948739	-1.942383	-3.018330
11	26	0	-1.096981	0.168248	0.225128
12	6	0	-3.430681	0.888067	-1.321257
13	6	0	-4.650363	1.447599	-1.690482
14	6	0	-3.281064	2.336668	0.513383
15	6	0	-5.184625	2.490800	-0.930606
16	1	0	-5.177992	1.071806	-2.561425
17	6	0	-4.487071	2.942722	0.192500
18	1	0	-2.719155	2.643490	1.390334
19	1	0	-6.135612	2.936546	-1.205886
20	1	0	-4.874695	3.741825	0.814742
21	6	0	-2.192871	-2.440835	0.790956
22	6	0	-2.488188	-3.650722	1.414622
23	6	0	-2.134844	-3.835504	2.752428
24	1	0	-3.000041	-4.434477	0.864994

25	6	0	-1.205328	-1.629274	2.750477
26	6	0	-1.487077	-2.802362	3.435178
27	1	0	-2.364791	-4.770080	3.254860
28	1	0	-0.699449	-0.804093	3.242268
29	1	0	-1.204402	-2.903561	4.477184
30	7	0	-2.749697	1.333658	-0.228619
31	7	0	-1.543537	-1.444990	1.450686
32	6	0	0.383013	-0.513434	-2.121511
33	1	0	1.239748	-0.903355	-2.675962
34	1	0	-0.002489	0.329892	-2.701147
35	7	0	0.841071	0.048013	-0.783686
36	6	0	1.625932	1.294394	-1.114590
37	1	0	2.504742	1.001598	-1.700764
38	1	0	0.995799	1.903930	-1.766121
39	6	0	1.672796	-0.972336	0.013686
40	1	0	1.685015	-0.610486	1.046438
41	1	0	1.084374	-1.892681	0.016440
42	6	0	3.100048	-1.249669	-0.422501
43	6	0	4.149687	-0.922968	0.461849
44	6	0	3.425726	-1.914025	-1.617236
45	6	0	5.481154	-1.202366	0.138151
46	1	0	3.917202	-0.533841	1.452590
47	6	0	4.757287	-2.179794	-1.946881
48	1	0	2.651928	-2.277510	-2.285951
49	6	0	5.788460	-1.813746	-1.079509
50	1	0	6.271571	-0.973240	0.846343
51	1	0	4.986345	-2.696494	-2.873413
52	1	0	6.819672	-2.035550	-1.334234
53	6	0	2.070646	2.199742	0.018779
54	6	0	1.317521	3.267242	0.494543
55	6	0	1.862690	4.158834	1.429954
56	1	0	0.322435	3.436545	0.095840
57	6	0	3.902711	2.910518	1.387614
58	6	0	3.172072	3.982270	1.880516
59	1	0	1.275788	5.001546	1.783051
60	1	0	4.927418	2.699946	1.674237
61	1	0	3.628898	4.665257	2.588399
62	7	0	3.339624	2.070514	0.492990
63	1	0	3.896324	1.268828	0.169010

1''$_{pt\text{-}A}$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1443.75517498 hartree

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Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	-2.177050	-0.822807	-1.100405
2	6	0	-2.930782	0.166226	-1.954268
3	1	0	-2.474626	0.202308	-2.949061
4	1	0	-3.956251	-0.183366	-2.104542
5	6	0	-3.079157	-1.866938	-0.507609
6	1	0	-4.017629	-1.376543	-0.223566
7	1	0	-3.327261	-2.631696	-1.252770
8	6	0	-1.029470	-1.441713	-1.844427
9	1	0	-0.750255	-2.361989	-1.328610
10	1	0	-1.332659	-1.716162	-2.861122
11	26	0	-1.329305	0.075951	0.413454
12	6	0	-2.926882	1.551731	-1.344913
13	6	0	-3.767210	2.559057	-1.814553
14	6	0	-1.987277	3.006134	0.222743
15	6	0	-3.698272	3.827527	-1.238948
16	1	0	-4.468294	2.352556	-2.617369
17	6	0	-2.790428	4.054351	-0.199192
18	1	0	-1.283110	3.137672	1.039450
19	1	0	-4.347088	4.624380	-1.589244
20	1	0	-2.715486	5.023265	0.282071
21	6	0	-2.438745	-2.469638	0.724971
22	6	0	-2.829147	-3.702841	1.237312
23	6	0	-2.270307	-4.147710	2.437037
24	1	0	-3.567074	-4.301920	0.713099
25	6	0	-0.969626	-2.136814	2.506119
26	6	0	-1.327718	-3.345350	3.086061
27	1	0	-2.565995	-5.103519	2.858467
28	1	0	-0.229723	-1.496175	2.975979
29	1	0	-0.874524	-3.652265	4.022234
30	7	0	-2.040866	1.770503	-0.336560
31	7	0	-1.506111	-1.694083	1.343903
32	6	0	0.122168	-0.451441	-1.885024
33	1	0	0.974987	-0.871553	-2.426007
34	1	0	-0.185545	0.455836	-2.410677
35	7	0	0.553797	-0.047446	-0.484482
36	6	0	1.313966	1.234484	-0.685600
37	1	0	2.088338	1.053117	-1.440024
38	1	0	0.609581	1.956390	-1.110489
39	6	0	1.459854	-1.157800	0.105366
40	1	0	1.687317	-0.864915	1.134042
41	1	0	0.823902	-2.039407	0.171746
42	6	0	2.732344	-1.473830	-0.641640

43	6	0	3.935647	-0.813346	-0.339243
44	6	0	2.749979	-2.495996	-1.607555
45	6	0	5.115151	-1.139587	-1.008389
46	1	0	3.968988	-0.069472	0.453691
47	6	0	3.928425	-2.821726	-2.279024
48	1	0	1.848783	-3.069389	-1.814249
49	6	0	5.110859	-2.138340	-1.985573
50	1	0	6.040982	-0.633269	-0.754851
51	1	0	3.928942	-3.619369	-3.014754
52	1	0	6.030465	-2.398948	-2.499463
53	6	0	2.024104	1.945662	0.456368
54	6	0	2.922012	2.969135	0.153590
55	6	0	3.552147	3.686314	1.172126
56	1	0	3.129930	3.199541	-0.886298
57	6	0	2.407137	2.357559	2.795005
58	6	0	3.292142	3.377410	2.514955
59	1	0	4.250842	4.479137	0.920828
60	1	0	2.156706	2.034706	3.799134
61	1	0	3.774704	3.910828	3.326694
62	7	0	1.801835	1.689898	1.771502
63	1	0	1.196277	0.917925	2.024015

1''$_{pt\text{-}A}$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1443.77853873 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.885546	-0.902753	-1.202826
2	6	0	-2.610789	-0.025342	-2.184669
3	1	0	-1.890388	0.340812	-2.922281
4	1	0	-3.352796	-0.611203	-2.737111
5	6	0	-2.813089	-1.937292	-0.628216
6	1	0	-3.809846	-1.486577	-0.563302
7	1	0	-2.887620	-2.794117	-1.307344
8	6	0	-0.644884	-1.516445	-1.780812
9	1	0	-0.370574	-2.361558	-1.145801
10	1	0	-0.849992	-1.915005	-2.781904
11	26	0	-1.263817	0.193643	0.302561
12	6	0	-3.243131	1.152128	-1.476434
13	6	0	-4.341348	1.836867	-1.984712
14	6	0	-3.108329	2.617514	0.343578
15	6	0	-4.821482	2.955022	-1.297103
16	1	0	-4.816735	1.504335	-2.902079

17	6	0	-4.193800	3.352015	-0.113242
18	1	0	-2.604654	2.880621	1.269092
19	1	0	-5.678540	3.502956	-1.676663
20	1	0	-4.544149	4.208991	0.451417
21	6	0	-2.378404	-2.355888	0.758639
22	6	0	-2.753647	-3.570443	1.323262
23	6	0	-2.409888	-3.835354	2.651268
24	1	0	-3.315525	-4.294001	0.741173
25	6	0	-1.334784	-1.696225	2.743875
26	6	0	-1.692390	-2.879119	3.375477
27	1	0	-2.699354	-4.773930	3.113956
28	1	0	-0.771620	-0.931216	3.269655
29	1	0	-1.413185	-3.047090	4.409798
30	7	0	-2.631791	1.539507	-0.323719
31	7	0	-1.667080	-1.431795	1.457973
32	6	0	0.482712	-0.493136	-1.862009
33	1	0	1.360869	-0.966167	-2.314103
34	1	0	0.190316	0.330792	-2.518684
35	7	0	0.859255	0.106844	-0.522017
36	6	0	1.649946	1.333294	-0.882419
37	1	0	2.427838	1.050275	-1.600542
38	1	0	0.967980	2.015325	-1.405275
39	6	0	1.701801	-0.898387	0.293175
40	1	0	1.949113	-0.398266	1.233944
41	1	0	1.021592	-1.715210	0.544255
42	6	0	2.952206	-1.439471	-0.358318
43	6	0	4.190795	-0.797451	-0.191351
44	6	0	2.910024	-2.636020	-1.095638
45	6	0	5.347394	-1.316890	-0.773254
46	1	0	4.266367	0.089635	0.432732
47	6	0	4.064987	-3.156060	-1.679636
48	1	0	1.977753	-3.189370	-1.188508
49	6	0	5.284433	-2.492337	-1.525390
50	1	0	6.300458	-0.819734	-0.623676
51	1	0	4.018222	-4.085623	-2.237608
52	1	0	6.185648	-2.901648	-1.970267
53	6	0	2.362078	2.156028	0.176842
54	6	0	3.477497	2.915589	-0.170563
55	6	0	4.077341	3.764096	0.763481
56	1	0	3.874839	2.842095	-1.177304
57	6	0	2.471043	3.076650	2.394175
58	6	0	3.569513	3.845615	2.066602
59	1	0	4.943298	4.354335	0.478004
60	1	0	2.017721	3.063209	3.378675

61	1	0	4.020668	4.487531	2.815272
62	7	0	1.904842	2.276030	1.449991
63	1	0	1.108966	1.716496	1.732439

1''$_{pt\text{-}B}$ (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1443.81548947 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.396382	-0.918255	-0.970206
2	6	0	-2.241888	-0.319464	-2.067099
3	1	0	-1.633069	0.432157	-2.577108
4	1	0	-2.453806	-1.101668	-2.807387
5	6	0	-2.145706	-2.012553	-0.274022
6	1	0	-3.133561	-1.622686	-0.007765
7	1	0	-2.302082	-2.860906	-0.952943
8	6	0	-0.147073	-1.484502	-1.625295
9	1	0	0.240813	-2.258714	-0.958237
10	1	0	-0.409752	-1.980666	-2.567953
11	26	0	-0.337299	0.138106	0.720554
12	6	0	-3.579021	0.298399	-1.697637
13	6	0	-4.784197	-0.394432	-1.730103
14	6	0	-4.788869	2.317754	-1.213123
15	6	0	-5.995167	0.270411	-1.489570
16	1	0	-4.785195	-1.450953	-1.975602
17	6	0	-5.998380	1.641912	-1.222975
18	1	0	-4.698854	3.385642	-1.047059
19	1	0	-6.930724	-0.280044	-1.530016
20	1	0	-6.919768	2.186986	-1.048101
21	6	0	-1.485762	-2.498076	1.005061
22	6	0	-1.696397	-3.792445	1.469504
23	6	0	-1.165558	-4.172036	2.705866
24	1	0	-2.274000	-4.496765	0.879266
25	6	0	-0.230470	-1.978048	2.911988
26	6	0	-0.424837	-3.246260	3.442965
27	1	0	-1.326752	-5.176983	3.083948
28	1	0	0.353213	-1.232629	3.443401
29	1	0	0.003629	-3.500906	4.406116
30	7	0	-3.639417	1.637400	-1.441535
31	7	0	-0.752873	-1.603866	1.718187
32	6	0	0.924462	-0.420623	-1.868249
33	1	0	1.782609	-0.874086	-2.374980
34	1	0	0.553144	0.359634	-2.537946

35	7	0	1.337120	0.209899	-0.577389
36	6	0	1.661715	1.662950	-0.707697
37	1	0	2.715533	1.801547	-0.967798
38	1	0	1.081561	2.073118	-1.542409
39	6	0	2.484617	-0.556803	0.113627
40	1	0	2.611569	-0.076101	1.089820
41	1	0	2.109344	-1.569689	0.289015
42	6	0	3.795853	-0.601264	-0.627342
43	6	0	4.775909	0.381569	-0.404509
44	6	0	4.079012	-1.652343	-1.516691
45	6	0	5.993207	0.335561	-1.084324
46	1	0	4.607801	1.162392	0.334478
47	6	0	5.296076	-1.697168	-2.196968
48	1	0	3.366734	-2.464152	-1.650415
49	6	0	6.250267	-0.698522	-1.987808
50	1	0	6.747879	1.092093	-0.895071
51	1	0	5.508280	-2.519240	-2.872830
52	1	0	7.201248	-0.739424	-2.508969
53	6	0	1.311793	2.449262	0.544354
54	6	0	2.011588	3.597090	0.903827
55	6	0	1.598386	4.334553	2.016505
56	1	0	2.871621	3.911188	0.321106
57	6	0	-0.165107	2.748037	2.343741
58	6	0	0.489320	3.903240	2.748326
59	1	0	2.138342	5.229560	2.310355
60	1	0	-1.023083	2.368999	2.890759
61	1	0	0.141170	4.445097	3.620812
62	7	0	0.232100	2.030458	1.263159
63	1	0	-2.780527	2.179803	-1.480500

1''$_{pt\text{-}B}$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1443.77206003 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.445932	-1.210773	-0.598129
2	6	0	-2.460728	-1.104585	-1.717999
3	1	0	-1.971058	-0.590624	-2.550808
4	1	0	-2.684009	-2.119049	-2.070408
5	6	0	-2.011087	-1.972866	0.560468
6	1	0	-3.022350	-1.601114	0.752139
7	1	0	-2.093559	-3.042054	0.328441
8	6	0	-0.247911	-1.955888	-1.169079
9	1	0	0.217969	-2.498156	-0.344659

10	1	0	-0.573844	-2.702809	-1.901842
11	26	0	-0.484602	0.470445	0.222599
12	6	0	-3.799876	-0.441721	-1.443817
13	6	0	-4.924584	-1.128209	-0.999178
14	6	0	-5.145971	1.535312	-1.691009
15	6	0	-6.160600	-0.475373	-0.884829
16	1	0	-4.849614	-2.186643	-0.774274
17	6	0	-6.272594	0.873955	-1.228634
18	1	0	-5.146890	2.571027	-2.012947
19	1	0	-7.033428	-1.027473	-0.548205
20	1	0	-7.217889	1.402401	-1.166171
21	6	0	-1.188284	-1.746747	1.807806
22	6	0	-1.212554	-2.625010	2.886069
23	6	0	-0.506290	-2.298593	4.046151
24	1	0	-1.778764	-3.548906	2.823590
25	6	0	0.209681	-0.277625	2.972667
26	6	0	0.209804	-1.100163	4.090979
27	1	0	-0.514103	-2.970052	4.899220
28	1	0	0.770577	0.648861	2.953434
29	1	0	0.769246	-0.808830	4.973218
30	7	0	-3.967849	0.871449	-1.777888
31	7	0	-0.475233	-0.590872	1.846286
32	6	0	0.748264	-0.985498	-1.791673
33	1	0	1.614655	-1.522566	-2.190738
34	1	0	0.300501	-0.440942	-2.628978
35	7	0	1.168731	0.003330	-0.748249
36	6	0	1.607171	1.316610	-1.330581
37	1	0	2.640462	1.255265	-1.685577
38	1	0	0.985021	1.536104	-2.207298
39	6	0	2.284176	-0.565784	0.163858
40	1	0	2.431472	0.189818	0.937661
41	1	0	1.859351	-1.449623	0.641355
42	6	0	3.584392	-0.895797	-0.520641
43	6	0	4.616851	0.056703	-0.586896
44	6	0	3.812258	-2.179223	-1.047856
45	6	0	5.831883	-0.255151	-1.196832
46	1	0	4.488400	1.033137	-0.124245
47	6	0	5.026700	-2.490310	-1.659318
48	1	0	3.056489	-2.955687	-0.946442
49	6	0	6.034243	-1.525801	-1.741366
50	1	0	6.626243	0.483447	-1.230563
51	1	0	5.195087	-3.487468	-2.052879
52	1	0	6.982833	-1.771019	-2.207983
53	6	0	1.428305	2.402608	-0.290332

54	6	0	2.171618	3.577695	-0.269774
55	6	0	1.886055	4.544053	0.698404
56	1	0	2.960602	3.736223	-0.997928
57	6	0	0.165202	3.108665	1.552179
58	6	0	0.864834	4.305938	1.622737
59	1	0	2.455726	5.467604	0.733736
60	1	0	-0.628742	2.876714	2.255882
61	1	0	0.617523	5.032078	2.389331
62	7	0	0.437266	2.169460	0.614659
63	1	0	-3.182869	1.377433	-2.179419

1''$_{pt\text{-}B}$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1443.79916438 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.130015	-1.475796	-0.422189
2	6	0	-1.865038	-1.432432	-1.745472
3	1	0	-1.216136	-0.941478	-2.476029
4	1	0	-2.000168	-2.463990	-2.089513
5	6	0	-1.993815	-2.067076	0.662019
6	1	0	-3.028017	-2.116120	0.309891
7	1	0	-1.690263	-3.100163	0.860657
8	6	0	0.133996	-2.303616	-0.635375
9	1	0	0.487853	-2.601287	0.355195
10	1	0	-0.101443	-3.222404	-1.185746
11	26	0	-0.248540	0.252600	0.281457
12	6	0	-3.233009	-0.779197	-1.793529
13	6	0	-4.396465	-1.500622	-2.031891
14	6	0	-4.506810	1.253285	-1.872963
15	6	0	-5.623413	-0.838682	-2.191333
16	1	0	-4.347170	-2.581311	-2.115712
17	6	0	-5.680421	0.554315	-2.108794
18	1	0	-4.456110	2.334516	-1.808707
19	1	0	-6.524591	-1.412501	-2.388000
20	1	0	-6.611779	1.095649	-2.236041
21	6	0	-1.964788	-1.252977	1.942015
22	6	0	-2.534016	-1.755018	3.110073
23	6	0	-2.526522	-0.973365	4.265639
24	1	0	-2.973836	-2.747662	3.118870
25	6	0	-1.376880	0.728095	3.033799
26	6	0	-1.936630	0.292972	4.225235
27	1	0	-2.964841	-1.350257	5.184714

28	1	0	-0.882139	1.689680	2.972529
29	1	0	-1.898258	0.927188	5.104120
30	7	0	-3.341513	0.578609	-1.726470
31	7	0	-1.394300	-0.018671	1.900419
32	6	0	1.208537	-1.493117	-1.363177
33	1	0	2.122711	-2.086973	-1.462499
34	1	0	0.895078	-1.228303	-2.376185
35	7	0	1.470793	-0.236053	-0.593753
36	6	0	1.883432	0.929770	-1.428398
37	1	0	2.954710	0.891818	-1.649490
38	1	0	1.357526	0.880284	-2.389360
39	6	0	2.494344	-0.471754	0.556891
40	1	0	2.532776	0.468693	1.111787
41	1	0	2.046693	-1.224030	1.212177
42	6	0	3.869789	-0.898765	0.117310
43	6	0	4.867753	0.059438	-0.133864
44	6	0	4.192963	-2.262497	0.003930
45	6	0	6.146465	-0.336735	-0.525508
46	1	0	4.661421	1.116550	0.020041
47	6	0	5.471868	-2.657515	-0.388308
48	1	0	3.459738	-3.023680	0.264015
49	6	0	6.446386	-1.694538	-0.662293
50	1	0	6.913431	0.409889	-0.704204
51	1	0	5.714213	-3.712782	-0.460421
52	1	0	7.444038	-2.002104	-0.958562
53	6	0	1.502851	2.208775	-0.714295
54	6	0	2.159477	3.415912	-0.929315
55	6	0	1.705848	4.566135	-0.279774
56	1	0	3.014285	3.456184	-1.596787
57	6	0	-0.006451	3.243037	0.748907
58	6	0	0.599942	4.478008	0.570192
59	1	0	2.208820	5.516069	-0.433332
60	1	0	-0.869763	3.133339	1.395442
61	1	0	0.216757	5.349178	1.090144
62	7	0	0.431767	2.120648	0.128018
63	1	0	-2.496985	1.126239	-1.579397

1''$_{pt\text{-}C}$ (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1443.81644775 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.275977	1.185505	-1.053740

2	6	0	2.263911	0.601271	-2.030754
3	1	0	1.714829	-0.052898	-2.715359
4	1	0	2.709869	1.389521	-2.648877
5	6	0	1.916506	2.440902	-0.517764
6	1	0	2.903521	2.157425	-0.138275
7	1	0	2.090192	3.128227	-1.356234
8	6	0	-0.024065	1.477067	-1.748391
9	1	0	-0.582266	2.172967	-1.121231
10	1	0	0.155906	1.976959	-2.709218
11	26	0	0.899756	-0.794107	0.134602
12	6	0	3.338890	-0.214717	-1.344194
13	6	0	4.656715	-0.244085	-1.785360
14	6	0	3.798996	-1.826042	0.289957
15	6	0	5.564161	-1.107908	-1.162494
16	1	0	4.970717	0.385700	-2.611681
17	6	0	5.127215	-1.912476	-0.108423
18	1	0	3.417923	-2.438090	1.101038
19	1	0	6.595939	-1.150899	-1.498040
20	1	0	5.799757	-2.597285	0.396479
21	6	0	1.187968	3.235355	0.549766
22	6	0	0.316073	4.283903	0.278235
23	6	0	-0.220927	5.051639	1.321588
24	1	0	0.081771	4.528776	-0.752147
25	6	0	1.009788	3.734222	2.894350
26	6	0	0.124972	4.771373	2.645889
27	1	0	-0.889411	5.877375	1.095466
28	1	0	1.359470	3.466943	3.885565
29	1	0	-0.260921	5.357816	3.472772
30	7	0	2.917603	-0.993696	-0.313649
31	7	0	1.499507	3.010188	1.859285
32	6	0	-0.863150	0.215559	-1.982395
33	1	0	-1.830718	0.506759	-2.406212
34	1	0	-0.386364	-0.443285	-2.713798
35	7	0	-1.042824	-0.555402	-0.718924
36	6	0	-1.470768	-1.966323	-0.965074
37	1	0	-2.543551	-2.017529	-1.175258
38	1	0	-0.948790	-2.334851	-1.856056
39	6	0	-2.001057	0.136848	0.264354
40	1	0	-1.963176	-0.454165	1.183388
41	1	0	-1.561185	1.113472	0.488096
42	6	0	-3.428410	0.288497	-0.202063
43	6	0	-4.389036	-0.677273	0.142011
44	6	0	-3.831977	1.405655	-0.952954
45	6	0	-5.712324	-0.545003	-0.280212

46	1	0	-4.110971	-1.520984	0.769867
47	6	0	-5.154036	1.537416	-1.377707
48	1	0	-3.121152	2.196471	-1.186046
49	6	0	-6.094033	0.558090	-1.047191
50	1	0	-6.447329	-1.292423	0.000519
51	1	0	-5.455316	2.406924	-1.952988
52	1	0	-7.124239	0.663703	-1.371438
53	6	0	-1.113808	-2.844146	0.220842
54	6	0	-1.830114	-3.994949	0.534047
55	6	0	-1.419263	-4.785023	1.610194
56	1	0	-2.696792	-4.271274	-0.057890
57	6	0	0.363072	-3.234622	1.999385
58	6	0	-0.305775	-4.395158	2.359528
59	1	0	-1.965427	-5.688009	1.865451
60	1	0	1.226092	-2.890255	2.560990
61	1	0	0.035984	-4.976445	3.208782
62	7	0	-0.023865	-2.473859	0.946097
63	1	0	2.190042	2.296574	2.078177

1''$_{pt\text{-}C}$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1443.76917273 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.078714	1.408786	-1.093248
2	6	0	2.155046	0.992401	-2.077898
3	1	0	1.666822	0.546433	-2.949241
4	1	0	2.695106	1.867073	-2.452658
5	6	0	1.471428	2.793255	-0.618817
6	1	0	2.499321	2.715109	-0.250425
7	1	0	1.499786	3.460184	-1.489582
8	6	0	-0.245102	1.419645	-1.817324
9	1	0	-0.953652	1.993103	-1.219367
10	1	0	-0.152775	1.921529	-2.788307
11	26	0	0.900064	-0.234738	0.244364
12	6	0	3.102045	-0.022034	-1.502116
13	6	0	4.392929	-0.196668	-1.988487
14	6	0	3.333016	-1.860572	-0.077919
15	6	0	5.167583	-1.250983	-1.499533
16	1	0	4.783087	0.472755	-2.748654
17	6	0	4.622579	-2.098811	-0.533051
18	1	0	2.879938	-2.491940	0.674135
19	1	0	6.176042	-1.408627	-1.869530

20	1	0	5.186687	-2.933594	-0.131668
21	6	0	0.624694	3.486914	0.433727
22	6	0	-0.499141	4.257026	0.154436
23	6	0	-1.142829	4.973754	1.173837
24	1	0	-0.852223	4.336793	-0.867860
25	6	0	0.484334	4.173926	2.734295
26	6	0	-0.650329	4.928205	2.480396
27	1	0	-2.010578	5.583675	0.939408
28	1	0	0.958084	4.109019	3.707890
29	1	0	-1.115787	5.486410	3.285689
30	7	0	2.576249	-0.835386	-0.548079
31	7	0	1.070287	3.486558	1.724664
32	6	0	-0.756562	-0.010055	-2.000761
33	1	0	-1.759189	-0.000322	-2.439523
34	1	0	-0.112325	-0.583683	-2.671726
35	7	0	-0.760476	-0.691704	-0.673566
36	6	0	-0.768986	-2.186603	-0.749278
37	1	0	-1.761315	-2.560473	-1.018757
38	1	0	-0.070259	-2.489394	-1.536756
39	6	0	-1.919555	-0.190081	0.222960
40	1	0	-1.795164	-0.690156	1.185228
41	1	0	-1.750420	0.880047	0.381315
42	6	0	-3.310635	-0.430708	-0.313908
43	6	0	-4.008106	-1.597846	0.040235
44	6	0	-3.945425	0.517975	-1.133104
45	6	0	-5.297737	-1.824951	-0.441160
46	1	0	-3.558486	-2.317933	0.720085
47	6	0	-5.234258	0.289983	-1.615140
48	1	0	-3.448417	1.455148	-1.376708
49	6	0	-5.908534	-0.885566	-1.275146
50	1	0	-5.831175	-2.725234	-0.153818
51	1	0	-5.717872	1.031916	-2.242263
52	1	0	-6.913840	-1.060244	-1.644561
53	6	0	-0.313503	-2.716364	0.592770
54	6	0	-0.690191	-3.952968	1.105449
55	6	0	-0.215245	-4.341223	2.361244
56	1	0	-1.345736	-4.602022	0.533635
57	6	0	0.950931	-2.250620	2.505424
58	6	0	0.610929	-3.471055	3.076927
59	1	0	-0.494757	-5.303626	2.778678
60	1	0	1.597244	-1.548678	3.024509
61	1	0	0.986796	-3.730322	4.060590
62	7	0	0.509834	-1.879899	1.281371
63	1	0	1.934895	2.995893	1.940431

1''$_{pt\text{-}C}$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1443.80703370 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.097442	1.213119	-1.152437
2	6	0	2.154095	0.740436	-2.126375
3	1	0	1.680667	0.043543	-2.825150
4	1	0	2.531784	1.579086	-2.722465
5	6	0	1.636678	2.493042	-0.548616
6	1	0	2.642479	2.272373	-0.179522
7	1	0	1.751482	3.220599	-1.361045
8	6	0	-0.221483	1.441445	-1.854173
9	1	0	-0.808456	2.120325	-1.234548
10	1	0	-0.062710	1.931367	-2.822199
11	26	0	0.873470	-0.538308	-0.056442
12	6	0	3.268824	0.038144	-1.384497
13	6	0	4.584976	0.039184	-1.829723
14	6	0	3.809040	-1.375950	0.391291
15	6	0	5.539054	-0.704964	-1.128603
16	1	0	4.862274	0.602889	-2.714863
17	6	0	5.142226	-1.421802	0.000888
18	1	0	3.467669	-1.931390	1.254986
19	1	0	6.572515	-0.722947	-1.460938
20	1	0	5.849711	-2.013405	0.571603
21	6	0	0.845184	3.178303	0.548628
22	6	0	-0.055742	4.212154	0.321648
23	6	0	-0.651362	4.886117	1.398531
24	1	0	-0.269289	4.520530	-0.696341
25	6	0	0.577860	3.501267	2.914363
26	6	0	-0.335101	4.524561	2.710060
27	1	0	-1.342716	5.702190	1.208737
28	1	0	0.904372	3.174969	3.895823
29	1	0	-0.766545	5.037261	3.563131
30	7	0	2.879204	-0.658729	-0.279773
31	7	0	1.125478	2.870315	1.848689
32	6	0	-0.973565	0.123726	-2.034141
33	1	0	-1.987538	0.315230	-2.400712
34	1	0	-0.479379	-0.510976	-2.774507
35	7	0	-1.005839	-0.623970	-0.734692
36	6	0	-1.266645	-2.089958	-0.931877
37	1	0	-2.336512	-2.282255	-1.053417

38	1	0	-0.769386	-2.407027	-1.855323
39	6	0	-2.012660	-0.023483	0.270348
40	1	0	-1.876805	-0.591144	1.194059
41	1	0	-1.678462	1.000499	0.461437
42	6	0	-3.457858	-0.043464	-0.159262
43	6	0	-4.291982	-1.109741	0.217546
44	6	0	-4.006847	1.016410	-0.901329
45	6	0	-5.633275	-1.130907	-0.166095
46	1	0	-3.902863	-1.911694	0.841156
47	6	0	-5.346980	0.994471	-1.287163
48	1	0	-3.397709	1.882137	-1.155824
49	6	0	-6.159484	-0.083333	-0.925549
50	1	0	-6.270395	-1.954679	0.139002
51	1	0	-5.761851	1.820753	-1.855344
52	1	0	-7.204016	-0.097355	-1.219485
53	6	0	-0.688182	-2.841958	0.241497
54	6	0	-1.182230	-4.063966	0.684497
55	6	0	-0.573754	-4.691288	1.773732
56	1	0	-2.032551	-4.517032	0.185218
57	6	0	0.953522	-2.849404	1.907386
58	6	0	0.503381	-4.064140	2.404806
59	1	0	-0.943553	-5.646709	2.133058
60	1	0	1.776174	-2.327010	2.382217
61	1	0	0.987629	-4.506539	3.268367
62	7	0	0.386508	-2.248877	0.834583
63	1	0	1.828062	2.160008	2.038881

Fe^{I} HNPy **2''$_A$** (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1444.19311388 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.675901	-1.253245	-1.159373
2	6	0	-2.577694	-0.569496	-2.109184
3	1	0	-1.970187	-0.126564	-2.905596
4	1	0	-3.254580	-1.277480	-2.606387
5	6	0	-2.354249	-2.365551	-0.454759
6	1	0	-3.393331	-2.060311	-0.279367
7	1	0	-2.392431	-3.276788	-1.068208
8	6	0	-0.393948	-1.669498	-1.768049
9	1	0	0.051258	-2.424596	-1.115632
10	1	0	-0.545350	-2.151669	-2.745485
11	26	0	-1.288408	0.172850	0.496581

12	6	0	-3.383631	0.551914	-1.472202
13	6	0	-4.598146	0.955784	-2.025456
14	6	0	-3.514755	2.239092	0.128263
15	6	0	-5.271475	2.050388	-1.484355
16	1	0	-5.007810	0.418933	-2.875143
17	6	0	-4.715066	2.709480	-0.387824
18	1	0	-3.065092	2.705848	0.998693
19	1	0	-6.216006	2.377655	-1.906976
20	1	0	-5.205849	3.560533	0.070672
21	6	0	-1.715680	-2.661595	0.889174
22	6	0	-1.718045	-3.945614	1.429263
23	6	0	-1.192752	-4.154907	2.705014
24	1	0	-2.130748	-4.770535	0.857452
25	6	0	-0.703064	-1.813025	2.804959
26	6	0	-0.676442	-3.065758	3.406649
27	1	0	-1.189338	-5.148248	3.141933
28	1	0	-0.320207	-0.939950	3.323535
29	1	0	-0.264302	-3.178464	4.403148
30	7	0	-2.848241	1.186104	-0.398126
31	7	0	-1.202500	-1.602636	1.567355
32	6	0	0.556554	-0.489808	-1.949217
33	1	0	1.460160	-0.832963	-2.468569
34	1	0	0.088060	0.256184	-2.597777
35	7	0	0.911611	0.200096	-0.670098
36	6	0	1.513660	1.503675	-1.041268
37	1	0	2.452290	1.368932	-1.594133
38	1	0	0.815361	2.014254	-1.716150
39	6	0	1.874865	-0.626866	0.165068
40	1	0	2.019561	-0.081095	1.102577
41	1	0	1.343581	-1.543839	0.424347
42	6	0	3.221415	-0.955862	-0.447630
43	6	0	4.334410	-0.131598	-0.218017
44	6	0	3.397121	-2.114040	-1.221942
45	6	0	5.579414	-0.437674	-0.768959
46	1	0	4.237686	0.739897	0.425866
47	6	0	4.639923	-2.422471	-1.776107
48	1	0	2.565342	-2.798129	-1.372392
49	6	0	5.732096	-1.580958	-1.555568
50	1	0	6.432562	0.204026	-0.571783
51	1	0	4.759373	-3.325334	-2.366582
52	1	0	6.701010	-1.824497	-1.979481
53	6	0	1.792359	2.454408	0.101560
54	6	0	2.836090	3.377434	0.086971
55	6	0	2.974169	4.286194	1.137458

56	1	0	3.531025	3.379420	-0.745523
57	6	0	1.057210	3.326943	2.197815
58	6	0	2.074595	4.262822	2.210999
59	1	0	3.784276	5.008718	1.123874
60	1	0	0.319247	3.227531	2.985848
61	1	0	2.163961	4.953601	3.041367
62	7	0	0.949294	2.471841	1.156369
63	1	0	0.175648	1.755229	1.135951

Fe^{I} HNPy **$2''_A$** (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1444.15940301 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.608084	-1.273240	-1.200795
2	6	0	-2.486860	-0.613615	-2.192801
3	1	0	-1.854781	-0.143428	-2.953527
4	1	0	-3.121226	-1.336378	-2.723756
5	6	0	-2.334168	-2.316153	-0.437054
6	1	0	-3.384469	-2.008028	-0.374944
7	1	0	-2.320847	-3.282975	-0.958113
8	6	0	-0.330230	-1.760540	-1.770453
9	1	0	0.074982	-2.504000	-1.079312
10	1	0	-0.478690	-2.272473	-2.732504
11	26	0	-1.083387	0.219508	0.248575
12	6	0	-3.340056	0.464066	-1.547689
13	6	0	-4.586607	0.811115	-2.064302
14	6	0	-3.520325	2.097072	0.100157
15	6	0	-5.308566	1.847344	-1.471430
16	1	0	-4.986461	0.274907	-2.918914
17	6	0	-4.764794	2.502861	-0.366940
18	1	0	-3.067613	2.569814	0.964984
19	1	0	-6.281001	2.131330	-1.860842
20	1	0	-5.293996	3.307913	0.130353
21	6	0	-1.817628	-2.469428	0.981864
22	6	0	-1.941416	-3.674769	1.670380
23	6	0	-1.554859	-3.740091	3.009327
24	1	0	-2.342857	-4.547833	1.165980
25	6	0	-0.940151	-1.430783	2.869496
26	6	0	-1.049493	-2.593792	3.623000
27	1	0	-1.648208	-4.669071	3.562660
28	1	0	-0.548263	-0.517463	3.305086
29	1	0	-0.742830	-2.597169	4.662923

30	7	0	-2.809236	1.101463	-0.472562
31	7	0	-1.308751	-1.359447	1.572882
32	6	0	0.662616	-0.616322	-1.969152
33	1	0	1.587764	-1.005408	-2.409978
34	1	0	0.251259	0.102672	-2.683564
35	7	0	0.956168	0.138778	-0.701749
36	6	0	1.596314	1.422625	-1.101369
37	1	0	2.558140	1.241287	-1.595709
38	1	0	0.940811	1.904406	-1.836973
39	6	0	1.870921	-0.658268	0.224967
40	1	0	1.990140	-0.052501	1.127917
41	1	0	1.306069	-1.544711	0.517914
42	6	0	3.227779	-1.056749	-0.317191
43	6	0	4.352740	-0.244353	-0.104146
44	6	0	3.400559	-2.271185	-1.001088
45	6	0	5.607747	-0.617499	-0.586841
46	1	0	4.255668	0.670569	0.475676
47	6	0	4.653398	-2.646593	-1.486688
48	1	0	2.557689	-2.945475	-1.133549
49	6	0	5.758142	-1.816548	-1.286126
50	1	0	6.469824	0.016244	-0.403531
51	1	0	4.770309	-3.591696	-2.007402
52	1	0	6.734604	-2.111586	-1.656607
53	6	0	1.832949	2.423835	0.009316
54	6	0	2.946810	3.259042	0.049838
55	6	0	3.053569	4.228339	1.049940
56	1	0	3.721113	3.148696	-0.701340
57	6	0	0.960624	3.500681	1.948820
58	6	0	2.049230	4.352116	2.016742
59	1	0	3.919598	4.882235	1.078567
60	1	0	0.136525	3.518768	2.653321
61	1	0	2.109454	5.092120	2.806416
62	7	0	0.885927	2.585098	0.959508
63	1	0	0.053745	1.919022	0.911352

Fe^{I} HNPy **2''$_A$** (sextet) E(B3LYP/ SDD-6-31G(d,p))= -1444.17595623 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.658962	-0.991486	-1.139021
2	6	0	-2.435726	-0.314869	-2.206475
3	1	0	-1.742422	0.264242	-2.825030

4	1	0	-2.919234	-1.042492	-2.872621
5	6	0	-2.490811	-2.051571	-0.502830
6	1	0	-3.535305	-1.722573	-0.531611
7	1	0	-2.438434	-2.986005	-1.075863
8	6	0	-0.383783	-1.571424	-1.645279
9	1	0	-0.050570	-2.305965	-0.908623
10	1	0	-0.563005	-2.121900	-2.579824
11	26	0	-1.241827	0.558888	0.450853
12	6	0	-3.464489	0.628321	-1.614432
13	6	0	-4.627109	0.981381	-2.296228
14	6	0	-4.020872	2.024189	0.164476
15	6	0	-5.503396	1.896530	-1.711260
16	1	0	-4.843200	0.547147	-3.267149
17	6	0	-5.196452	2.427391	-0.457025
18	1	0	-3.735192	2.408728	1.139313
19	1	0	-6.414312	2.186629	-2.225155
20	1	0	-5.854155	3.136472	0.032940
21	6	0	-2.120807	-2.287513	0.945355
22	6	0	-2.307001	-3.521712	1.565389
23	6	0	-2.051005	-3.638297	2.932331
24	1	0	-2.654853	-4.373792	0.990266
25	6	0	-1.433087	-1.325361	2.949509
26	6	0	-1.610889	-2.518654	3.639998
27	1	0	-2.193558	-4.588915	3.436432
28	1	0	-1.085215	-0.426663	3.450272
29	1	0	-1.405835	-2.566823	4.703536
30	7	0	-3.170998	1.142913	-0.400322
31	7	0	-1.679752	-1.209706	1.629412
32	6	0	0.710865	-0.536236	-1.894167
33	1	0	1.547847	-1.037554	-2.398390
34	1	0	0.344111	0.224968	-2.589394
35	7	0	1.172362	0.166886	-0.667509
36	6	0	1.946806	1.353496	-1.102192
37	1	0	2.843631	1.060285	-1.663706
38	1	0	1.312220	1.926420	-1.790645
39	6	0	1.972485	-0.723858	0.253388
40	1	0	2.196636	-0.125701	1.141705
41	1	0	1.297633	-1.516874	0.585526
42	6	0	3.248814	-1.324698	-0.302617
43	6	0	4.483309	-0.683827	-0.115619
44	6	0	3.231241	-2.550933	-0.986599
45	6	0	5.661444	-1.235065	-0.621197
46	1	0	4.531180	0.236969	0.460855
47	6	0	4.406675	-3.104297	-1.495532

48	1	0	2.297805	-3.097424	-1.100250
49	6	0	5.623870	-2.443454	-1.319316
50	1	0	6.609356	-0.732151	-0.456594
51	1	0	4.374887	-4.056585	-2.015489
52	1	0	6.539856	-2.876878	-1.707758
53	6	0	2.390218	2.313428	-0.019614
54	6	0	3.614840	2.976522	-0.064761
55	6	0	3.925669	3.936497	0.901181
56	1	0	4.317007	2.740051	-0.856350
57	6	0	1.808355	3.546160	1.937802
58	6	0	3.012761	4.226565	1.920924
59	1	0	4.878437	4.455049	0.859950
60	1	0	1.035964	3.699197	2.683464
61	1	0	3.230450	4.962669	2.685991
62	7	0	1.539952	2.630282	0.983235
63	1	0	0.596017	2.153903	1.000199

Fe^{I} HNPy **$2''_B$** (sextet) E(B3LYP/ SDD-6-31G(d,p))= -1444.20007881 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.192095	-1.521953	-1.237800
2	6	0	-2.093088	-1.086095	-2.360853
3	1	0	-1.460586	-0.600037	-3.114619
4	1	0	-2.565595	-1.946788	-2.848379
5	6	0	-1.860850	-2.540684	-0.390016
6	1	0	-2.942977	-2.419226	-0.510282
7	1	0	-1.618906	-3.557554	-0.722357
8	6	0	0.148073	-1.974982	-1.710303
9	1	0	0.567349	-2.625938	-0.939171
10	1	0	0.058240	-2.581497	-2.621337
11	26	0	-0.821693	0.297692	0.027093
12	6	0	-3.122643	-0.138217	-1.834518
13	6	0	-4.467438	-0.373609	-1.741251
14	6	0	-3.464796	1.990760	-0.637201
15	6	0	-5.346045	0.541349	-1.116823
16	1	0	-4.857490	-1.296636	-2.161471
17	6	0	-4.796716	1.723539	-0.556191
18	1	0	-3.009565	2.904701	-0.276139
19	1	0	-6.410072	0.346640	-1.074362
20	1	0	-5.439918	2.446690	-0.065321
21	6	0	-1.554283	-2.376913	1.085732
22	6	0	-1.662652	-3.446705	1.973070

23	6	0	-1.476634	-3.225038	3.337246
24	1	0	-1.895710	-4.438462	1.599033
25	6	0	-1.073101	-0.919628	2.842867
26	6	0	-1.180122	-1.934990	3.782848
27	1	0	-1.560558	-4.046444	4.041827
28	1	0	-0.830162	0.095492	3.141005
29	1	0	-1.029797	-1.719604	4.834656
30	7	0	-2.542452	1.067659	-1.262869
31	7	0	-1.254097	-1.129510	1.519147
32	6	0	1.088513	-0.796265	-1.975094
33	1	0	2.068420	-1.168419	-2.293813
34	1	0	0.701650	-0.184805	-2.795722
35	7	0	1.210871	0.081435	-0.774988
36	6	0	1.652469	1.457989	-1.121187
37	1	0	2.735065	1.504956	-1.278428
38	1	0	1.183109	1.738891	-2.071818
39	6	0	2.105360	-0.520223	0.306506
40	1	0	2.021331	0.145348	1.170428
41	1	0	1.652354	-1.472474	0.591687
42	6	0	3.558742	-0.715770	-0.059538
43	6	0	4.504441	0.283175	0.223182
44	6	0	3.998177	-1.911246	-0.650803
45	6	0	5.848697	0.105118	-0.105494
46	1	0	4.194779	1.193432	0.732220
47	6	0	5.341905	-2.090654	-0.980597
48	1	0	3.295371	-2.722162	-0.829063
49	6	0	6.267588	-1.079521	-0.714554
50	1	0	6.570226	0.881898	0.127107
51	1	0	5.668400	-3.022872	-1.430405
52	1	0	7.314097	-1.221644	-0.964323
53	6	0	1.222947	2.449312	-0.055245
54	6	0	1.935797	3.619842	0.198009
55	6	0	1.452605	4.520781	1.147202
56	1	0	2.854160	3.821487	-0.343765
57	6	0	-0.384845	3.034875	1.530088
58	6	0	0.269703	4.223312	1.827250
59	1	0	1.993400	5.438221	1.356864
60	1	0	-1.306370	2.762511	2.036613
61	1	0	-0.136784	4.894334	2.575601
62	7	0	0.076380	2.162947	0.606335
63	1	0	-2.010529	1.568863	-1.985478

Fe^{I} HNPy **2''$_B$** (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1444.17535337 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.294307	-1.306499	-0.995456
2	6	0	-2.071931	-0.902175	-2.200938
3	1	0	-1.398711	-0.364681	-2.875606
4	1	0	-2.425786	-1.786539	-2.747367
5	6	0	-2.104406	-2.261980	-0.183990
6	1	0	-3.161572	-2.001572	-0.312495
7	1	0	-1.991655	-3.287981	-0.556791
8	6	0	-0.003751	-1.931916	-1.451377
9	1	0	0.371665	-2.533433	-0.619791
10	1	0	-0.183245	-2.618841	-2.290571
11	26	0	-0.497993	0.218676	0.352112
12	6	0	-3.260326	-0.006877	-1.926859
13	6	0	-4.494888	-0.145887	-2.552400
14	6	0	-4.039789	1.935796	-0.797595
15	6	0	-5.507824	0.783963	-2.296260
16	1	0	-4.659715	-0.970210	-3.237949
17	6	0	-5.280104	1.840156	-1.408412
18	1	0	-3.776010	2.715334	-0.091388
19	1	0	-6.471796	0.681028	-2.784597
20	1	0	-6.047873	2.574105	-1.191979
21	6	0	-1.797462	-2.193413	1.297505
22	6	0	-2.061153	-3.272839	2.138305
23	6	0	-1.863944	-3.129383	3.512006
24	1	0	-2.420052	-4.209976	1.724756
25	6	0	-1.131195	-0.887618	3.100335
26	6	0	-1.396407	-1.910052	4.003381
27	1	0	-2.067141	-3.956416	4.184730
28	1	0	-0.735943	0.065560	3.434779
29	1	0	-1.226318	-1.754943	5.062860
30	7	0	-3.082564	1.029810	-1.078168
31	7	0	-1.327464	-1.014705	1.769576
32	6	0	1.031671	-0.872877	-1.843967
33	1	0	1.941307	-1.364304	-2.206630
34	1	0	0.663531	-0.259031	-2.671220
35	7	0	1.307599	0.015407	-0.685815
36	6	0	1.661443	1.411560	-1.048580
37	1	0	2.706101	1.506232	-1.364790
38	1	0	1.040246	1.709045	-1.902003
39	6	0	2.340822	-0.584202	0.260662
40	1	0	2.367078	0.069429	1.135619

41	1	0	1.936498	-1.543040	0.595352
42	6	0	3.732770	-0.769960	-0.302007
43	6	0	4.690789	0.251143	-0.194099
44	6	0	4.106210	-1.978623	-0.911219
45	6	0	5.974717	0.082464	-0.713372
46	1	0	4.442532	1.172927	0.327179
47	6	0	5.389729	-2.149628	-1.431295
48	1	0	3.401445	-2.806465	-0.952663
49	6	0	6.323386	-1.115618	-1.340215
50	1	0	6.706751	0.877959	-0.615270
51	1	0	5.665094	-3.092777	-1.892605
52	1	0	7.324076	-1.249916	-1.738302
53	6	0	1.366784	2.336165	0.119401
54	6	0	2.076958	3.517019	0.324989
55	6	0	1.731545	4.346812	1.391776
56	1	0	2.891702	3.778866	-0.342288
57	6	0	0.019200	2.774959	1.967853
58	6	0	0.682823	3.966848	2.230604
59	1	0	2.275258	5.269239	1.568698
60	1	0	-0.801105	2.442384	2.596282
61	1	0	0.385483	4.577226	3.075982
62	7	0	0.344751	1.966116	0.935874
63	1	0	-2.134113	1.041288	-0.554314

Fe^{I} HNPy **$2''_B$** (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1444.20445641 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.394701	-1.083343	-1.125190
2	6	0	-2.095909	-0.457479	-2.270350
3	1	0	-1.377174	0.163930	-2.814052
4	1	0	-2.452690	-1.217437	-2.979947
5	6	0	-2.254508	-2.137189	-0.527094
6	1	0	-3.281373	-1.753084	-0.494040
7	1	0	-2.278214	-3.034330	-1.162182
8	6	0	-0.091687	-1.669857	-1.595071
9	1	0	0.230701	-2.383971	-0.832269
10	1	0	-0.248582	-2.243206	-2.520418
11	26	0	-0.515759	0.136263	0.617981
12	6	0	-3.270244	0.421887	-1.895526
13	6	0	-4.470216	0.438434	-2.598842
14	6	0	-4.071171	2.171819	-0.489637
15	6	0	-5.473603	1.344483	-2.241919

16	1	0	-4.614551	-0.250089	-3.424387
17	6	0	-5.273489	2.225436	-1.174105
18	1	0	-3.829827	2.808059	0.354316
19	1	0	-6.408897	1.359385	-2.792706
20	1	0	-6.033971	2.937888	-0.875996
21	6	0	-1.851826	-2.511145	0.886049
22	6	0	-2.195218	-3.754090	1.416758
23	6	0	-1.894271	-4.032059	2.749478
24	1	0	-2.695161	-4.490924	0.796070
25	6	0	-0.919344	-1.851471	2.908963
26	6	0	-1.247598	-3.058787	3.512725
27	1	0	-2.156540	-4.992035	3.182595
28	1	0	-0.400662	-1.073835	3.460087
29	1	0	-0.993070	-3.231305	4.552407
30	7	0	-3.120179	1.292434	-0.869631
31	7	0	-1.212928	-1.571798	1.618952
32	6	0	1.005489	-0.621955	-1.818419
33	1	0	1.879001	-1.116058	-2.258092
34	1	0	0.680197	0.116514	-2.556130
35	7	0	1.355781	0.088351	-0.561040
36	6	0	1.644368	1.531239	-0.762517
37	1	0	2.674665	1.705732	-1.090851
38	1	0	0.988734	1.894681	-1.562888
39	6	0	2.451391	-0.608411	0.221383
40	1	0	2.520347	-0.083528	1.179273
41	1	0	2.083287	-1.615923	0.438087
42	6	0	3.812853	-0.681032	-0.434450
43	6	0	4.759533	0.336526	-0.234226
44	6	0	4.169104	-1.780843	-1.231098
45	6	0	6.013705	0.274443	-0.842499
46	1	0	4.527849	1.167679	0.428142
47	6	0	5.422546	-1.844945	-1.841212
48	1	0	3.476404	-2.611138	-1.351390
49	6	0	6.343903	-0.812961	-1.653914
50	1	0	6.737956	1.064669	-0.671026
51	1	0	5.685316	-2.705892	-2.447798
52	1	0	7.321839	-0.865267	-2.121687
53	6	0	1.342351	2.333010	0.488317
54	6	0	2.142243	3.397638	0.895116
55	6	0	1.792571	4.124940	2.034178
56	1	0	3.032028	3.649274	0.327348
57	6	0	-0.113774	2.694795	2.271776
58	6	0	0.644960	3.762324	2.738602
59	1	0	2.408351	4.954100	2.367474

60	1	0	-1.018854	2.386243	2.784932
61	1	0	0.338117	4.293268	3.632811
62	7	0	0.216131	1.988258	1.167308
63	1	0	-2.227181	1.217941	-0.302771

Fe^{I} HNPy **2''$_c$** (sextet) E(B3LYP/ SDD-6-31G(d,p))= -1444.20184961 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.233038	-1.752625	-0.929381
2	6	0	-2.290849	-1.546319	-1.944456
3	1	0	-1.826559	-1.137185	-2.848953
4	1	0	-2.757135	-2.495547	-2.238529
5	6	0	-1.646069	-2.769246	0.100079
6	1	0	-2.733888	-2.672594	0.221669
7	1	0	-1.450832	-3.789193	-0.250545
8	6	0	0.086397	-2.075857	-1.541749
9	1	0	0.669853	-2.617299	-0.794634
10	1	0	-0.031308	-2.746506	-2.402772
11	26	0	-0.964159	0.190479	0.171605
12	6	0	-3.345297	-0.562252	-1.475676
13	6	0	-4.647312	-0.592920	-1.972567
14	6	0	-3.824276	1.351386	-0.230446
15	6	0	-5.551671	0.393886	-1.580730
16	1	0	-4.945154	-1.376277	-2.662044
17	6	0	-5.131190	1.389624	-0.696015
18	1	0	-3.454331	2.105116	0.457727
19	1	0	-6.568764	0.386167	-1.959719
20	1	0	-5.801323	2.177101	-0.370165
21	6	0	-0.946650	-2.506192	1.393527
22	6	0	-0.014328	-3.312509	1.989578
23	6	0	0.650741	-2.934778	3.177828
24	1	0	0.209231	-4.268410	1.523979
25	6	0	-0.583177	-0.849239	3.183225
26	6	0	0.340463	-1.672313	3.748964
27	1	0	1.366923	-3.597308	3.647051
28	1	0	-0.885593	0.098687	3.610867
29	1	0	0.827770	-1.350200	4.663472
30	7	0	-2.943658	0.395409	-0.605048
31	7	0	-1.263803	-1.201646	1.956663
32	6	0	0.825886	-0.807535	-1.974197
33	1	0	1.800338	-1.069735	-2.400495

34	1	0	0.263415	-0.293402	-2.759849
35	7	0	0.976005	0.141288	-0.832845
36	6	0	1.199146	1.539871	-1.286918
37	1	0	2.237387	1.699561	-1.595911
38	1	0	0.571772	1.717308	-2.168736
39	6	0	2.055162	-0.290283	0.157797
40	1	0	1.999187	0.417275	0.989293
41	1	0	1.750909	-1.264299	0.547660
42	6	0	3.466458	-0.351738	-0.380012
43	6	0	4.318166	0.759827	-0.275326
44	6	0	3.965205	-1.529465	-0.959852
45	6	0	5.623463	0.706219	-0.765442
46	1	0	3.970397	1.663568	0.220429
47	6	0	5.269736	-1.584595	-1.451267
48	1	0	3.343452	-2.420970	-1.004026
49	6	0	6.098372	-0.464216	-1.360555
50	1	0	6.273395	1.570243	-0.669730
51	1	0	5.643686	-2.503861	-1.890755
52	1	0	7.115560	-0.508989	-1.736202
53	6	0	0.806247	2.526645	-0.203074
54	6	0	1.410498	3.777257	-0.087367
55	6	0	0.968184	4.660062	0.897675
56	1	0	2.214584	4.052789	-0.761924
57	6	0	-0.611750	2.998779	1.584669
58	6	0	-0.062165	4.262958	1.752514
59	1	0	1.425233	5.638961	1.002189
60	1	0	-1.407221	2.647996	2.235911
61	1	0	-0.428981	4.914653	2.537510
62	7	0	-0.195718	2.145355	0.624179
63	1	0	-2.278732	-1.126923	2.099285

Fe^{I} HNPy **2''$_c$** (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1444.18367237 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.206557	1.236748	-1.209771
2	6	0	2.177356	0.675179	-2.202811
3	1	0	1.626679	0.010281	-2.874651
4	1	0	2.617798	1.466451	-2.824006
5	6	0	1.835804	2.448973	-0.607502
6	1	0	2.879001	2.198283	-0.384697
7	1	0	1.852873	3.273366	-1.331819

8	6	0	-0.103841	1.584388	-1.850590
9	1	0	-0.604455	2.303128	-1.196212
10	1	0	0.051171	2.084927	-2.815697
11	26	0	0.840615	-0.495918	-0.050796
12	6	0	3.247148	-0.116259	-1.483849
13	6	0	4.556545	-0.201310	-1.946091
14	6	0	3.717285	-1.543924	0.287698
15	6	0	5.471488	-0.995036	-1.250892
16	1	0	4.855487	0.341356	-2.837037
17	6	0	5.043256	-1.675366	-0.112124
18	1	0	3.345895	-2.071879	1.157499
19	1	0	6.498049	-1.077666	-1.592963
20	1	0	5.718604	-2.303093	0.458304
21	6	0	1.203985	2.946898	0.672614
22	6	0	1.016370	4.293831	0.965526
23	6	0	0.519969	4.666247	2.218883
24	1	0	1.264826	5.044457	0.222972
25	6	0	0.398044	2.355957	2.831060
26	6	0	0.207498	3.686891	3.166974
27	1	0	0.375296	5.716421	2.452407
28	1	0	0.176138	1.530151	3.498187
29	1	0	-0.177859	3.948164	4.145893
30	7	0	2.826276	-0.779663	-0.376167
31	7	0	0.889611	2.032870	1.618248
32	6	0	-0.982465	0.345844	-2.035789
33	1	0	-1.963430	0.644083	-2.423126
34	1	0	-0.539695	-0.324314	-2.777182
35	7	0	-1.097259	-0.409760	-0.755729
36	6	0	-1.417325	-1.853653	-0.971439
37	1	0	-2.485463	-2.012146	-1.151293
38	1	0	-0.883112	-2.185157	-1.868354
39	6	0	-2.080225	0.225476	0.217235
40	1	0	-1.998518	-0.352099	1.141875
41	1	0	-1.705123	1.230148	0.429271
42	6	0	-3.523449	0.297560	-0.230406
43	6	0	-4.421921	-0.732786	0.089239
44	6	0	-4.001730	1.410227	-0.940760
45	6	0	-5.754584	-0.668176	-0.319092
46	1	0	-4.084885	-1.578878	0.683777
47	6	0	-5.333600	1.476507	-1.351114
48	1	0	-3.338404	2.246080	-1.154084
49	6	0	-6.210155	0.433139	-1.046583
50	1	0	-6.439295	-1.469233	-0.059088
51	1	0	-5.689832	2.345173	-1.895788

52	1	0	-7.247720	0.485976	-1.360415
53	6	0	-0.932580	-2.652762	0.217047
54	6	0	-1.569574	-3.807309	0.662609
55	6	0	-1.041538	-4.500868	1.752716
56	1	0	-2.465550	-4.157082	0.160177
57	6	0	0.681404	-2.839937	1.878143
58	6	0	0.101302	-4.000810	2.376746
59	1	0	-1.519373	-5.405882	2.113444
60	1	0	1.562783	-2.414899	2.346767
61	1	0	0.538240	-4.496634	3.236332
62	7	0	0.194769	-2.176384	0.807890
63	1	0	0.957392	0.994204	1.304224

Fe^{I} HNPy **2''$_c$** (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1444.20073742 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.428802	1.165615	-1.158701
2	6	0	2.329743	0.498858	-2.136779
3	1	0	1.716627	-0.138891	-2.780509
4	1	0	2.823113	1.228208	-2.794815
5	6	0	2.146513	2.319266	-0.577769
6	1	0	3.168570	1.993649	-0.345820
7	1	0	2.238699	3.142215	-1.301682
8	6	0	0.141156	1.584896	-1.778845
9	1	0	-0.312536	2.329655	-1.119039
10	1	0	0.316145	2.087998	-2.741257
11	26	0	0.886660	-0.861151	0.101688
12	6	0	3.360738	-0.363755	-1.437802
13	6	0	4.677395	-0.453832	-1.881950
14	6	0	3.773137	-1.906762	0.253938
15	6	0	5.561860	-1.310411	-1.223013
16	1	0	5.004760	0.134174	-2.733279
17	6	0	5.101675	-2.047890	-0.132798
18	1	0	3.371905	-2.471336	1.088924
19	1	0	6.591582	-1.396676	-1.554853
20	1	0	5.753631	-2.724006	0.408757
21	6	0	1.564603	2.884507	0.699318
22	6	0	1.630973	4.236088	1.026923
23	6	0	1.176100	4.674842	2.272720
24	1	0	2.044312	4.937632	0.310420
25	6	0	0.583066	2.425266	2.825408

26	6	0	0.646688	3.758480	3.188518
27	1	0	1.232234	5.728578	2.527579
28	1	0	0.181875	1.644310	3.461385
29	1	0	0.285782	4.071635	4.161332
30	7	0	2.912656	-1.084219	-0.382055
31	7	0	1.037967	2.036683	1.613573
32	6	0	-0.836978	0.424585	-2.000720
33	1	0	-1.751978	0.825813	-2.454413
34	1	0	-0.419654	-0.282949	-2.722764
35	7	0	-1.125834	-0.324920	-0.754155
36	6	0	-1.655540	-1.684603	-1.034566
37	1	0	-2.710360	-1.662248	-1.329587
38	1	0	-1.093583	-2.096472	-1.881484
39	6	0	-2.037887	0.428834	0.188155
40	1	0	-2.064356	-0.152744	1.113983
41	1	0	-1.538268	1.373513	0.419754
42	6	0	-3.447906	0.699838	-0.294064
43	6	0	-4.489727	-0.188861	0.014888
44	6	0	-3.749934	1.855767	-1.031315
45	6	0	-5.791205	0.055937	-0.425068
46	1	0	-4.287618	-1.066755	0.624379
47	6	0	-5.049880	2.102113	-1.474380
48	1	0	-2.971322	2.585965	-1.242634
49	6	0	-6.071921	1.198615	-1.176564
50	1	0	-6.587114	-0.637342	-0.171668
51	1	0	-5.267477	3.002771	-2.039856
52	1	0	-7.084629	1.392001	-1.515471
53	6	0	-1.458816	-2.595886	0.161994
54	6	0	-2.360862	-3.609904	0.477235
55	6	0	-2.094187	-4.446630	1.561596
56	1	0	-3.256491	-3.740893	-0.121315
57	6	0	-0.082868	-3.202622	1.937047
58	6	0	-0.934840	-4.236268	2.308806
59	1	0	-2.782400	-5.244585	1.821596
60	1	0	0.829149	-3.004327	2.490931
61	1	0	-0.692105	-4.857998	3.163235
62	7	0	-0.329706	-2.398567	0.881998
63	1	0	0.954595	1.024087	1.344188

Fe^{III}-H **2''$_D$** (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1444.20870188 hartree

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Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	7	0	0.857205	-0.751593	1.458195
2	6	0	1.945240	-0.004192	2.141183
3	1	0	1.595257	1.019133	2.315708
4	1	0	2.176035	-0.439674	3.122353
5	6	0	1.193785	-2.204822	1.371592
6	1	0	2.283537	-2.307273	1.371145
7	1	0	0.828323	-2.744125	2.253131
8	6	0	-0.482483	-0.552374	2.096625
9	1	0	-1.057203	-1.468250	1.944300
10	1	0	-0.375374	-0.422985	3.180593
11	26	0	0.794707	-0.007019	-0.590373
12	6	0	3.178795	0.010926	1.258559
13	6	0	4.471945	0.081308	1.771982
14	6	0	3.988315	-0.073340	-0.924425
15	6	0	5.551242	0.082580	0.885829
16	1	0	4.632608	0.126382	2.844390
17	6	0	5.306868	-0.003167	-0.486024
18	1	0	3.746276	-0.141226	-1.980434
19	1	0	6.567769	0.136424	1.262598
20	1	0	6.118793	-0.019932	-1.204524
21	6	0	0.670571	-2.827071	0.098462
22	6	0	0.412981	-4.192069	-0.003303
23	6	0	0.034481	-4.725488	-1.235805
24	1	0	0.514270	-4.828317	0.869910
25	6	0	0.178237	-2.522206	-2.166323
26	6	0	-0.079576	-3.875949	-2.337270
27	1	0	-0.167409	-5.787461	-1.333668
28	1	0	0.097605	-1.823655	-2.990280
29	1	0	-0.365764	-4.250201	-3.313732
30	7	0	2.943979	-0.055991	-0.071984
31	7	0	0.541544	-2.001602	-0.971296
32	6	0	-1.228450	0.634074	1.497254
33	1	0	-2.218535	0.719821	1.960815
34	1	0	-0.691844	1.562378	1.711882
35	7	0	-1.348228	0.505459	0.015228
36	6	0	-1.649998	1.824287	-0.587101
37	1	0	-1.949365	1.656536	-1.628147
38	1	0	-2.497265	2.313233	-0.092642
39	6	0	-2.384935	-0.518867	-0.406515
40	1	0	-2.296742	-0.598134	-1.494031
41	1	0	-2.071536	-1.478340	0.009870
42	6	0	-3.816722	-0.221650	-0.015860
43	6	0	-4.658664	0.496912	-0.878815

44	6	0	-4.339246	-0.686746	1.201563
45	6	0	-5.979965	0.767406	-0.522334
46	1	0	-4.291383	0.825938	-1.848153
47	6	0	-5.659943	-0.415563	1.561185
48	1	0	-3.722150	-1.290321	1.864119
49	6	0	-6.480326	0.317366	0.701390
50	1	0	-6.621977	1.315580	-1.204549
51	1	0	-6.051817	-0.787548	2.502549
52	1	0	-7.510182	0.521951	0.975980
53	6	0	-0.438546	2.723084	-0.578851
54	6	0	-0.563514	4.111540	-0.623095
55	6	0	0.581897	4.899460	-0.703348
56	1	0	-1.550623	4.561599	-0.600889
57	6	0	1.879976	2.886094	-0.673282
58	6	0	1.828561	4.271593	-0.731863
59	1	0	0.504435	5.981214	-0.744429
60	1	0	2.826530	2.362736	-0.699204
61	1	0	2.748238	4.841662	-0.800060
62	7	0	0.770452	2.118902	-0.586849
63	1	0	1.019282	0.220391	-2.076428

Fe^{III}-H **2''$_D$** (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1444.21153170 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.832836	-0.677665	1.570492
2	6	0	1.979750	0.088395	2.121167
3	1	0	1.664357	1.128210	2.260281
4	1	0	2.300916	-0.291529	3.099698
5	6	0	1.140554	-2.137333	1.550191
6	1	0	2.224864	-2.270079	1.622413
7	1	0	0.710321	-2.642019	2.422480
8	6	0	-0.488704	-0.406268	2.214269
9	1	0	-1.067941	-1.331074	2.172961
10	1	0	-0.369855	-0.154095	3.275063
11	26	0	0.719446	0.024602	-0.456031
12	6	0	3.109117	0.015841	1.111469
13	6	0	4.456750	0.027414	1.458052
14	6	0	3.643934	-0.136508	-1.162009
15	6	0	5.419764	-0.042100	0.447892
16	1	0	4.748196	0.083642	2.501838
17	6	0	5.007183	-0.131312	-0.881714

18	1	0	3.270130	-0.192661	-2.178205
19	1	0	6.475775	-0.035156	0.698569
20	1	0	5.723444	-0.195304	-1.693162
21	6	0	0.678559	-2.774514	0.262622
22	6	0	0.491391	-4.148786	0.136072
23	6	0	0.164788	-4.678916	-1.112188
24	1	0	0.607737	-4.793189	1.001535
25	6	0	0.217055	-2.453211	-2.001240
26	6	0	0.033221	-3.815703	-2.200755
27	1	0	0.017470	-5.747482	-1.232371
28	1	0	0.115871	-1.742937	-2.812586
29	1	0	-0.212943	-4.185479	-3.189752
30	7	0	2.716596	-0.060922	-0.187130
31	7	0	0.527732	-1.936572	-0.789949
32	6	0	-1.232908	0.707014	1.488912
33	1	0	-2.258060	0.788290	1.865565
34	1	0	-0.744112	1.666376	1.668272
35	7	0	-1.251781	0.472991	-0.000256
36	6	0	-1.550982	1.757879	-0.695456
37	1	0	-1.718734	1.530048	-1.753450
38	1	0	-2.467942	2.212097	-0.306831
39	6	0	-2.273854	-0.587654	-0.400584
40	1	0	-2.134815	-0.733806	-1.474226
41	1	0	-1.974849	-1.511411	0.096248
42	6	0	-3.718710	-0.267658	-0.090569
43	6	0	-4.521070	0.401580	-1.028298
44	6	0	-4.297893	-0.679173	1.120796
45	6	0	-5.859491	0.678419	-0.749407
46	1	0	-4.108583	0.686224	-1.993360
47	6	0	-5.636075	-0.401945	1.401992
48	1	0	-3.710725	-1.246553	1.840102
49	6	0	-6.416787	0.282993	0.468743
50	1	0	-6.470464	1.188327	-1.487441
51	1	0	-6.071927	-0.732543	2.339386
52	1	0	-7.460058	0.492262	0.682358
53	6	0	-0.377778	2.686612	-0.570425
54	6	0	-0.509161	4.069502	-0.666458
55	6	0	0.630900	4.868107	-0.605410
56	1	0	-1.493372	4.508259	-0.793158
57	6	0	1.922847	2.864857	-0.336826
58	6	0	1.869376	4.249707	-0.437871
59	1	0	0.553995	5.947613	-0.684814
60	1	0	2.872538	2.363477	-0.213115
61	1	0	2.786598	4.825352	-0.384697

62	7	0	0.822772	2.084022	-0.398069
63	1	0	0.658827	0.349062	-1.916207

Fe^{III}-H **2''$_D$** (sextet) E(B3LYP/ SDD-6-31G(d,p))= -1444.19676827 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.864493	-0.817565	1.485468
2	6	0	1.963607	-0.038447	2.107560
3	1	0	1.605907	0.982238	2.284383
4	1	0	2.250477	-0.450982	3.083782
5	6	0	1.203321	-2.263343	1.432547
6	1	0	2.294027	-2.360524	1.416815
7	1	0	0.857666	-2.782310	2.334818
8	6	0	-0.461659	-0.585848	2.126308
9	1	0	-1.060137	-1.486097	1.972156
10	1	0	-0.356824	-0.459348	3.211613
11	26	0	0.773843	0.044894	-0.662646
12	6	0	3.157600	-0.007294	1.172366
13	6	0	4.475446	0.005387	1.620914
14	6	0	3.864499	0.015842	-1.056938
15	6	0	5.511303	0.031860	0.683548
16	1	0	4.688410	-0.013004	2.684852
17	6	0	5.202562	0.030678	-0.678017
18	1	0	3.567499	0.013696	-2.101532
19	1	0	6.545406	0.040641	1.013509
20	1	0	5.979356	0.036340	-1.434405
21	6	0	0.661981	-2.927900	0.185881
22	6	0	0.411228	-4.297622	0.137182
23	6	0	0.023157	-4.874135	-1.073051
24	1	0	0.526648	-4.903665	1.030172
25	6	0	0.144008	-2.700598	-2.073529
26	6	0	-0.105395	-4.061995	-2.200658
27	1	0	-0.174084	-5.939782	-1.133379
28	1	0	0.050708	-2.022637	-2.914902
29	1	0	-0.398364	-4.470129	-3.161485
30	7	0	2.865784	0.006003	-0.149749
31	7	0	0.515680	-2.140555	-0.902627
32	6	0	-1.177853	0.625074	1.533254
33	1	0	-2.176746	0.717342	1.974844
34	1	0	-0.634603	1.543496	1.771198
35	7	0	-1.278896	0.529295	0.044874

36	6	0	-1.600738	1.858553	-0.541320
37	1	0	-1.865512	1.698903	-1.592497
38	1	0	-2.478064	2.298415	-0.055487
39	6	0	-2.305302	-0.500717	-0.413849
40	1	0	-2.183082	-0.571246	-1.498039
41	1	0	-1.999644	-1.458824	0.008225
42	6	0	-3.745172	-0.202299	-0.059205
43	6	0	-4.569887	0.496994	-0.954329
44	6	0	-4.295266	-0.656609	1.150412
45	6	0	-5.902565	0.759391	-0.636607
46	1	0	-4.179749	0.815742	-1.918098
47	6	0	-5.627362	-0.392890	1.470908
48	1	0	-3.691740	-1.247597	1.836206
49	6	0	-6.430997	0.320893	0.579554
50	1	0	-6.531274	1.291866	-1.343163
51	1	0	-6.041192	-0.756768	2.405980
52	1	0	-7.469714	0.519077	0.823774
53	6	0	-0.426117	2.803635	-0.487650
54	6	0	-0.601041	4.186318	-0.501359
55	6	0	0.520197	5.013099	-0.549363
56	1	0	-1.602062	4.604595	-0.481806
57	6	0	1.887484	3.046947	-0.540034
58	6	0	1.789383	4.431173	-0.572481
59	1	0	0.406140	6.092308	-0.567186
60	1	0	2.853368	2.556752	-0.553697
61	1	0	2.688107	5.036289	-0.611987
62	7	0	0.803414	2.242059	-0.494964
63	1	0	0.617294	0.076415	-2.309166

Fe^{III}-H **2''$_E$** (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1444.21455186 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.267481	1.496916	-1.398152
2	6	0	2.544538	1.121216	-2.077398
3	1	0	2.477120	1.268519	-3.161057
4	1	0	3.331239	1.789104	-1.711412
5	6	0	1.249892	2.941853	-1.015565
6	1	0	2.270827	3.232896	-0.748860
7	1	0	0.935338	3.576610	-1.851976
8	6	0	0.060986	1.155622	-2.244997
9	1	0	-0.727769	1.863367	-1.981777

10	1	0	0.290053	1.312646	-3.304986
11	26	0	1.107952	0.411529	0.309735
12	6	0	2.960056	-0.285921	-1.735256
13	6	0	3.887710	-0.989110	-2.500509
14	6	0	2.927258	-1.972828	-0.131182
15	6	0	4.345962	-2.224826	-2.047188
16	1	0	4.255626	-0.564334	-3.428829
17	6	0	3.863234	-2.718848	-0.833784
18	1	0	2.532931	-2.320310	0.814689
19	1	0	5.072987	-2.786898	-2.624544
20	1	0	4.204277	-3.666978	-0.433626
21	6	0	0.380065	3.146118	0.198709
22	6	0	-0.200494	4.371918	0.511693
23	6	0	-0.887989	4.510949	1.717845
24	1	0	-0.103576	5.207253	-0.174083
25	6	0	-0.389945	2.214485	2.192036
26	6	0	-0.978119	3.413592	2.574753
27	1	0	-1.341823	5.460086	1.984235
28	1	0	-0.443704	1.336417	2.823603
29	1	0	-1.497067	3.478996	3.524388
30	7	0	2.464027	-0.783341	-0.576399
31	7	0	0.271093	2.075032	1.024398
32	6	0	-0.425201	-0.273558	-2.002869
33	1	0	-1.327930	-0.464609	-2.593267
34	1	0	0.327717	-0.997739	-2.322308
35	7	0	-0.666685	-0.454309	-0.545111
36	6	0	-0.578751	-1.860536	-0.068681
37	1	0	-1.520315	-2.399390	-0.211765
38	1	0	0.179546	-2.379537	-0.664576
39	6	0	-1.982426	0.168489	-0.091981
40	1	0	-1.993871	0.081751	0.997251
41	1	0	-1.927767	1.232878	-0.324609
42	6	0	-3.240553	-0.433394	-0.675257
43	6	0	-3.917290	-1.464312	-0.003235
44	6	0	-3.783439	0.055708	-1.874693
45	6	0	-5.083650	-2.016895	-0.533491
46	1	0	-3.549992	-1.816332	0.958432
47	6	0	-4.949018	-0.496066	-2.407230
48	1	0	-3.314602	0.894778	-2.384299
49	6	0	-5.596056	-1.538916	-1.741161
50	1	0	-5.599963	-2.807372	0.001895
51	1	0	-5.360059	-0.102816	-3.331574
52	1	0	-6.506542	-1.963653	-2.151521
53	6	0	-0.156327	-1.876691	1.388552

54	6	0	-0.548830	-2.877262	2.275087
55	6	0	-0.057063	-2.865478	3.581573
56	1	0	-1.228690	-3.655224	1.943374
57	6	0	1.165089	-0.875165	3.038999
58	6	0	0.816559	-1.848266	3.969122
59	1	0	-0.352426	-3.637294	4.285249
60	1	0	1.844719	-0.067389	3.287155
61	1	0	1.224262	-1.804673	4.972911
62	7	0	0.689317	-0.883177	1.775234
63	1	0	2.308898	0.950372	1.015623

Fe^{III}-H **2''$_E$** (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1444.20845559 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.367103	1.652690	-1.236514
2	6	0	2.632947	1.286913	-1.913683
3	1	0	2.579436	1.484697	-2.991815
4	1	0	3.430237	1.926402	-1.520208
5	6	0	1.380067	3.042483	-0.720046
6	1	0	2.404957	3.286701	-0.421800
7	1	0	1.090861	3.768122	-1.491080
8	6	0	0.160010	1.397316	-2.089159
9	1	0	-0.625585	2.080763	-1.758586
10	1	0	0.373093	1.645392	-3.136946
11	26	0	1.078101	0.296506	0.531338
12	6	0	3.060085	-0.146808	-1.669371
13	6	0	4.001378	-0.761623	-2.495652
14	6	0	3.030499	-1.996541	-0.256304
15	6	0	4.469899	-2.032409	-2.168842
16	1	0	4.369018	-0.242211	-3.375005
17	6	0	3.980504	-2.659443	-1.020654
18	1	0	2.621333	-2.443063	0.642795
19	1	0	5.208070	-2.522989	-2.795283
20	1	0	4.325763	-3.642761	-0.721792
21	6	0	0.502360	3.202844	0.505803
22	6	0	-0.014243	4.443250	0.877874
23	6	0	-0.718371	4.558399	2.076036
24	1	0	0.144422	5.307540	0.240916
25	6	0	-0.373896	2.216764	2.431528
26	6	0	-0.897762	3.424464	2.871488
27	1	0	-1.120087	5.518226	2.384875

28	1	0	-0.494585	1.306064	3.008903
29	1	0	-1.435276	3.471532	3.811826
30	7	0	2.568479	-0.768221	-0.577766
31	7	0	0.306522	2.106249	1.270629
32	6	0	-0.337120	-0.047010	-1.996014
33	1	0	-1.220412	-0.174758	-2.631077
34	1	0	0.426459	-0.735761	-2.365095
35	7	0	-0.633994	-0.404007	-0.577762
36	6	0	-0.622346	-1.874054	-0.332182
37	1	0	-1.558651	-2.339590	-0.655480
38	1	0	0.179938	-2.311757	-0.936088
39	6	0	-1.947583	0.200320	-0.087245
40	1	0	-2.005449	-0.036495	0.978400
41	1	0	-1.845391	1.283170	-0.167396
42	6	0	-3.201953	-0.261127	-0.793702
43	6	0	-3.944463	-1.345244	-0.298496
44	6	0	-3.675688	0.415789	-1.929262
45	6	0	-5.110947	-1.762720	-0.940365
46	1	0	-3.627511	-1.846719	0.613355
47	6	0	-4.840777	-0.000971	-2.573484
48	1	0	-3.150699	1.294304	-2.297905
49	6	0	-5.556021	-1.095811	-2.083581
50	1	0	-5.679661	-2.596516	-0.541077
51	1	0	-5.198220	0.536470	-3.446054
52	1	0	-6.466489	-1.416057	-2.579832
53	6	0	-0.347638	-2.169523	1.130493
54	6	0	-0.878297	-3.281220	1.780612
55	6	0	-0.525416	-3.526919	3.109350
56	1	0	-1.555983	-3.944716	1.253441
57	6	0	0.841523	-1.560518	3.049078
58	6	0	0.349585	-2.652286	3.755549
59	1	0	-0.929766	-4.388007	3.632168
60	1	0	1.530401	-0.856021	3.503638
61	1	0	0.648253	-2.809626	4.785917
62	7	0	0.501093	-1.319361	1.764761
63	1	0	2.288470	0.731180	1.339445

Fe^{III}-H **2''$_E$** (sextet) E(B3LYP/ SDD-6-31G(d,p))= -1444.19078950 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.410952	1.616177	-1.178422
2	6	0	2.625292	1.232210	-1.951451

3	1	0	2.474269	1.401559	-3.024071
4	1	0	3.448182	1.888428	-1.648906
5	6	0	1.508861	3.016262	-0.676012
6	1	0	2.536945	3.182554	-0.336068
7	1	0	1.311718	3.740921	-1.475994
8	6	0	0.151613	1.433321	-1.978204
9	1	0	-0.597534	2.112986	-1.567068
10	1	0	0.324834	1.741577	-3.016590
11	26	0	1.199860	0.289085	0.641014
12	6	0	3.073352	-0.190905	-1.698839
13	6	0	3.990587	-0.819056	-2.541241
14	6	0	3.100243	-2.006920	-0.238449
15	6	0	4.472317	-2.081144	-2.199060
16	1	0	4.329942	-0.319511	-3.443112
17	6	0	4.025209	-2.683561	-1.019822
18	1	0	2.725997	-2.429140	0.687424
19	1	0	5.191052	-2.584448	-2.837971
20	1	0	4.386436	-3.657908	-0.710747
21	6	0	0.587208	3.249544	0.500569
22	6	0	0.120654	4.518875	0.836355
23	6	0	-0.631437	4.677990	2.000526
24	1	0	0.351252	5.368597	0.201914
25	6	0	-0.415352	2.325483	2.390939
26	6	0	-0.900905	3.561879	2.795821
27	1	0	-0.999674	5.658855	2.283912
28	1	0	-0.598265	1.429131	2.974877
29	1	0	-1.476492	3.645329	3.710757
30	7	0	2.622427	-0.787735	-0.576549
31	7	0	0.306500	2.170421	1.262043
32	6	0	-0.371356	-0.000823	-1.944425
33	1	0	-1.252509	-0.080664	-2.591354
34	1	0	0.379728	-0.686313	-2.345288
35	7	0	-0.683118	-0.415175	-0.550379
36	6	0	-0.683784	-1.888298	-0.382326
37	1	0	-1.618059	-2.338186	-0.734185
38	1	0	0.124167	-2.304575	-0.994490
39	6	0	-1.988581	0.179430	-0.041164
40	1	0	-2.055175	-0.103520	1.012950
41	1	0	-1.875909	1.264063	-0.070464
42	6	0	-3.246923	-0.233188	-0.771962
43	6	0	-4.001520	-1.333949	-0.335116
44	6	0	-3.709786	0.503408	-1.874259
45	6	0	-5.169053	-1.707899	-1.001534
46	1	0	-3.693438	-1.883337	0.551841

47	6	0	-4.876120	0.130725	-2.542984
48	1	0	-3.175344	1.394531	-2.196601
49	6	0	-5.603532	-0.980354	-2.111352
50	1	0	-5.746987	-2.555298	-0.646473
51	1	0	-5.225107	0.714581	-3.388770
52	1	0	-6.515060	-1.266709	-2.626039
53	6	0	-0.426215	-2.242852	1.066292
54	6	0	-0.965870	-3.370912	1.678610
55	6	0	-0.632472	-3.650575	3.005754
56	1	0	-1.636384	-4.018874	1.123647
57	6	0	0.737272	-1.684732	3.016515
58	6	0	0.232594	-2.792613	3.687183
59	1	0	-1.044738	-4.524356	3.500651
60	1	0	1.423762	-0.990840	3.490314
61	1	0	0.514996	-2.975067	4.718003
62	7	0	0.412547	-1.414438	1.733067
63	1	0	2.292122	0.506612	1.881037

Fe^{III}-H **2''$_F$** (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1444.20833685 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.110832	-1.912444	0.407698
2	6	0	1.973469	-1.780373	1.616300
3	1	0	1.702742	-2.534373	2.365176
4	1	0	3.007473	-1.998151	1.325993
5	6	0	1.823219	-2.637857	-0.672550
6	1	0	2.276884	-3.571139	-0.314823
7	1	0	1.090734	-2.906225	-1.440977
8	6	0	-0.230696	-2.479793	0.723463
9	1	0	-0.626641	-2.928540	-0.189443
10	1	0	-0.153661	-3.282854	1.467143
11	26	0	0.772045	0.130571	-0.414956
12	6	0	1.967952	-0.401208	2.242453
13	6	0	2.443212	-0.208400	3.540703
14	6	0	1.658859	1.891130	1.972778
15	6	0	2.530239	1.084998	4.050865
16	1	0	2.747396	-1.061834	4.138347
17	6	0	2.137044	2.158347	3.247585
18	1	0	1.331067	2.690962	1.317743
19	1	0	2.900179	1.253832	5.057241
20	1	0	2.194410	3.181267	3.602257

21	6	0	2.877737	-1.745301	-1.297474
22	6	0	4.039729	-2.254524	-1.872982
23	6	0	4.940639	-1.379512	-2.480564
24	1	0	4.232062	-3.322271	-1.848106
25	6	0	3.490956	0.428569	-1.880557
26	6	0	4.663090	-0.011480	-2.482006
27	1	0	5.847917	-1.758926	-2.939716
28	1	0	3.240958	1.484223	-1.850528
29	1	0	5.340160	0.703612	-2.935427
30	7	0	1.567248	0.637114	1.474541
31	7	0	2.614982	-0.418332	-1.302524
32	6	0	-1.182934	-1.394853	1.231384
33	1	0	-2.156081	-1.836898	1.470407
34	1	0	-0.794501	-0.953878	2.153477
35	7	0	-1.318124	-0.313322	0.219311
36	6	0	-1.759440	0.976286	0.807873
37	1	0	-2.838653	0.986672	0.991641
38	1	0	-1.265092	1.099677	1.777896
39	6	0	-2.229599	-0.713647	-0.940915
40	1	0	-2.167842	0.101921	-1.664788
41	1	0	-1.770157	-1.584553	-1.411473
42	6	0	-3.670104	-1.001837	-0.587173
43	6	0	-4.638854	0.013252	-0.647267
44	6	0	-4.079007	-2.299572	-0.238614
45	6	0	-5.972090	-0.252783	-0.333425
46	1	0	-4.356295	1.011401	-0.974678
47	6	0	-5.411250	-2.567885	0.076475
48	1	0	-3.360813	-3.116748	-0.244377
49	6	0	-6.358333	-1.542494	0.036946
50	1	0	-6.711102	0.539909	-0.393868
51	1	0	-5.712790	-3.577729	0.335957
52	1	0	-7.396393	-1.752195	0.274185
53	6	0	-1.366014	2.123325	-0.103313
54	6	0	-2.133334	3.280421	-0.224618
55	6	0	-1.698546	4.302942	-1.068426
56	1	0	-3.060610	3.372330	0.331486
57	6	0	0.200234	2.951945	-1.619443
58	6	0	-0.511682	4.133771	-1.783738
59	1	0	-2.283953	5.210372	-1.177543
60	1	0	1.116448	2.770581	-2.172014
61	1	0	-0.147518	4.894766	-2.464729
62	7	0	-0.206686	1.973041	-0.784952
63	1	0	0.295752	-0.313261	-1.778702

Fe^{III}-H **2''$_F$** (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1444.21159966 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.040711	-1.954807	0.005370
2	6	0	1.944948	-2.099838	1.196511
3	1	0	1.687421	-3.005606	1.756090
4	1	0	2.967473	-2.243781	0.832387
5	6	0	1.736206	-2.442218	-1.225349
6	1	0	2.180841	-3.433535	-1.078190
7	1	0	0.992740	-2.519442	-2.024395
8	6	0	-0.296762	-2.598327	0.241986
9	1	0	-0.714295	-2.864211	-0.730868
10	1	0	-0.189421	-3.526379	0.814285
11	26	0	0.655934	0.003177	-0.370292
12	6	0	1.949688	-0.890504	2.100807
13	6	0	2.507631	-0.943899	3.378429
14	6	0	1.551049	1.387903	2.311063
15	6	0	2.590252	0.226947	4.129606
16	1	0	2.878807	-1.884481	3.772897
17	6	0	2.110934	1.419102	3.581436
18	1	0	1.155487	2.287328	1.851429
19	1	0	3.023722	0.210732	5.124539
20	1	0	2.163631	2.353766	4.128386
21	6	0	2.778538	-1.415540	-1.600190
22	6	0	3.964985	-1.728446	-2.255484
23	6	0	4.861499	-0.704166	-2.565269
24	1	0	4.183596	-2.758467	-2.517598
25	6	0	3.350793	0.841409	-1.528248
26	6	0	4.553487	0.601299	-2.183933
27	1	0	5.789690	-0.925223	-3.082256
28	1	0	3.083879	1.839031	-1.199905
29	1	0	5.230273	1.424044	-2.385042
30	7	0	1.462310	0.255201	1.580762
31	7	0	2.469958	-0.139347	-1.253564
32	6	0	-1.215714	-1.614769	0.965920
33	1	0	-2.211178	-2.044660	1.110997
34	1	0	-0.817054	-1.369393	1.953470
35	7	0	-1.283290	-0.354982	0.159793
36	6	0	-1.642937	0.855724	0.956044
37	1	0	-2.720687	0.903471	1.136566
38	1	0	-1.148481	0.789376	1.929527

39	6	0	-2.249064	-0.498659	-1.033457
40	1	0	-2.133175	0.415782	-1.616225
41	1	0	-1.862687	-1.312856	-1.646460
42	6	0	-3.697447	-0.735257	-0.679409
43	6	0	-4.586746	0.344177	-0.546453
44	6	0	-4.198732	-2.039697	-0.535010
45	6	0	-5.930615	0.128048	-0.240683
46	1	0	-4.234880	1.359130	-0.717492
47	6	0	-5.542084	-2.257996	-0.228665
48	1	0	-3.546106	-2.895074	-0.696074
49	6	0	-6.407992	-1.173526	-0.073169
50	1	0	-6.607667	0.971541	-0.150252
51	1	0	-5.916036	-3.271923	-0.128406
52	1	0	-7.454841	-1.343039	0.157452
53	6	0	-1.159761	2.073872	0.198460
54	6	0	-1.813242	3.302406	0.235310
55	6	0	-1.313250	4.364381	-0.520450
56	1	0	-2.706913	3.419848	0.839521
57	6	0	0.414124	2.899761	-1.307452
58	6	0	-0.187024	4.154145	-1.315342
59	1	0	-1.807804	5.330291	-0.505457
60	1	0	1.270323	2.688071	-1.936325
61	1	0	0.217376	4.940346	-1.942909
62	7	0	-0.039851	1.883664	-0.548271
63	1	0	0.206251	-0.183397	-1.772781

Fe^{III}-H **2''$_F$** (sextet) E(B3LYP/ SDD-6-31G(d,p))= -1444.18590860 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.122641	-1.872169	0.402347
2	6	0	1.937178	-1.692489	1.641543
3	1	0	1.616616	-2.409953	2.405478
4	1	0	2.977104	-1.942414	1.406151
5	6	0	1.900560	-2.612822	-0.632954
6	1	0	2.298822	-3.553531	-0.233480
7	1	0	1.216615	-2.859860	-1.451469
8	6	0	-0.209414	-2.488204	0.682312
9	1	0	-0.577729	-2.920979	-0.249908
10	1	0	-0.116035	-3.308048	1.404937
11	26	0	0.708826	0.076832	-0.602643
12	6	0	1.931033	-0.289963	2.213869
13	6	0	2.388068	-0.061227	3.513789

14	6	0	1.635717	1.986566	1.867686
15	6	0	2.476847	1.247158	3.982698
16	1	0	2.677302	-0.897051	4.143217
17	6	0	2.100474	2.295085	3.138703
18	1	0	1.319580	2.767970	1.184751
19	1	0	2.834245	1.446950	4.987905
20	1	0	2.159642	3.328979	3.459897
21	6	0	3.016785	-1.743863	-1.174811
22	6	0	4.212808	-2.276405	-1.649863
23	6	0	5.170164	-1.418385	-2.193682
24	1	0	4.389667	-3.345938	-1.599402
25	6	0	3.702089	0.413572	-1.723897
26	6	0	4.912091	-0.047579	-2.229739
27	1	0	6.105309	-1.814161	-2.576720
28	1	0	3.465346	1.473443	-1.724370
29	1	0	5.632181	0.653483	-2.636470
30	7	0	1.547050	0.718970	1.407519
31	7	0	2.771751	-0.414096	-1.211956
32	6	0	-1.187026	-1.434998	1.200900
33	1	0	-2.152566	-1.895751	1.433600
34	1	0	-0.808940	-0.991411	2.126062
35	7	0	-1.343448	-0.349842	0.190981
36	6	0	-1.766170	0.943001	0.793194
37	1	0	-2.837366	0.942276	1.019211
38	1	0	-1.232452	1.070080	1.740900
39	6	0	-2.276769	-0.749468	-0.954893
40	1	0	-2.228027	0.065445	-1.680189
41	1	0	-1.822937	-1.615494	-1.437811
42	6	0	-3.707464	-1.039094	-0.565228
43	6	0	-4.677294	-0.023609	-0.590399
44	6	0	-4.106723	-2.340609	-0.219502
45	6	0	-6.002146	-0.293717	-0.246091
46	1	0	-4.404044	0.977347	-0.916944
47	6	0	-5.430637	-2.612623	0.126332
48	1	0	-3.388826	-3.157288	-0.253579
49	6	0	-6.378526	-1.587296	0.121165
50	1	0	-6.742945	0.498846	-0.280845
51	1	0	-5.725402	-3.625331	0.382335
52	1	0	-7.410279	-1.799845	0.382144
53	6	0	-1.418477	2.093608	-0.129075
54	6	0	-2.213262	3.231459	-0.244631
55	6	0	-1.814973	4.259619	-1.101358
56	1	0	-3.134038	3.306816	0.324346
57	6	0	0.106956	2.954930	-1.678444

58	6	0	-0.636680	4.117512	-1.836626
59	1	0	-2.423752	5.152369	-1.204355
60	1	0	1.019175	2.791108	-2.244174
61	1	0	-0.303108	4.884752	-2.526143
62	7	0	-0.264985	1.971571	-0.831601
63	1	0	0.345066	-0.582445	-2.083373

2''$_{dp}$ (quartet) E(B3LYP/ SDD-6-31G(d,p))= -1443.92243105 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.339693	-1.489384	-1.189977
2	6	0	-2.223372	-0.956729	-2.241261
3	1	0	-1.599103	-0.424602	-2.967583
4	1	0	-2.738604	-1.755737	-2.796265
5	6	0	-2.018130	-2.502848	-0.364406
6	1	0	-3.077167	-2.224926	-0.308780
7	1	0	-1.975968	-3.506081	-0.815065
8	6	0	-0.026987	-1.936890	-1.695049
9	1	0	0.412048	-2.587918	-0.932975
10	1	0	-0.125923	-2.545592	-2.608192
11	26	0	-0.924160	0.317592	0.238150
12	6	0	-3.229354	0.021593	-1.671282
13	6	0	-4.518430	0.131757	-2.180383
14	6	0	-3.626875	1.741593	-0.164612
15	6	0	-5.390171	1.088758	-1.652804
16	1	0	-4.836384	-0.526341	-2.983297
17	6	0	-4.928292	1.908757	-0.622721
18	1	0	-3.228309	2.375546	0.621694
19	1	0	-6.399577	1.189508	-2.037330
20	1	0	-5.560764	2.671179	-0.180923
21	6	0	-1.473313	-2.534276	1.048156
22	6	0	-1.376334	-3.715970	1.775520
23	6	0	-0.927678	-3.674290	3.099315
24	1	0	-1.651902	-4.657882	1.311544
25	6	0	-0.709510	-1.300156	2.858214
26	6	0	-0.589132	-2.439380	3.648969
27	1	0	-0.846133	-4.585404	3.683015
28	1	0	-0.461126	-0.319185	3.252013
29	1	0	-0.238845	-2.352104	4.671728
30	7	0	-2.778704	0.810923	-0.660949
31	7	0	-1.136474	-1.331105	1.576762

32	6	0	0.914605	-0.758389	-1.978378
33	1	0	1.863921	-1.141576	-2.374839
34	1	0	0.485641	-0.127389	-2.761704
35	7	0	1.114527	0.088012	-0.781098
36	6	0	1.402320	1.503178	-1.114769
37	1	0	2.431181	1.652215	-1.466037
38	1	0	0.734626	1.781983	-1.939370
39	6	0	2.113698	-0.482632	0.185808
40	1	0	2.062357	0.137531	1.085428
41	1	0	1.750832	-1.474535	0.468000
42	6	0	3.549256	-0.576521	-0.294024
43	6	0	4.444566	0.484775	-0.089422
44	6	0	4.021459	-1.733843	-0.931958
45	6	0	5.764482	0.403950	-0.534954
46	1	0	4.111199	1.372642	0.442434
47	6	0	5.340616	-1.818013	-1.379692
48	1	0	3.359715	-2.587449	-1.059798
49	6	0	6.213508	-0.745875	-1.187172
50	1	0	6.444842	1.232645	-0.362915
51	1	0	5.689220	-2.723438	-1.867245
52	1	0	7.241420	-0.811690	-1.530195
53	6	0	1.115598	2.415703	0.060566
54	6	0	1.899414	3.533799	0.331371
55	6	0	1.572646	4.364733	1.405308
56	1	0	2.759488	3.747520	-0.295652
57	6	0	-0.274152	2.905114	1.860364
58	6	0	0.463148	4.034966	2.187282
59	1	0	2.171738	5.241085	1.629040
60	1	0	-1.145065	2.621639	2.444341
61	1	0	0.170697	4.641860	3.037320
62	7	0	0.026430	2.100401	0.812661

2''$_{dp}$ (doublet) E(B3LYP/ SDD-6-31G(d,p))= -1443.89469477 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.194795	-1.626225	-1.029843
2	6	0	-2.211558	-1.372153	-2.081139
3	1	0	-1.702014	-0.899714	-2.928927
4	1	0	-2.660178	-2.304224	-2.454360
5	6	0	-1.716714	-2.574567	-0.007213
6	1	0	-2.793787	-2.396338	0.078185

7	1	0	-1.583858	-3.618429	-0.322254
8	6	0	0.119949	-2.067133	-1.579858
9	1	0	0.621004	-2.642584	-0.797025
10	1	0	-0.010296	-2.741060	-2.438259
11	26	0	-0.896136	0.186470	-0.133012
12	6	0	-3.267200	-0.428279	-1.548667
13	6	0	-4.566737	-0.413109	-2.040764
14	6	0	-3.720692	1.353388	-0.137308
15	6	0	-5.471053	0.539201	-1.565427
16	1	0	-4.863943	-1.135672	-2.794624
17	6	0	-5.028794	1.441263	-0.598018
18	1	0	-3.353873	2.036597	0.619211
19	1	0	-6.488713	0.572951	-1.939396
20	1	0	-5.687363	2.202610	-0.193988
21	6	0	-1.089630	-2.319586	1.344837
22	6	0	-0.880038	-3.333749	2.274029
23	6	0	-0.384446	-3.008112	3.539510
24	1	0	-1.110038	-4.362671	2.014397
25	6	0	-0.333587	-0.716288	2.830254
26	6	0	-0.112746	-1.669488	3.820404
27	1	0	-0.216438	-3.780140	4.283099
28	1	0	-0.122833	0.333778	3.010392
29	1	0	0.269668	-1.362878	4.788230
30	7	0	-2.832487	0.436464	-0.586596
31	7	0	-0.809297	-1.017663	1.604600
32	6	0	0.980397	-0.863200	-1.975291
33	1	0	1.957687	-1.203426	-2.340218
34	1	0	0.504664	-0.322232	-2.798604
35	7	0	1.100892	0.076860	-0.828525
36	6	0	1.303545	1.493600	-1.236937
37	1	0	2.345501	1.714347	-1.497301
38	1	0	0.697518	1.664311	-2.134965
39	6	0	2.123716	-0.358933	0.189522
40	1	0	2.012654	0.321065	1.037371
41	1	0	1.819152	-1.346749	0.541305
42	6	0	3.567670	-0.389526	-0.268980
43	6	0	4.392338	0.735699	-0.114312
44	6	0	4.122002	-1.549827	-0.831289
45	6	0	5.722095	0.713044	-0.536606
46	1	0	3.996240	1.629138	0.362738
47	6	0	5.451150	-1.576174	-1.255696
48	1	0	3.517932	-2.450416	-0.916127
49	6	0	6.252358	-0.441711	-1.114878
50	1	0	6.346632	1.591330	-0.403688

51	1	0	5.863897	-2.484587	-1.683988
52	1	0	7.287995	-0.462408	-1.439789
53	6	0	0.808461	2.402601	-0.135038
54	6	0	1.419165	3.608492	0.189157
55	6	0	0.877583	4.405958	1.200621
56	1	0	2.308778	3.919597	-0.349509
57	6	0	-0.811773	2.726151	1.497800
58	6	0	-0.256977	3.946733	1.868278
59	1	0	1.335521	5.353431	1.464117
60	1	0	-1.683656	2.330686	2.008387
61	1	0	-0.709878	4.519308	2.670545
62	7	0	-0.311362	1.954906	0.504853

3''$_A$ (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1444.81658160 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.788020	-1.001559	-1.208802
2	6	0	-2.559850	-0.221675	-2.203327
3	1	0	-1.857652	0.259828	-2.891626
4	1	0	-3.198920	-0.869636	-2.817753
5	6	0	-2.644244	-2.041226	-0.584520
6	1	0	-3.667205	-1.649113	-0.545123
7	1	0	-2.679229	-2.950526	-1.199110
8	6	0	-0.537839	-1.578384	-1.761628
9	1	0	-0.214532	-2.371091	-1.082323
10	1	0	-0.716275	-2.053624	-2.737066
11	26	0	-1.124612	0.421880	0.443997
12	6	0	-3.385460	0.858306	-1.529722
13	6	0	-4.565992	1.345777	-2.085751
14	6	0	-3.536572	2.365097	0.240333
15	6	0	-5.237314	2.388050	-1.444523
16	1	0	-4.952600	0.918315	-3.005381
17	6	0	-4.713519	2.909444	-0.260666
18	1	0	-3.090218	2.726216	1.161894
19	1	0	-6.158610	2.782681	-1.861231
20	1	0	-5.207959	3.715583	0.269455
21	6	0	-2.220241	-2.366577	0.832677
22	6	0	-2.489832	-3.602002	1.418269
23	6	0	-2.172463	-3.797938	2.762931
24	1	0	-2.947762	-4.393573	0.833817
25	6	0	-1.340821	-1.553319	2.828536

26	6	0	-1.591410	-2.753433	3.483919
27	1	0	-2.377505	-4.751049	3.240056
28	1	0	-0.889158	-0.708851	3.339802
29	1	0	-1.335903	-2.863726	4.531758
30	7	0	-2.883087	1.361588	-0.380415
31	7	0	-1.642958	-1.362976	1.528019
32	6	0	0.561429	-0.530838	-1.924342
33	1	0	1.432371	-0.998216	-2.398841
34	1	0	0.219560	0.255282	-2.603719
35	7	0	0.961313	0.135580	-0.642494
36	6	0	1.723945	1.358561	-1.040686
37	1	0	2.543146	1.080023	-1.714515
38	1	0	1.038424	1.990229	-1.619270
39	6	0	1.785620	-0.787617	0.243149
40	1	0	2.001013	-0.223973	1.154635
41	1	0	1.117964	-1.600957	0.536844
42	6	0	3.066032	-1.352103	-0.339144
43	6	0	4.296882	-0.713188	-0.123870
44	6	0	3.057431	-2.556038	-1.062735
45	6	0	5.479139	-1.241379	-0.644086
46	1	0	4.339832	0.185787	0.484982
47	6	0	4.237051	-3.085838	-1.586339
48	1	0	2.127899	-3.104474	-1.196531
49	6	0	5.450095	-2.424811	-1.384011
50	1	0	6.424115	-0.740706	-0.457370
51	1	0	4.211770	-4.020564	-2.137442
52	1	0	6.369660	-2.840157	-1.783586
53	6	0	2.333174	2.233823	0.038101
54	6	0	3.572002	2.845803	-0.149445
55	6	0	4.061804	3.740364	0.804821
56	1	0	4.147589	2.622260	-1.040609
57	6	0	2.093963	3.377835	2.107643
58	6	0	3.316023	4.011203	1.955296
59	1	0	5.023751	4.219618	0.652231
60	1	0	1.445067	3.521623	2.964715
61	1	0	3.671913	4.695720	2.716394
62	7	0	1.642647	2.530450	1.161036
63	1	0	0.675293	2.070658	1.322408
64	1	0	-0.519387	1.518577	1.591905

3''$_A$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1444.77999292hartree

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Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	-1.665376	-1.412911	-0.982592
2	6	0	-2.673624	-1.063481	-2.020678
3	1	0	-2.143000	-0.659169	-2.891003
4	1	0	-3.225546	-1.946639	-2.368265
5	6	0	-2.285238	-2.241241	0.094768
6	1	0	-3.365352	-2.062357	0.084983
7	1	0	-2.142677	-3.311111	-0.096541
8	6	0	-0.430282	-2.042115	-1.528998
9	1	0	-0.026240	-2.703199	-0.759767
10	1	0	-0.653090	-2.669895	-2.401160
11	26	0	-1.150059	0.404833	-0.148996
12	6	0	-3.613580	-0.014944	-1.455617
13	6	0	-4.920110	0.152217	-1.902712
14	6	0	-3.841700	1.745847	0.055672
15	6	0	-5.701747	1.164825	-1.342716
16	1	0	-5.319856	-0.498077	-2.674037
17	6	0	-5.153619	1.972602	-0.346193
18	1	0	-3.365060	2.343946	0.823086
19	1	0	-6.723431	1.315096	-1.676435
20	1	0	-5.729542	2.766307	0.116171
21	6	0	-1.758211	-1.841237	1.452028
22	6	0	-1.835129	-2.676910	2.563907
23	6	0	-1.430612	-2.193076	3.807655
24	1	0	-2.215865	-3.687499	2.456240
25	6	0	-0.895612	-0.110700	2.745083
26	6	0	-0.960095	-0.882618	3.899139
27	1	0	-1.486125	-2.825107	4.687961
28	1	0	-0.538294	0.911617	2.761749
29	1	0	-0.645801	-0.460831	4.847225
30	7	0	-3.080851	0.772564	-0.485316
31	7	0	-1.278216	-0.577447	1.538547
32	6	0	0.591726	-0.978138	-1.908948
33	1	0	1.501730	-1.452648	-2.294205
34	1	0	0.190614	-0.360100	-2.720204
35	7	0	0.912215	-0.054576	-0.763652
36	6	0	1.670774	1.083274	-1.379423
37	1	0	2.551665	0.695895	-1.903183
38	1	0	1.019567	1.532186	-2.139738
39	6	0	1.743311	-0.748505	0.308424
40	1	0	1.874166	-0.013855	1.106631
41	1	0	1.111263	-1.537168	0.718239
42	6	0	3.086640	-1.315948	-0.105343

43	6	0	4.269012	-0.597899	0.132427
44	6	0	3.189985	-2.597551	-0.672059
45	6	0	5.512629	-1.125551	-0.218236
46	1	0	4.222316	0.366988	0.630067
47	6	0	4.430661	-3.126479	-1.028465
48	1	0	2.300604	-3.207338	-0.810668
49	6	0	5.594827	-2.387378	-0.809468
50	1	0	6.417341	-0.561272	-0.014209
51	1	0	4.490226	-4.120622	-1.459973
52	1	0	6.561246	-2.801629	-1.078115
53	6	0	2.145284	2.204076	-0.477559
54	6	0	3.413434	2.767213	-0.605678
55	6	0	3.757105	3.884164	0.160357
56	1	0	4.121882	2.334917	-1.303200
57	6	0	1.585311	3.830379	1.156424
58	6	0	2.833342	4.425003	1.058936
59	1	0	4.741597	4.329324	0.055870
60	1	0	0.803752	4.186070	1.819007
61	1	0	3.071725	5.290114	1.666704
62	7	0	1.281422	2.760382	0.397254
63	1	0	0.282368	2.316171	0.459112
64	1	0	-0.911881	1.833182	0.505514

3''$_A$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1444.80601258 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.718277	-1.094380	-1.188290
2	6	0	-2.517203	-0.337922	-2.195017
3	1	0	-1.829230	0.105996	-2.921155
4	1	0	-3.178040	-1.006544	-2.760236
5	6	0	-2.555504	-2.159299	-0.562242
6	1	0	-3.575241	-1.767207	-0.471999
7	1	0	-2.609037	-3.047729	-1.204321
8	6	0	-0.472382	-1.665407	-1.774864
9	1	0	-0.122672	-2.449041	-1.098529
10	1	0	-0.674823	-2.144019	-2.742800
11	26	0	-1.141108	0.211721	0.335038
12	6	0	-3.295043	0.773534	-1.528348
13	6	0	-4.480545	1.283885	-2.048519
14	6	0	-3.333403	2.311161	0.221182
15	6	0	-5.096735	2.356692	-1.401301
16	1	0	-4.914923	0.850986	-2.943790

17	6	0	-4.512803	2.879825	-0.247651
18	1	0	-2.848111	2.665169	1.123396
19	1	0	-6.021551	2.771472	-1.789421
20	1	0	-4.964065	3.707443	0.287874
21	6	0	-2.056493	-2.502652	0.821626
22	6	0	-2.292256	-3.736143	1.422745
23	6	0	-1.888299	-3.930719	2.744687
24	1	0	-2.790629	-4.526471	0.870825
25	6	0	-1.050054	-1.685403	2.754262
26	6	0	-1.261107	-2.885785	3.424110
27	1	0	-2.064496	-4.882210	3.236188
28	1	0	-0.571411	-0.840597	3.236647
29	1	0	-0.940663	-2.994547	4.454115
30	7	0	-2.729013	1.280528	-0.406057
31	7	0	-1.431430	-1.495400	1.475009
32	6	0	0.592831	-0.590600	-1.950628
33	1	0	1.494402	-1.033684	-2.389228
34	1	0	0.240968	0.166330	-2.656988
35	7	0	0.912593	0.110287	-0.663978
36	6	0	1.581680	1.390603	-1.035697
37	1	0	2.476641	1.187415	-1.636372
38	1	0	0.885855	1.946883	-1.675720
39	6	0	1.805656	-0.746547	0.227686
40	1	0	1.954241	-0.176544	1.148266
41	1	0	1.212612	-1.621837	0.499392
42	6	0	3.139621	-1.183976	-0.341959
43	6	0	4.298613	-0.419885	-0.134645
44	6	0	3.254694	-2.394105	-1.045703
45	6	0	5.530238	-0.835197	-0.642417
46	1	0	4.247279	0.489514	0.458527
47	6	0	4.484081	-2.811704	-1.556201
48	1	0	2.384152	-3.033646	-1.173176
49	6	0	5.623440	-2.028713	-1.360956
50	1	0	6.419221	-0.238545	-0.463091
51	1	0	4.555676	-3.753164	-2.091523
52	1	0	6.582057	-2.356282	-1.750233
53	6	0	2.003187	2.324329	0.081017
54	6	0	3.150160	3.110151	-0.024091
55	6	0	3.453958	4.037548	0.974822
56	1	0	3.797955	2.994125	-0.885950
57	6	0	1.491131	3.362111	2.156485
58	6	0	2.615147	4.166997	2.086134
59	1	0	4.344451	4.652320	0.888751
60	1	0	0.785394	3.386380	2.979615

61	1	0	2.828387	4.872904	2.880311
62	7	0	1.218174	2.486057	1.167730
63	1	0	0.328916	1.880674	1.263135
64	1	0	-0.804506	1.183380	1.538505

3''$_B$ (quinete) E(B3LYP/ SDD-6-31G(d,p))= -1444.81520364 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.607546	-1.181132	-0.574432
2	6	0	-2.555427	-1.129307	-1.719271
3	1	0	-2.039311	-0.644958	-2.555358
4	1	0	-2.801922	-2.147872	-2.052378
5	6	0	-2.226657	-1.838837	0.598776
6	1	0	-3.240374	-1.438640	0.717489
7	1	0	-2.337108	-2.922258	0.444204
8	6	0	-0.386728	-1.924458	-1.018030
9	1	0	0.060718	-2.382419	-0.133519
10	1	0	-0.662561	-2.750575	-1.688697
11	26	0	-0.533932	0.854197	0.314257
12	6	0	-3.870102	-0.406321	-1.506169
13	6	0	-5.086523	-0.950759	-1.909531
14	6	0	-4.983542	1.585889	-0.846799
15	6	0	-6.261118	-0.201830	-1.785714
16	1	0	-5.113696	-1.951782	-2.325725
17	6	0	-6.213133	1.085961	-1.247599
18	1	0	-4.847530	2.570416	-0.412380
19	1	0	-7.207812	-0.625245	-2.106327
20	1	0	-7.106121	1.690172	-1.137744
21	6	0	-1.478596	-1.583235	1.894368
22	6	0	-1.558219	-2.495717	2.946419
23	6	0	-0.946484	-2.194548	4.162851
24	1	0	-2.097625	-3.428130	2.814356
25	6	0	-0.210310	-0.133340	3.198701
26	6	0	-0.261990	-0.985776	4.294285
27	1	0	-1.002349	-2.892296	4.992356
28	1	0	0.321355	0.811475	3.251895
29	1	0	0.226527	-0.708655	5.221620
30	7	0	-3.869130	0.843814	-0.989415
31	7	0	-0.801304	-0.418731	2.017690
32	6	0	0.637760	-1.026068	-1.711828
33	1	0	1.434105	-1.646226	-2.139278

34	1	0	0.172298	-0.490113	-2.544580
35	7	0	1.191582	-0.017739	-0.770847
36	6	0	1.778539	1.149779	-1.480407
37	1	0	2.746380	0.903681	-1.930186
38	1	0	1.101284	1.421657	-2.299108
39	6	0	2.201315	-0.621716	0.197446
40	1	0	2.473347	0.181350	0.886410
41	1	0	1.666986	-1.372229	0.783692
42	6	0	3.444515	-1.226551	-0.416399
43	6	0	4.599660	-0.450738	-0.604125
44	6	0	3.482453	-2.584383	-0.771827
45	6	0	5.750753	-1.009080	-1.161018
46	1	0	4.610191	0.589419	-0.286538
47	6	0	4.632277	-3.144803	-1.329047
48	1	0	2.618505	-3.219235	-0.586542
49	6	0	5.766176	-2.355415	-1.530696
50	1	0	6.638728	-0.398806	-1.292404
51	1	0	4.648383	-4.197841	-1.591781
52	1	0	6.663443	-2.791895	-1.957626
53	6	0	1.905806	2.337007	-0.544239
54	6	0	2.876093	3.321809	-0.718453
55	6	0	2.886537	4.421994	0.139660
56	1	0	3.606797	3.229908	-1.515528
57	6	0	0.994795	3.480843	1.265740
58	6	0	1.927525	4.505149	1.150311
59	1	0	3.632411	5.201584	0.021574
60	1	0	0.224220	3.507210	2.030523
61	1	0	1.900819	5.343801	1.836851
62	7	0	0.984825	2.415241	0.441133
63	1	0	-2.934861	1.266693	-0.644342
64	1	0	-1.834237	1.839218	-0.124962

3''$_B$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1444.78148567 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.426743	-1.341825	-0.408052
2	6	0	-2.433158	-1.464069	-1.505921
3	1	0	-1.972442	-1.065309	-2.417657
4	1	0	-2.634327	-2.525549	-1.700122
5	6	0	-1.969783	-1.871407	0.878301
6	1	0	-2.991203	-1.497250	0.998685

7	1	0	-2.026571	-2.967759	0.864917
8	6	0	-0.207602	-2.141699	-0.813642
9	1	0	0.259719	-2.502548	0.104386
10	1	0	-0.503701	-3.026739	-1.390414
11	26	0	-0.616743	0.551430	0.052405
12	6	0	-3.780881	-0.788271	-1.329519
13	6	0	-4.936125	-1.338251	-1.880916
14	6	0	-5.025203	1.084198	-0.578378
15	6	0	-6.146727	-0.646705	-1.785235
16	1	0	-4.888573	-2.297378	-2.385282
17	6	0	-6.196303	0.584210	-1.125711
18	1	0	-4.970321	2.021834	-0.035702
19	1	0	-7.046932	-1.071408	-2.218264
20	1	0	-7.121391	1.140865	-1.030673
21	6	0	-1.144239	-1.381501	2.044540
22	6	0	-1.110616	-2.052424	3.264518
23	6	0	-0.407433	-1.491622	4.330595
24	1	0	-1.634620	-2.996067	3.377799
25	6	0	0.188441	0.326841	2.884577
26	6	0	0.248254	-0.275963	4.135835
27	1	0	-0.372327	-1.993883	5.291746
28	1	0	0.692673	1.265232	2.687177
29	1	0	0.805165	0.200043	4.935123
30	7	0	-3.869946	0.402334	-0.699802
31	7	0	-0.491723	-0.210848	1.851503
32	6	0	0.784240	-1.291608	-1.599656
33	1	0	1.640307	-1.900695	-1.911469
34	1	0	0.322121	-0.909297	-2.515683
35	7	0	1.199403	-0.132821	-0.763411
36	6	0	1.628222	1.047536	-1.568533
37	1	0	2.663029	0.955505	-1.913482
38	1	0	1.001316	1.095540	-2.468107
39	6	0	2.275566	-0.500811	0.247809
40	1	0	2.421016	0.391446	0.861475
41	1	0	1.847696	-1.265190	0.898389
42	6	0	3.596650	-0.971938	-0.316424
43	6	0	4.635909	-0.060897	-0.565605
44	6	0	3.826778	-2.335584	-0.561124
45	6	0	5.858439	-0.495845	-1.078520
46	1	0	4.501028	0.991833	-0.327118
47	6	0	5.048065	-2.772868	-1.074861
48	1	0	3.059153	-3.067926	-0.319652
49	6	0	6.063154	-1.851856	-1.341387
50	1	0	6.654963	0.219317	-1.258160

51	1	0	5.212903	-3.830999	-1.251862
52	1	0	7.016120	-2.191737	-1.734053
53	6	0	1.422622	2.312540	-0.760166
54	6	0	2.204952	3.452875	-0.920273
55	6	0	1.898323	4.595417	-0.179558
56	1	0	3.038246	3.445198	-1.615169
57	6	0	0.074581	3.391618	0.807648
58	6	0	0.814145	4.563500	0.698980
59	1	0	2.495936	5.494971	-0.286971
60	1	0	-0.783901	3.315534	1.465471
61	1	0	0.540887	5.430876	1.289349
62	7	0	0.372618	2.281243	0.100384
63	1	0	-2.960369	0.803956	-0.213637
64	1	0	-1.977180	1.261299	0.447846

3''$_B$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1444.79520562 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.392595	-1.143368	-0.861540
2	6	0	-2.340904	-0.795452	-1.954095
3	1	0	-1.832243	-0.096467	-2.628004
4	1	0	-2.567649	-1.690146	-2.550778
5	6	0	-1.997230	-2.153840	0.054417
6	1	0	-3.008454	-1.822459	0.311122
7	1	0	-2.096415	-3.123452	-0.452576
8	6	0	-0.138536	-1.713405	-1.476727
9	1	0	0.310560	-2.376871	-0.735380
10	1	0	-0.387875	-2.332770	-2.348642
11	26	0	-0.570746	0.461161	0.420301
12	6	0	-3.670356	-0.175267	-1.563707
13	6	0	-4.805334	-0.359258	-2.350609
14	6	0	-4.901045	1.255903	-0.124651
15	6	0	-5.995276	0.291943	-2.017242
16	1	0	-4.756072	-1.005969	-3.220048
17	6	0	-6.048100	1.113501	-0.887402
18	1	0	-4.849829	1.857471	0.776268
19	1	0	-6.878347	0.151915	-2.632761
20	1	0	-6.958778	1.625626	-0.599339
21	6	0	-1.207261	-2.304998	1.338438
22	6	0	-1.275289	-3.472506	2.097464
23	6	0	-0.606621	-3.524882	3.320330
24	1	0	-1.847398	-4.322879	1.739901

25	6	0	0.153591	-1.289388	2.915486
26	6	0	0.117661	-2.408797	3.740135
27	1	0	-0.649208	-4.420373	3.931801
28	1	0	0.714531	-0.404633	3.201073
29	1	0	0.651428	-2.403426	4.683888
30	7	0	-3.762709	0.626418	-0.480497
31	7	0	-0.492776	-1.233036	1.734865
32	6	0	0.849573	-0.623533	-1.869918
33	1	0	1.728411	-1.071088	-2.347262
34	1	0	0.398318	0.042350	-2.611525
35	7	0	1.228229	0.196560	-0.682214
36	6	0	1.633006	1.578571	-1.083035
37	1	0	2.684842	1.621500	-1.380914
38	1	0	1.044684	1.865228	-1.962375
39	6	0	2.320838	-0.458784	0.154046
40	1	0	2.437421	0.178104	1.035772
41	1	0	1.913743	-1.409816	0.500875
42	6	0	3.658492	-0.672503	-0.517517
43	6	0	4.670500	0.296748	-0.424881
44	6	0	3.931296	-1.862919	-1.211020
45	6	0	5.907273	0.098649	-1.039690
46	1	0	4.502683	1.199490	0.158549
47	6	0	5.166823	-2.062865	-1.827705
48	1	0	3.186142	-2.655051	-1.245039
49	6	0	6.153822	-1.078274	-1.749415
50	1	0	6.682113	0.853740	-0.952311
51	1	0	5.364649	-2.991035	-2.354498
52	1	0	7.117663	-1.235997	-2.222703
53	6	0	1.327368	2.560366	0.021368
54	6	0	2.072417	3.713924	0.246530
55	6	0	1.664022	4.601832	1.243592
56	1	0	2.955586	3.913872	-0.351007
57	6	0	-0.177974	3.140620	1.709970
58	6	0	0.520323	4.309904	1.987692
59	1	0	2.231695	5.506593	1.436552
60	1	0	-1.073157	2.864170	2.254344
61	1	0	0.171247	4.974010	2.770291
62	7	0	0.216544	2.278305	0.748101
63	1	0	-2.893570	0.743774	0.165634
64	1	0	-1.932637	0.868515	1.099137

3''$_c$ (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1444.81723079 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.491882	1.077035	-1.072833
2	6	0	2.311577	0.303046	-2.046282
3	1	0	1.632795	-0.230156	-2.717805
4	1	0	2.908532	0.971358	-2.681647
5	6	0	2.340996	2.191009	-0.569363
6	1	0	3.252411	1.741120	-0.157808
7	1	0	2.654515	2.832261	-1.405351
8	6	0	0.231774	1.566379	-1.693237
9	1	0	-0.195494	2.317340	-1.023789
10	1	0	0.425001	2.070603	-2.652177
11	26	0	0.813468	-0.669919	0.470845
12	6	0	3.203271	-0.721460	-1.377412
13	6	0	4.479632	-1.012539	-1.853310
14	6	0	3.373959	-2.381404	0.242069
15	6	0	5.212897	-2.036563	-1.250562
16	1	0	4.890953	-0.451672	-2.686286
17	6	0	4.648813	-2.736683	-0.184513
18	1	0	2.899892	-2.894630	1.072553
19	1	0	6.208419	-2.280650	-1.607486
20	1	0	5.183030	-3.538843	0.311981
21	6	0	1.749471	3.100863	0.487770
22	6	0	1.746235	4.486998	0.358173
23	6	0	1.295609	5.286238	1.414129
24	1	0	2.105939	4.939552	-0.559301
25	6	0	0.851326	3.307458	2.678287
26	6	0	0.842896	4.691773	2.593732
27	1	0	1.300652	6.367090	1.313754
28	1	0	0.515594	2.756710	3.550399
29	1	0	0.491039	5.283876	3.430547
30	7	0	2.660029	-1.396221	-0.339367
31	7	0	1.297893	2.566509	1.646756
32	6	0	-0.777514	0.438194	-1.925384
33	1	0	-1.698079	0.863105	-2.341579
34	1	0	-0.397518	-0.259762	-2.675843
35	7	0	-1.059115	-0.338823	-0.687964
36	6	0	-1.579488	-1.696516	-1.014010
37	1	0	-2.619667	-1.656261	-1.354588
38	1	0	-0.983816	-2.091228	-1.845772
39	6	0	-1.998716	0.402366	0.254618
40	1	0	-2.031154	-0.184759	1.175960
41	1	0	-1.505872	1.347261	0.498945

42	6	0	-3.401255	0.660523	-0.250601
43	6	0	-4.433393	-0.252573	0.018181
44	6	0	-3.708888	1.831054	-0.962357
45	6	0	-5.730856	-0.016442	-0.437537
46	1	0	-4.227715	-1.141629	0.609794
47	6	0	-5.005187	2.068394	-1.420787
48	1	0	-2.938829	2.579421	-1.138343
49	6	0	-6.017035	1.141202	-1.163914
50	1	0	-6.520058	-0.727586	-0.214681
51	1	0	-5.228364	2.980573	-1.965139
52	1	0	-7.027188	1.327967	-1.513976
53	6	0	-1.440283	-2.633694	0.168176
54	6	0	-2.317422	-3.694741	0.386199
55	6	0	-2.097397	-4.543485	1.471641
56	1	0	-3.156399	-3.852176	-0.283827
57	6	0	-0.191445	-3.211355	2.043387
58	6	0	-1.016665	-4.295489	2.319540
59	1	0	-2.765360	-5.378231	1.658747
60	1	0	0.647650	-2.964870	2.687484
61	1	0	-0.819602	-4.921861	3.182258
62	7	0	-0.389010	-2.403478	0.983026
63	1	0	1.260054	1.489603	1.744200
64	1	0	1.139236	0.133907	1.919680

3''$_c$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1444.78177182 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.224292	1.106669	-1.172694
2	6	0	2.151007	0.429286	-2.140198
3	1	0	1.564285	-0.283128	-2.732028
4	1	0	2.583968	1.142755	-2.853861
5	6	0	1.949229	2.300756	-0.641850
6	1	0	2.929125	1.958389	-0.293358
7	1	0	2.130027	3.013561	-1.456836
8	6	0	-0.069986	1.515568	-1.808927
9	1	0	-0.524992	2.266673	-1.158689
10	1	0	0.103012	1.994554	-2.782117
11	26	0	0.815480	-0.605610	-0.028503
12	6	0	3.235221	-0.297129	-1.366375
13	6	0	4.544776	-0.406030	-1.821852
14	6	0	3.736362	-1.483087	0.564002
15	6	0	5.474898	-1.099732	-1.044201

16	1	0	4.833253	0.044114	-2.766260
17	6	0	5.063406	-1.638437	0.173769
18	1	0	3.386577	-1.876013	1.510570
19	1	0	6.501972	-1.204095	-1.378485
20	1	0	5.755150	-2.169188	0.818332
21	6	0	1.291250	3.054304	0.492052
22	6	0	1.245583	4.444672	0.541234
23	6	0	0.732553	5.080889	1.676004
24	1	0	1.617562	5.024923	-0.296154
25	6	0	0.310777	2.937995	2.650409
26	6	0	0.260364	4.320337	2.748768
27	1	0	0.701345	6.165067	1.719831
28	1	0	-0.041544	2.268572	3.427589
29	1	0	-0.141676	4.785704	3.641228
30	7	0	2.824502	-0.840131	-0.190539
31	7	0	0.819640	2.355731	1.548037
32	6	0	-1.015893	0.326613	-1.971006
33	1	0	-1.991021	0.675109	-2.329125
34	1	0	-0.633355	-0.355177	-2.736431
35	7	0	-1.136599	-0.441377	-0.694205
36	6	0	-1.535011	-1.860249	-0.956775
37	1	0	-2.616991	-1.959835	-1.084885
38	1	0	-1.076074	-2.173052	-1.902317
39	6	0	-2.082460	0.213626	0.300777
40	1	0	-1.987157	-0.370238	1.218922
41	1	0	-1.668429	1.203205	0.506737
42	6	0	-3.531837	0.327707	-0.114785
43	6	0	-4.453503	-0.672628	0.234041
44	6	0	-3.994285	1.448323	-0.823665
45	6	0	-5.792857	-0.572125	-0.144239
46	1	0	-4.127443	-1.522825	0.829051
47	6	0	-5.332697	1.550633	-1.204504
48	1	0	-3.312371	2.263682	-1.057330
49	6	0	-6.232348	0.536073	-0.871210
50	1	0	-6.494846	-1.350049	0.138971
51	1	0	-5.676006	2.425183	-1.748121
52	1	0	-7.274863	0.617141	-1.161800
53	6	0	-1.019899	-2.745890	0.151336
54	6	0	-1.683046	-3.896337	0.569227
55	6	0	-1.116039	-4.681019	1.573707
56	1	0	-2.628169	-4.171077	0.112480
57	6	0	0.690804	-3.109177	1.675859
58	6	0	0.091321	-4.274129	2.140710
59	1	0	-1.612529	-5.583960	1.913921

60	1	0	1.615187	-2.750437	2.110312
61	1	0	0.562406	-4.842278	2.934916
62	7	0	0.163971	-2.357746	0.688965
63	1	0	0.815377	1.271313	1.461798
64	1	0	0.728955	-0.029644	1.383438

3''$_c$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1444.79461573 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.317158	1.163015	-1.048643
2	6	0	2.215816	0.536999	-2.083979
3	1	0	1.583375	0.010844	-2.803791
4	1	0	2.750694	1.309557	-2.648618
5	6	0	2.053412	2.363509	-0.530415
6	1	0	2.997431	1.997085	-0.113363
7	1	0	2.304380	3.022698	-1.370893
8	6	0	0.019753	1.558533	-1.694227
9	1	0	-0.483896	2.254632	-1.019532
10	1	0	0.199878	2.094457	-2.636167
11	26	0	0.821328	-0.447470	0.290637
12	6	0	3.167569	-0.464089	-1.481767
13	6	0	4.465131	-0.656928	-1.945846
14	6	0	3.373353	-2.214340	0.027611
15	6	0	5.231673	-1.684365	-1.390151
16	1	0	4.867654	-0.024431	-2.730333
17	6	0	4.674688	-2.479697	-0.389663
18	1	0	2.903345	-2.802139	0.808698
19	1	0	6.246045	-1.858542	-1.734490
20	1	0	5.234731	-3.289135	0.064926
21	6	0	1.366314	3.224667	0.509829
22	6	0	1.200040	4.597565	0.350230
23	6	0	0.665908	5.358172	1.396182
24	1	0	1.498635	5.071695	-0.578386
25	6	0	0.469024	3.364107	2.701291
26	6	0	0.296033	4.736992	2.590685
27	1	0	0.542716	6.430010	1.276688
28	1	0	0.207073	2.797571	3.588535
29	1	0	-0.116196	5.300290	3.419892
30	7	0	2.630572	-1.226414	-0.504525
31	7	0	0.992315	2.663039	1.680506
32	6	0	-0.872381	0.339409	-1.944762

33	1	0	-1.834952	0.664016	-2.355221
34	1	0	-0.425257	-0.324426	-2.689090
35	7	0	-1.040381	-0.429235	-0.682999
36	6	0	-1.292764	-1.885470	-0.885512
37	1	0	-2.329798	-2.086416	-1.174258
38	1	0	-0.653548	-2.226870	-1.708430
39	6	0	-2.090052	0.190336	0.232550
40	1	0	-2.037733	-0.361162	1.174111
41	1	0	-1.754588	1.209365	0.442024
42	6	0	-3.507205	0.204637	-0.294729
43	6	0	-4.379047	-0.863189	-0.027375
44	6	0	-3.990879	1.299759	-1.028420
45	6	0	-5.688335	-0.851642	-0.509292
46	1	0	-4.042433	-1.695757	0.586114
47	6	0	-5.299674	1.313043	-1.511871
48	1	0	-3.352470	2.164023	-1.200253
49	6	0	-6.147916	0.233264	-1.258765
50	1	0	-6.353341	-1.680528	-0.288235
51	1	0	-5.661113	2.169315	-2.072472
52	1	0	-7.168110	0.245176	-1.628732
53	6	0	-0.925682	-2.633169	0.381884
54	6	0	-1.551362	-3.811610	0.778469
55	6	0	-1.137311	-4.439901	1.954456
56	1	0	-2.351420	-4.228442	0.175459
57	6	0	0.455864	-2.674738	2.264372
58	6	0	-0.121121	-3.857768	2.713148
59	1	0	-1.610559	-5.360941	2.279258
60	1	0	1.234563	-2.168250	2.824049
61	1	0	0.216313	-4.303807	3.641960
62	7	0	0.076440	-2.081308	1.114315
63	1	0	1.088784	1.569350	1.746715
64	1	0	1.207428	0.286790	1.713093

3''$_{dp\text{-}A}$ (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1444.50966923 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.870635	-0.829247	1.427049
2	6	0	1.958528	-0.041074	2.030537
3	1	0	1.605248	0.989186	2.150585
4	1	0	2.230317	-0.405490	3.033703
5	6	0	1.199462	-2.269372	1.410745

6	1	0	2.286339	-2.369425	1.321564
7	1	0	0.918232	-2.757662	2.355293
8	6	0	-0.452341	-0.585063	2.043091
9	1	0	-1.062107	-1.473306	1.858739
10	1	0	-0.373039	-0.483529	3.136409
11	26	0	0.804279	-0.021638	-0.877168
12	6	0	3.181970	-0.041845	1.129529
13	6	0	4.480204	-0.002839	1.639283
14	6	0	3.979308	-0.065569	-1.049959
15	6	0	5.556624	0.011924	0.751670
16	1	0	4.642347	0.009819	2.712562
17	6	0	5.303224	-0.024179	-0.619643
18	1	0	3.722992	-0.091689	-2.105537
19	1	0	6.575278	0.041446	1.125577
20	1	0	6.110082	-0.023942	-1.344164
21	6	0	0.578093	-2.991858	0.232402
22	6	0	0.221153	-4.338990	0.299729
23	6	0	-0.241707	-4.973159	-0.853721
24	1	0	0.311725	-4.881349	1.235940
25	6	0	0.021498	-2.893369	-2.013595
26	6	0	-0.335928	-4.239776	-2.035746
27	1	0	-0.523073	-6.021344	-0.827847
28	1	0	-0.040019	-2.263707	-2.896845
29	1	0	-0.685219	-4.694153	-2.956457
30	7	0	2.940850	-0.070022	-0.196564
31	7	0	0.464127	-2.280353	-0.903485
32	6	0	-1.156447	0.647182	1.472749
33	1	0	-2.133716	0.760032	1.961942
34	1	0	-0.579932	1.544156	1.712886
35	7	0	-1.292816	0.583374	-0.001360
36	6	0	-1.542392	1.922667	-0.568814
37	1	0	-1.762828	1.785358	-1.634475
38	1	0	-2.420485	2.405179	-0.118380
39	6	0	-2.337557	-0.391616	-0.462435
40	1	0	-2.242009	-0.437112	-1.551296
41	1	0	-2.049823	-1.374070	-0.083225
42	6	0	-3.772704	-0.088228	-0.072688
43	6	0	-4.597370	0.678821	-0.909217
44	6	0	-4.314911	-0.587150	1.121617
45	6	0	-5.916645	0.959764	-0.552242
46	1	0	-4.211396	1.043085	-1.858121
47	6	0	-5.633417	-0.307067	1.483653
48	1	0	-3.708907	-1.219917	1.766359
49	6	0	-6.435901	0.471999	0.648596

50	1	0	-6.541765	1.549072	-1.216347
51	1	0	-6.036450	-0.705938	2.409743
52	1	0	-7.463795	0.685860	0.924927
53	6	0	-0.343275	2.840384	-0.466412
54	6	0	-0.505728	4.228122	-0.468120
55	6	0	0.622577	5.044150	-0.470279
56	1	0	-1.503546	4.655292	-0.473872
57	6	0	1.957952	3.059069	-0.442324
58	6	0	1.883867	4.447615	-0.460886
59	1	0	0.520061	6.124822	-0.477684
60	1	0	2.917889	2.553475	-0.433017
61	1	0	2.791177	5.041620	-0.464307
62	7	0	0.872871	2.264593	-0.442720
63	1	0	0.656671	0.075166	-2.543846

3''$_{dp\text{-}A}$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1444.49703534 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.860407	-0.657397	1.567893
2	6	0	2.021357	0.103223	2.075433
3	1	0	1.718132	1.149516	2.188728
4	1	0	2.363995	-0.250238	3.060258
5	6	0	1.153084	-2.115227	1.550311
6	1	0	2.238780	-2.251159	1.581243
7	1	0	0.754978	-2.614835	2.442793
8	6	0	-0.451964	-0.375792	2.208997
9	1	0	-1.023652	-1.307511	2.194324
10	1	0	-0.333820	-0.097998	3.265596
11	26	0	0.758282	0.027401	-0.459813
12	6	0	3.144067	-0.002975	1.053763
13	6	0	4.491066	0.005333	1.404917
14	6	0	3.675171	-0.200427	-1.204079
15	6	0	5.457135	-0.082014	0.399506
16	1	0	4.778592	0.076991	2.449191
17	6	0	5.040688	-0.190270	-0.926152
18	1	0	3.291204	-0.272605	-2.215378
19	1	0	6.512913	-0.073437	0.650726
20	1	0	5.755829	-0.266619	-1.737821
21	6	0	0.643140	-2.762911	0.284208
22	6	0	0.395240	-4.131801	0.196591
23	6	0	0.030107	-4.678054	-1.033020

24	1	0	0.494805	-4.757466	1.078206
25	6	0	0.174926	-2.471847	-1.967721
26	6	0	-0.072272	-3.830527	-2.135972
27	1	0	-0.166827	-5.741152	-1.127330
28	1	0	0.103537	-1.765130	-2.785477
29	1	0	-0.344816	-4.208887	-3.115055
30	7	0	2.741309	-0.102864	-0.240446
31	7	0	0.518173	-1.934841	-0.777951
32	6	0	-1.231733	0.712210	1.472247
33	1	0	-2.243960	0.786536	1.889372
34	1	0	-0.751525	1.678829	1.634729
35	7	0	-1.270930	0.467747	-0.003367
36	6	0	-1.523895	1.741969	-0.718295
37	1	0	-1.626694	1.495678	-1.781028
38	1	0	-2.452196	2.225351	-0.387643
39	6	0	-2.288805	-0.568550	-0.393127
40	1	0	-2.147062	-0.729701	-1.464444
41	1	0	-2.005390	-1.496783	0.107410
42	6	0	-3.741508	-0.249024	-0.095607
43	6	0	-4.533979	0.434678	-1.030202
44	6	0	-4.335020	-0.658634	1.108154
45	6	0	-5.871560	0.724196	-0.758708
46	1	0	-4.107265	0.727106	-1.986431
47	6	0	-5.672400	-0.370440	1.384356
48	1	0	-3.752623	-1.228084	1.829405
49	6	0	-6.442238	0.327121	0.452233
50	1	0	-6.470674	1.249270	-1.496549
51	1	0	-6.114821	-0.699638	2.319747
52	1	0	-7.484335	0.547794	0.661909
53	6	0	-0.352564	2.670225	-0.558003
54	6	0	-0.489472	4.052223	-0.666065
55	6	0	0.641577	4.861342	-0.583531
56	1	0	-1.474353	4.481495	-0.820010
57	6	0	1.929875	2.863189	-0.265686
58	6	0	1.876184	4.247921	-0.379776
59	1	0	0.560385	5.939716	-0.672913
60	1	0	2.878893	2.365891	-0.112690
61	1	0	2.790476	4.826597	-0.305947
62	7	0	0.843324	2.067411	-0.353840
63	1	0	0.698927	0.286836	-1.984430

3''$_{dp\text{-}A}$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1444.49542330 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.867058	-0.708373	1.395093
2	6	0	1.905132	0.095258	2.075014
3	1	0	1.529302	1.120696	2.163690
4	1	0	2.095538	-0.268384	3.096864
5	6	0	1.256802	-2.139284	1.344738
6	1	0	2.348385	-2.197428	1.298061
7	1	0	0.952259	-2.673956	2.255100
8	6	0	-0.467587	-0.553756	2.031997
9	1	0	-1.021699	-1.478804	1.853789
10	1	0	-0.370409	-0.452583	3.122853
11	26	0	0.791909	-0.050860	-0.776860
12	6	0	3.194995	0.095192	1.275514
13	6	0	4.447070	0.187153	1.885762
14	6	0	4.157077	-0.033266	-0.824454
15	6	0	5.589172	0.175574	1.084564
16	1	0	4.525142	0.259393	2.966246
17	6	0	5.444365	0.055618	-0.297699
18	1	0	3.988273	-0.122447	-1.894518
19	1	0	6.574832	0.247170	1.533712
20	1	0	6.305974	0.028966	-0.955890
21	6	0	0.712969	-2.821384	0.112341
22	6	0	0.433766	-4.185279	0.085536
23	6	0	0.033913	-4.777997	-1.112916
24	1	0	0.536256	-4.774225	0.991454
25	6	0	0.205637	-2.620414	-2.146559
26	6	0	-0.074507	-3.979975	-2.249653
27	1	0	-0.185616	-5.840053	-1.155113
28	1	0	0.131923	-1.953187	-2.996088
29	1	0	-0.374818	-4.394454	-3.205565
30	7	0	3.054626	-0.005356	-0.058707
31	7	0	0.586243	-2.040010	-0.988004
32	6	0	-1.256577	0.625818	1.467766
33	1	0	-2.215536	0.707671	1.999465
34	1	0	-0.713219	1.556400	1.655344
35	7	0	-1.435932	0.491874	0.010565
36	6	0	-1.656616	1.786747	-0.644450
37	1	0	-1.887753	1.579871	-1.697091
38	1	0	-2.512685	2.337141	-0.228397
39	6	0	-2.469293	-0.510488	-0.384934
40	1	0	-2.397205	-0.606956	-1.472739
41	1	0	-2.168640	-1.474426	0.034098

42	6	0	-3.900791	-0.202600	0.017287
43	6	0	-4.737524	0.548139	-0.821968
44	6	0	-4.421939	-0.669540	1.233359
45	6	0	-6.048757	0.843362	-0.447447
46	1	0	-4.367420	0.889065	-1.785817
47	6	0	-5.732613	-0.375425	1.612784
48	1	0	-3.805001	-1.287601	1.882175
49	6	0	-6.547547	0.386572	0.774129
50	1	0	-6.683799	1.419752	-1.113532
51	1	0	-6.119724	-0.749608	2.555845
52	1	0	-7.569246	0.611613	1.064259
53	6	0	-0.423600	2.656076	-0.614318
54	6	0	-0.538502	4.046982	-0.600463
55	6	0	0.605534	4.835023	-0.686677
56	1	0	-1.523164	4.498056	-0.531022
57	6	0	1.876860	2.805700	-0.769124
58	6	0	1.840012	4.195028	-0.780148
59	1	0	0.534851	5.918005	-0.683700
60	1	0	2.818865	2.280227	-0.845422
61	1	0	2.765163	4.755222	-0.860209
62	7	0	0.775127	2.031532	-0.680286
63	1	0	0.724966	0.186550	-2.320002

3''$_{dp\text{-}B}$ (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1444.50261938 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.492456	1.590279	-1.132625
2	6	0	2.767332	1.191249	-1.764326
3	1	0	2.787278	1.457352	-2.831364
4	1	0	3.568995	1.762587	-1.282762
5	6	0	1.526591	3.002658	-0.690628
6	1	0	2.507677	3.183688	-0.237021
7	1	0	1.425691	3.699681	-1.535734
8	6	0	0.313842	1.335000	-2.005797
9	1	0	-0.472024	2.030799	-1.702607
10	1	0	0.557817	1.571766	-3.052138
11	26	0	1.336019	0.390183	0.855036
12	6	0	3.122143	-0.274376	-1.589041
13	6	0	4.011360	-0.900634	-2.465671
14	6	0	3.039750	-2.154623	-0.244391
15	6	0	4.426832	-2.202485	-2.193883

16	1	0	4.378050	-0.369870	-3.338859
17	6	0	3.939593	-2.841280	-1.052943
18	1	0	2.628195	-2.610451	0.651297
19	1	0	5.121406	-2.707376	-2.857894
20	1	0	4.243557	-3.849917	-0.795677
21	6	0	0.479567	3.308854	0.364731
22	6	0	-0.025381	4.600523	0.526175
23	6	0	-0.892977	4.860608	1.585594
24	1	0	0.266061	5.388089	-0.161742
25	6	0	-0.706033	2.555963	2.203250
26	6	0	-1.236566	3.818755	2.447430
27	1	0	-1.293101	5.858427	1.735497
28	1	0	-0.950917	1.712185	2.841749
29	1	0	-1.905093	3.975754	3.286689
30	7	0	2.629261	-0.901349	-0.506776
31	7	0	0.130402	2.299679	1.183780
32	6	0	-0.219215	-0.098908	-1.925498
33	1	0	-1.044886	-0.205598	-2.642711
34	1	0	0.557067	-0.800191	-2.238635
35	7	0	-0.623170	-0.444560	-0.550188
36	6	0	-0.586050	-1.889621	-0.276291
37	1	0	-1.465015	-2.419144	-0.666601
38	1	0	0.288084	-2.304020	-0.789290
39	6	0	-1.934887	0.156780	-0.145920
40	1	0	-2.045299	-0.035841	0.925042
41	1	0	-1.843484	1.238297	-0.255510
42	6	0	-3.168200	-0.329731	-0.884944
43	6	0	-3.923907	-1.405062	-0.393123
44	6	0	-3.598074	0.301522	-2.062434
45	6	0	-5.057487	-1.855122	-1.071637
46	1	0	-3.635449	-1.879080	0.542225
47	6	0	-4.729736	-0.146286	-2.745308
48	1	0	-3.058782	1.168461	-2.437238
49	6	0	-5.458870	-1.230532	-2.253841
50	1	0	-5.633133	-2.684677	-0.671987
51	1	0	-5.049042	0.358492	-3.652152
52	1	0	-6.342932	-1.576577	-2.780414
53	6	0	-0.432737	-2.162466	1.208241
54	6	0	-1.045001	-3.251900	1.829016
55	6	0	-0.810206	-3.484575	3.184734
56	1	0	-1.692858	-3.906438	1.254370
57	6	0	0.603173	-1.550665	3.195109
58	6	0	0.030758	-2.618231	3.882176
59	1	0	-1.277684	-4.326228	3.686383

60	1	0	1.275121	-0.847911	3.679944
61	1	0	0.242336	-2.760820	4.936186
62	7	0	0.375955	-1.324041	1.888727
63	1	0	2.477860	0.781265	2.014917

3''$_{dp\text{-}B}$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1444.49929713 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.320571	1.474396	-1.411675
2	6	0	2.619386	1.086154	-2.013026
3	1	0	2.635305	1.252367	-3.099057
4	1	0	3.387845	1.726943	-1.568931
5	6	0	1.270501	2.914711	-1.051640
6	1	0	2.271300	3.199619	-0.713648
7	1	0	1.009877	3.550330	-1.909333
8	6	0	0.151883	1.083481	-2.267026
9	1	0	-0.652480	1.794269	-2.061567
10	1	0	0.401099	1.186472	-3.331672
11	26	0	1.151933	0.450415	0.346382
12	6	0	2.990892	-0.335765	-1.670500
13	6	0	3.925310	-1.048517	-2.418340
14	6	0	2.880489	-2.024062	-0.094821
15	6	0	4.353777	-2.296126	-1.967839
16	1	0	4.321212	-0.619579	-3.333561
17	6	0	3.827034	-2.784160	-0.772925
18	1	0	2.453854	-2.374191	0.837467
19	1	0	5.085648	-2.866545	-2.530277
20	1	0	4.137035	-3.740886	-0.367104
21	6	0	0.325652	3.139216	0.105208
22	6	0	-0.283840	4.370048	0.336411
23	6	0	-1.037779	4.552662	1.495488
24	1	0	-0.155895	5.176763	-0.378515
25	6	0	-0.543024	2.277915	2.071634
26	6	0	-1.159672	3.485159	2.383537
27	1	0	-1.514671	5.505635	1.700104
28	1	0	-0.625258	1.423019	2.733196
29	1	0	-1.728562	3.576560	3.302332
30	7	0	2.446611	-0.822168	-0.528765
31	7	0	0.185833	2.090141	0.954010
32	6	0	-0.339640	-0.340183	-1.977031
33	1	0	-1.211036	-0.559755	-2.607180
34	1	0	0.433305	-1.065754	-2.236495

35	7	0	-0.636691	-0.474569	-0.531803
36	6	0	-0.532649	-1.848269	0.008059
37	1	0	-1.449367	-2.431804	-0.136248
38	1	0	0.262153	-2.365067	-0.538359
39	6	0	-1.952633	0.146652	-0.146364
40	1	0	-1.993989	0.119054	0.945193
41	1	0	-1.911204	1.200097	-0.427170
42	6	0	-3.201809	-0.490840	-0.723041
43	6	0	-3.885079	-1.495337	-0.019989
44	6	0	-3.726520	-0.066600	-1.953806
45	6	0	-5.036839	-2.082784	-0.545281
46	1	0	-3.526696	-1.803342	0.959607
47	6	0	-4.877448	-0.651836	-2.483251
48	1	0	-3.247589	0.746626	-2.494328
49	6	0	-5.531118	-1.667081	-1.782769
50	1	0	-5.554131	-2.854950	0.016186
51	1	0	-5.270204	-0.306982	-3.434993
52	1	0	-6.429314	-2.119898	-2.191098
53	6	0	-0.155736	-1.795263	1.477710
54	6	0	-0.589178	-2.746321	2.399159
55	6	0	-0.138372	-2.677418	3.718722
56	1	0	-1.267560	-3.532191	2.082103
57	6	0	1.124192	-0.730698	3.105832
58	6	0	0.735885	-1.651361	4.075609
59	1	0	-0.463369	-3.410042	4.450518
60	1	0	1.809417	0.081574	3.322294
61	1	0	1.116759	-1.560194	5.086970
62	7	0	0.689361	-0.790096	1.830730
63	1	0	2.404461	1.076859	0.991851

3''$_{dp\text{-}B}$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1444.48775308 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.423577	1.730576	-1.164075
2	6	0	2.687581	1.365619	-1.816044
3	1	0	2.672101	1.591624	-2.893235
4	1	0	3.483072	1.981073	-1.381854
5	6	0	1.439408	3.069576	-0.552800
6	1	0	2.444260	3.237664	-0.151068
7	1	0	1.242400	3.869977	-1.282629
8	6	0	0.230723	1.506084	-2.010704
9	1	0	-0.560403	2.172121	-1.655633

10	1	0	0.430117	1.786837	-3.056684
11	26	0	1.149734	0.309331	0.681492
12	6	0	3.099866	-0.081702	-1.604196
13	6	0	4.036749	-0.675038	-2.453530
14	6	0	3.069562	-1.955972	-0.251993
15	6	0	4.503239	-1.955842	-2.169941
16	1	0	4.399354	-0.129293	-3.319451
17	6	0	4.014689	-2.606583	-1.036522
18	1	0	2.663180	-2.423435	0.638288
19	1	0	5.234372	-2.432853	-2.814841
20	1	0	4.354406	-3.599514	-0.762937
21	6	0	0.471870	3.186621	0.609770
22	6	0	-0.096552	4.413020	0.955915
23	6	0	-0.891737	4.503391	2.096851
24	1	0	0.092025	5.285620	0.338224
25	6	0	-0.510989	2.165060	2.444577
26	6	0	-1.098621	3.354253	2.860226
27	1	0	-1.338195	5.449869	2.384302
28	1	0	-0.645410	1.247685	3.009436
29	1	0	-1.704429	3.372947	3.759438
30	7	0	2.605459	-0.720837	-0.526503
31	7	0	0.252748	2.070786	1.338799
32	6	0	-0.256815	0.055309	-1.971127
33	1	0	-1.114116	-0.060582	-2.646680
34	1	0	0.531282	-0.603117	-2.343893
35	7	0	-0.584137	-0.369649	-0.587013
36	6	0	-0.556606	-1.846322	-0.442601
37	1	0	-1.448427	-2.321617	-0.867919
38	1	0	0.306655	-2.214380	-1.006514
39	6	0	-1.898032	0.188037	-0.103269
40	1	0	-1.979658	-0.099268	0.948430
41	1	0	-1.810125	1.274984	-0.121853
42	6	0	-3.147937	-0.238209	-0.849914
43	6	0	-3.888780	-1.355543	-0.434637
44	6	0	-3.614654	0.498078	-1.949745
45	6	0	-5.043670	-1.743657	-1.115283
46	1	0	-3.571847	-1.912529	0.444001
47	6	0	-4.768239	0.113051	-2.633970
48	1	0	-3.085239	1.395298	-2.261948
49	6	0	-5.482101	-1.013415	-2.221347
50	1	0	-5.606992	-2.607571	-0.775430
51	1	0	-5.115734	0.698188	-3.480046
52	1	0	-6.382773	-1.311530	-2.749045
53	6	0	-0.378075	-2.245685	1.007872

54	6	0	-1.004468	-3.359221	1.566679
55	6	0	-0.746359	-3.686130	2.899283
56	1	0	-1.681524	-3.958949	0.966618
57	6	0	0.725951	-1.797981	3.002548
58	6	0	0.132626	-2.889789	3.632556
59	1	0	-1.224768	-4.547125	3.355546
60	1	0	1.433001	-1.154872	3.517713
61	1	0	0.362512	-3.108708	4.669571
62	7	0	0.476724	-1.477875	1.719961
63	1	0	2.335425	0.645763	1.601197

3''$_{dp\text{-}C}$ (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1444.49924549 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.238482	-1.789995	0.490355
2	6	0	2.003277	-1.484602	1.717082
3	1	0	1.697171	-2.143381	2.541642
4	1	0	3.060249	-1.706508	1.532399
5	6	0	2.047379	-2.565115	-0.475990
6	1	0	2.418001	-3.507007	-0.044739
7	1	0	1.393934	-2.815610	-1.319728
8	6	0	-0.071303	-2.417394	0.777416
9	1	0	-0.420432	-2.887642	-0.144471
10	1	0	0.024898	-3.215031	1.530187
11	26	0	0.725827	0.089700	-0.766969
12	6	0	1.930711	-0.038248	2.173333
13	6	0	2.367542	0.305416	3.457630
14	6	0	1.530911	2.180193	1.665888
15	6	0	2.388611	1.644417	3.833925
16	1	0	2.690878	-0.470644	4.144912
17	6	0	1.967771	2.607100	2.914413
18	1	0	1.180873	2.889887	0.923667
19	1	0	2.727290	1.932780	4.824179
20	1	0	1.971841	3.663727	3.158418
21	6	0	3.205154	-1.743868	-1.011268
22	6	0	4.402706	-2.341257	-1.407467
23	6	0	5.403970	-1.545792	-1.962994
24	1	0	4.543782	-3.410758	-1.285903
25	6	0	3.964593	0.342112	-1.658571
26	6	0	5.182477	-0.175040	-2.092039
27	1	0	6.341695	-1.988132	-2.284389
28	1	0	3.749781	1.404176	-1.737994

29	1	0	5.934710	0.482210	-2.514246
30	7	0	1.505410	0.885458	1.295281
31	7	0	2.993968	-0.419371	-1.131566
32	6	0	-1.103552	-1.391923	1.259300
33	1	0	-2.023400	-1.913864	1.553287
34	1	0	-0.729606	-0.889326	2.156469
35	7	0	-1.357578	-0.362595	0.227403
36	6	0	-1.840476	0.912907	0.792150
37	1	0	-2.898273	0.870561	1.081771
38	1	0	-1.265754	1.113744	1.703132
39	6	0	-2.244206	-0.851598	-0.888595
40	1	0	-2.241421	-0.068657	-1.650330
41	1	0	-1.739760	-1.704172	-1.346614
42	6	0	-3.665333	-1.215388	-0.506122
43	6	0	-4.691897	-0.260011	-0.565224
44	6	0	-3.995105	-2.521624	-0.112347
45	6	0	-6.001086	-0.590228	-0.212348
46	1	0	-4.468454	0.744696	-0.916084
47	6	0	-5.302835	-2.856122	0.242166
48	1	0	-3.228099	-3.292699	-0.107778
49	6	0	-6.307918	-1.888376	0.199307
50	1	0	-6.783123	0.160950	-0.271417
51	1	0	-5.539088	-3.873771	0.538333
52	1	0	-7.326874	-2.148437	0.469054
53	6	0	-1.615732	2.054343	-0.182199
54	6	0	-2.530010	3.100323	-0.319845
55	6	0	-2.257187	4.129038	-1.221049
56	1	0	-3.442973	3.101081	0.267169
57	6	0	-0.224210	2.996683	-1.780334
58	6	0	-1.083242	4.075079	-1.971929
59	1	0	-2.955678	4.950813	-1.344486
60	1	0	0.692501	2.899509	-2.354815
61	1	0	-0.838026	4.844082	-2.696074
62	7	0	-0.472417	2.014787	-0.897128
63	1	0	0.480768	-0.418930	-2.340528

3''$_{dp\text{-}C}$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1444.49385030 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.056627	-1.987077	-0.029074
2	6	0	1.903843	-2.133206	1.190157

3	1	0	1.600243	-3.014115	1.769791
4	1	0	2.935081	-2.319858	0.872355
5	6	0	1.805300	-2.416620	-1.240045
6	1	0	2.266640	-3.407747	-1.121073
7	1	0	1.091090	-2.455033	-2.066710
8	6	0	-0.281977	-2.615376	0.147660
9	1	0	-0.683825	-2.823902	-0.845272
10	1	0	-0.208609	-3.573498	0.681120
11	26	0	0.654176	-0.021174	-0.425949
12	6	0	1.917205	-0.901169	2.066349
13	6	0	2.487137	-0.933636	3.340410
14	6	0	1.520077	1.368101	2.243047
15	6	0	2.573401	0.244301	4.078147
16	1	0	2.863824	-1.869942	3.740838
17	6	0	2.086936	1.422878	3.511023
18	1	0	1.122807	2.260956	1.772171
19	1	0	3.013937	0.243749	5.069964
20	1	0	2.139160	2.368535	4.039357
21	6	0	2.852087	-1.366018	-1.544608
22	6	0	4.065312	-1.667730	-2.156141
23	6	0	4.970290	-0.640112	-2.425992
24	1	0	4.295151	-2.695630	-2.418491
25	6	0	3.412530	0.878979	-1.419434
26	6	0	4.638063	0.657181	-2.041918
27	1	0	5.917435	-0.852115	-2.911240
28	1	0	3.128314	1.871529	-1.087150
29	1	0	5.314426	1.487930	-2.210879
30	7	0	1.419876	0.230002	1.525028
31	7	0	2.517163	-0.098100	-1.188955
32	6	0	-1.214266	-1.659364	0.906194
33	1	0	-2.192305	-2.129525	1.062344
34	1	0	-0.802332	-1.439083	1.894982
35	7	0	-1.317041	-0.383910	0.151132
36	6	0	-1.639707	0.812229	0.964993
37	1	0	-2.708297	0.895738	1.194526
38	1	0	-1.107338	0.729547	1.917159
39	6	0	-2.273952	-0.497751	-1.019636
40	1	0	-2.148406	0.416424	-1.600861
41	1	0	-1.902364	-1.303230	-1.651561
42	6	0	-3.733463	-0.718605	-0.673976
43	6	0	-4.608419	0.368264	-0.518560
44	6	0	-4.257434	-2.014816	-0.547340
45	6	0	-5.954982	0.168761	-0.211422
46	1	0	-4.236747	1.379744	-0.664967

47	6	0	-5.603158	-2.219440	-0.239511
48	1	0	-3.614065	-2.874947	-0.717950
49	6	0	-6.453713	-1.126714	-0.063538
50	1	0	-6.616805	1.022582	-0.100784
51	1	0	-5.989743	-3.230289	-0.150846
52	1	0	-7.502141	-1.284135	0.170315
53	6	0	-1.159980	2.034670	0.204460
54	6	0	-1.819010	3.261030	0.258434
55	6	0	-1.332760	4.335273	-0.487409
56	1	0	-2.707935	3.365282	0.872661
57	6	0	0.393316	2.880680	-1.298593
58	6	0	-0.210085	4.134507	-1.289282
59	1	0	-1.831110	5.298816	-0.458141
60	1	0	1.248298	2.675488	-1.932378
61	1	0	0.190919	4.928764	-1.909383
62	7	0	-0.045357	1.847363	-0.553684
63	1	0	0.201697	-0.317252	-1.867158

3''$_{dp\text{-}C}$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1444.48944592 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.137903	-1.900571	0.410455
2	6	0	1.932262	-1.714137	1.643046
3	1	0	1.604847	-2.408522	2.429180
4	1	0	2.975545	-1.974343	1.429546
5	6	0	1.903651	-2.609330	-0.633158
6	1	0	2.318154	-3.564533	-0.276272
7	1	0	1.212770	-2.829642	-1.453534
8	6	0	-0.191336	-2.493240	0.669741
9	1	0	-0.560452	-2.904777	-0.271895
10	1	0	-0.123709	-3.329594	1.382446
11	26	0	0.820441	0.152312	-0.558809
12	6	0	1.929720	-0.297010	2.184555
13	6	0	2.381546	-0.045237	3.482334
14	6	0	1.631613	1.965936	1.805861
15	6	0	2.463824	1.267123	3.939071
16	1	0	2.669624	-0.874701	4.121051
17	6	0	2.087103	2.296753	3.076101
18	1	0	1.315762	2.735640	1.110267
19	1	0	2.814399	1.481590	4.943569
20	1	0	2.137240	3.336954	3.378594

21	6	0	3.013077	-1.732358	-1.176276
22	6	0	4.212734	-2.264294	-1.647582
23	6	0	5.172218	-1.410750	-2.190230
24	1	0	4.386565	-3.334314	-1.591097
25	6	0	3.689845	0.412778	-1.729663
26	6	0	4.905227	-0.042699	-2.229957
27	1	0	6.110120	-1.804889	-2.568071
28	1	0	3.446197	1.470978	-1.740138
29	1	0	5.621769	0.662736	-2.635956
30	7	0	1.543151	0.695945	1.354910
31	7	0	2.756195	-0.407631	-1.215342
32	6	0	-1.181301	-1.451525	1.201060
33	1	0	-2.123904	-1.948572	1.467080
34	1	0	-0.789464	-1.011754	2.123559
35	7	0	-1.374455	-0.369110	0.219624
36	6	0	-1.774720	0.911012	0.823636
37	1	0	-2.839730	0.948070	1.088731
38	1	0	-1.207833	1.034891	1.753093
39	6	0	-2.270893	-0.753987	-0.921425
40	1	0	-2.209585	0.058880	-1.648225
41	1	0	-1.815569	-1.618095	-1.407825
42	6	0	-3.718059	-1.045711	-0.571656
43	6	0	-4.684518	-0.028398	-0.602652
44	6	0	-4.131811	-2.343314	-0.232419
45	6	0	-6.015489	-0.291191	-0.274995
46	1	0	-4.396428	0.973772	-0.911485
47	6	0	-5.461310	-2.611002	0.097043
48	1	0	-3.413250	-3.159648	-0.250878
49	6	0	-6.405409	-1.582871	0.083138
50	1	0	-6.749715	0.508199	-0.311531
51	1	0	-5.762048	-3.622973	0.351492
52	1	0	-7.441219	-1.790327	0.333716
53	6	0	-1.434491	2.059087	-0.106604
54	6	0	-2.257563	3.178243	-0.237366
55	6	0	-1.883402	4.209516	-1.097523
56	1	0	-3.182512	3.230963	0.328181
57	6	0	0.070820	2.935493	-1.638536
58	6	0	-0.695588	4.082016	-1.817651
59	1	0	-2.511479	5.087067	-1.213157
60	1	0	0.992176	2.788512	-2.193869
61	1	0	-0.368868	4.848006	-2.512240
62	7	0	-0.276145	1.945283	-0.793823
63	1	0	0.326074	-0.302519	-1.943433

TS''$_A$ (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1444.81170512 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.766377	-1.078557	-1.235047
2	6	0	-2.540503	-0.289476	-2.221227
3	1	0	-1.843018	0.149626	-2.941864
4	1	0	-3.222500	-0.924422	-2.800907
5	6	0	-2.614343	-2.110056	-0.587115
6	1	0	-3.640512	-1.725348	-0.557539
7	1	0	-2.641321	-3.033399	-1.180044
8	6	0	-0.505087	-1.643857	-1.782955
9	1	0	-0.178641	-2.434142	-1.102054
10	1	0	-0.670997	-2.116202	-2.761154
11	26	0	-1.059630	0.314926	0.352718
12	6	0	-3.303766	0.837689	-1.548473
13	6	0	-4.473970	1.362155	-2.091794
14	6	0	-3.360124	2.391194	0.190497
15	6	0	-5.089259	2.446123	-1.463891
16	1	0	-4.895963	0.930512	-2.993713
17	6	0	-4.521954	2.972292	-0.302264
18	1	0	-2.886180	2.755071	1.096790
19	1	0	-6.001094	2.869364	-1.873267
20	1	0	-4.971911	3.810510	0.217567
21	6	0	-2.190463	-2.402023	0.839441
22	6	0	-2.475189	-3.620696	1.451875
23	6	0	-2.162482	-3.792350	2.800937
24	1	0	-2.941643	-4.419171	0.883812
25	6	0	-1.301936	-1.558387	2.821670
26	6	0	-1.569355	-2.740439	3.501271
27	1	0	-2.379819	-4.732798	3.297374
28	1	0	-0.837932	-0.712324	3.318740
29	1	0	-1.315830	-2.831940	4.551378
30	7	0	-2.757891	1.347240	-0.418833
31	7	0	-1.600463	-1.390142	1.515876
32	6	0	0.579141	-0.575941	-1.926818
33	1	0	1.476403	-1.027892	-2.363023
34	1	0	0.244373	0.197001	-2.624101
35	7	0	0.927161	0.112401	-0.635009
36	6	0	1.632544	1.384736	-1.015204
37	1	0	2.468067	1.140529	-1.680991
38	1	0	0.919619	1.975391	-1.603534

39	6	0	1.793424	-0.776913	0.258768
40	1	0	1.992253	-0.192439	1.159807
41	1	0	1.160311	-1.616563	0.557445
42	6	0	3.086897	-1.298211	-0.331216
43	6	0	4.288918	-0.591630	-0.171462
44	6	0	3.119413	-2.532515	-1.001227
45	6	0	5.483289	-1.088691	-0.694242
46	1	0	4.299807	0.338021	0.390034
47	6	0	4.311869	-3.030790	-1.526297
48	1	0	2.213154	-3.127681	-1.090435
49	6	0	5.495777	-2.305407	-1.378900
50	1	0	6.406471	-0.535393	-0.553125
51	1	0	4.320097	-3.989564	-2.034938
52	1	0	6.426041	-2.695269	-1.779415
53	6	0	2.169319	2.272146	0.093637
54	6	0	3.372841	2.957818	-0.086052
55	6	0	3.805342	3.856044	0.891642
56	1	0	3.962594	2.792806	-0.981500
57	6	0	1.851972	3.322496	2.159097
58	6	0	3.034866	4.042593	2.039660
59	1	0	4.735810	4.398753	0.758442
60	1	0	1.205590	3.417890	3.027413
61	1	0	3.340035	4.726484	2.823500
62	7	0	1.437588	2.472862	1.205231
63	1	0	0.215877	1.825500	1.443076
64	1	0	-0.591966	1.424958	1.683890

TS''$_A$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1444.77570418 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.628277	-1.448181	-0.940381
2	6	0	-2.644761	-1.147994	-1.989417
3	1	0	-2.121547	-0.766838	-2.874387
4	1	0	-3.181768	-2.052223	-2.302689
5	6	0	-2.239258	-2.250448	0.165873
6	1	0	-3.319647	-2.073910	0.161628
7	1	0	-2.093411	-3.323169	-0.002535
8	6	0	-0.390580	-2.091388	-1.476988
9	1	0	0.022126	-2.723769	-0.689110
10	1	0	-0.622220	-2.746276	-2.325555
11	26	0	-1.131753	0.365141	-0.174415

12	6	0	-3.597001	-0.096764	-1.454249
13	6	0	-4.902972	0.048893	-1.909531
14	6	0	-3.849749	1.691024	0.022499
15	6	0	-5.696486	1.065190	-1.373418
16	1	0	-5.293279	-0.620620	-2.669141
17	6	0	-5.161195	1.897439	-0.389749
18	1	0	-3.390106	2.309899	0.784475
19	1	0	-6.717936	1.199326	-1.714696
20	1	0	-5.746718	2.694069	0.055151
21	6	0	-1.694682	-1.814091	1.504073
22	6	0	-1.746800	-2.618108	2.639870
23	6	0	-1.314295	-2.099320	3.860237
24	1	0	-2.128107	-3.631683	2.568855
25	6	0	-0.797661	-0.048436	2.729536
26	6	0	-0.837529	-0.788619	3.905077
27	1	0	-1.350015	-2.706644	4.758796
28	1	0	-0.425755	0.969110	2.714218
29	1	0	-0.496708	-0.342957	4.832805
30	7	0	-3.075265	0.715606	-0.497710
31	7	0	-1.214095	-0.548430	1.547723
32	6	0	0.614908	-1.025988	-1.889629
33	1	0	1.537657	-1.495696	-2.247966
34	1	0	0.213300	-0.441939	-2.725493
35	7	0	0.903509	-0.065985	-0.767899
36	6	0	1.621111	1.094259	-1.402288
37	1	0	2.511809	0.723250	-1.920561
38	1	0	0.952583	1.501371	-2.171870
39	6	0	1.765263	-0.710681	0.314788
40	1	0	1.893006	0.053907	1.083529
41	1	0	1.159068	-1.502152	0.757629
42	6	0	3.110886	-1.264360	-0.107982
43	6	0	4.279074	-0.500078	0.038488
44	6	0	3.230680	-2.578065	-0.591964
45	6	0	5.523654	-1.018679	-0.321483
46	1	0	4.221491	0.497476	0.464350
47	6	0	4.472607	-3.097979	-0.956986
48	1	0	2.353964	-3.218406	-0.657793
49	6	0	5.621790	-2.315297	-0.829185
50	1	0	6.417859	-0.417156	-0.191187
51	1	0	4.545535	-4.116832	-1.323993
52	1	0	6.589907	-2.720895	-1.104892
53	6	0	2.040188	2.235412	-0.496155
54	6	0	3.273050	2.868409	-0.662210
55	6	0	3.575573	3.987353	0.116784

56	1	0	3.982110	2.493840	-1.392796
57	6	0	1.438571	3.761363	1.165275
58	6	0	2.645434	4.443276	1.051850
59	1	0	4.526786	4.495496	-0.005898
60	1	0	0.669265	4.073316	1.866489
61	1	0	2.845155	5.307817	1.674799
62	7	0	1.154791	2.692111	0.405146
63	1	0	-0.133394	2.067834	0.427900
64	1	0	-1.019014	1.847011	0.497879

TS''$_A$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1444.79881233 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.651825	-1.107801	-1.220501
2	6	0	-2.423972	-0.314313	-2.224990
3	1	0	-1.718353	0.132564	-2.931419
4	1	0	-3.084849	-0.963906	-2.810557
5	6	0	-2.522578	-2.176344	-0.637614
6	1	0	-3.537627	-1.770424	-0.557261
7	1	0	-2.573522	-3.042756	-1.307924
8	6	0	-0.400993	-1.689015	-1.801081
9	1	0	-0.066577	-2.478699	-1.123807
10	1	0	-0.604201	-2.157279	-2.772801
11	26	0	-1.081260	0.115315	0.299335
12	6	0	-3.193084	0.792926	-1.542395
13	6	0	-4.348428	1.353805	-2.077413
14	6	0	-3.233960	2.281381	0.252459
15	6	0	-4.950117	2.424697	-1.413466
16	1	0	-4.769904	0.962950	-2.997788
17	6	0	-4.382301	2.897988	-0.229908
18	1	0	-2.763558	2.604445	1.174446
19	1	0	-5.851298	2.878750	-1.813133
20	1	0	-4.821795	3.724937	0.316251
21	6	0	-2.050415	-2.564045	0.742610
22	6	0	-2.310911	-3.807438	1.310766
23	6	0	-1.917842	-4.042043	2.629740
24	1	0	-2.817656	-4.575591	0.735781
25	6	0	-1.037067	-1.814463	2.702275
26	6	0	-1.273259	-3.027249	3.338902
27	1	0	-2.112923	-5.002687	3.095689
28	1	0	-0.535927	-0.997927	3.210626
29	1	0	-0.956174	-3.169547	4.365825

30	7	0	-2.645004	1.249249	-0.388865
31	7	0	-1.413710	-1.583841	1.426847
32	6	0	0.665880	-0.613341	-1.947113
33	1	0	1.591093	-1.057214	-2.329626
34	1	0	0.348952	0.130276	-2.682855
35	7	0	0.912402	0.104822	-0.653851
36	6	0	1.510973	1.434519	-1.002234
37	1	0	2.423832	1.277667	-1.587995
38	1	0	0.792841	1.941764	-1.657603
39	6	0	1.834355	-0.701486	0.261607
40	1	0	1.958598	-0.099674	1.164336
41	1	0	1.274607	-1.595951	0.546155
42	6	0	3.182029	-1.102985	-0.299546
43	6	0	4.303031	-0.270262	-0.157190
44	6	0	3.346198	-2.346354	-0.931981
45	6	0	5.545738	-0.656592	-0.660675
46	1	0	4.213029	0.672684	0.374922
47	6	0	4.587401	-2.734447	-1.437022
48	1	0	2.505097	-3.032707	-1.007668
49	6	0	5.688414	-1.885754	-1.307716
50	1	0	6.405645	-0.006183	-0.534865
51	1	0	4.698361	-3.701710	-1.916777
52	1	0	6.656604	-2.188411	-1.693515
53	6	0	1.836961	2.372416	0.144555
54	6	0	2.940929	3.224361	0.060865
55	6	0	3.166352	4.152638	1.078486
56	1	0	3.610704	3.164337	-0.790840
57	6	0	1.221725	3.312627	2.185223
58	6	0	2.292410	4.200079	2.165116
59	1	0	4.016628	4.825100	1.024918
60	1	0	0.513358	3.296610	3.009770
61	1	0	2.436438	4.902126	2.978639
62	7	0	1.001386	2.432807	1.194926
63	1	0	-0.161808	1.460553	1.348084
64	1	0	-0.844399	0.993216	1.664848

TS''$_B$ (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1444.80950663 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.505568	-1.120086	-0.732390
2	6	0	-2.401463	-0.866337	-1.905473

3	1	0	-1.845986	-0.240164	-2.610944
4	1	0	-2.602535	-1.816440	-2.418571
5	6	0	-2.206620	-1.927671	0.298338
6	1	0	-3.227337	-1.542394	0.391690
7	1	0	-2.294906	-2.978572	-0.009923
8	6	0	-0.284713	-1.842267	-1.215704
9	1	0	0.136042	-2.384296	-0.365635
10	1	0	-0.558406	-2.595499	-1.966850
11	26	0	-0.508677	0.655912	0.407581
12	6	0	-3.734581	-0.201813	-1.619440
13	6	0	-4.910607	-0.688494	-2.191051
14	6	0	-4.899727	1.576620	-0.653059
15	6	0	-6.108235	0.002466	-1.986766
16	1	0	-4.891250	-1.589531	-2.795277
17	6	0	-6.106703	1.156879	-1.205218
18	1	0	-4.831988	2.463636	-0.028939
19	1	0	-7.029009	-0.360897	-2.431887
20	1	0	-7.015173	1.719846	-1.023195
21	6	0	-1.556582	-1.843757	1.665375
22	6	0	-1.719842	-2.863903	2.601807
23	6	0	-1.191066	-2.708608	3.882856
24	1	0	-2.259417	-3.765645	2.330935
25	6	0	-0.361331	-0.568421	3.210998
26	6	0	-0.500831	-1.535959	4.196302
27	1	0	-1.313584	-3.491926	4.624187
28	1	0	0.178655	0.353397	3.404058
29	1	0	-0.074270	-1.374833	5.179851
30	7	0	-3.753531	0.913714	-0.864719
31	7	0	-0.876152	-0.713379	1.968833
32	6	0	0.763645	-0.894651	-1.798907
33	1	0	1.591513	-1.474869	-2.220524
34	1	0	0.336811	-0.311149	-2.619124
35	7	0	1.251188	0.055419	-0.761114
36	6	0	1.803343	1.307171	-1.343764
37	1	0	2.812294	1.155517	-1.741125
38	1	0	1.166655	1.599121	-2.187443
39	6	0	2.258954	-0.589082	0.189220
40	1	0	2.474696	0.163070	0.952309
41	1	0	1.739727	-1.410674	0.688241
42	6	0	3.543594	-1.085439	-0.434098
43	6	0	4.668244	-0.248652	-0.516320
44	6	0	3.650159	-2.404364	-0.904108
45	6	0	5.857409	-0.707777	-1.083656
46	1	0	4.625686	0.758370	-0.107428

47	6	0	4.838326	-2.864995	-1.472030
48	1	0	2.810776	-3.088706	-0.799952
49	6	0	5.941336	-2.014278	-1.569158
50	1	0	6.721290	-0.052538	-1.133195
51	1	0	4.908018	-3.889211	-1.824392
52	1	0	6.868110	-2.373850	-2.004601
53	6	0	1.787979	2.422717	-0.316755
54	6	0	2.684288	3.488700	-0.360972
55	6	0	2.563831	4.515524	0.575747
56	1	0	3.459305	3.513975	-1.120123
57	6	0	0.694882	3.352396	1.517577
58	6	0	1.549667	4.447477	1.532956
59	1	0	3.251046	5.355453	0.559158
60	1	0	-0.114043	3.263392	2.236816
61	1	0	1.421280	5.225536	2.276941
62	7	0	0.812278	2.355444	0.616280
63	1	0	-2.572860	1.405073	-0.224236
64	1	0	-1.883183	1.792412	0.235662

TS''$_B$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1444.77944050 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.401215	-1.368256	-0.488755
2	6	0	-2.398761	-1.414228	-1.604398
3	1	0	-1.913343	-0.986607	-2.489511
4	1	0	-2.618281	-2.461750	-1.846919
5	6	0	-1.958260	-1.986319	0.750816
6	1	0	-2.986335	-1.632130	0.875475
7	1	0	-2.001411	-3.079629	0.664654
8	6	0	-0.173601	-2.129355	-0.933452
9	1	0	0.298329	-2.539670	-0.038363
10	1	0	-0.458365	-2.979987	-1.564421
11	26	0	-0.626737	0.488890	0.093942
12	6	0	-3.721898	-0.700326	-1.394181
13	6	0	-4.886559	-1.182529	-1.991328
14	6	0	-4.886351	1.146566	-0.543177
15	6	0	-6.072071	-0.454960	-1.863987
16	1	0	-4.866771	-2.110862	-2.552903
17	6	0	-6.075833	0.732292	-1.129727
18	1	0	-4.818488	2.048581	0.058096
19	1	0	-6.983834	-0.816892	-2.328421
20	1	0	-6.978619	1.319533	-1.005986

21	6	0	-1.152690	-1.564610	1.956968
22	6	0	-1.131685	-2.304684	3.136797
23	6	0	-0.439185	-1.807520	4.240605
24	1	0	-1.657052	-3.252801	3.189687
25	6	0	0.171866	0.093194	2.912640
26	6	0	0.219552	-0.582999	4.125853
27	1	0	-0.414414	-2.365429	5.170973
28	1	0	0.676676	1.042176	2.776472
29	1	0	0.768038	-0.155899	4.957877
30	7	0	-3.749722	0.445009	-0.688394
31	7	0	-0.497289	-0.384651	1.843369
32	6	0	0.800921	-1.214813	-1.664649
33	1	0	1.679698	-1.777110	-1.997585
34	1	0	0.335269	-0.796262	-2.562261
35	7	0	1.174414	-0.088967	-0.761408
36	6	0	1.572091	1.143590	-1.505496
37	1	0	2.606004	1.089013	-1.860178
38	1	0	0.937211	1.226679	-2.396699
39	6	0	2.267073	-0.481569	0.228410
40	1	0	2.390160	0.379712	0.889077
41	1	0	1.861634	-1.292760	0.834411
42	6	0	3.597447	-0.884241	-0.364837
43	6	0	4.608984	0.068018	-0.571164
44	6	0	3.865814	-2.227325	-0.676047
45	6	0	5.841643	-0.305889	-1.107353
46	1	0	4.445390	1.103438	-0.280446
47	6	0	5.097489	-2.603328	-1.212766
48	1	0	3.120637	-2.992747	-0.469470
49	6	0	6.084429	-1.641106	-1.436219
50	1	0	6.616721	0.439784	-1.253405
51	1	0	5.292245	-3.646307	-1.441485
52	1	0	7.045463	-1.933624	-1.846897
53	6	0	1.346923	2.355038	-0.625445
54	6	0	2.094904	3.524045	-0.730539
55	6	0	1.770188	4.612437	0.080722
56	1	0	2.915751	3.580600	-1.437874
57	6	0	-0.000262	3.301855	1.027475
58	6	0	0.704209	4.498680	0.974806
59	1	0	2.340692	5.533447	0.016113
60	1	0	-0.840935	3.166013	1.699042
61	1	0	0.418829	5.321651	1.620375
62	7	0	0.313439	2.243889	0.249098
63	1	0	-2.675048	0.822044	-0.004048
64	1	0	-1.996336	1.168008	0.622789

TS''$_B$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1444.79209343 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.376403	-1.136989	-0.927675
2	6	0	-2.322880	-0.704508	-2.000742
3	1	0	-1.788385	-0.000546	-2.647961
4	1	0	-2.578281	-1.569926	-2.626576
5	6	0	-2.012888	-2.176451	-0.065090
6	1	0	-3.025864	-1.839532	0.175953
7	1	0	-2.111009	-3.122726	-0.613184
8	6	0	-0.137158	-1.704911	-1.571965
9	1	0	0.312053	-2.397293	-0.856989
10	1	0	-0.401803	-2.289706	-2.462214
11	26	0	-0.562981	0.398863	0.344045
12	6	0	-3.620802	-0.051342	-1.555550
13	6	0	-4.771300	-0.182859	-2.333905
14	6	0	-4.751151	1.357194	-0.068382
15	6	0	-5.931593	0.498238	-1.960847
16	1	0	-4.759201	-0.806188	-3.222229
17	6	0	-5.925132	1.285353	-0.808213
18	1	0	-4.681962	1.934744	0.849123
19	1	0	-6.831668	0.407563	-2.560546
20	1	0	-6.808648	1.823251	-0.483753
21	6	0	-1.253800	-2.382242	1.229401
22	6	0	-1.341983	-3.576348	1.943893
23	6	0	-0.699131	-3.675288	3.177772
24	1	0	-1.909422	-4.410749	1.544022
25	6	0	0.071074	-1.427560	2.875563
26	6	0	0.017905	-2.577665	3.655813
27	1	0	-0.756797	-4.592772	3.754545
28	1	0	0.624040	-0.553874	3.207656
29	1	0	0.530326	-2.609395	4.610815
30	7	0	-3.635583	0.710028	-0.446077
31	7	0	-0.547673	-1.327164	1.683314
32	6	0	0.852863	-0.606201	-1.933901
33	1	0	1.752304	-1.035496	-2.386899
34	1	0	0.418030	0.069556	-2.675196
35	7	0	1.188743	0.196544	-0.718107
36	6	0	1.581010	1.598134	-1.070259
37	1	0	2.626423	1.652136	-1.387613
38	1	0	0.969461	1.918265	-1.921683

39	6	0	2.273739	-0.466718	0.133614
40	1	0	2.349124	0.139919	1.040309
41	1	0	1.875984	-1.438141	0.430518
42	6	0	3.632618	-0.623073	-0.508008
43	6	0	4.614821	0.369356	-0.356142
44	6	0	3.955741	-1.784388	-1.228721
45	6	0	5.873428	0.221736	-0.939728
46	1	0	4.406578	1.249784	0.247967
47	6	0	5.213385	-1.933038	-1.814284
48	1	0	3.233551	-2.594109	-1.308819
49	6	0	6.171190	-0.926293	-1.676844
50	1	0	6.625290	0.993184	-0.806857
51	1	0	5.450717	-2.838993	-2.362826
52	1	0	7.152120	-1.044644	-2.125807
53	6	0	1.299695	2.518779	0.092056
54	6	0	2.028067	3.676641	0.347121
55	6	0	1.643441	4.500105	1.406598
56	1	0	2.879344	3.929762	-0.275982
57	6	0	-0.140935	2.969665	1.875898
58	6	0	0.541574	4.139827	2.184048
59	1	0	2.197365	5.408093	1.622831
60	1	0	-1.002633	2.645560	2.447984
61	1	0	0.213086	4.752291	3.016099
62	7	0	0.228441	2.170992	0.850629
63	1	0	-2.558367	0.750071	0.419391
64	1	0	-1.937714	0.788730	1.142978

TS''$_C$ (quintet) E(B3LYP/ SDD-6-31G(d,p))= -1444.81209247 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.362043	1.234399	-1.049614
2	6	0	2.323177	0.641742	-2.022183
3	1	0	1.761219	0.031191	-2.736374
4	1	0	2.823284	1.422423	-2.610320
5	6	0	2.012828	2.440938	-0.448157
6	1	0	2.961334	2.106348	-0.013014
7	1	0	2.261860	3.155197	-1.244474
8	6	0	0.071601	1.574673	-1.713790
9	1	0	-0.458462	2.272277	-1.062051
10	1	0	0.240738	2.097019	-2.666051
11	26	0	0.924109	-0.604166	0.326605
12	6	0	3.348698	-0.246624	-1.349582

13	6	0	4.663493	-0.337565	-1.798903
14	6	0	3.742302	-1.875050	0.272606
15	6	0	5.532376	-1.240495	-1.183587
16	1	0	5.001361	0.285816	-2.620187
17	6	0	5.063519	-2.025593	-0.129409
18	1	0	3.336194	-2.459747	1.091773
19	1	0	6.560604	-1.326340	-1.520478
20	1	0	5.706460	-2.737196	0.376036
21	6	0	1.225076	3.179866	0.615351
22	6	0	1.006443	4.554751	0.529532
23	6	0	0.367488	5.215247	1.583206
24	1	0	1.342304	5.105700	-0.342796
25	6	0	0.190783	3.114167	2.711542
26	6	0	-0.047268	4.485873	2.696522
27	1	0	0.199493	6.286326	1.532142
28	1	0	-0.108093	2.488218	3.548063
29	1	0	-0.541639	4.962875	3.535267
30	7	0	2.897965	-1.006433	-0.323762
31	7	0	0.810996	2.491988	1.698432
32	6	0	-0.787321	0.333530	-1.969072
33	1	0	-1.744713	0.637536	-2.406854
34	1	0	-0.304486	-0.319280	-2.701731
35	7	0	-0.995678	-0.463134	-0.727006
36	6	0	-1.376714	-1.870830	-1.034614
37	1	0	-2.426427	-1.941277	-1.338027
38	1	0	-0.773209	-2.205755	-1.886792
39	6	0	-1.999550	0.185932	0.221782
40	1	0	-1.979837	-0.411010	1.137601
41	1	0	-1.594196	1.169154	0.472553
42	6	0	-3.417368	0.311978	-0.288086
43	6	0	-4.359409	-0.695461	-0.024675
44	6	0	-3.829507	1.448861	-1.001643
45	6	0	-5.670406	-0.583892	-0.488941
46	1	0	-4.074445	-1.559796	0.570978
47	6	0	-5.139715	1.561501	-1.467902
48	1	0	-3.133439	2.267355	-1.171989
49	6	0	-6.060065	0.541624	-1.217755
50	1	0	-6.390140	-1.366455	-0.270492
51	1	0	-5.445658	2.448786	-2.013067
52	1	0	-7.081104	0.631606	-1.574387
53	6	0	-1.098525	-2.778360	0.147571
54	6	0	-1.843659	-3.929429	0.395202
55	6	0	-1.500414	-4.740041	1.477828
56	1	0	-2.677289	-4.185106	-0.250722

57	6	0	0.257197	-3.198253	1.993600
58	6	0	-0.432438	-4.366348	2.295333
59	1	0	-2.065073	-5.643142	1.686595
60	1	0	1.079098	-2.856159	2.615645
61	1	0	-0.143528	-4.960289	3.155097
62	7	0	-0.057930	-2.424790	0.934443
63	1	0	0.982200	1.096652	1.766719
64	1	0	1.081259	0.174760	1.911483

TS''$_c$ (singlet) E(B3LYP/ SDD-6-31G(d,p))= -1444.77609959 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.162357	1.168220	-1.175099
2	6	0	2.140013	0.562410	-2.138928
3	1	0	1.612179	-0.184361	-2.745413
4	1	0	2.530623	1.311021	-2.839672
5	6	0	1.794725	2.403281	-0.605919
6	1	0	2.792245	2.124070	-0.253894
7	1	0	1.929832	3.136057	-1.411266
8	6	0	-0.147829	1.506436	-1.822893
9	1	0	-0.641592	2.237415	-1.179825
10	1	0	0.009243	1.986101	-2.797597
11	26	0	0.851957	-0.544130	-0.044448
12	6	0	3.261117	-0.089396	-1.352124
13	6	0	4.580622	-0.115322	-1.789640
14	6	0	3.822112	-1.198773	0.610555
15	6	0	5.547389	-0.723684	-0.986025
16	1	0	4.849285	0.338235	-2.738118
17	6	0	5.161823	-1.262691	0.240566
18	1	0	3.492077	-1.591359	1.564464
19	1	0	6.583871	-0.759039	-1.305606
20	1	0	5.882821	-1.722621	0.907002
21	6	0	1.049019	3.058283	0.536691
22	6	0	0.909084	4.443793	0.614753
23	6	0	0.313899	5.003445	1.748510
24	1	0	1.268721	5.076294	-0.190392
25	6	0	0.021485	2.791002	2.612661
26	6	0	-0.136020	4.165669	2.768853
27	1	0	0.203455	6.080054	1.830526
28	1	0	-0.316860	2.087745	3.368780
29	1	0	-0.600805	4.562843	3.664256
30	7	0	2.876789	-0.642636	-0.171622

31	7	0	0.602829	2.263393	1.525042
32	6	0	-1.021807	0.266100	-1.980169
33	1	0	-2.019222	0.549578	-2.332958
34	1	0	-0.600941	-0.398632	-2.740852
35	7	0	-1.093814	-0.500938	-0.695347
36	6	0	-1.438576	-1.935049	-0.953403
37	1	0	-2.519897	-2.076406	-1.037741
38	1	0	-1.008187	-2.224113	-1.919481
39	6	0	-2.064742	0.115582	0.308783
40	1	0	-1.953666	-0.480159	1.218336
41	1	0	-1.681211	1.113550	0.527602
42	6	0	-3.514803	0.184508	-0.109172
43	6	0	-4.405408	-0.847630	0.228587
44	6	0	-4.010966	1.299403	-0.804717
45	6	0	-5.747274	-0.783472	-0.148526
46	1	0	-4.055512	-1.692981	0.817149
47	6	0	-5.351922	1.364914	-1.184093
48	1	0	-3.354932	2.138668	-1.026688
49	6	0	-6.220082	0.319367	-0.862621
50	1	0	-6.425570	-1.584835	0.126747
51	1	0	-5.722188	2.235475	-1.716167
52	1	0	-7.264863	0.372569	-1.151442
53	6	0	-0.842970	-2.807377	0.122761
54	6	0	-1.418256	-4.011345	0.519794
55	6	0	-0.776473	-4.786906	1.485051
56	1	0	-2.354467	-4.333734	0.076188
57	6	0	0.929102	-3.107242	1.593952
58	6	0	0.418234	-4.321872	2.034646
59	1	0	-1.205623	-5.729743	1.808429
60	1	0	1.843601	-2.708941	2.013883
61	1	0	0.946510	-4.883296	2.796924
62	7	0	0.326478	-2.359596	0.646546
63	1	0	0.693245	0.800364	1.328652
64	1	0	0.705495	-0.092144	1.459572

TS''$_C$ (triplet) E(B3LYP/ SDD-6-31G(d,p))= -1444.79259113 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.240369	1.223718	-1.046448
2	6	0	2.196931	0.676184	-2.069859
3	1	0	1.624299	0.078945	-2.785847

4	1	0	2.660584	1.489077	-2.640926
5	6	0	1.887726	2.455076	-0.472095
6	1	0	2.839549	2.133444	-0.036905
7	1	0	2.122303	3.143723	-1.292762
8	6	0	-0.067202	1.558785	-1.705312
9	1	0	-0.608193	2.229309	-1.034606
10	1	0	0.097954	2.104834	-2.643537
11	26	0	0.852386	-0.442213	0.216121
12	6	0	3.234462	-0.212422	-1.432834
13	6	0	4.543979	-0.309709	-1.892464
14	6	0	3.603362	-1.861942	0.162103
15	6	0	5.402984	-1.231219	-1.289416
16	1	0	4.885559	0.317851	-2.708988
17	6	0	4.923515	-2.022648	-0.246039
18	1	0	3.190675	-2.455370	0.969996
19	1	0	6.429092	-1.327481	-1.629568
20	1	0	5.557052	-2.751035	0.247385
21	6	0	1.106039	3.234462	0.566951
22	6	0	0.867663	4.600882	0.427870
23	6	0	0.240298	5.296141	1.466696
24	1	0	1.180215	5.119586	-0.472437
25	6	0	0.110778	3.244330	2.690245
26	6	0	-0.143913	4.610962	2.619090
27	1	0	0.057634	6.362041	1.374208
28	1	0	-0.162256	2.646611	3.555114
29	1	0	-0.627532	5.118909	3.445823
30	7	0	2.771069	-0.973914	-0.415266
31	7	0	0.720972	2.595588	1.688344
32	6	0	-0.890655	0.297250	-1.964891
33	1	0	-1.875562	0.567115	-2.360796
34	1	0	-0.411465	-0.333016	-2.718604
35	7	0	-1.003496	-0.496330	-0.707910
36	6	0	-1.213636	-1.956824	-0.943761
37	1	0	-2.253400	-2.179946	-1.203847
38	1	0	-0.593604	-2.254250	-1.797634
39	6	0	-2.063702	0.066012	0.239503
40	1	0	-1.980888	-0.512370	1.162682
41	1	0	-1.755333	1.087459	0.474251
42	6	0	-3.485615	0.048362	-0.271898
43	6	0	-4.322428	-1.050166	-0.016992
44	6	0	-4.009951	1.145135	-0.974892
45	6	0	-5.637871	-1.066090	-0.481706
46	1	0	-3.954512	-1.885200	0.574941
47	6	0	-5.324870	1.130643	-1.441010

48	1	0	-3.399270	2.031271	-1.135286
49	6	0	-6.138214	0.021265	-1.200938
50	1	0	-6.276014	-1.918197	-0.270157
51	1	0	-5.718409	1.988177	-1.977480
52	1	0	-7.163307	0.011900	-1.557146
53	6	0	-0.778110	-2.724236	0.287066
54	6	0	-1.344262	-3.936517	0.671258
55	6	0	-0.869505	-4.576391	1.817378
56	1	0	-2.146091	-4.369629	0.082346
57	6	0	0.661106	-2.757434	2.125035
58	6	0	0.144944	-3.972130	2.561292
59	1	0	-1.296009	-5.523258	2.132572
60	1	0	1.432530	-2.235426	2.681419
61	1	0	0.526071	-4.425252	3.469515
62	7	0	0.225411	-2.151942	1.001125
63	1	0	0.910855	1.294367	1.710798
64	1	0	1.062045	0.316956	1.745134
