Supporting information:

Mechanism of Photocatalytic CO_2 Reduction to HCO_2H by a Robust Multifunctional Iridium Complex

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Contents

1. Additional computational results

Table S1. The experimental and calculated ΔE (V) in water for related reactions

Reaction	ΔE_{exp} (V)	ΔE_{cal} (V)
$CO_2 + 2e^- + 2H^+ = HCO_2H$ [a]	-0.61	-0.47
$CO_2 + 2e^- + 2H^+ = H_2O + CO$ [a]	-0.53	-0.54
$2e^- + 2H^+ = H_2$	-0.41	-0.34

[a]The concentration correction of 1.9 kcal mol^{-1} at 298.15 K was added, which originates from the free energy change from 1 atm (24.5 L mol^{-1} for ideal gas) to 1 M (1 mol L^{-1} in water). The correction for water (standard concentration of 55.56 mol L^{-1}) is 4.3 kcal mol^{-1}, respectively. It should be noted that the redox potentials are sensitive to the reaction solvent.

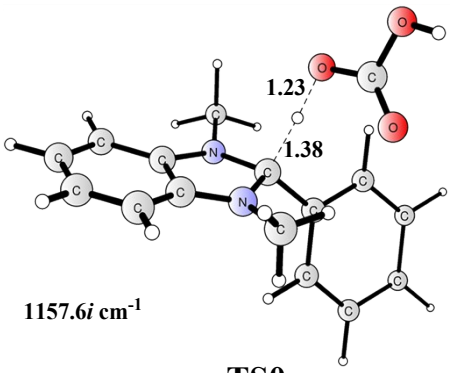
Table S2. The energies for some intermediates in their low-spin and high-spin state.

Species	Relative Gibbs free energy (in kcal mol^{-1})	
	low-spin state	high-spin state
Cl-3-H	0.0	59.7
Cl-2-H	0.0	61.5
3-H	0.0	51.8
2-H	0.0	57.8
1-H	0.0	12.6
1-OCHO	0.0	18.1
1	0.0	18.4

The energies of critical intermediates at their low spin-state and high-spin state have been calculated and the results indicated that, for each species, the low-spin state is thermodynamically much more favored over the high-spin state. Therefore, unless otherwise mentioned, the energies and structures reported are in their low-spin state.

2. The nature of the BIH

$$HCO_3^- + BIH^{\bullet+} \xrightarrow[\Delta G = 1.2 \text{ kcal mol}^{-1}]{\Delta G^{\ddagger} = 7.8 \text{ kcal mol}^{-1}} BI^{\bullet} + H_2CO_3$$



TS0

Figure S1. Optimized structure of **TS0**. Distances are given in Ångström, and the imaginary frequency for **TS0** is shown.

Table S3. The computed pK_as of the related species in the reaction medium.

Species	pK_a
H_2CO_3	13.4
BIH-H$^+$	4.1
BIH$^{\bullet+}$	13.7
HCO_2H	12.9
^{1}3-H	19.8
^{3}3-H	-4.7

3. Several possible conformers of ^{1}Cl-3-H.

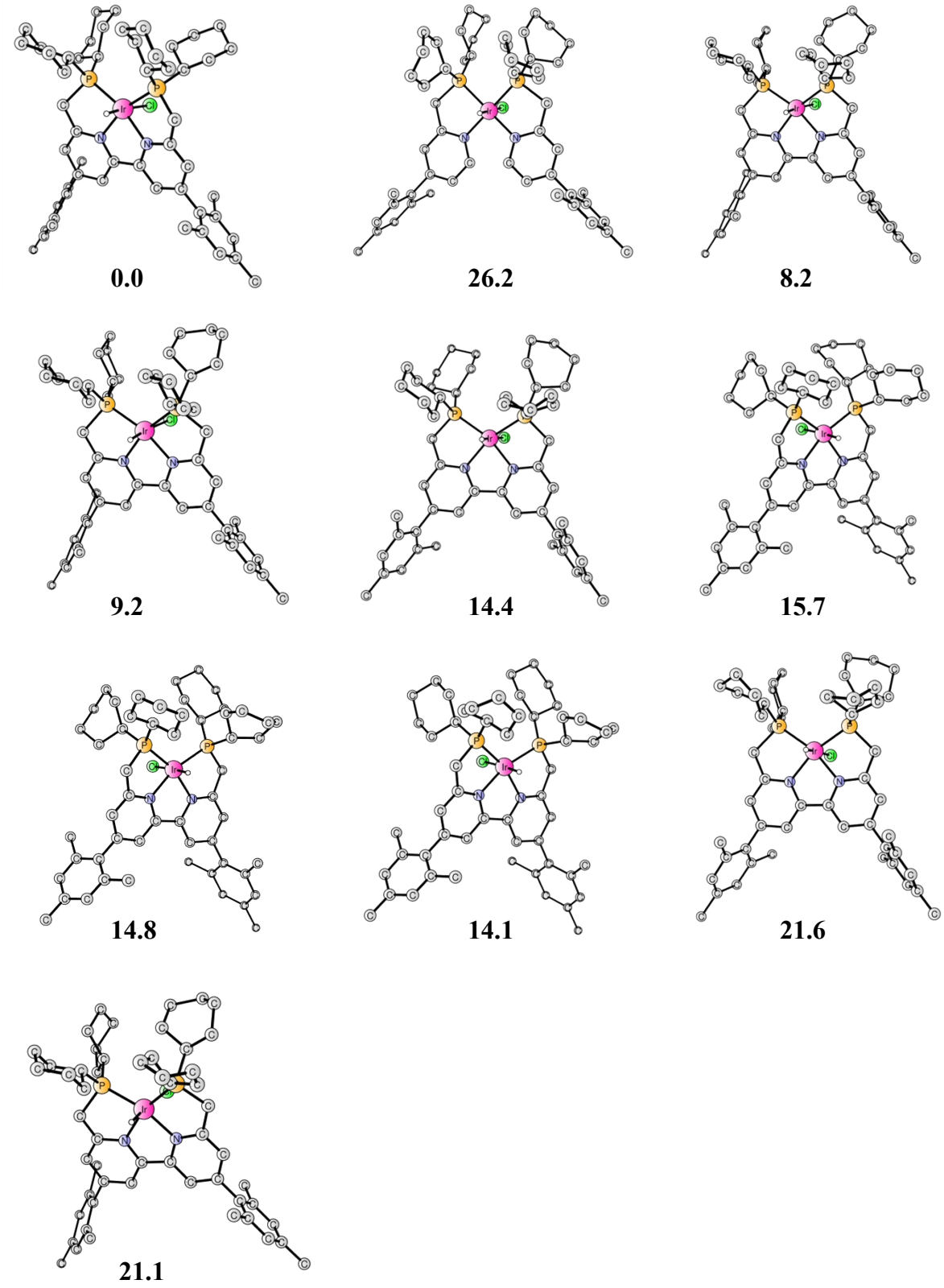


Figure S2. Relative Gibbs free energies (in kcal mol^{-1}) of possible conformers of **^{1}Cl-3-H**. Unimportant hydrogen atoms are omitted for clarity.

4. The computed UV-Vis absorption spectra.

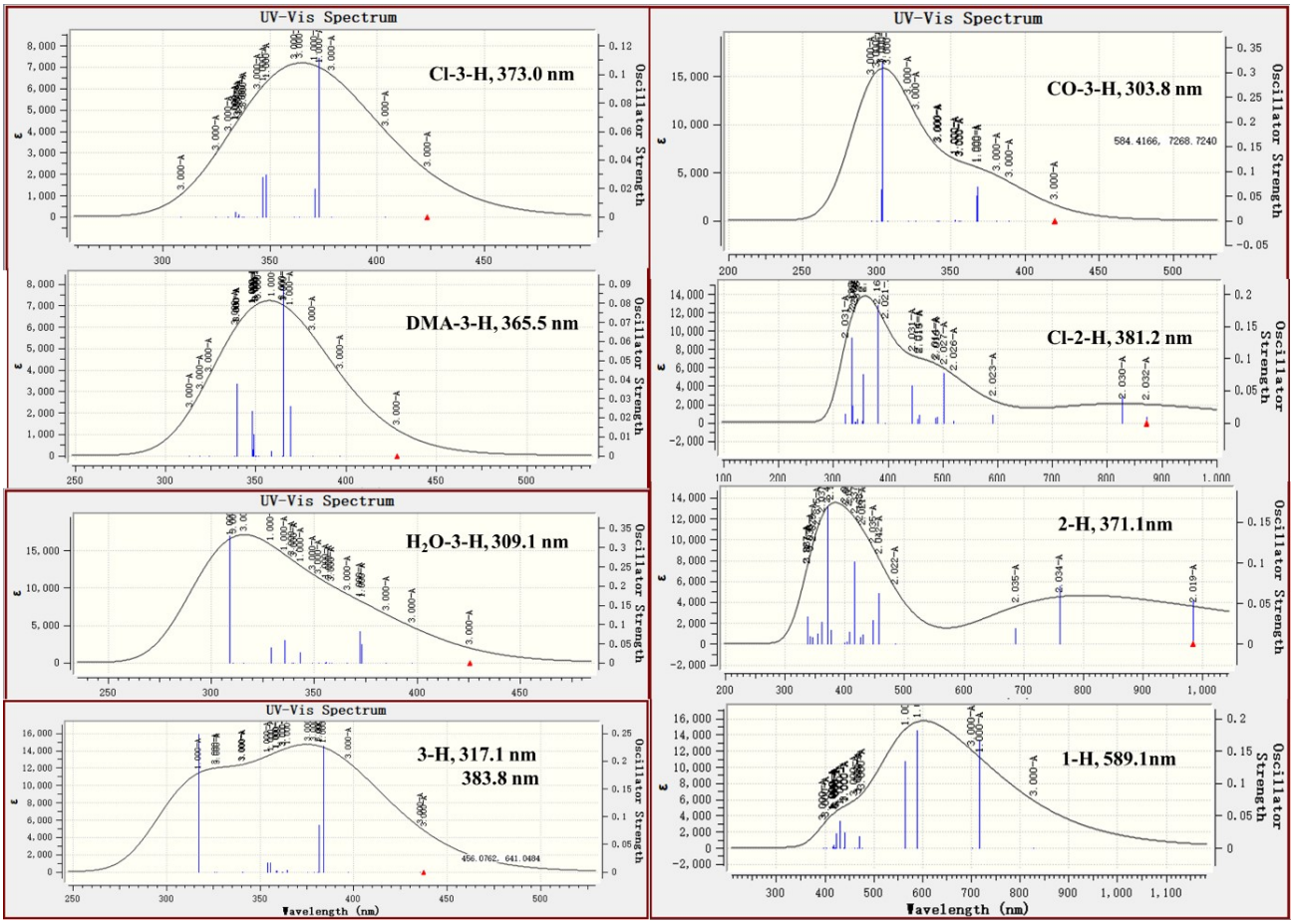


Figure S3. The computed UV-Vis absorption spectra for the possible complexes in the reaction medium.

5. Redox properties of Ir complex Mes-IrPCY2

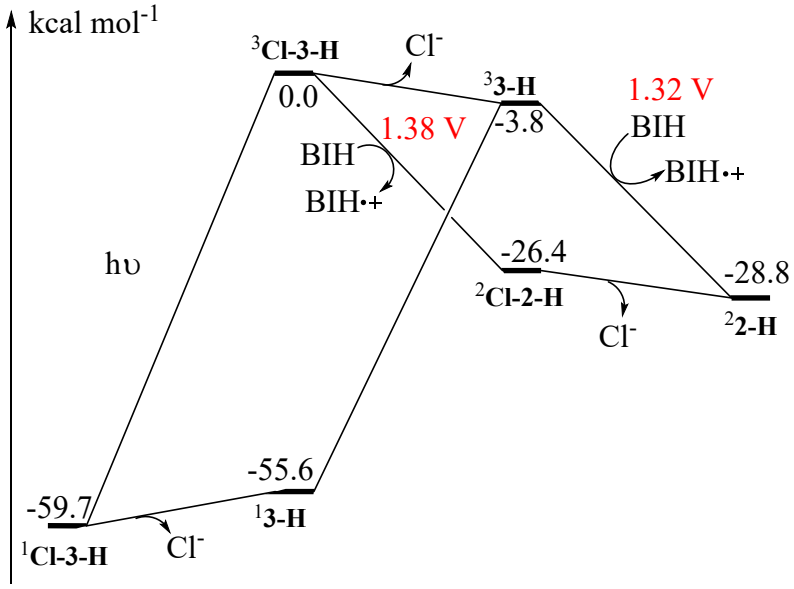
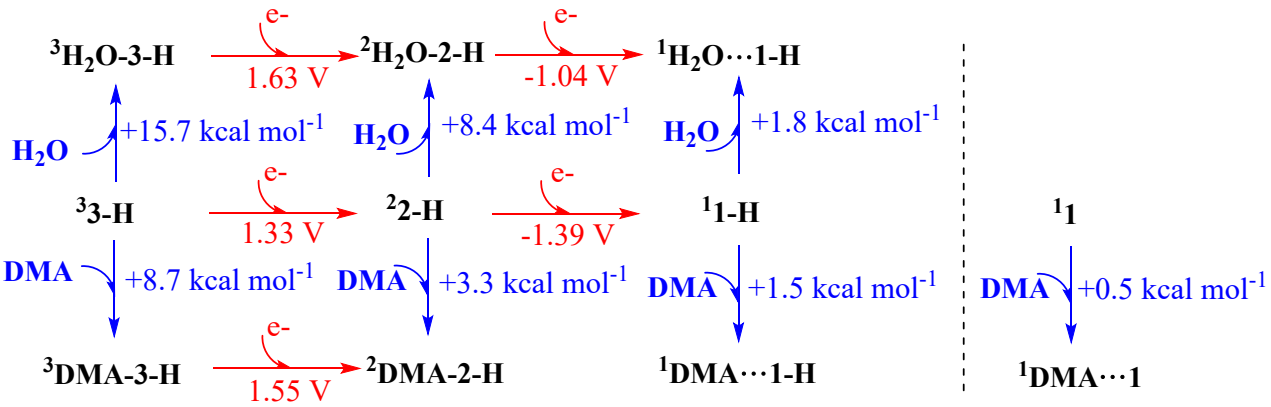
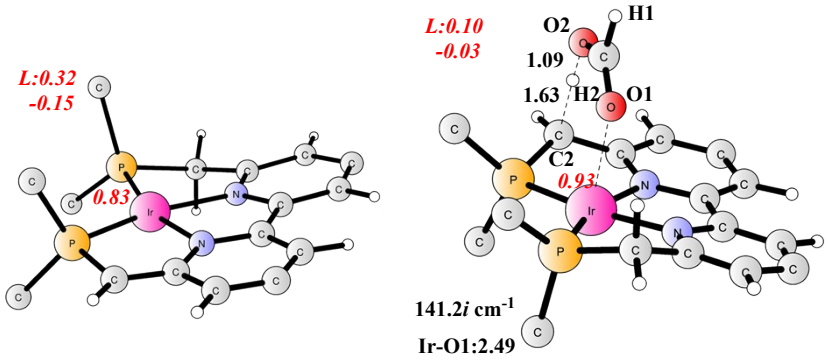


Figure S4. Gibbs free energy diagram (in kcal mol^{-1}) for the first reduction step of the catalyst in DMA.



Scheme S1. Possible solvent coordination manners to critical iridium species including **3-H**, **2-H**, **1-H**, and **1**, and related redox potentials (in red) and reaction free energies (in blue).

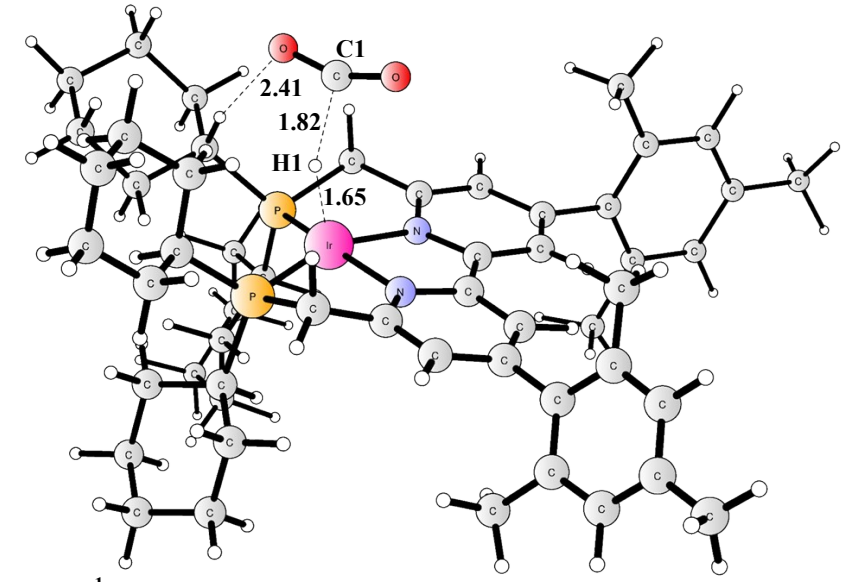
6. Pathway I.



^{2}2(-H) ^{2}TS3

Figure S5. The optimized structures of ^{2}**2(-H)** (total charge of +1) and ^{2}**TS3** (total charge of +1). The spin multiplicities of the species are indicated by the numbers in the left superscript. Distances are given in Ångstroms. The spin populations of Ir and the ligand are shown in red italic and the imaginary frequencies for all transition states are also shown. For clarity, the four Cy groups are shown with only one C atom, two trimethylphenyl groups and unimportant hydrogen atoms are not shown.

7. Pathway II.



^{1}TS4

Figure S6. The whole optimized structures of **^{1}TS4** (total charge of 0). The spin multiplicities of the species are indicated by the numbers in the left superscript. Distances are given in Ångstroms. The imaginary frequency is also shown.

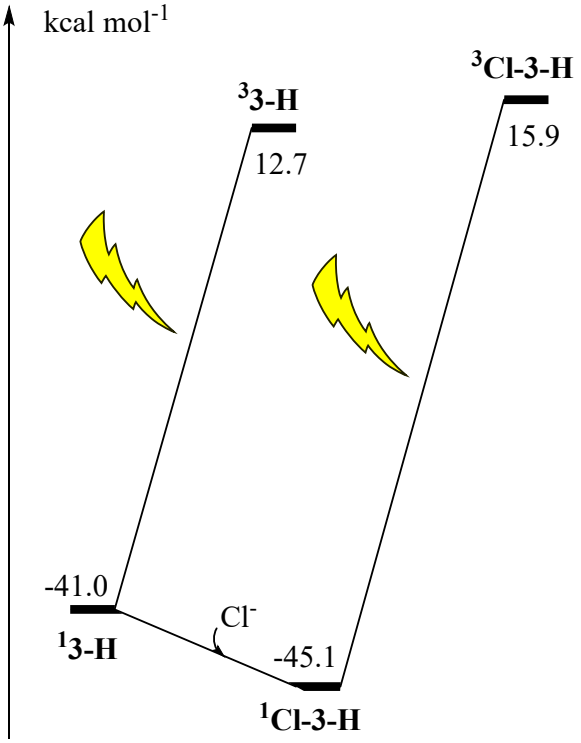


Figure S7. Gibbs free energy diagram (in kcal mol^{-1}) for the starting of the second catalytic cycle.

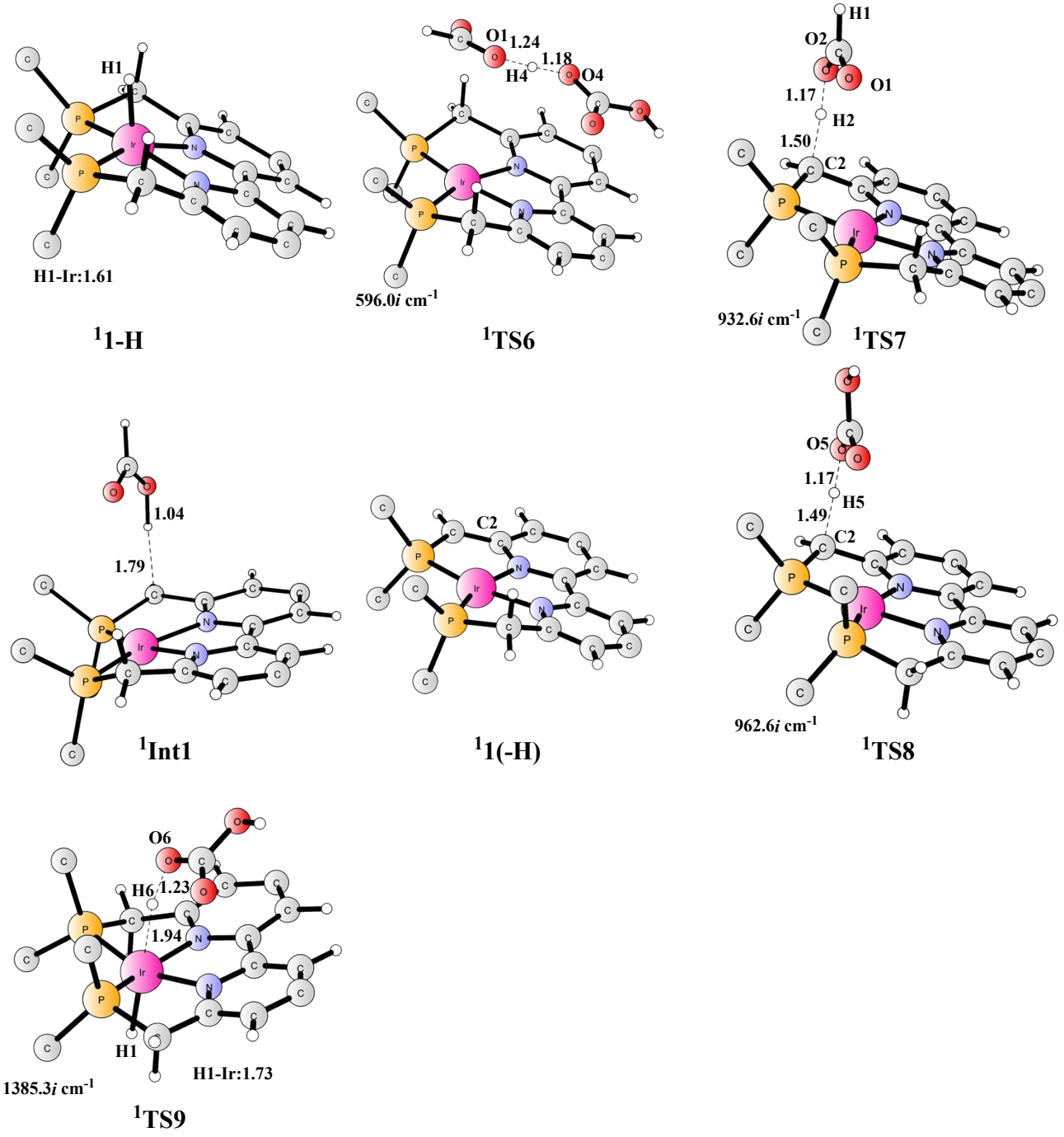
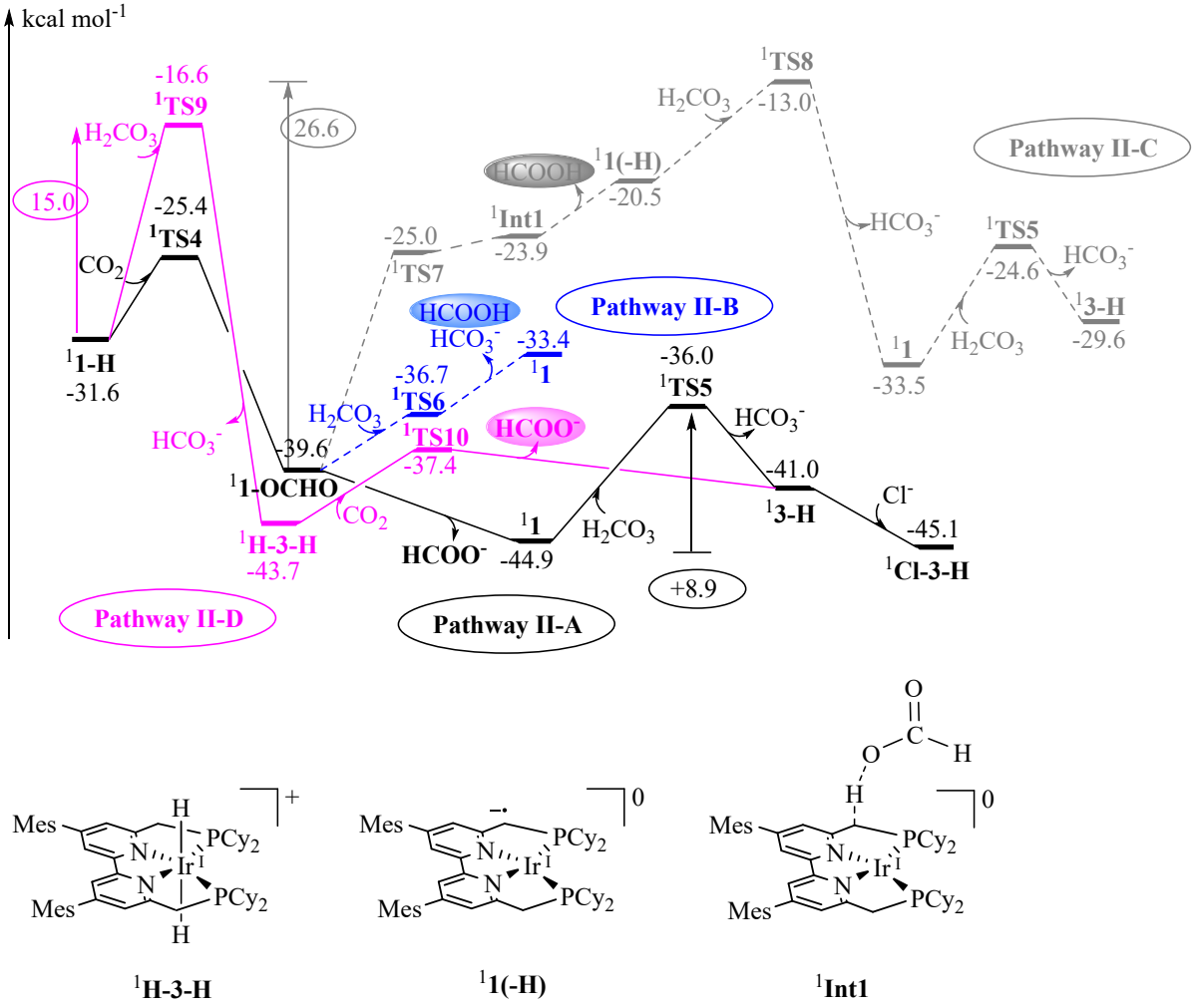


Figure S8. The optimized structures of ^{1}**1-H** (total charge of 0), ^{1}**TS6** (total charge of 0), ^{1}**TS7** (total charge of 0), ^{1}**Int1**(total charge of 0), ^{1}**1(-H)** (total charge of 0), ^{1}**TS8** (total charge of 0), and ^{1}**TS9** (total charge of 0). The spin multiplicities of the species are indicated by the numbers in the left superscript. Distances are given in Ångstroms. The imaginary frequencies for all transition states are also shown. For clarity, the four Cy groups are shown with only one C atom, two trimethylphenyl groups and unimportant hydrogen atoms are not shown.



1H-3-H **1(-H)** **1Int1**

Figure S9. Gibbs free energy diagram (in kcal mol^{-1}) for the reduction of CO_2 from **^{1}1-H** complex.

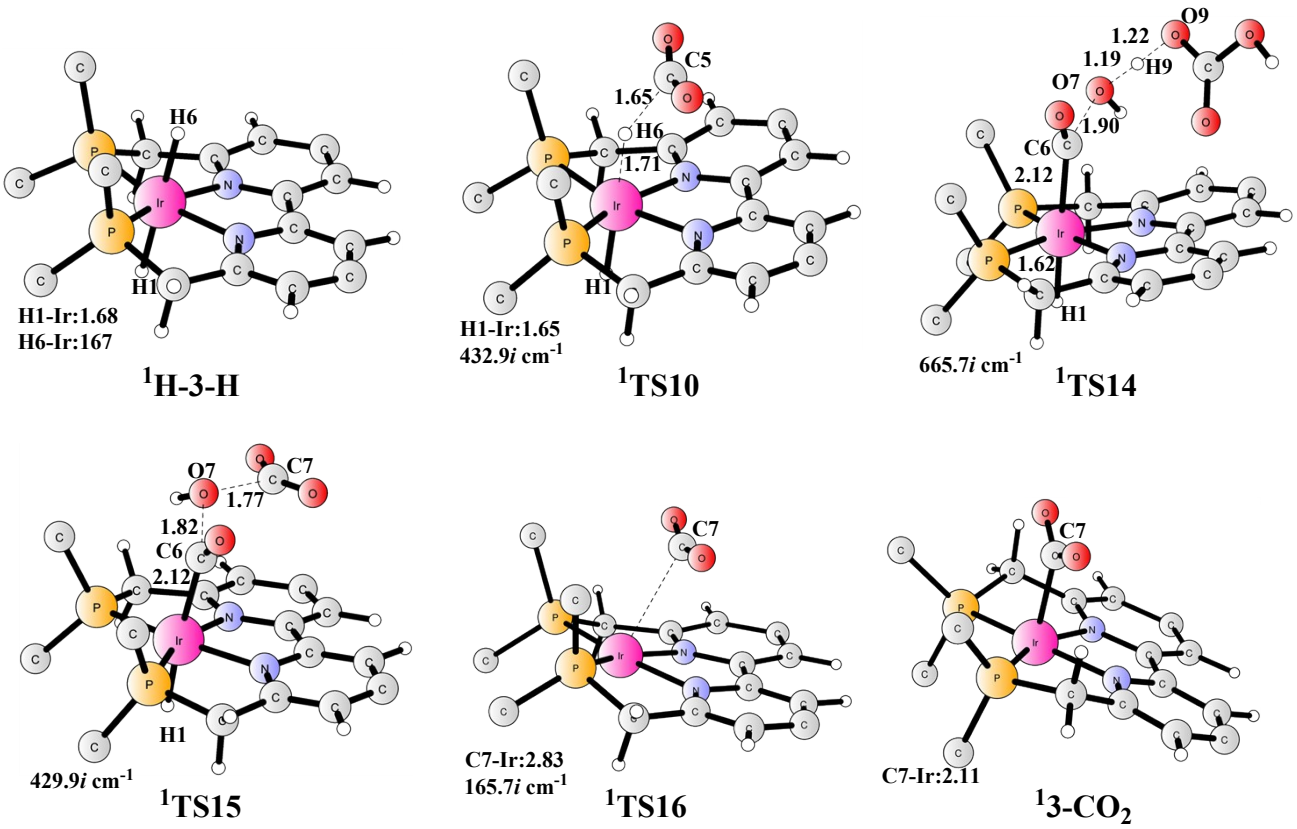
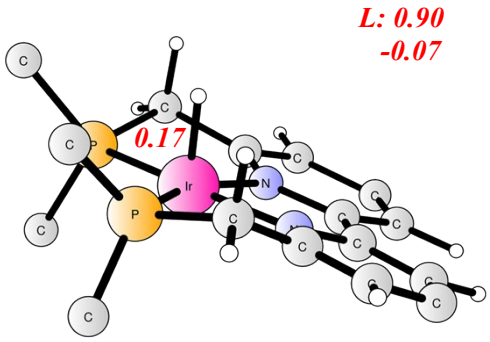


Figure S10. The optimized structures of ^{1}**H-3-H** (total charge of +1), ^{1}**TS10** (total charge of +1), ^{1}**TS14** (total charge of +1), ^{1}**TS15** (total charge of +1), ^{1}**TS16** (total charge of +1) and ^{1}**3-CO$_2$** (total charge of +1). The spin multiplicities of the species are indicated by the numbers in the left superscript. Distances are given in Ångstroms. The imaginary frequencies for all transition states are also shown. For clarity, the four Cy groups are shown with only one C atom, two trimethylphenyl groups and unimportant hydrogen atoms are not shown. It should be pointed out that, for ^{1}**H-3-H**, a small imaginary frequency (35.6i) corresponding to a low energy torsion mode could not be eliminated after many attempts, and it does not affect the conclusion in the present work.

Table S4. The barriers (in kcal mol^{-1}) for **TS4** and **TS11** calculated with different functionals.

Transition state	Barriers (in kcal mol^{-1})		
	B3LYP-D3	M06-D3	TPSSh-D3
TS4	6.2	9.7	5.4
TS11	8.1	10.0	6.0



^{2}2-H

Figure S11. The optimized structure of **^{2}2-H** (total charge of +1). The spin multiplicities of the species are indicated by the numbers in the left superscript. Distances are given in Ångstroms. The spin populations of Ir and the ligand are shown in red italic and the imaginary frequencies for all transition states are also shown. For clarity, the four Cy groups are shown with only one C atom, two trimethylphenyl groups and unimportant hydrogen atoms are not shown.

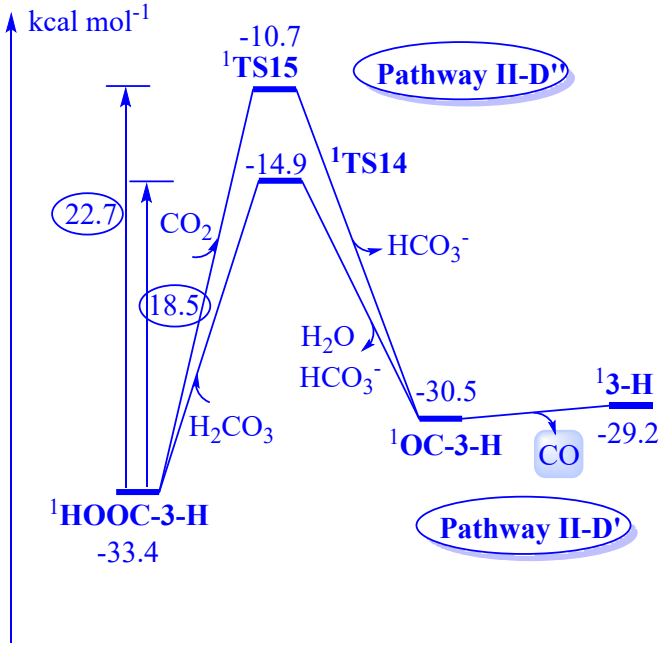


Figure S12. Gibbs free energy diagram (in kcal mol^{-1}) for the formation of CO from the ^{1}**HOOC-3-H** complex.

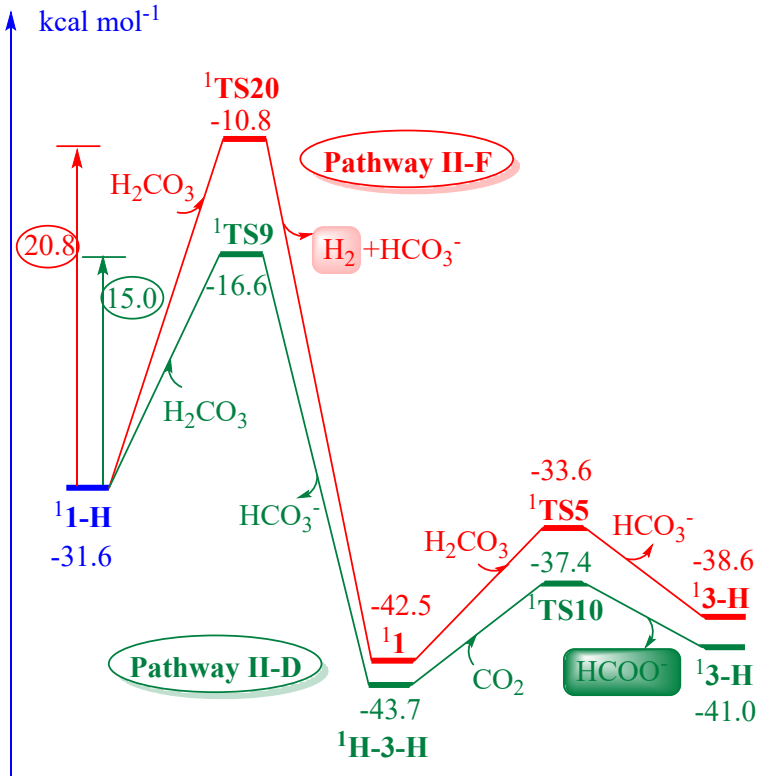


Figure S13. Gibbs free energy diagram (in kcal mol^{-1}) for the comparison of pathway II-D and pathway II-F from the **^{1}1-H** complex.

8. Pathway III.

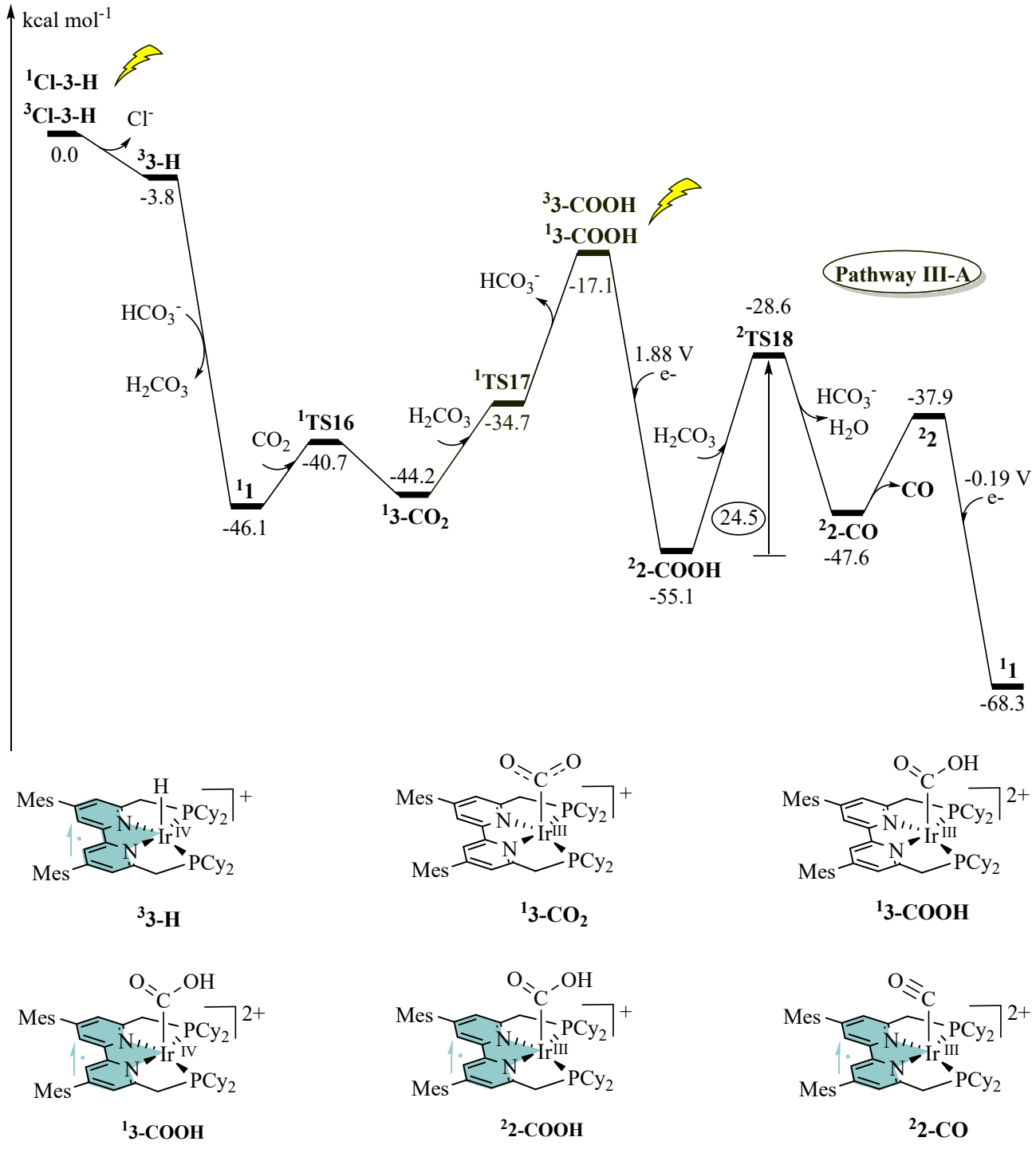


Figure S14. Gibbs free energy diagram (in kcal mol^{-1}) for the reduction of CO_2 to CO involving the deprotonation of **Cl-3-H** under photoexcitation.

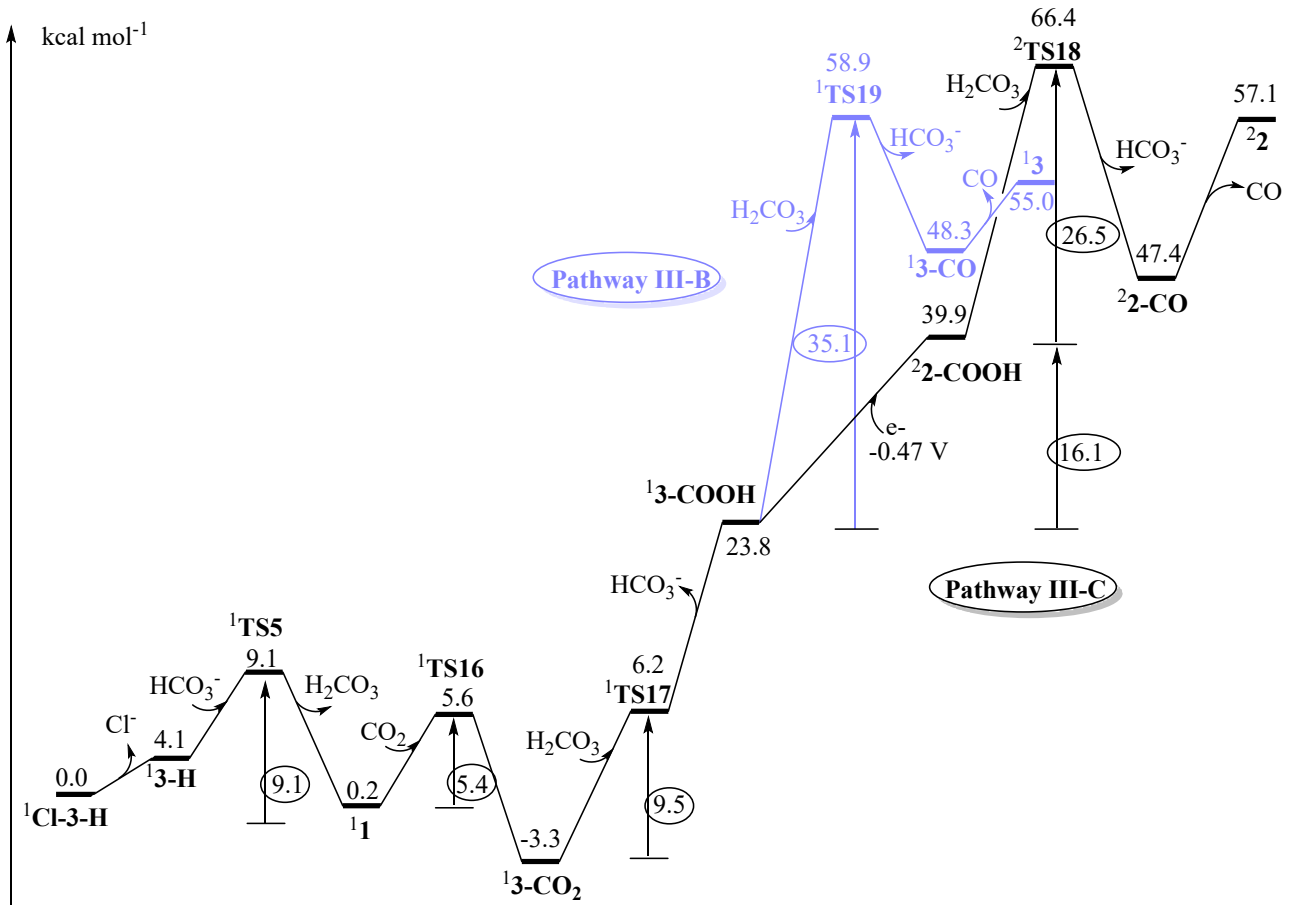


Figure S15. Gibbs free energy diagram (in kcal mol^{-1}) for the reduction of CO_2 to CO involving the deprotonation of **Cl-3-H** in dark.

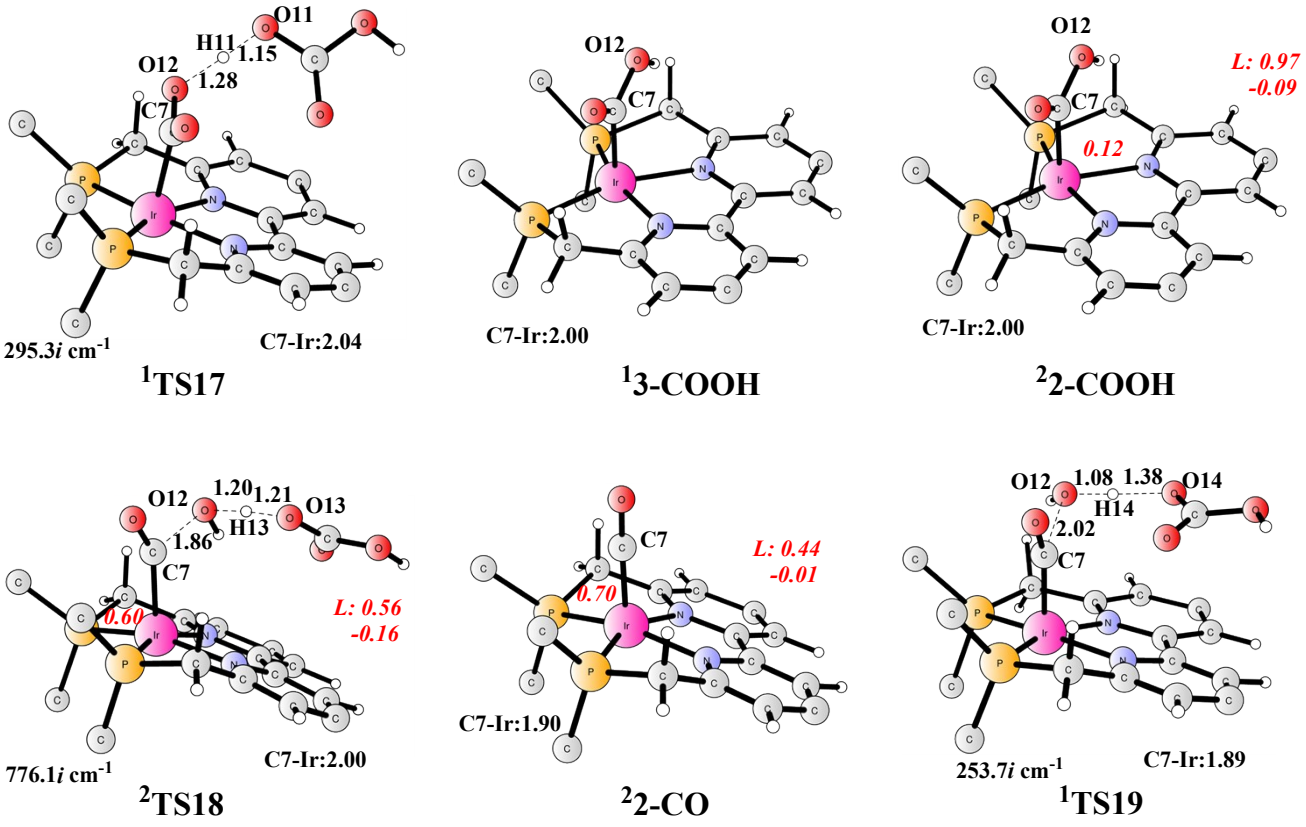


Figure S16. The optimized structures of ^{1}**TS17** (total charge of +1), ^{1}**3-COOH** (total charge of +2), ^{2}**2-COOH** (total charge of +1), ^{2}**TS18** (total charge of +1), ^{2}**2-CO** (total charge of +2), and ^{1}**TS19** (total charge of +2). The spin multiplicities of the species are indicated by the numbers in the left superscript. Distances are given in Ångstroms. The spin populations of Ir and the ligand are shown in red italic and the imaginary frequencies for all transition states are also shown. For clarity, the four Cy groups are shown with only one C atom, two trimethylphenyl groups and unimportant hydrogen atoms are not shown.

Hydricity, $\Delta G°_{H-}$, is defined as the heterolytic bond dissociation free energy of the hydride dissociation reaction, namely, $MH \rightarrow M^+ + H^-$, which measures the strength of the $M^+–H^-$ interaction in a hydride donor. By definition, a MH complex with a more positive value of hydricity ($\Delta G°_{H-}$) corresponds to a lower hydride donating ability (less hydridic).

We have calculated the hydricity ($\Delta G°_{H-}$) [1-6] of critical intermediates, including $HCOO^-$, BIH, and Ir-H at different oxidation states (including **3-H**, **2-H**, and **1-H**). The results suggest an hydricity order of **3-H (**148.0 kcal mol^{-1}**)** > **2-H (**67.2 kcal mol^{-1}**)** > BIH (53.3 kcal mol^{-1}) > $HCOO^-$ (52.6 kcal mol^{-1}) > **1-H (**34.7 kcal mol^{-1}**)** by using the formula developed by Muckerman[1] et al. The order of hydricity calculated with the method developed by Ye[2] et al is the same as above: **3-H (**124.0 kcal mol^{-1}**)** > **2-H (**50.1 kcal mol^{-1}**)** > BIH (37.4 kcal mol^{-1}) > $HCOO^-$ (36.7 kcal mol^{-1}) > **1-H (**20.4 kcal mol^{-1}**)**, albert with different absolute values. Therefore, these results suggest an order of the hydride donor ability as **3-H** < **2-H** < $HCOO^-$ < BIH < **1-H**. Clearly, **3-H** is the most suitable one for CO_2 reduction to produce formate via direct hydride transfer.

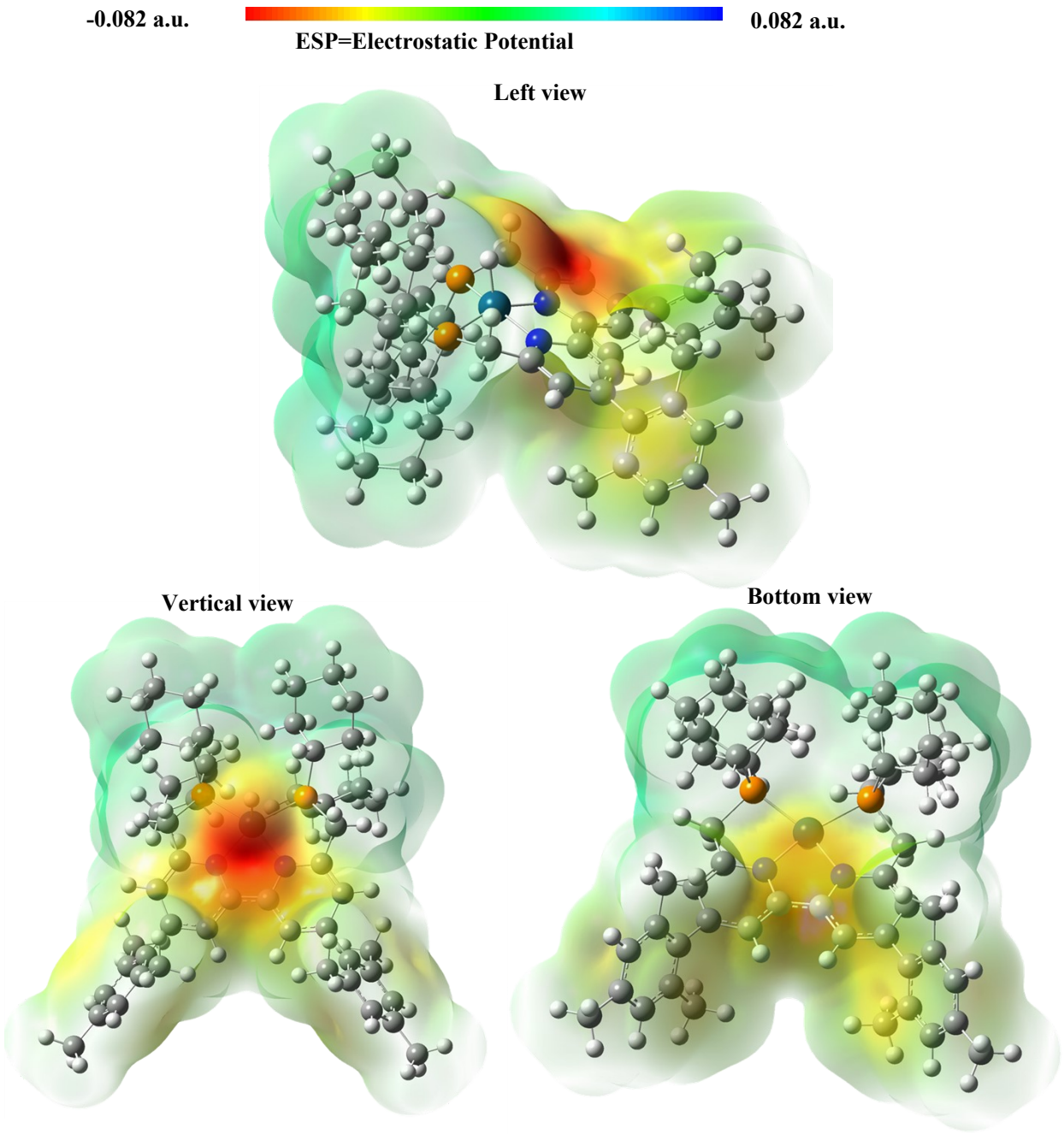


Figure S17. Left view (up), vertical view (down left), and bottom view (down right) of electrostatic potential for **[1]1-H**. The isosurface plot is depicted at 0.001 au. The electrostatic potential on the hydride (red) is more negative than that on Ir center (yellow).

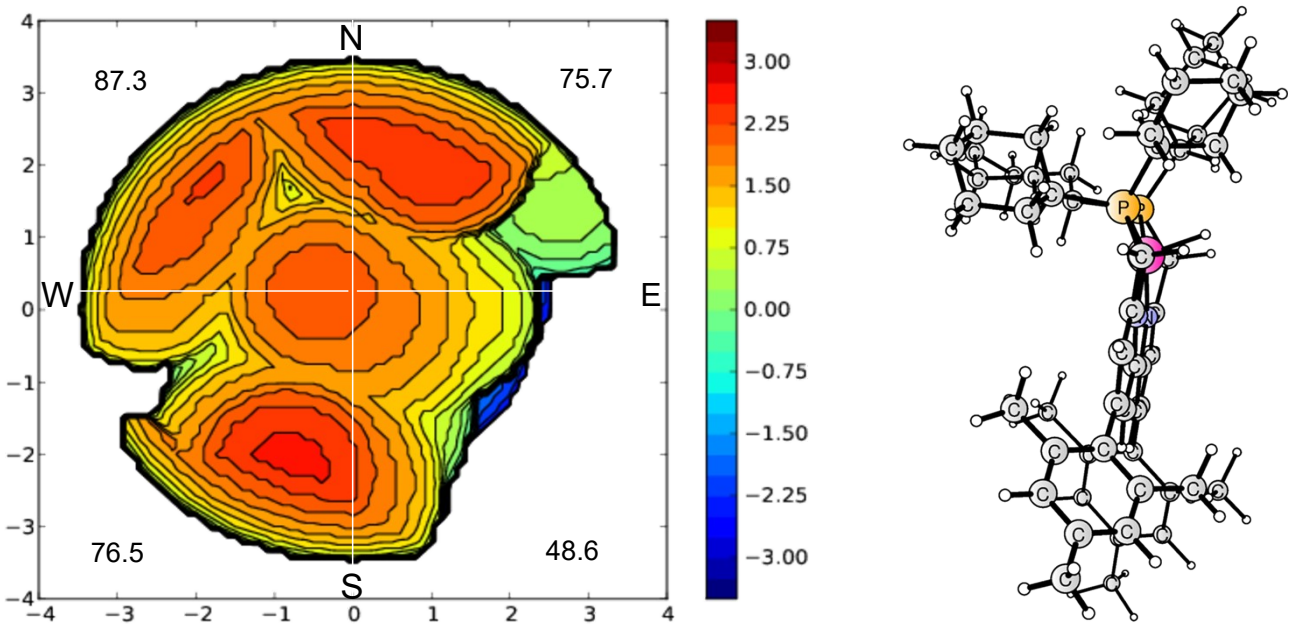


Figure S18. The steric contour map analysis for the active species ^{1}**1-H**.

9. Energies.

Table S5. Table of energies.

Species	Opt（hartree）	Gibbs energy correction (hartree)	Large basis set (hartree)	The lowest frequency (cm^{-1})
^{1}Cl-3-H	-3460.23743	1.08434	-3460.89946	8.8*i*
^{3}Cl-3-H	-3460.13761	1.08226	-3460.80225	11.2*i*
^{2}Cl-2-H	-3460.33292	1.07869	-3461.00112	9.8*i*
^{2}2-H	-2999.95635	1.08116	-3000.58650	12.5*i*
^{1}1-H	-3000.05209	1.07945	-3000.68557	11.1*i*
^{2}Cl-2	-3459.60654	1.07487	-3460.26945	12.4*i*
^{2}2	-2999.22280	1.07525	-2999.84863	12.0*i*
^{2}2-OCHO	-3188.54551	1.09360	-3189.24347	11.3*i*
^{2}2(-H)	-2998.71939	1.06192	-2999.35067	12.0*i*
^{1}1-OCHO	-3188.66519	1.08985	-3189.37493	13.7*i*
^{1}1	-2999.36468	1.07405	-2999.99219	9.8*i*
^{1}3-H	-2999.84735	1.08530	-3000.47308	8.2*i*
$^{1}O_2$C-3-H	-3188.66234	1.09221	-3189.36305	11.9*i*
^{1}HOOC-3-H	-3189.16283	1.10673	-3189.85775	10.7*i*
^{3}HOOC-3-H	-3189.08001	1.10249	-3189.77762	11.0*i*
^{2}HOOC-2-H	-3189.25857	1.10045	-3189.95948	9.2*i*
^{2}OC-2-H	-3113.29416	1.08675	-3113.96461	9.7*i*
^{1}H-3-H	-3000.56804	1.09302	-3001.19435	-35.9*i*
^{2}TS1	-3648.90161	1.08506	-3649.64101	-1373.9*i*
^{2}TS2	-3188.53636	1.08598	-3189.23830	-687.1*i*
^{2}TS3	-3188.51229	1.08941	-3189.20962	-141.2*i*
^{1}TS4	-3188.63894	1.08342	-3189.34579	-478.9*i*
^{1}TS5	-3264.40904	1.10569	-3265.13961	-476.2*i*
^{1}TS6	-3453.72763	1.12508	-3454.53559	-5960*i*
^{1}TS7	-3188.64493	1.08721	-3189.34903	-932.6*i*
^{1}TS8	-3263.89302	1.08996	-3264.62975	-962.6*i*
^{1}TS9	-3265.09025	1.10988	-3265.82214	-1385.3*i*
^{1}TS10	-3189.15692	1.099442	-3189.85685	-432.9*i*
^{1}TS11	-3188.64389	1.088745	-3189.34813	-207.6*i*
^{1}TS12	-3453.71931	1.12386	-3454.52408	-321.7*i*
^{1}TS13	-3454.28413	1.13172	-3455.09315	-684.3*i*
^{1}TS14	-3454.18762	1.13867	-3454.99029	-665.7*i*

^{1}TS15	-3377.72450	1.11438	-3378.49545	-429.9*i*
^{1}TS16	-3187.96029	1.08429	-3188.65993	-165.7*i*
^{1}TS17	-3453.02006	1.11733	-3453.82201	-295.3*i*
^{2}TS18	-3453.56827	1.12539	-3454.37044	-776.1*i*
^{1}TS19	-3453.43435	1.13932	-3454.23604	-253.7*i*
^{1}TS20	-3265.07291	1.10702	-3265.80100	-603.9*i*

10. Cartesian coordinates.

^{1}Cl-3-H E(opt)= -3460.23743 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.742842	-0.078179	-0.274087
2	1	0	-1.013343	-0.146994	-1.822842
3	15	0	-1.970034	-2.034825	-0.090445
4	15	0	-2.066613	1.832845	-0.216752
5	6	0	2.106043	-0.753731	-0.350669
6	6	0	0.762427	-2.700944	-0.399915
7	6	0	3.264233	-1.520304	-0.284772
8	6	0	1.899092	-3.504263	-0.307559
9	6	0	3.169273	-2.919070	-0.247369
10	1	0	4.237328	-1.044949	-0.258162
11	1	0	1.790333	-4.582795	-0.289510
12	6	0	2.070406	0.726033	-0.381430
13	6	0	0.638646	2.601734	-0.551693
14	6	0	3.187129	1.550667	-0.303971
15	6	0	1.732022	3.463112	-0.466540
16	6	0	3.024914	2.943167	-0.332308
17	1	0	4.177755	1.125067	-0.202023
18	1	0	1.572428	4.534637	-0.509266
19	6	0	4.396067	-3.761784	-0.149142
20	6	0	4.826053	-4.507537	-1.266456
21	6	0	5.118422	-3.803398	1.061934
22	6	0	5.982417	-5.286921	-1.150796
23	6	0	6.264588	-4.602650	1.134647

24	6	0	6.712508	-5.352201	0.041165
25	1	0	6.321923	-5.854425	-2.014437
26	1	0	6.820190	-4.640832	2.068993
27	6	0	4.205620	3.847070	-0.216783
28	6	0	5.108549	3.964772	-1.293593
29	6	0	4.413185	4.571404	0.975930
30	6	0	6.209308	4.818339	-1.158861
31	6	0	5.531832	5.406393	1.069761
32	6	0	6.438845	5.547119	0.013255
33	1	0	6.903940	4.915041	-1.990276
34	1	0	5.700590	5.956711	1.992758
35	6	0	7.934154	-6.231280	0.153877
36	1	0	7.660146	-7.238769	0.493022
37	1	0	8.440236	-6.340344	-0.810556
38	1	0	8.651749	-5.829929	0.876456
39	6	0	4.073260	-4.459981	-2.576358
40	1	0	3.090621	-4.938427	-2.493859
41	1	0	3.897219	-3.428287	-2.901363
42	1	0	4.628965	-4.974560	-3.364870
43	6	0	4.666958	-3.014595	2.269804
44	1	0	4.776422	-1.935554	2.110534
45	1	0	3.609887	-3.195527	2.495378
46	1	0	5.253584	-3.281942	3.152853
47	6	0	4.898026	3.197847	-2.578889
48	1	0	5.031634	2.119861	-2.431529
49	1	0	3.884643	3.340960	-2.970812
50	1	0	5.607706	3.519679	-3.345770
51	6	0	3.464303	4.441325	2.145361
52	1	0	2.481550	4.869627	1.916799
53	1	0	3.297307	3.391583	2.412395

54	1	0	3.856799	4.957928	3.025370
55	6	0	7.617181	6.483337	0.125834
56	1	0	8.447917	6.161148	-0.509786
57	1	0	7.341131	7.498402	-0.188093
58	1	0	7.978198	6.550661	1.157093
59	7	0	0.888602	-1.360263	-0.398927
60	7	0	0.828036	1.270106	-0.485175
61	6	0	-0.627656	-3.254046	-0.575591
62	6	0	-0.771446	3.069042	-0.788987
63	1	0	-0.764732	-3.452207	-1.646090
64	1	0	-0.740873	-4.209944	-0.058451
65	1	0	-0.934701	4.068189	-0.383232
66	1	0	-0.908351	3.143223	-1.875182
67	17	0	-0.079297	0.015141	2.250944
68	6	0	-2.458881	-2.537475	1.629255
69	6	0	-3.304833	-1.466169	2.345671
70	6	0	-3.116141	-3.924157	1.767327
71	1	0	-1.479286	-2.563167	2.127614
72	6	0	-3.489984	-1.827911	3.827132
73	1	0	-4.289458	-1.391987	1.869529
74	1	0	-2.818937	-0.494162	2.257208
75	6	0	-3.285761	-4.286387	3.252406
76	1	0	-4.104617	-3.901845	1.293537
77	1	0	-2.529715	-4.696045	1.256938
78	6	0	-4.105694	-3.223540	3.997315
79	1	0	-4.116083	-1.070589	4.314764
80	1	0	-2.510721	-1.799235	4.325605
81	1	0	-3.764593	-5.269245	3.339704
82	1	0	-2.293089	-4.373182	3.716547
83	1	0	-4.183861	-3.479623	5.060942

84	1	0	-5.129834	-3.216255	3.596948
85	6	0	-3.319485	-2.345348	-1.327566
86	6	0	-3.644619	-3.818706	-1.655861
87	6	0	-4.607161	-1.573623	-0.978962
88	1	0	-2.889136	-1.891058	-2.231680
89	6	0	-4.650982	-3.890579	-2.817365
90	1	0	-4.078328	-4.309834	-0.779205
91	1	0	-2.738778	-4.373428	-1.920494
92	6	0	-5.610125	-1.648542	-2.139668
93	1	0	-5.061311	-2.017209	-0.084325
94	1	0	-4.376126	-0.531625	-0.739110
95	6	0	-5.931696	-3.104343	-2.504546
96	1	0	-4.888344	-4.939467	-3.032035
97	1	0	-4.184010	-3.478150	-3.723119
98	1	0	-6.525786	-1.106381	-1.874252
99	1	0	-5.182127	-1.142320	-3.014886
100	1	0	-6.617834	-3.139765	-3.359365
101	1	0	-6.450287	-3.581931	-1.660921
102	6	0	-2.657708	2.341342	1.483236
103	6	0	-2.323149	3.780508	1.921325
104	6	0	-4.154252	2.028962	1.700490
105	1	0	-2.082034	1.669399	2.128356
106	6	0	-2.724195	3.991972	3.391680
107	1	0	-2.849997	4.504365	1.286695
108	1	0	-1.250445	3.973223	1.811022
109	6	0	-4.527080	2.225878	3.177351
110	1	0	-4.767901	2.700996	1.088261
111	1	0	-4.387193	1.006434	1.386388
112	6	0	-4.199689	3.651758	3.642169
113	1	0	-2.514806	5.028038	3.684198

114	1	0	-2.094710	3.350163	4.024381
115	1	0	-5.592615	2.010084	3.321835
116	1	0	-3.969088	1.503089	3.789061
117	1	0	-4.440152	3.771718	4.705488
118	1	0	-4.832948	4.362184	3.091445
119	6	0	-3.472202	2.123131	-1.400021
120	6	0	-3.836854	3.618903	-1.537358
121	6	0	-3.231660	1.483925	-2.781379
122	1	0	-4.323173	1.605950	-0.941111
123	6	0	-5.054416	3.804890	-2.456105
124	1	0	-2.987161	4.164723	-1.966595
125	1	0	-4.038607	4.060148	-0.557015
126	6	0	-4.443602	1.697105	-3.703001
127	1	0	-2.340713	1.928690	-3.245969
128	1	0	-3.033306	0.414296	-2.668937
129	6	0	-4.809950	3.180690	-3.835459
130	1	0	-5.281774	4.873503	-2.551010
131	1	0	-5.931885	3.332054	-1.992477
132	1	0	-4.236191	1.260917	-4.687736
133	1	0	-5.303547	1.153036	-3.290158
134	1	0	-5.696321	3.297808	-4.470573
135	1	0	-3.988697	3.715970	-4.333434

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^{3}Cl-3-H E(opt)= -3460.137613 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.716388	-0.105611	-0.197211
2	1	0	-1.142856	-0.329858	-1.698353

3	15	0	-1.910717	-2.167087	0.037365
4	15	0	-2.087197	1.813594	-0.330309
5	6	0	2.139608	-0.761117	-0.415046
6	6	0	0.853068	-2.753402	-0.175435
7	6	0	3.329418	-1.519152	-0.343141
8	6	0	2.006337	-3.521762	-0.073833
9	6	0	3.271901	-2.891537	-0.152126
10	1	0	4.288692	-1.024209	-0.441872
11	1	0	1.930267	-4.596058	0.047249
12	6	0	2.054195	0.655684	-0.577771
13	6	0	0.539075	2.519082	-0.947247
14	6	0	3.117342	1.566801	-0.459060
15	6	0	1.572519	3.405960	-0.838052
16	6	0	2.911060	2.934118	-0.565398
17	1	0	4.107274	1.188386	-0.231210
18	1	0	1.385317	4.464434	-0.971740
19	6	0	4.521547	-3.702055	-0.047998
20	6	0	4.966647	-4.452923	-1.155354
21	6	0	5.248145	-3.713303	1.160140
22	6	0	6.139883	-5.206126	-1.034191
23	6	0	6.414490	-4.483212	1.240381
24	6	0	6.875874	-5.237641	0.155923
25	1	0	6.488470	-5.779225	-1.890700
26	1	0	6.975101	-4.494027	2.172633
27	6	0	4.018493	3.904476	-0.387196
28	6	0	5.158917	3.858114	-1.226059
29	6	0	3.937138	4.886686	0.633162
30	6	0	6.181551	4.794151	-1.036146
31	6	0	4.989806	5.792333	0.791154
32	6	0	6.118637	5.769817	-0.036224

33	1	0	7.049358	4.762767	-1.691522
34	1	0	4.931593	6.530216	1.588610
35	6	0	8.118059	-6.087174	0.275468
36	1	0	7.867221	-7.103493	0.606267
37	1	0	8.635700	-6.178302	-0.684857
38	1	0	8.819398	-5.672082	1.006237
39	6	0	4.204112	-4.433957	-2.459695
40	1	0	3.200189	-4.858499	-2.344011
41	1	0	4.072059	-3.410029	-2.828473
42	1	0	4.726150	-5.008324	-3.229839
43	6	0	4.779200	-2.914878	2.354602
44	1	0	4.820277	-1.837302	2.158332
45	1	0	3.738560	-3.148928	2.607502
46	1	0	5.397222	-3.120878	3.232878
47	6	0	5.297393	2.840667	-2.337060
48	1	0	5.618139	1.864489	-1.954641
49	1	0	4.352360	2.680487	-2.865040
50	1	0	6.045587	3.166507	-3.065454
51	6	0	2.765227	4.952044	1.588107
52	1	0	1.891363	5.428989	1.129477
53	1	0	2.449742	3.955640	1.914288
54	1	0	3.026215	5.534172	2.476531
55	6	0	7.220906	6.785916	0.131811
56	1	0	8.173821	6.413144	-0.256371
57	1	0	6.986160	7.711105	-0.410742
58	1	0	7.359012	7.055958	1.183912
59	7	0	0.927928	-1.415476	-0.302278
60	7	0	0.750017	1.168411	-0.771218
61	6	0	-0.518561	-3.373848	-0.240447
62	6	0	-0.879343	2.904168	-1.248596

63	1	0	-0.643036	-3.772647	-1.253365
64	1	0	-0.604958	-4.221101	0.445172
65	1	0	-1.056630	3.964759	-1.069942
66	1	0	-1.075919	2.710912	-2.310174
67	17	0	-0.133826	0.079474	2.249823
68	6	0	-2.487534	-2.453149	1.782538
69	6	0	-3.371860	-1.313303	2.326071
70	6	0	-3.150103	-3.824261	2.024601
71	1	0	-1.533968	-2.422705	2.327410
72	6	0	-3.644162	-1.516960	3.824093
73	1	0	-4.325690	-1.292976	1.787601
74	1	0	-2.881447	-0.352572	2.163737
75	6	0	-3.409149	-4.020510	3.528845
76	1	0	-4.105834	-3.865655	1.490103
77	1	0	-2.526984	-4.639978	1.642762
78	6	0	-4.272945	-2.888977	4.102188
79	1	0	-4.296183	-0.714154	4.188979
80	1	0	-2.696155	-1.432161	4.373599
81	1	0	-3.892107	-4.991714	3.690202
82	1	0	-2.446521	-4.050201	4.058135
83	1	0	-4.417798	-3.031098	5.179864
84	1	0	-5.269545	-2.929073	3.639618
85	6	0	-3.202929	-2.611709	-1.219234
86	6	0	-3.416732	-4.125567	-1.452903
87	6	0	-4.553349	-1.920380	-0.939432
88	1	0	-2.780192	-2.187014	-2.140805
89	6	0	-4.396254	-4.348209	-2.617684
90	1	0	-3.824485	-4.586903	-0.547882
91	1	0	-2.472235	-4.630382	-1.675497
92	6	0	-5.522658	-2.145358	-2.109619

93	1	0	-4.990425	-2.346402	-0.028973
94	1	0	-4.415017	-0.851004	-0.758021
95	6	0	-5.735742	-3.640776	-2.376022
96	1	0	-4.549701	-5.424347	-2.761116
97	1	0	-3.944686	-3.964582	-3.543503
98	1	0	-6.477531	-1.650842	-1.895720
99	1	0	-5.113203	-1.672424	-3.011258
100	1	0	-6.401311	-3.783285	-3.235779
101	1	0	-6.234067	-4.096369	-1.508532
102	6	0	-2.483070	2.593318	1.320610
103	6	0	-2.077860	4.075050	1.457312
104	6	0	-3.949038	2.370970	1.754165
105	1	0	-1.850042	2.019084	2.005113
106	6	0	-2.306903	4.556132	2.899950
107	1	0	-2.664416	4.692292	0.765304
108	1	0	-1.022496	4.206177	1.195540
109	6	0	-4.149012	2.845687	3.201774
110	1	0	-4.622322	2.937085	1.099818
111	1	0	-4.225374	1.316027	1.663358
112	6	0	-3.751203	4.319477	3.361335
113	1	0	-2.048590	5.619127	2.976651
114	1	0	-1.621748	4.013611	3.566723
115	1	0	-5.194536	2.695537	3.496495
116	1	0	-3.536146	2.226823	3.872163
117	1	0	-3.872490	4.636353	4.404179
118	1	0	-4.429233	4.941374	2.759359
119	6	0	-3.606161	1.885154	-1.395605
120	6	0	-4.031065	3.344741	-1.689397
121	6	0	-3.455090	1.094441	-2.710927
122	1	0	-4.392529	1.408055	-0.797879

123	6	0	-5.331275	3.381780	-2.507711
124	1	0	-3.239970	3.844071	-2.262724
125	1	0	-4.159575	3.909812	-0.762319
126	6	0	-4.753728	1.150281	-3.531774
127	1	0	-2.636138	1.520026	-3.306091
128	1	0	-3.189559	0.055022	-2.504167
129	6	0	-5.188840	2.593157	-3.814853
130	1	0	-5.602246	4.424253	-2.713135
131	1	0	-6.146672	2.951902	-1.908981
132	1	0	-4.617509	0.596472	-4.468342
133	1	0	-5.549503	0.639882	-2.974052
134	1	0	-6.133395	2.602633	-4.371896
135	1	0	-4.438143	3.082265	-4.451938

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^{2}Cl-2-H E(opt)= -3460.332922 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.743347	-0.074654	-0.299036
2	1	0	-0.996573	-0.120874	-1.847946
3	15	0	-1.956671	-2.041688	-0.128864
4	15	0	-2.056633	1.842161	-0.204683
5	6	0	2.112528	-0.719271	-0.380518
6	6	0	0.767753	-2.704444	-0.442614
7	6	0	3.277838	-1.527298	-0.300480
8	6	0	1.890656	-3.512574	-0.346160
9	6	0	3.178883	-2.904830	-0.270471
10	1	0	4.254168	-1.056524	-0.255835
11	1	0	1.788220	-4.591754	-0.346901

12	6	0	2.076595	0.707402	-0.398271
13	6	0	0.638190	2.620988	-0.537909
14	6	0	3.197230	1.573934	-0.307082
15	6	0	1.717167	3.485825	-0.446925
16	6	0	3.032162	2.945854	-0.314718
17	1	0	4.192055	1.152729	-0.211596
18	1	0	1.561605	4.557725	-0.487439
19	6	0	4.398942	-3.761191	-0.168365
20	6	0	4.968643	-4.316235	-1.332670
21	6	0	4.973478	-4.019388	1.093091
22	6	0	6.108877	-5.119962	-1.215917
23	6	0	6.113185	-4.829208	1.168358
24	6	0	6.694900	-5.390464	0.025923
25	1	0	6.550721	-5.542483	-2.116068
26	1	0	6.556424	-5.026626	2.142285
27	6	0	4.205151	3.860479	-0.184429
28	6	0	5.098655	4.029466	-1.263125
29	6	0	4.418599	4.558251	1.024441
30	6	0	6.190029	4.894403	-1.114509
31	6	0	5.522853	5.411088	1.132967
32	6	0	6.419538	5.595333	0.074152
33	1	0	6.876311	5.024323	-1.948821
34	1	0	5.690210	5.939541	2.069338
35	6	0	7.903246	-6.289525	0.133453
36	1	0	7.603057	-7.337231	0.266183
37	1	0	8.520719	-6.241852	-0.769311
38	1	0	8.528126	-6.021074	0.991374
39	6	0	4.367150	-4.037540	-2.690395
40	1	0	3.331130	-4.390920	-2.748540
41	1	0	4.343033	-2.961808	-2.900487

42	1	0	4.937705	-4.526975	-3.484670
43	6	0	4.370872	-3.433072	2.348810
44	1	0	4.424486	-2.338352	2.345027
45	1	0	3.309950	-3.693671	2.440242
46	1	0	4.888797	-3.794245	3.241824
47	6	0	4.890153	3.298245	-2.569993
48	1	0	5.063121	2.221521	-2.461890
49	1	0	3.863880	3.416583	-2.935391
50	1	0	5.571780	3.670737	-3.340138
51	6	0	3.487452	4.373589	2.200586
52	1	0	2.478974	4.740616	1.978531
53	1	0	3.383371	3.313990	2.461830
54	1	0	3.854850	4.907881	3.081260
55	6	0	7.583852	6.547952	0.202111
56	1	0	8.416207	6.254242	-0.445404
57	1	0	7.292083	7.566608	-0.085408
58	1	0	7.951093	6.596162	1.232446
59	7	0	0.875933	-1.358864	-0.433769
60	7	0	0.810868	1.282725	-0.485200
61	6	0	-0.624743	-3.256551	-0.639073
62	6	0	-0.776212	3.089857	-0.774325
63	1	0	-0.766265	-3.425770	-1.713945
64	1	0	-0.744566	-4.224856	-0.146268
65	1	0	-0.946069	4.086255	-0.363398
66	1	0	-0.923154	3.166235	-1.859024
67	17	0	-0.083597	-0.021906	2.288347
68	6	0	-2.441727	-2.574268	1.585426
69	6	0	-3.292082	-1.518537	2.319221
70	6	0	-3.084626	-3.968115	1.714092
71	1	0	-1.460361	-2.595272	2.080715

72	6	0	-3.469243	-1.897641	3.797390
73	1	0	-4.279719	-1.444539	1.848700
74	1	0	-2.811003	-0.543159	2.239275
75	6	0	-3.244020	-4.348126	3.195920
76	1	0	-4.076170	-3.952541	1.245920
77	1	0	-2.493190	-4.728774	1.192501
78	6	0	-4.071146	-3.300910	3.955221
79	1	0	-4.100410	-1.151784	4.296521
80	1	0	-2.488556	-1.865642	4.292827
81	1	0	-3.712437	-5.336769	3.276549
82	1	0	-2.248426	-4.429109	3.655003
83	1	0	-4.143498	-3.569045	5.016441
84	1	0	-5.096852	-3.299285	3.558447
85	6	0	-3.322662	-2.343491	-1.355290
86	6	0	-3.654349	-3.810919	-1.701058
87	6	0	-4.607092	-1.573601	-0.991328
88	1	0	-2.900628	-1.879178	-2.258681
89	6	0	-4.667808	-3.867712	-2.857266
90	1	0	-4.083790	-4.312439	-0.827929
91	1	0	-2.750892	-4.364193	-1.977137
92	6	0	-5.617731	-1.631219	-2.146444
93	1	0	-5.057833	-2.026650	-0.099481
94	1	0	-4.372374	-0.534953	-0.739255
95	6	0	-5.944709	-3.081715	-2.528061
96	1	0	-4.909912	-4.913220	-3.083693
97	1	0	-4.205253	-3.445703	-3.760976
98	1	0	-6.531234	-1.090846	-1.869453
99	1	0	-5.194043	-1.114623	-3.017878
100	1	0	-6.635988	-3.105152	-3.379313
101	1	0	-6.459978	-3.568330	-1.687419

102	6	0	-2.636661	2.334572	1.506434
103	6	0	-2.309430	3.771236	1.957940
104	6	0	-4.127025	2.007721	1.741283
105	1	0	-2.047529	1.659981	2.137235
106	6	0	-2.692983	3.964055	3.435537
107	1	0	-2.850363	4.498604	1.338887
108	1	0	-1.240112	3.975057	1.835182
109	6	0	-4.484288	2.185650	3.224442
110	1	0	-4.755117	2.680055	1.143660
111	1	0	-4.355294	0.986310	1.419776
112	6	0	-4.162461	3.609026	3.701068
113	1	0	-2.488370	4.998381	3.738097
114	1	0	-2.050692	3.320177	4.053174
115	1	0	-5.546281	1.959742	3.380627
116	1	0	-3.912827	1.461156	3.821665
117	1	0	-4.390927	3.715734	4.768575
118	1	0	-4.808318	4.320260	3.165992
119	6	0	-3.482534	2.151164	-1.363645
120	6	0	-3.857462	3.645700	-1.476333
121	6	0	-3.257064	1.533144	-2.757411
122	1	0	-4.326969	1.622579	-0.905154
123	6	0	-5.085051	3.841269	-2.379813
124	1	0	-3.014360	4.202876	-1.904289
125	1	0	-4.051667	4.070960	-0.487276
126	6	0	-4.479863	1.753212	-3.662821
127	1	0	-2.373358	1.987482	-3.226765
128	1	0	-3.051649	0.462927	-2.662538
129	6	0	-4.853571	3.237126	-3.770430
130	1	0	-5.317984	4.910218	-2.457887
131	1	0	-5.956285	3.358699	-1.914108

132	1	0	-4.282509	1.331928	-4.656239
133	1	0	-5.333193	1.199775	-3.248190
134	1	0	-5.747037	3.360194	-4.394626
135	1	0	-4.039437	3.782249	-4.269558

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^{2}2-H E(opt)= -2999.95634475 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.794340	-0.079026	-0.396533
2	1	0	-1.117332	-0.137107	-1.914557
3	15	0	-1.964461	-2.061805	-0.140550
4	15	0	-2.080883	1.839269	-0.212721
5	6	0	2.065443	-0.719803	-0.352992
6	6	0	0.727257	-2.708124	-0.505823
7	6	0	3.227120	-1.518750	-0.261539
8	6	0	1.850888	-3.504039	-0.409098
9	6	0	3.134194	-2.900127	-0.271344
10	1	0	4.199836	-1.044803	-0.186575
11	1	0	1.755716	-4.583078	-0.455088
12	6	0	2.023361	0.716742	-0.371471
13	6	0	0.578605	2.621616	-0.592135
14	6	0	3.133612	1.582901	-0.270662
15	6	0	1.652099	3.482547	-0.495888
16	6	0	2.965059	2.957046	-0.311304
17	1	0	4.127218	1.166092	-0.150813
18	1	0	1.496295	4.552309	-0.576371
19	6	0	4.352356	-3.756286	-0.156652
20	6	0	4.924343	-4.323555	-1.314056

21	6	0	4.921487	-4.002063	1.109822
22	6	0	6.062070	-5.128558	-1.184455
23	6	0	6.058224	-4.814453	1.196990
24	6	0	6.642229	-5.388776	0.062273
25	1	0	6.506731	-5.560242	-2.078721
26	1	0	6.496855	-5.004045	2.174453
27	6	0	4.130203	3.878877	-0.173797
28	6	0	5.075461	3.990444	-1.215368
29	6	0	4.284300	4.640136	1.005826
30	6	0	6.158954	4.863806	-1.058965
31	6	0	5.384096	5.496819	1.123348
32	6	0	6.331563	5.625909	0.101079
33	1	0	6.884408	4.951229	-1.865052
34	1	0	5.506893	6.073421	2.037855
35	6	0	7.846905	-6.290676	0.183367
36	1	0	7.541786	-7.335230	0.328764
37	1	0	8.465941	-6.256830	-0.718858
38	1	0	8.470984	-6.013921	1.039176
39	6	0	4.330606	-4.056309	-2.677449
40	1	0	3.305297	-4.437305	-2.749801
41	1	0	4.281183	-2.981108	-2.885586
42	1	0	4.922802	-4.529025	-3.465854
43	6	0	4.315910	-3.403803	2.358552
44	1	0	4.383108	-2.309792	2.352273
45	1	0	3.251662	-3.652770	2.444193
46	1	0	4.823674	-3.767516	3.256240
47	6	0	4.932021	3.192872	-2.491874
48	1	0	5.117015	2.125689	-2.324554
49	1	0	3.921050	3.276375	-2.905858
50	1	0	5.640752	3.538772	-3.249672

51	6	0	3.295440	4.521708	2.143068
52	1	0	2.310828	4.914981	1.864975
53	1	0	3.145124	3.475633	2.433997
54	1	0	3.640430	5.073772	3.021755
55	6	0	7.490294	6.583778	0.237694
56	1	0	8.337749	6.280630	-0.385120
57	1	0	7.201788	7.596130	-0.074068
58	1	0	7.833460	6.651825	1.275270
59	7	0	0.829094	-1.350844	-0.431390
60	7	0	0.753870	1.274088	-0.480141
61	6	0	-0.660751	-3.246105	-0.761764
62	6	0	-0.833381	3.061807	-0.884307
63	1	0	-0.808414	-3.316390	-1.847413
64	1	0	-0.785292	-4.250421	-0.348551
65	1	0	-1.016958	4.087007	-0.559168
66	1	0	-0.980607	3.034031	-1.972105
67	6	0	-2.176236	-2.578689	1.637061
68	6	0	-2.787744	-1.470831	2.515618
69	6	0	-2.898915	-3.920044	1.863653
70	1	0	-1.126369	-2.701435	1.947545
71	6	0	-2.757574	-1.867679	3.999162
72	1	0	-3.825771	-1.291824	2.210359
73	1	0	-2.243633	-0.533220	2.366232
74	6	0	-2.853876	-4.313511	3.349451
75	1	0	-3.946136	-3.819328	1.554030
76	1	0	-2.454424	-4.711088	1.249743
77	6	0	-3.454427	-3.214438	4.237199
78	1	0	-3.228058	-1.080442	4.600768
79	1	0	-1.710919	-1.937939	4.328967
80	1	0	-3.388903	-5.259456	3.496888

81	1	0	-1.809362	-4.489412	3.643646
82	1	0	-3.384922	-3.498032	5.294305
83	1	0	-4.524451	-3.111367	4.005944
84	6	0	-3.470847	-2.381074	-1.169882
85	6	0	-3.821870	-3.850814	-1.477043
86	6	0	-4.692946	-1.621153	-0.615870
87	1	0	-3.184171	-1.904021	-2.118760
88	6	0	-5.000058	-3.915947	-2.464183
89	1	0	-4.099980	-4.371047	-0.555074
90	1	0	-2.956557	-4.375302	-1.896519
91	6	0	-5.868162	-1.697695	-1.601503
92	1	0	-4.992376	-2.067509	0.340782
93	1	0	-4.432346	-0.576693	-0.415523
94	6	0	-6.223224	-3.153628	-1.934616
95	1	0	-5.257949	-4.963579	-2.660703
96	1	0	-4.689007	-3.479553	-3.424075
97	1	0	-6.737565	-1.175468	-1.183903
98	1	0	-5.593688	-1.170473	-2.525269
99	1	0	-7.038365	-3.187972	-2.667527
100	1	0	-6.591960	-3.651527	-1.026310
101	6	0	-2.402680	2.313305	1.571732
102	6	0	-2.032819	3.755752	1.971320
103	6	0	-3.840986	1.969077	2.011513
104	1	0	-1.721202	1.645761	2.116558
105	6	0	-2.217768	3.954475	3.485696
106	1	0	-2.663655	4.468579	1.425501
107	1	0	-0.993228	3.972094	1.703430
108	6	0	-4.001009	2.156222	3.527174
109	1	0	-4.546489	2.632323	1.495555
110	1	0	-4.097849	0.943933	1.727565

111	6	0	-3.634633	3.586482	3.946964
112	1	0	-1.986133	4.993151	3.750726
113	1	0	-1.491031	3.322488	4.016118
114	1	0	-5.030623	1.920981	3.822537
115	1	0	-3.348626	1.442042	4.049248
116	1	0	-3.719791	3.699217	5.034552
117	1	0	-4.353597	4.286792	3.498158
118	6	0	-3.626542	2.162626	-1.185194
119	6	0	-3.998640	3.658207	-1.271230
120	6	0	-3.562138	1.521779	-2.585987
121	1	0	-4.414079	1.645577	-0.622748
122	6	0	-5.318801	3.850749	-2.034339
123	1	0	-3.202180	4.202222	-1.795402
124	1	0	-4.078841	4.091685	-0.269414
125	6	0	-4.880749	1.734720	-3.345952
126	1	0	-2.737297	1.968023	-3.158822
127	1	0	-3.348747	0.451973	-2.496764
128	6	0	-5.254517	3.220473	-3.431758
129	1	0	-5.550148	4.920415	-2.104981
130	1	0	-6.135000	3.385396	-1.463519
131	1	0	-4.801642	1.298833	-4.349309
132	1	0	-5.682058	1.191549	-2.826379
133	1	0	-6.213804	3.342080	-3.949200
134	1	0	-4.500324	3.749871	-4.031704

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^{1}1-H E(opt)= -3000.05209389 hartree

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

1	77	0	-0.815870	-0.066110	-0.644611
2	1	0	-1.416124	-0.118936	-2.140302
3	15	0	-1.943795	-2.037239	-0.255311
4	15	0	-2.070500	1.819525	-0.165757
5	6	0	2.060088	-0.694873	-0.571108
6	6	0	0.711193	-2.690635	-0.701765
7	6	0	3.215139	-1.513150	-0.444658
8	6	0	1.821212	-3.482807	-0.574286
9	6	0	3.120480	-2.886743	-0.414105
10	1	0	4.186253	-1.038373	-0.347770
11	1	0	1.720123	-4.562033	-0.615381
12	6	0	2.019948	0.718654	-0.538144
13	6	0	0.562075	2.639646	-0.572681
14	6	0	3.129588	1.593555	-0.393578
15	6	0	1.628423	3.486011	-0.430978
16	6	0	2.962417	2.958234	-0.311318
17	1	0	4.126102	1.168899	-0.330609
18	1	0	1.466882	4.558628	-0.431242
19	6	0	4.321093	-3.748509	-0.213392
20	6	0	5.322382	-3.832317	-1.205523
21	6	0	4.460213	-4.488838	0.984198
22	6	0	6.438149	-4.650877	-0.984734
23	6	0	5.590935	-5.291917	1.166019
24	6	0	6.591458	-5.390476	0.191774
25	1	0	7.204391	-4.714221	-1.754802
26	1	0	5.697433	-5.849442	2.094625
27	6	0	4.117902	3.878321	-0.109845
28	6	0	5.114975	4.012380	-1.102167
29	6	0	4.219766	4.627735	1.086497
30	6	0	6.186682	4.887893	-0.882608

31	6	0	5.307546	5.488747	1.266225
32	6	0	6.301737	5.637184	0.292054
33	1	0	6.948466	4.989582	-1.653073
34	1	0	5.385215	6.052377	2.194004
35	6	0	7.785176	-6.291250	0.399830
36	1	0	7.541268	-7.332735	0.152451
37	1	0	8.628233	-5.994497	-0.231874
38	1	0	8.118238	-6.279440	1.443209
39	6	0	5.210138	-3.061767	-2.502079
40	1	0	4.210180	-3.153944	-2.939231
41	1	0	5.390763	-1.990852	-2.354386
42	1	0	5.939002	-3.422353	-3.234004
43	6	0	3.422554	-4.400186	2.080335
44	1	0	3.186302	-3.357567	2.321770
45	1	0	2.479266	-4.874591	1.786239
46	1	0	3.773101	-4.891644	2.992493
47	6	0	5.046985	3.238658	-2.400306
48	1	0	5.318139	2.185788	-2.260798
49	1	0	4.037089	3.249149	-2.823356
50	1	0	5.733962	3.659992	-3.140360
51	6	0	3.190530	4.489185	2.185791
52	1	0	2.230795	4.937623	1.904538
53	1	0	2.988936	3.436372	2.413296
54	1	0	3.530011	4.978764	3.103185
55	6	0	7.446939	6.599799	0.495652
56	1	0	8.315991	6.324810	-0.110339
57	1	0	7.159759	7.620424	0.210411
58	1	0	7.758492	6.635448	1.545001
59	7	0	0.800774	-1.314272	-0.638140
60	7	0	0.725251	1.267519	-0.563308

61	6	0	-0.679318	-3.218486	-0.955641
62	6	0	-0.856363	3.096932	-0.793085
63	1	0	-0.862131	-3.226651	-2.039364
64	1	0	-0.799585	-4.241102	-0.588986
65	1	0	-1.029033	4.100500	-0.400649
66	1	0	-1.048379	3.128063	-1.874878
67	6	0	-2.077096	-2.617230	1.518914
68	6	0	-2.668979	-1.557280	2.463973
69	6	0	-2.755421	-3.981739	1.743198
70	1	0	-1.011500	-2.723834	1.778189
71	6	0	-2.546537	-1.996021	3.931082
72	1	0	-3.727145	-1.397761	2.221820
73	1	0	-2.156421	-0.603384	2.312146
74	6	0	-2.617153	-4.422607	3.210186
75	1	0	-3.821366	-3.896984	1.498897
76	1	0	-2.331533	-4.743942	1.080060
77	6	0	-3.192645	-3.368400	4.166276
78	1	0	-3.002945	-1.241336	4.583346
79	1	0	-1.481455	-2.046278	4.200214
80	1	0	-3.119629	-5.386689	3.356890
81	1	0	-1.553556	-4.580295	3.439564
82	1	0	-3.055099	-3.682310	5.208265
83	1	0	-4.276802	-3.288302	4.000013
84	6	0	-3.510734	-2.376126	-1.198502
85	6	0	-3.884127	-3.840212	-1.501945
86	6	0	-4.704976	-1.614921	-0.588296
87	1	0	-3.273685	-1.895425	-2.158875
88	6	0	-5.097639	-3.888060	-2.447158
89	1	0	-4.134404	-4.368037	-0.576379
90	1	0	-3.037638	-4.367864	-1.955586

91	6	0	-5.919371	-1.671134	-1.527145
92	1	0	-4.970721	-2.068477	0.375454
93	1	0	-4.429643	-0.573772	-0.388055
94	6	0	-6.295235	-3.120820	-1.867247
95	1	0	-5.372986	-4.931308	-2.644751
96	1	0	-4.817651	-3.445021	-3.413630
97	1	0	-6.770390	-1.152223	-1.068874
98	1	0	-5.678632	-1.130061	-2.453084
99	1	0	-7.135993	-3.140808	-2.571457
100	1	0	-6.636396	-3.626891	-0.952541
101	6	0	-2.327254	2.187360	1.665094
102	6	0	-1.898218	3.588124	2.149407
103	6	0	-3.753571	1.854485	2.149280
104	1	0	-1.643141	1.468569	2.134022
105	6	0	-2.009182	3.685545	3.680981
106	1	0	-2.530077	4.357068	1.687072
107	1	0	-0.865848	3.795494	1.848747
108	6	0	-3.841061	1.937780	3.680242
109	1	0	-4.462972	2.571219	1.716681
110	1	0	-4.056255	0.859726	1.806857
111	6	0	-3.414847	3.324820	4.180778
112	1	0	-1.734357	4.696179	4.007257
113	1	0	-1.279704	2.997772	4.132393
114	1	0	-4.862597	1.708535	4.007770
115	1	0	-3.186136	1.173028	4.120620
116	1	0	-3.449513	3.363725	5.276443
117	1	0	-4.131423	4.073962	3.814070
118	6	0	-3.677451	2.263173	-1.003555
119	6	0	-4.017131	3.767430	-0.944823
120	6	0	-3.755761	1.741586	-2.451173

121	1	0	-4.436455	1.720583	-0.425671
122	6	0	-5.397758	4.045981	-1.560463
123	1	0	-3.258228	4.332486	-1.501979
124	1	0	-3.991031	4.129501	0.087264
125	6	0	-5.133422	2.032759	-3.067077
126	1	0	-2.975136	2.220002	-3.059277
127	1	0	-3.557116	0.665955	-2.471004
128	6	0	-5.483885	3.525310	-3.001081
129	1	0	-5.607242	5.122271	-1.528177
130	1	0	-6.168582	3.553819	-0.950060
131	1	0	-5.156252	1.678526	-4.105132
132	1	0	-5.894979	1.458387	-2.520372
133	1	0	-6.485805	3.700829	-3.411701
134	1	0	-4.779986	4.089396	-3.630002

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^{2}Cl-2 E(opt)= -3459.606539 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.748825	-0.040425	-0.256504
2	15	0	-1.992535	-1.989815	-0.114850
3	15	0	-2.053351	1.877597	-0.205719
4	6	0	2.095783	-0.748853	-0.332422
5	6	0	0.729743	-2.679468	-0.446114
6	6	0	3.244516	-1.531351	-0.279093
7	6	0	1.856346	-3.498472	-0.369655
8	6	0	3.131922	-2.928718	-0.283027
9	1	0	4.223513	-1.069953	-0.229517
10	1	0	1.737028	-4.576109	-0.388080

11	6	0	2.077951	0.731679	-0.326486
12	6	0	0.671872	2.631334	-0.443519
13	6	0	3.205511	1.538271	-0.221044
14	6	0	1.777732	3.473733	-0.331718
15	6	0	3.063859	2.933336	-0.215991
16	1	0	4.190002	1.096816	-0.126074
17	1	0	1.633237	4.548269	-0.342233
18	6	0	4.349737	-3.787846	-0.203259
19	6	0	4.886046	-4.351266	-1.378284
20	6	0	4.955539	-4.022005	1.047563
21	6	0	6.032081	-5.148356	-1.279847
22	6	0	6.097937	-4.828338	1.101150
23	6	0	6.650387	-5.401455	-0.050068
24	1	0	6.452634	-5.578972	-2.185945
25	1	0	6.567278	-5.012126	2.065109
26	6	0	4.257325	3.818886	-0.089773
27	6	0	5.157266	3.940710	-1.169008
28	6	0	4.478495	4.525818	1.110886
29	6	0	6.267912	4.780348	-1.028469
30	6	0	5.606477	5.347705	1.210140
31	6	0	6.510172	5.492313	0.151394
32	1	0	6.960001	4.880006	-1.861680
33	1	0	5.785000	5.884821	2.139074
34	6	0	7.864656	-6.293936	0.036717
35	1	0	7.570722	-7.339815	0.194350
36	1	0	8.455352	-6.258346	-0.884135
37	1	0	8.511956	-6.009964	0.872551
38	6	0	4.248410	-4.091039	-2.722995
39	1	0	3.229538	-4.493043	-2.768339
40	1	0	4.173189	-3.016613	-2.927992

41	1	0	4.827629	-4.550530	-3.528357
42	6	0	4.382756	-3.420682	2.309680
43	1	0	4.413814	-2.325143	2.282046
44	1	0	3.331838	-3.702341	2.444769
45	1	0	4.939064	-3.751118	3.190930
46	6	0	4.933183	3.193825	-2.463941
47	1	0	5.062884	2.113156	-2.333856
48	1	0	3.917625	3.347389	-2.846086
49	1	0	5.638563	3.523823	-3.231379
50	6	0	3.533313	4.391994	2.282863
51	1	0	2.557112	4.841232	2.066762
52	1	0	3.349224	3.340938	2.532687
53	1	0	3.939011	4.886717	3.169468
54	6	0	7.698167	6.415629	0.269098
55	1	0	8.525706	6.087996	-0.367971
56	1	0	7.432828	7.434980	-0.040198
57	1	0	8.059588	6.474237	1.300711
58	7	0	0.870231	-1.338666	-0.404868
59	7	0	0.841003	1.293518	-0.426630
60	6	0	-0.666238	-3.209341	-0.650084
61	6	0	-0.730096	3.139337	-0.654921
62	1	0	-0.804044	-3.359776	-1.728269
63	1	0	-0.792083	-4.185578	-0.175299
64	1	0	-0.880336	4.098530	-0.156796
65	1	0	-0.850151	3.326046	-1.729048
66	17	0	-0.039885	0.047161	2.360923
67	6	0	-2.441142	-2.540767	1.603842
68	6	0	-3.264116	-1.489479	2.374760
69	6	0	-3.093605	-3.931234	1.722832
70	1	0	-1.447745	-2.579124	2.073887

71	6	0	-3.409933	-1.893755	3.849740
72	1	0	-4.261564	-1.399446	1.928935
73	1	0	-2.776627	-0.516444	2.301471
74	6	0	-3.223685	-4.334723	3.201282
75	1	0	-4.094422	-3.898487	1.275887
76	1	0	-2.520107	-4.688152	1.176503
77	6	0	-4.022996	-3.293105	3.996863
78	1	0	-4.021344	-1.150243	4.376015
79	1	0	-2.417626	-1.880508	4.322301
80	1	0	-3.699941	-5.320036	3.274683
81	1	0	-2.218944	-4.433403	3.636303
82	1	0	-4.073970	-3.579031	5.054582
83	1	0	-5.057161	-3.274176	3.623465
84	6	0	-3.375181	-2.273404	-1.325539
85	6	0	-3.701299	-3.736055	-1.696261
86	6	0	-4.656175	-1.523411	-0.909606
87	1	0	-2.977766	-1.783360	-2.227162
88	6	0	-4.747565	-3.775978	-2.823573
89	1	0	-4.099071	-4.261567	-0.822302
90	1	0	-2.800916	-4.272726	-2.011901
91	6	0	-5.699998	-1.566500	-2.035082
92	1	0	-5.075574	-1.999192	-0.014541
93	1	0	-4.424427	-0.487883	-0.642596
94	6	0	-6.022273	-3.011641	-2.439756
95	1	0	-4.985331	-4.818625	-3.066592
96	1	0	-4.315521	-3.328785	-3.730248
97	1	0	-6.610073	-1.043566	-1.716944
98	1	0	-5.309441	-1.024740	-2.907084
99	1	0	-6.737623	-3.024015	-3.270966
100	1	0	-6.507609	-3.522249	-1.595641

101	6	0	-2.777271	2.342483	1.451325
102	6	0	-2.593698	3.802139	1.908322
103	6	0	-4.256858	1.913846	1.558748
104	1	0	-2.193489	1.711218	2.131797
105	6	0	-3.122217	3.980172	3.342742
106	1	0	-3.126357	4.482048	1.231483
107	1	0	-1.535109	4.081767	1.881623
108	6	0	-4.757681	2.078102	3.000971
109	1	0	-4.870270	2.538578	0.897411
110	1	0	-4.385172	0.878209	1.230920
111	6	0	-4.581174	3.524837	3.482146
112	1	0	-3.017509	5.029157	3.645257
113	1	0	-2.494771	3.389002	4.024863
114	1	0	-5.810681	1.777865	3.063647
115	1	0	-4.192915	1.401270	3.657417
116	1	0	-4.910954	3.624807	4.523363
117	1	0	-5.224411	4.183296	2.880750
118	6	0	-3.350502	2.143145	-1.508519
119	6	0	-3.802282	3.609558	-1.668773
120	6	0	-2.898226	1.542274	-2.855753
121	1	0	-4.210377	1.558406	-1.160515
122	6	0	-4.901082	3.728587	-2.737508
123	1	0	-2.947515	4.229520	-1.968869
124	1	0	-4.165102	4.004228	-0.714759
125	6	0	-3.997607	1.684386	-3.919877
126	1	0	-1.992361	2.056258	-3.205962
127	1	0	-2.634003	0.486559	-2.722061
128	6	0	-4.443436	3.143970	-4.080331
129	1	0	-5.188577	4.780425	-2.854275
130	1	0	-5.795850	3.190136	-2.394021

131	1	0	-3.640093	1.283277	-4.876043
132	1	0	-4.862644	1.076021	-3.622989
133	1	0	-5.248890	3.215603	-4.821170
134	1	0	-3.603184	3.739458	-4.465591

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^{2}2 E(opt)= -2999.22279505 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.787990	-0.058765	-0.297777
2	15	0	-1.979863	-2.042188	-0.081248
3	15	0	-2.096838	1.864749	-0.236720
4	6	0	2.070336	-0.736797	-0.232226
5	6	0	0.731552	-2.687100	-0.422538
6	6	0	3.227651	-1.505090	-0.178853
7	6	0	1.869641	-3.490515	-0.353876
8	6	0	3.134476	-2.904671	-0.228920
9	1	0	4.200085	-1.032485	-0.109821
10	1	0	1.767935	-4.568259	-0.414757
11	6	0	2.033998	0.746868	-0.236479
12	6	0	0.610433	2.629465	-0.482522
13	6	0	3.146663	1.571340	-0.121608
14	6	0	1.703269	3.487883	-0.365955
15	6	0	2.988465	2.964951	-0.178188
16	1	0	4.133671	1.147332	0.016717
17	1	0	1.551496	4.559106	-0.435656
18	6	0	4.363081	-3.749649	-0.175789
19	6	0	4.882936	-4.297380	-1.366008
20	6	0	4.992879	-3.989739	1.061970

21	6	0	6.037553	-5.084610	-1.294928
22	6	0	6.142392	-4.787076	1.087531
23	6	0	6.679233	-5.344471	-0.078676
24	1	0	6.446056	-5.502354	-2.212404
25	1	0	6.629440	-4.976830	2.041419
26	6	0	4.170511	3.865856	-0.055010
27	6	0	5.092486	3.957448	-1.118325
28	6	0	4.358496	4.615569	1.124922
29	6	0	6.193359	4.810538	-0.982222
30	6	0	5.478438	5.448315	1.220993
31	6	0	6.404628	5.563385	0.177963
32	1	0	6.902194	4.887968	-1.803543
33	1	0	5.632373	6.018176	2.134615
34	6	0	7.901717	-6.227838	-0.022123
35	1	0	7.618261	-7.277400	0.129972
36	1	0	8.475569	-6.178498	-0.952893
37	1	0	8.561294	-5.947188	0.805121
38	6	0	4.221353	-4.031423	-2.698114
39	1	0	3.213612	-4.460985	-2.739216
40	1	0	4.114712	-2.956256	-2.884222
41	1	0	4.803094	-4.461694	-3.517578
42	6	0	4.435832	-3.409625	2.340956
43	1	0	4.451464	-2.313565	2.325761
44	1	0	3.391952	-3.708822	2.492887
45	1	0	5.013425	-3.742035	3.207543
46	6	0	4.901383	3.165877	-2.391701
47	1	0	5.026311	2.090281	-2.221062
48	1	0	3.896384	3.306896	-2.805459
49	1	0	5.627023	3.468793	-3.151222
50	6	0	3.386382	4.515425	2.277917

51	1	0	2.409145	4.938798	2.018312
52	1	0	3.213455	3.472831	2.568351
53	1	0	3.761458	5.053924	3.152312
54	6	0	7.583883	6.498142	0.291731
55	1	0	8.417907	6.170284	-0.336512
56	1	0	7.311231	7.511542	-0.030327
57	1	0	7.938427	6.571746	1.324823
58	7	0	0.853872	-1.345467	-0.332901
59	7	0	0.795112	1.295382	-0.391041
60	6	0	-0.655045	-3.229243	-0.668891
61	6	0	-0.789762	3.096164	-0.789128
62	1	0	-0.789690	-3.338312	-1.752683
63	1	0	-0.775781	-4.222085	-0.227571
64	1	0	-0.968717	4.102389	-0.407195
65	1	0	-0.886159	3.151983	-1.880873
66	6	0	-2.213250	-2.535553	1.697146
67	6	0	-2.846926	-1.421702	2.553485
68	6	0	-2.930607	-3.879313	1.926933
69	1	0	-1.166922	-2.646422	2.023591
70	6	0	-2.827050	-1.802194	4.041556
71	1	0	-3.883846	-1.260986	2.236380
72	1	0	-2.314626	-0.478064	2.398775
73	6	0	-2.899941	-4.255973	3.417427
74	1	0	-3.974184	-3.787048	1.603037
75	1	0	-2.473835	-4.673975	1.326967
76	6	0	-3.516565	-3.151380	4.287048
77	1	0	-3.309704	-1.011940	4.629185
78	1	0	-1.783199	-1.860634	4.382233
79	1	0	-3.431286	-5.203251	3.568323
80	1	0	-1.857777	-4.422988	3.724668

81	1	0	-3.454800	-3.423029	5.347652
82	1	0	-4.584913	-3.058215	4.044724
83	6	0	-3.461053	-2.362546	-1.142172
84	6	0	-3.806992	-3.835622	-1.439956
85	6	0	-4.689105	-1.595648	-0.610512
86	1	0	-3.157259	-1.893049	-2.090082
87	6	0	-4.975671	-3.910173	-2.437508
88	1	0	-4.093247	-4.346461	-0.515327
89	1	0	-2.937278	-4.362907	-1.846382
90	6	0	-5.854565	-1.684808	-1.606322
91	1	0	-4.997707	-2.030228	0.348401
92	1	0	-4.429398	-0.549101	-0.420629
93	6	0	-6.204512	-3.144708	-1.926356
94	1	0	-5.229814	-4.960041	-2.625944
95	1	0	-4.655995	-3.482687	-3.398511
96	1	0	-6.727556	-1.159199	-1.201089
97	1	0	-5.573336	-1.167461	-2.533741
98	1	0	-7.013112	-3.188188	-2.665784
99	1	0	-6.579997	-3.633344	-1.015891
100	6	0	-2.623460	2.340707	1.490413
101	6	0	-2.401284	3.808940	1.902351
102	6	0	-4.077321	1.903393	1.769233
103	1	0	-1.963004	1.724093	2.115886
104	6	0	-2.768447	4.006391	3.383599
105	1	0	-3.014788	4.469997	1.277761
106	1	0	-1.355645	4.096362	1.749785
107	6	0	-4.418477	2.089128	3.254410
108	1	0	-4.759404	2.517114	1.167353
109	1	0	-4.234257	0.862658	1.470810
110	6	0	-4.199385	3.544104	3.691339

111	1	0	-2.639495	5.060992	3.654853
112	1	0	-2.063751	3.431682	4.001594
113	1	0	-5.456480	1.785599	3.435387
114	1	0	-3.782346	1.424729	3.856135
115	1	0	-4.411165	3.657851	4.761274
116	1	0	-4.910460	4.189698	3.156415
117	6	0	-3.509321	2.112169	-1.403456
118	6	0	-3.947769	3.581651	-1.562587
119	6	0	-3.205651	1.460689	-2.768579
120	1	0	-4.335450	1.553435	-0.946189
121	6	0	-5.153006	3.686821	-2.511006
122	1	0	-3.116428	4.169545	-1.973217
123	1	0	-4.197790	4.012303	-0.587967
124	6	0	-4.413681	1.584027	-3.710120
125	1	0	-2.338901	1.954444	-3.229392
126	1	0	-2.939484	0.406246	-2.628936
127	6	0	-4.854686	3.045128	-3.872872
128	1	0	-5.431915	4.739902	-2.635625
129	1	0	-6.014533	3.181073	-2.052418
130	1	0	-4.168360	1.144883	-4.684528
131	1	0	-5.247448	0.999507	-3.297816
132	1	0	-5.736395	3.104590	-4.522085
133	1	0	-4.054439	3.611165	-4.370935

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^{1}2-OCHO E(opt)= -3188.54550755 hartree

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	77	-0.000992926	0.001788960	-0.002264541

2	1	-0.000132797	0.000532453	-0.001110431
3	15	-0.000121331	-0.001083205	-0.000460247
4	15	0.001207849	-0.000779337	0.002048313
5	6	-0.000205296	-0.000373208	0.000149813
6	6	0.000378980	0.001803771	-0.000716672
7	6	-0.000026717	0.000770065	-0.000015109
8	6	0.000304724	-0.000484600	-0.000593454
9	6	-0.000234065	-0.000274520	0.000000588
10	1	0.000152285	0.000066259	-0.000438608
11	1	-0.000136034	0.000048395	0.000422901
12	6	-0.000339602	0.000082616	0.000028664
13	6	-0.000414353	-0.000271970	-0.000107232
14	6	0.000073165	-0.000303774	0.000267132
15	6	0.000039767	0.000255598	0.000150310
16	6	-0.000166860	-0.000040438	-0.000151149
17	1	-0.000188880	0.000008397	0.000246588
18	1	0.000048386	0.000006541	0.000067254
19	6	0.000046850	-0.000062153	0.000005555
20	6	-0.000055931	-0.000167487	0.000028730
21	6	-0.000035816	0.000044792	-0.000046415
22	6	-0.000031286	0.000023040	-0.000023661
23	6	-0.000007603	0.000016004	0.000007511
24	6	0.000024923	0.000005159	-0.000025694
25	1	0.000019140	0.000020083	0.000007900
26	1	-0.000018299	-0.000006644	-0.000009301
27	6	0.000040689	-0.000020623	0.000317554
28	6	-0.000046054	-0.000048928	0.000001909
29	6	0.000037972	-0.000021843	-0.000114643
30	6	-0.000038320	-0.000032588	-0.000095413
31	6	0.000015655	0.000036084	-0.000050147

32	6	-0.000008688	0.000078306	0.000125433
33	1	-0.000046537	-0.000047215	-0.000000396
34	1	0.000039172	0.000005389	0.000001629
35	6	0.000005217	0.000008792	0.000005852
36	1	-0.000009504	0.000003327	0.000010153
37	1	-0.000008581	-0.000008301	-0.000003863
38	1	-0.000009257	-0.000010577	0.000018860
39	6	0.000080231	0.000022301	-0.000021972
40	1	0.000026044	0.000005330	-0.000003423
41	1	-0.000006687	0.000003895	-0.000029983
42	1	-0.000017922	-0.000007164	0.000009013
43	6	-0.000031157	-0.000051570	0.000006739
44	1	0.000033868	-0.000006593	0.000018915
45	1	0.000015200	0.000036751	0.000037555
46	1	-0.000008507	-0.000006734	0.000014123
47	6	0.000011955	-0.000072305	-0.000097845
48	1	0.000018587	0.000021488	-0.000078361
49	1	0.000013309	0.000011577	-0.000007140
50	1	0.000013811	-0.000004762	0.000007632
51	6	0.000085563	-0.000035057	-0.000036379
52	1	-0.000035813	0.000018263	-0.000047180
53	1	-0.000025448	0.000000096	-0.000028293
54	1	0.000003664	-0.000026829	-0.000009887
55	6	0.000004009	-0.000001323	0.000047731
56	1	-0.000010529	-0.000013036	-0.000004986
57	1	-0.000007960	-0.000013110	-0.000000938
58	1	0.000018956	-0.000002425	-0.000003212
59	7	0.000418305	-0.001609021	0.001723528
60	7	0.000970887	-0.000266428	0.000220420
61	6	-0.000346150	0.002134247	-0.000457808

62	6	0.000063030	-0.000181532	-0.000216937
63	1	-0.000073800	-0.002047900	0.001362654
64	1	-0.000093729	-0.000125167	0.000013778
65	1	-0.000169504	0.000302215	-0.000091350
66	1	-0.000263093	-0.000012721	-0.000039013
67	6	0.000424744	-0.000219180	-0.000865699
68	6	0.000000843	0.000246282	0.000386025
69	6	0.000144480	-0.000047098	0.000376207
70	1	0.000074005	0.000154059	0.000028022
71	6	-0.000046597	0.000113718	-0.000010019
72	1	-0.000265345	-0.000085603	-0.000340652
73	1	-0.000064765	0.000061890	0.000182579
74	6	0.000006533	-0.000092739	0.000010224
75	1	-0.000178461	0.000033867	-0.000301602
76	1	-0.000024776	-0.000007174	0.000046764
77	6	-0.000058670	0.000025277	-0.000139430
78	1	-0.000039221	-0.000054058	0.000090487
79	1	-0.000015734	0.000014750	-0.000032937
80	1	-0.000020075	0.000067483	0.000043694
81	1	0.000008326	-0.000017610	-0.000012444
82	1	0.000026148	-0.000005490	0.000028217
83	1	0.000015675	0.000001915	0.000018458
84	6	0.000471853	0.000299001	0.000929026
85	6	0.000269055	-0.000285464	-0.000160846
86	6	0.000084302	-0.000149466	-0.000368118
87	1	0.000259898	0.000361033	-0.000515999
88	6	-0.000073076	0.000057245	-0.000112178
89	1	0.000040127	0.000054126	0.000426997
90	1	-0.000323209	-0.000044121	-0.000010766
91	6	-0.000195590	0.000052815	-0.000058009

92	1	0.000153193	-0.000021307	0.000279186
93	1	-0.000038987	0.000172665	-0.000038420
94	6	0.000153052	-0.000014348	0.000191952
95	1	-0.000065572	0.000037614	0.000034037
96	1	0.000039575	-0.000053584	0.000047685
97	1	-0.000067655	-0.000058275	-0.000075053
98	1	-0.000011396	-0.000057867	0.000084409
99	1	0.000034670	0.000019222	-0.000033836
100	1	-0.000009810	0.000029677	-0.000007514
101	6	-0.000785463	0.000803938	-0.000114557
102	6	-0.000161054	0.000393680	-0.000106804
103	6	-0.000141630	-0.000110212	-0.000113473
104	1	0.000237759	-0.000052670	-0.000146564
105	6	-0.000170041	-0.000283545	-0.000035329
106	1	0.000194857	-0.000017892	0.000184202
107	1	0.000037205	-0.000138368	-0.000131107
108	6	0.000076553	0.000034120	0.000032250
109	1	-0.000051999	-0.000264982	0.000326795
110	1	0.000158801	-0.000169556	0.000019031
111	6	0.000155706	0.000020370	0.000120980
112	1	0.000064162	-0.000038435	-0.000188345
113	1	0.000008077	0.000004778	0.000063382
114	1	-0.000000013	-0.000035362	-0.000114019
115	1	0.000017881	0.000026513	0.000036589
116	1	-0.000103438	-0.000008550	0.000008432
117	1	-0.000014539	0.000002678	-0.000011034
118	6	0.000056499	-0.001490258	-0.001836962
119	6	0.000404268	0.000339372	0.000131330
120	6	-0.000267152	0.000449439	0.001655829
121	1	-0.000083909	-0.000424178	0.000145304

122	6	-0.000010783	0.000131318	-0.000142719
123	1	0.000160484	0.000009830	-0.000025545
124	1	-0.000083268	0.000211125	-0.000459431
125	6	-0.000131402	0.000196400	0.000104981
126	1	0.000615870	0.000404294	-0.000070274
127	1	-0.000889642	-0.000341626	-0.000196517
128	6	-0.000020396	-0.000129976	0.000116869
129	1	0.000085894	-0.000045740	0.000092676
130	1	-0.000092943	0.000003895	0.000094543
131	1	-0.000011024	-0.000158333	-0.000096008
132	1	0.000318409	0.000185975	-0.000054445
133	1	0.000080182	-0.000135354	-0.000112091
134	1	0.000031657	-0.000025118	-0.000037145
135	6	0.001058975	-0.002366051	0.001734357
136	8	-0.000027042	0.002100386	0.000859646
137	8	-0.001272200	0.000689734	-0.001828326

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^{2}2(-H) E(opt)= -2998.719393 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.769817	-0.097878	-0.163443
2	15	0	-1.961525	-2.105180	0.010909
3	15	0	-2.059132	1.851773	-0.160988
4	6	0	2.092519	-0.794013	-0.111393
5	6	0	0.683213	-2.758323	-0.153983
6	6	0	3.248462	-1.548986	-0.070152
7	6	0	1.883133	-3.552540	-0.108716
8	6	0	3.128706	-2.969980	-0.061732

9	1	0	4.226481	-1.085227	-0.050972
10	1	0	1.785598	-4.633750	-0.100034
11	6	0	2.069493	0.688931	-0.156126
12	6	0	0.664369	2.581333	-0.424875
13	6	0	3.193574	1.508132	-0.100811
14	6	0	1.766134	3.431761	-0.366371
15	6	0	3.050979	2.898955	-0.194949
16	1	0	4.179233	1.075232	0.018168
17	1	0	1.624492	4.501293	-0.474541
18	6	0	4.363345	-3.810038	0.011449
19	6	0	4.927257	-4.340477	-1.165831
20	6	0	4.965653	-4.057105	1.262234
21	6	0	6.087452	-5.118784	-1.071257
22	6	0	6.123798	-4.841073	1.314502
23	6	0	6.698593	-5.383752	0.159324
24	1	0	6.524785	-5.525079	-1.980877
25	1	0	6.587876	-5.032208	2.279876
26	6	0	4.246452	3.789486	-0.139915
27	6	0	5.138862	3.829523	-1.231518
28	6	0	4.477865	4.582394	1.003507
29	6	0	6.252721	4.673769	-1.160292
30	6	0	5.609080	5.405250	1.035457
31	6	0	6.505902	5.468728	-0.037156
32	1	0	6.938695	4.710313	-2.003739
33	1	0	5.795406	6.008580	1.921266
34	6	0	7.928366	-6.255570	0.244178
35	1	0	7.654328	-7.305350	0.412029
36	1	0	8.513091	-6.216749	-0.680370
37	1	0	8.576592	-5.954817	1.073695
38	6	0	4.297789	-4.069769	-2.512554

39	1	0	3.293546	-4.503752	-2.578817
40	1	0	4.187141	-2.993755	-2.691276
41	1	0	4.901744	-4.488981	-3.322082
42	6	0	4.369614	-3.490522	2.529840
43	1	0	4.341941	-2.394879	2.503817
44	1	0	3.335301	-3.827058	2.667126
45	1	0	4.945776	-3.794225	3.408218
46	6	0	4.903600	2.991223	-2.467251
47	1	0	5.032170	1.922469	-2.260520
48	1	0	3.885350	3.118989	-2.851672
49	1	0	5.603594	3.263045	-3.261912
50	6	0	3.538329	4.538448	2.186645
51	1	0	2.557690	4.960244	1.937778
52	1	0	3.364430	3.509941	2.523078
53	1	0	3.942735	5.107522	3.028026
54	6	0	7.698138	6.393168	0.004815
55	1	0	8.516111	6.021651	-0.620386
56	1	0	7.431953	7.391492	-0.366159
57	1	0	8.073567	6.516888	1.025652
58	7	0	0.860129	-1.380646	-0.146026
59	7	0	0.832210	1.248171	-0.284231
60	6	0	-0.615657	-3.262679	-0.193052
61	6	0	-0.730554	3.050189	-0.742930
62	1	0	-0.775931	-4.335333	-0.159722
63	1	0	-0.898089	4.073136	-0.403491
64	1	0	-0.822725	3.063771	-1.836470
65	6	0	-2.660883	-2.436750	1.717470
66	6	0	-3.499249	-1.284197	2.298760
67	6	0	-3.389325	-3.785423	1.870329
68	1	0	-1.732596	-2.489527	2.306753

69	6	0	-3.871159	-1.555460	3.764915
70	1	0	-4.417051	-1.154640	1.713811
71	1	0	-2.935919	-0.350496	2.223573
72	6	0	-3.748391	-4.048613	3.342209
73	1	0	-4.312846	-3.766529	1.279114
74	1	0	-2.771766	-4.602618	1.479520
75	6	0	-4.588050	-2.903184	3.925314
76	1	0	-4.498165	-0.739128	4.144314
77	1	0	-2.954051	-1.559839	4.371707
78	1	0	-4.287209	-5.000217	3.428469
79	1	0	-2.822382	-4.153357	3.925534
80	1	0	-4.811274	-3.093247	4.982255
81	1	0	-5.553132	-2.862106	3.399718
82	6	0	-3.236886	-2.438201	-1.306385
83	6	0	-3.484686	-3.923281	-1.641518
84	6	0	-4.566697	-1.699867	-1.062810
85	1	0	-2.758725	-1.982686	-2.187067
86	6	0	-4.419864	-4.052884	-2.855389
87	1	0	-3.940800	-4.429391	-0.783314
88	1	0	-2.534212	-4.427533	-1.846421
89	6	0	-5.492936	-1.833260	-2.281361
90	1	0	-5.066007	-2.132128	-0.187114
91	1	0	-4.383260	-0.643908	-0.837981
92	6	0	-5.742921	-3.306715	-2.632058
93	1	0	-4.608912	-5.112822	-3.065372
94	1	0	-3.916941	-3.638556	-3.741063
95	1	0	-6.441691	-1.318009	-2.086869
96	1	0	-5.029037	-1.330924	-3.140886
97	1	0	-6.378602	-3.383900	-3.522626
98	1	0	-6.291972	-3.785270	-1.808230

99	6	0	-2.629014	2.441674	1.526596
100	6	0	-2.229219	3.881267	1.906382
101	6	0	-4.142987	2.224195	1.741264
102	1	0	-2.095491	1.765148	2.207935
103	6	0	-2.637064	4.189477	3.357194
104	1	0	-2.716357	4.592705	1.226981
105	1	0	-1.148051	4.020476	1.800705
106	6	0	-4.526748	2.513585	3.200104
107	1	0	-4.703699	2.902953	1.087356
108	1	0	-4.435114	1.206043	1.469270
109	6	0	-4.131562	3.941242	3.600879
110	1	0	-2.376078	5.226983	3.598396
111	1	0	-2.050698	3.549853	4.032312
112	1	0	-5.604276	2.360737	3.335100
113	1	0	-4.018178	1.793741	3.856835
114	1	0	-4.379773	4.126278	4.652959
115	1	0	-4.718127	4.655658	3.005663
116	6	0	-3.435935	2.130943	-1.373096
117	6	0	-3.791160	3.613798	-1.608075
118	6	0	-3.137933	1.416166	-2.707305
119	1	0	-4.302782	1.634467	-0.918722
120	6	0	-4.977237	3.741174	-2.577654
121	1	0	-2.924921	4.132115	-2.039126
122	1	0	-4.022132	4.110848	-0.660650
123	6	0	-4.322358	1.557529	-3.676293
124	1	0	-2.242156	1.854780	-3.168924
125	1	0	-2.919841	0.357914	-2.526063
126	6	0	-4.691250	3.029382	-3.907175
127	1	0	-5.200561	4.800898	-2.750266
128	1	0	-5.870180	3.298904	-2.113408

129	1	0	-4.083006	1.066698	-4.627457
130	1	0	-5.189757	1.030664	-3.256667
131	1	0	-5.559699	3.102814	-4.572873
132	1	0	-3.858053	3.536156	-4.415032

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^{1}1-OCHO E(opt)= -3188.66519242 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.735106	0.012713	-0.187726
2	1	0	-2.475642	-1.404402	-4.271840
3	15	0	-1.930396	-1.887001	0.265498
4	15	0	-1.994205	1.916848	-0.182557
5	6	0	2.102636	-0.705548	-0.170558
6	6	0	0.718450	-2.631726	-0.164399
7	6	0	3.247707	-1.492592	-0.099952
8	6	0	1.844548	-3.450067	-0.074599
9	6	0	3.126346	-2.887400	-0.041208
10	1	0	4.230246	-1.035235	-0.099197
11	1	0	1.719832	-4.527325	-0.049995
12	6	0	2.087286	0.768482	-0.262027
13	6	0	0.681617	2.648495	-0.576569
14	6	0	3.208796	1.588650	-0.181471
15	6	0	1.779635	3.500361	-0.490561
16	6	0	3.063290	2.978696	-0.276575
17	1	0	4.190515	1.157934	-0.024273
18	1	0	1.634491	4.570129	-0.594589
19	6	0	4.340033	-3.753176	0.033173
20	6	0	4.888487	-4.287113	-1.150048

21	6	0	4.930130	-4.024336	1.283384
22	6	0	6.029235	-5.092875	-1.060003
23	6	0	6.069238	-4.836205	1.329479
24	6	0	6.632270	-5.381288	0.169775
25	1	0	6.457672	-5.502498	-1.972224
26	1	0	6.527366	-5.046614	2.293482
27	6	0	4.244308	3.880441	-0.143119
28	6	0	5.177255	3.981525	-1.195337
29	6	0	4.422068	4.621928	1.043922
30	6	0	6.277117	4.833760	-1.042714
31	6	0	5.539305	5.456551	1.157036
32	6	0	6.475898	5.579614	0.124301
33	1	0	6.995186	4.916070	-1.855703
34	1	0	5.683231	6.020931	2.075858
35	6	0	7.841553	-6.281798	0.245897
36	1	0	7.541361	-7.332133	0.354805
37	1	0	8.451425	-6.211825	-0.660474
38	1	0	8.472660	-6.034167	1.105357
39	6	0	4.263781	-3.988429	-2.492698
40	1	0	3.233670	-4.359701	-2.546276
41	1	0	4.217395	-2.909146	-2.679983
42	1	0	4.832642	-4.450332	-3.304141
43	6	0	4.344226	-3.450504	2.552086
44	1	0	4.355701	-2.354230	2.537475
45	1	0	3.297735	-3.751884	2.679484
46	1	0	4.902998	-3.783005	3.431109
47	6	0	4.996935	3.195454	-2.473374
48	1	0	5.095849	2.117542	-2.300778
49	1	0	4.002256	3.355460	-2.904941
50	1	0	5.742225	3.484551	-3.219328

51	6	0	3.439486	4.510802	2.187217
52	1	0	2.459725	4.921951	1.917700
53	1	0	3.274715	3.465851	2.474186
54	1	0	3.799189	5.052447	3.066301
55	6	0	7.653005	6.515130	0.256760
56	1	0	8.497119	6.188103	-0.358436
57	1	0	7.385747	7.528951	-0.068676
58	1	0	7.991714	6.588049	1.295297
59	7	0	0.865156	-1.283282	-0.183290
60	7	0	0.843852	1.310420	-0.424549
61	6	0	-0.682097	-3.151519	-0.324655
62	6	0	-0.717964	3.110595	-0.882324
63	1	0	-0.886200	-3.244533	-1.407195
64	1	0	-0.803560	-4.132724	0.142462
65	1	0	-0.874233	4.149086	-0.586175
66	1	0	-0.854849	3.063619	-1.970355
67	6	0	-2.074042	-2.270867	2.089241
68	6	0	-2.675860	-1.109777	2.904181
69	6	0	-2.763884	-3.599588	2.450349
70	1	0	-1.012661	-2.352265	2.372135
71	6	0	-2.581238	-1.386917	4.412211
72	1	0	-3.728833	-0.974576	2.627582
73	1	0	-2.157433	-0.178529	2.657170
74	6	0	-2.652036	-3.877427	3.958704
75	1	0	-3.825012	-3.537668	2.179635
76	1	0	-2.334152	-4.431566	1.881336
77	6	0	-3.238684	-2.723333	4.783855
78	1	0	-3.044719	-0.563709	4.970154
79	1	0	-1.521281	-1.411787	4.704491
80	1	0	-3.161090	-4.818306	4.201577

81	1	0	-1.592975	-4.011722	4.221928
82	1	0	-3.120979	-2.922269	5.856132
83	1	0	-4.319259	-2.658229	4.590262
84	6	0	-3.490497	-2.293447	-0.653169
85	6	0	-3.860857	-3.780226	-0.816269
86	6	0	-4.690011	-1.475788	-0.139358
87	1	0	-3.230043	-1.932545	-1.655713
88	6	0	-5.050376	-3.914010	-1.781751
89	1	0	-4.132220	-4.216095	0.151136
90	1	0	-3.007163	-4.341018	-1.206443
91	6	0	-5.881924	-1.617212	-1.098521
92	1	0	-4.981358	-1.834605	0.856746
93	1	0	-4.415829	-0.421110	-0.031455
94	6	0	-6.258188	-3.091065	-1.309913
95	1	0	-5.328060	-4.970304	-1.887756
96	1	0	-4.732659	-3.565825	-2.774082
97	1	0	-6.741447	-1.052774	-0.715684
98	1	0	-5.612620	-1.170544	-2.065685
99	1	0	-7.080795	-3.173489	-2.031156
100	1	0	-6.627278	-3.506575	-0.360802
101	6	0	-2.449291	2.564113	1.522455
102	6	0	-2.177421	4.053981	1.806828
103	6	0	-3.896798	2.187338	1.900631
104	1	0	-1.778300	1.986808	2.171676
105	6	0	-2.477828	4.381944	3.280252
106	1	0	-2.798457	4.682085	1.155933
107	1	0	-1.132219	4.300971	1.591859
108	6	0	-4.174063	2.504729	3.377166
109	1	0	-4.596252	2.760045	1.278376
110	1	0	-4.083336	1.127989	1.699993

111	6	0	-3.905233	3.985146	3.680711
112	1	0	-2.312538	5.451134	3.461033
113	1	0	-1.762848	3.839246	3.915320
114	1	0	-5.210189	2.243762	3.625121
115	1	0	-3.527895	1.877885	4.008079
116	1	0	-4.072610	4.194526	4.744324
117	1	0	-4.622112	4.601700	3.119481
118	6	0	-3.475838	2.158277	-1.281130
119	6	0	-3.883860	3.626354	-1.511830
120	6	0	-3.281811	1.415724	-2.618263
121	1	0	-4.290927	1.655804	-0.744747
122	6	0	-5.141681	3.714055	-2.392269
123	1	0	-3.062509	4.159697	-2.008890
124	1	0	-4.061585	4.130215	-0.556527
125	6	0	-4.540058	1.516901	-3.493109
126	1	0	-2.430965	1.850181	-3.161534
127	1	0	-3.031062	0.366767	-2.430064
128	6	0	-4.948829	2.977950	-3.725284
129	1	0	-5.397896	4.766016	-2.568304
130	1	0	-5.988370	3.266908	-1.851766
131	1	0	-4.367630	1.008337	-4.449642
132	1	0	-5.364297	0.986433	-2.995819
133	1	0	-5.866909	3.027336	-4.323550
134	1	0	-4.164063	3.484308	-4.305836
135	6	0	-1.533547	-1.844442	-3.819950
136	8	0	-0.495522	-1.156698	-3.957059
137	8	0	-1.689797	-2.967064	-3.266558

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[1]1 E(opt) = -2999.36468051 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.777259	-0.050981	-0.324968
2	15	0	-1.964844	-1.993279	-0.131862
3	15	0	-2.066689	1.834489	-0.189734
4	6	0	2.066974	-0.731356	-0.308255
5	6	0	0.719404	-2.669276	-0.505757
6	6	0	3.219518	-1.507874	-0.239070
7	6	0	1.850072	-3.478867	-0.418847
8	6	0	3.120313	-2.904971	-0.277326
9	1	0	4.192557	-1.038446	-0.154007
10	1	0	1.739647	-4.556555	-0.470774
11	6	0	2.035512	0.745374	-0.294841
12	6	0	0.611577	2.628291	-0.476658
13	6	0	3.151669	1.567760	-0.181501
14	6	0	1.705651	3.482489	-0.359746
15	6	0	2.996900	2.960410	-0.204619
16	1	0	4.139134	1.137010	-0.067683
17	1	0	1.550897	4.554986	-0.403060
18	6	0	4.340163	-3.758904	-0.176399
19	6	0	4.894702	-4.329995	-1.339618
20	6	0	4.930456	-3.984330	1.083925
21	6	0	6.040906	-5.124111	-1.220111
22	6	0	6.073444	-4.788178	1.158899
23	6	0	6.642749	-5.368233	0.019507
24	1	0	6.474917	-5.559635	-2.117505
25	1	0	6.529478	-4.965186	2.130534
26	6	0	4.178676	3.861846	-0.079518
27	6	0	5.094653	3.969454	-1.146975

28	6	0	4.374213	4.599814	1.107008
29	6	0	6.194517	4.823801	-1.008734
30	6	0	5.491902	5.435773	1.205089
31	6	0	6.411172	5.565193	0.157792
32	1	0	6.898175	4.912023	-1.833555
33	1	0	5.649827	5.996475	2.123802
34	6	0	7.856755	-6.258549	0.129144
35	1	0	7.562035	-7.303434	0.291954
36	1	0	8.458997	-6.230098	-0.784444
37	1	0	8.493234	-5.966868	0.970650
38	6	0	4.277189	-4.080417	-2.695823
39	1	0	3.265589	-4.497797	-2.759473
40	1	0	4.189279	-3.007526	-2.903180
41	1	0	4.877591	-4.532019	-3.490135
42	6	0	4.340088	-3.378400	2.335964
43	1	0	4.381722	-2.283255	2.310492
44	1	0	3.284537	-3.650977	2.452064
45	1	0	4.877626	-3.714462	3.226756
46	6	0	4.898753	3.192242	-2.428640
47	1	0	5.036811	2.116005	-2.273453
48	1	0	3.887811	3.326935	-2.829573
49	1	0	5.612936	3.512850	-3.191950
50	6	0	3.411335	4.484650	2.266546
51	1	0	2.432956	4.914185	2.022073
52	1	0	3.237331	3.438206	2.541770
53	1	0	3.795109	5.008616	3.146137
54	6	0	7.587973	6.503117	0.273221
55	1	0	8.424179	6.176886	-0.353121
56	1	0	7.314042	7.515741	-0.050376
57	1	0	7.940601	6.578364	1.306870

58	7	0	0.839354	-1.321423	-0.417983
59	7	0	0.786431	1.285423	-0.416897
60	6	0	-0.668821	-3.201878	-0.752044
61	6	0	-0.792064	3.104750	-0.739298
62	1	0	-0.815884	-3.284498	-1.836448
63	1	0	-0.790974	-4.203277	-0.330696
64	1	0	-0.960801	4.101055	-0.327375
65	1	0	-0.918243	3.186145	-1.826347
66	6	0	-2.206013	-2.567439	1.631324
67	6	0	-2.837253	-1.488141	2.532054
68	6	0	-2.919717	-3.918925	1.820687
69	1	0	-1.159946	-2.688940	1.954307
70	6	0	-2.813583	-1.919106	4.006219
71	1	0	-3.875609	-1.315253	2.224327
72	1	0	-2.303016	-0.541613	2.405063
73	6	0	-2.882357	-4.349090	3.296893
74	1	0	-3.965801	-3.819899	1.506447
75	1	0	-2.466030	-4.693032	1.191782
76	6	0	-3.498440	-3.277904	4.207878
77	1	0	-3.296081	-1.151197	4.623527
78	1	0	-1.768611	-1.986718	4.342182
79	1	0	-3.409874	-5.303161	3.417747
80	1	0	-1.838398	-4.523238	3.594482
81	1	0	-3.432708	-3.586977	5.258197
82	1	0	-4.568109	-3.179462	3.972663
83	6	0	-3.465820	-2.325209	-1.178494
84	6	0	-3.800867	-3.792628	-1.513673
85	6	0	-4.700768	-1.589719	-0.620230
86	1	0	-3.182788	-1.829853	-2.119286
87	6	0	-4.973771	-3.855005	-2.507472

88	1	0	-4.077750	-4.332428	-0.602790
89	1	0	-2.928748	-4.301531	-1.938232
90	6	0	-5.872325	-1.663033	-1.610506
91	1	0	-4.999756	-2.054476	0.327843
92	1	0	-4.454005	-0.545705	-0.400808
93	6	0	-6.208479	-3.117071	-1.970306
94	1	0	-5.218446	-4.902034	-2.723939
95	1	0	-4.664217	-3.397865	-3.458230
96	1	0	-6.749623	-1.159025	-1.186735
97	1	0	-5.602241	-1.116621	-2.524713
98	1	0	-7.020701	-3.149178	-2.706670
99	1	0	-6.574240	-3.634935	-1.071919
100	6	0	-2.589606	2.311558	1.550498
101	6	0	-2.361727	3.773805	1.979554
102	6	0	-4.040634	1.874426	1.841988
103	1	0	-1.927940	1.688640	2.166635
104	6	0	-2.714665	3.957295	3.466316
105	1	0	-2.977855	4.445855	1.369128
106	1	0	-1.316783	4.061536	1.821454
107	6	0	-4.368362	2.043909	3.332333
108	1	0	-4.731547	2.493241	1.255332
109	1	0	-4.200922	0.836414	1.534897
110	6	0	-4.143464	3.493982	3.782713
111	1	0	-2.581598	5.008676	3.749069
112	1	0	-2.005759	3.374506	4.071911
113	1	0	-5.405013	1.739613	3.521510
114	1	0	-3.726811	1.373036	3.921210
115	1	0	-4.346177	3.597695	4.855627
116	1	0	-4.858453	4.145926	3.260450
117	6	0	-3.513803	2.148066	-1.314577

118	6	0	-3.947111	3.623791	-1.416849
119	6	0	-3.262123	1.543253	-2.711141
120	1	0	-4.334759	1.581632	-0.856939
121	6	0	-5.181313	3.771361	-2.321918
122	1	0	-3.124169	4.218541	-1.835064
123	1	0	-4.163073	4.028940	-0.423561
124	6	0	-4.498722	1.702693	-3.609005
125	1	0	-2.407687	2.047914	-3.183690
126	1	0	-2.991713	0.485745	-2.615156
127	6	0	-4.934945	3.170709	-3.712441
128	1	0	-5.455073	4.830263	-2.404357
129	1	0	-6.032759	3.258641	-1.851842
130	1	0	-4.289781	1.292633	-4.604705
131	1	0	-5.323368	1.110660	-3.188176
132	1	0	-5.837399	3.257135	-4.329789
133	1	0	-4.147243	3.746618	-4.219435

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^{1}3-H E(opt) = -2999.847354 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.792715	-0.085891	-0.272959
2	1	0	-0.949305	-0.172421	-1.802310
3	15	0	-1.970321	-2.074274	-0.068830
4	15	0	-2.105429	1.830449	-0.264410
5	6	0	2.063790	-0.741237	-0.202813
6	6	0	0.742137	-2.702281	-0.390117
7	6	0	3.227261	-1.498870	-0.148461
8	6	0	1.886314	-3.495425	-0.317123

9	6	0	3.147913	-2.900287	-0.193888
10	1	0	4.194887	-1.015773	-0.088032
11	1	0	1.791376	-4.573824	-0.371681
12	6	0	2.014415	0.741172	-0.228440
13	6	0	0.580633	2.602883	-0.550637
14	6	0	3.120023	1.576763	-0.136774
15	6	0	1.666423	3.472633	-0.462967
16	6	0	2.953942	2.966935	-0.243051
17	1	0	4.108439	1.162851	0.019313
18	1	0	1.507600	4.538124	-0.583481
19	6	0	4.382322	-3.734151	-0.140584
20	6	0	4.784351	-4.461701	-1.281486
21	6	0	5.141743	-3.788400	1.047947
22	6	0	5.947771	-5.235546	-1.209881
23	6	0	6.292345	-4.583679	1.075723
24	6	0	6.711917	-5.315436	-0.040716
25	1	0	6.265903	-5.787111	-2.091739
26	1	0	6.874238	-4.633174	1.993326
27	6	0	4.128541	3.878649	-0.142438
28	6	0	5.113281	3.867641	-1.154001
29	6	0	4.249610	4.743528	0.966179
30	6	0	6.205452	4.734090	-1.038357
31	6	0	5.364958	5.584739	1.044492
32	6	0	6.350517	5.599471	0.051587
33	1	0	6.960986	4.733052	-1.820889
34	1	0	5.466640	6.242484	1.904745
35	6	0	7.939557	-6.190550	0.023673
36	1	0	7.680058	-7.201361	0.364283
37	1	0	8.412523	-6.290591	-0.958296
38	1	0	8.679786	-5.792191	0.724708

39	6	0	4.001323	-4.402765	-2.573687
40	1	0	3.049625	-4.940464	-2.494269
41	1	0	3.761786	-3.371369	-2.854729
42	1	0	4.568931	-4.854550	-3.391628
43	6	0	4.727112	-3.021266	2.283037
44	1	0	4.865080	-1.941581	2.152693
45	1	0	3.669638	-3.181248	2.521113
46	1	0	5.320007	-3.328281	3.148817
47	6	0	5.002653	2.957054	-2.356156
48	1	0	5.186275	1.909815	-2.089388
49	1	0	4.005158	3.000932	-2.806922
50	1	0	5.732847	3.235340	-3.120806
51	6	0	3.215911	4.761279	2.069598
52	1	0	2.278911	5.222838	1.736781
53	1	0	2.969400	3.749424	2.409840
54	1	0	3.577285	5.330412	2.930317
55	6	0	7.524535	6.543442	0.138163
56	1	0	8.414834	6.120112	-0.337660
57	1	0	7.302674	7.489709	-0.372133
58	1	0	7.769820	6.784021	1.177286
59	7	0	0.852939	-1.359946	-0.301758
60	7	0	0.771276	1.275732	-0.396244
61	6	0	-0.638475	-3.255219	-0.641809
62	6	0	-0.818625	3.036817	-0.896634
63	1	0	-0.765169	-3.368758	-1.726091
64	1	0	-0.757049	-4.246247	-0.196108
65	1	0	-1.011757	4.064524	-0.586370
66	1	0	-0.912642	3.007928	-1.989861
67	6	0	-2.207174	-2.542190	1.715094
68	6	0	-2.844875	-1.413173	2.548916

69	6	0	-2.927127	-3.882087	1.959710
70	1	0	-1.162779	-2.649569	2.048667
71	6	0	-2.841497	-1.770803	4.042621
72	1	0	-3.877484	-1.251933	2.218318
73	1	0	-2.307325	-0.473904	2.386323
74	6	0	-2.910552	-4.233968	3.456376
75	1	0	-3.967481	-3.794943	1.624534
76	1	0	-2.464273	-4.685835	1.376810
77	6	0	-3.535549	-3.115110	4.301485
78	1	0	-3.329088	-0.970779	4.612604
79	1	0	-1.801414	-1.825583	4.395158
80	1	0	-3.443605	-5.178569	3.617413
81	1	0	-1.871479	-4.395944	3.776439
82	1	0	-3.485733	-3.369855	5.366859
83	1	0	-4.601016	-3.024703	4.045921
84	6	0	-3.445998	-2.398168	-1.131002
85	6	0	-3.792615	-3.874078	-1.414088
86	6	0	-4.674715	-1.624256	-0.611753
87	1	0	-3.135863	-1.939646	-2.081484
88	6	0	-4.955879	-3.956160	-2.417447
89	1	0	-4.085048	-4.374373	-0.485578
90	1	0	-2.921789	-4.407196	-1.810370
91	6	0	-5.832726	-1.719200	-1.615507
92	1	0	-4.990630	-2.051577	0.347995
93	1	0	-4.413015	-0.577311	-0.427677
94	6	0	-6.185482	-3.181294	-1.922395
95	1	0	-5.211991	-5.007313	-2.595524
96	1	0	-4.629054	-3.540404	-3.381128
97	1	0	-6.706838	-1.185939	-1.222934
98	1	0	-5.541538	-1.213114	-2.545709

99	1	0	-6.989039	-3.229752	-2.666970
100	1	0	-6.568949	-3.659075	-1.009506
101	6	0	-2.534007	2.345361	1.480811
102	6	0	-2.220661	3.808057	1.854117
103	6	0	-3.990715	1.980849	1.838616
104	1	0	-1.872985	1.709335	2.086364
105	6	0	-2.505506	4.048794	3.346620
106	1	0	-2.831493	4.487294	1.246558
107	1	0	-1.171069	4.040903	1.645977
108	6	0	-4.249965	2.213199	3.334388
109	1	0	-4.673736	2.612282	1.257008
110	1	0	-4.208494	0.941870	1.572867
111	6	0	-3.941042	3.664122	3.728501
112	1	0	-2.311951	5.100179	3.590450
113	1	0	-1.801361	3.450146	3.942136
114	1	0	-5.291278	1.964050	3.570518
115	1	0	-3.617856	1.530878	3.920186
116	1	0	-4.098090	3.809194	4.804040
117	1	0	-4.643686	4.333217	3.211716
118	6	0	-3.573844	2.085874	-1.358518
119	6	0	-3.961828	3.571902	-1.513372
120	6	0	-3.383228	1.404924	-2.729172
121	1	0	-4.391277	1.569240	-0.840859
122	6	0	-5.217627	3.717137	-2.387042
123	1	0	-3.135268	4.118441	-1.985228
124	1	0	-4.131406	4.026171	-0.532209
125	6	0	-4.638215	1.575975	-3.599627
126	1	0	-2.520370	1.847657	-3.245858
127	1	0	-3.163705	0.341439	-2.590310
128	6	0	-5.025476	3.052479	-3.756323

129	1	0	-5.460485	4.779813	-2.505391
130	1	0	-6.069495	3.250462	-1.872472
131	1	0	-4.470157	1.114845	-4.580249
132	1	0	-5.471467	1.034156	-3.131939
133	1	0	-5.939828	3.142975	-4.354826
134	1	0	-4.232198	3.579800	-4.305384

$^1O_2$C-3-H E(opt) = -3188.66234278 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.715878	-0.086647	-0.338230
2	1	0	-0.943419	-0.170004	-2.032824
3	15	0	-1.921006	-2.041641	-0.141809
4	15	0	-2.076989	1.787106	-0.202264
5	6	0	2.147790	-0.717754	-0.400312
6	6	0	0.822030	-2.675786	-0.441541
7	6	0	3.314308	-1.475328	-0.334899
8	6	0	1.965831	-3.466715	-0.361518
9	6	0	3.234087	-2.872699	-0.305750
10	1	0	4.281523	-0.989019	-0.292021
11	1	0	1.867306	-4.546697	-0.352576
12	6	0	2.093873	0.755809	-0.389092
13	6	0	0.629626	2.612285	-0.443983
14	6	0	3.198268	1.595439	-0.270807
15	6	0	1.708479	3.483697	-0.315198
16	6	0	3.014071	2.982317	-0.218026
17	1	0	4.195923	1.180363	-0.194505
18	1	0	1.530358	4.553284	-0.293549

19	6	0	4.467624	-3.707145	-0.218007
20	6	0	5.334083	-3.799644	-1.327596
21	6	0	4.762460	-4.396451	0.977277
22	6	0	6.484057	-4.590227	-1.222306
23	6	0	5.926668	-5.170564	1.040633
24	6	0	6.797672	-5.284390	-0.048585
25	1	0	7.150075	-4.665910	-2.079151
26	1	0	6.160050	-5.694101	1.965255
27	6	0	4.179047	3.899360	-0.052825
28	6	0	5.088596	4.081896	-1.115494
29	6	0	4.369936	4.571019	1.173557
30	6	0	6.176530	4.943298	-0.933094
31	6	0	5.475030	5.417874	1.314383
32	6	0	6.387520	5.620532	0.272890
33	1	0	6.875862	5.087985	-1.753725
34	1	0	5.629239	5.927313	2.263160
35	6	0	8.026811	-6.156885	0.030073
36	1	0	7.799928	-7.182083	-0.290440
37	1	0	8.825809	-5.783974	-0.618654
38	1	0	8.412551	-6.215131	1.052832
39	6	0	5.034253	-3.071936	-2.618363
40	1	0	4.008385	-3.257726	-2.955721
41	1	0	5.137499	-1.986741	-2.503357
42	1	0	5.716092	-3.388781	-3.412326
43	6	0	3.856385	-4.294447	2.182986
44	1	0	3.626778	-3.250940	2.426222
45	1	0	2.897073	-4.795837	2.010370
46	1	0	4.319962	-4.755122	3.059629
47	6	0	4.899931	3.373403	-2.437532
48	1	0	5.068916	2.294319	-2.344762

49	1	0	3.881404	3.501926	-2.820666
50	1	0	5.596927	3.755970	-3.188239
51	6	0	3.418340	4.371991	2.331239
52	1	0	2.431730	4.801043	2.121942
53	1	0	3.259935	3.308404	2.542739
54	1	0	3.802823	4.846377	3.238300
55	6	0	7.551485	6.567401	0.436952
56	1	0	8.396677	6.277723	-0.195426
57	1	0	7.267938	7.589290	0.153128
58	1	0	7.895241	6.603657	1.475659
59	7	0	0.932360	-1.331450	-0.450768
60	7	0	0.838178	1.279550	-0.461094
61	6	0	-0.561133	-3.251768	-0.603886
62	6	0	-0.785677	3.078523	-0.652845
63	1	0	-0.697747	-3.476074	-1.669458
64	1	0	-0.656060	-4.198675	-0.065939
65	1	0	-0.960876	4.041476	-0.170617
66	1	0	-0.914009	3.239036	-1.731387
67	6	0	-2.476271	-2.609276	1.540704
68	6	0	-3.316734	-1.553585	2.282843
69	6	0	-3.158346	-3.987374	1.608512
70	1	0	-1.508849	-2.651604	2.055763
71	6	0	-3.543659	-1.971059	3.743715
72	1	0	-4.289181	-1.430749	1.790251
73	1	0	-2.808200	-0.588354	2.248103
74	6	0	-3.364532	-4.407843	3.073802
75	1	0	-4.137626	-3.936521	1.117225
76	1	0	-2.572462	-4.748014	1.079876
77	6	0	-4.184407	-3.362348	3.843216
78	1	0	-4.169352	-1.225009	4.249589

79	1	0	-2.575358	-1.978667	4.263582
80	1	0	-3.859583	-5.386125	3.114085
81	1	0	-2.383194	-4.527102	3.554696
82	1	0	-4.292516	-3.659923	4.893598
83	1	0	-5.198783	-3.322051	3.419944
84	6	0	-3.240118	-2.356772	-1.420718
85	6	0	-3.567256	-3.819556	-1.786922
86	6	0	-4.532659	-1.579919	-1.102545
87	1	0	-2.784168	-1.891561	-2.305837
88	6	0	-4.530140	-3.859612	-2.986721
89	1	0	-4.038587	-4.325259	-0.938726
90	1	0	-2.656660	-4.378108	-2.028277
91	6	0	-5.498603	-1.622803	-2.295977
92	1	0	-5.020313	-2.030517	-0.228659
93	1	0	-4.299600	-0.543734	-0.840435
94	6	0	-5.815448	-3.068163	-2.705216
95	1	0	-4.769732	-4.901222	-3.233337
96	1	0	-4.026736	-3.432503	-3.865870
97	1	0	-6.420917	-1.082475	-2.049201
98	1	0	-5.039611	-1.097382	-3.144437
99	1	0	-6.470306	-3.080423	-3.585112
100	1	0	-6.368486	-3.559388	-1.891615
101	6	0	-2.810976	2.231989	1.467387
102	6	0	-2.569960	3.667099	1.974651
103	6	0	-4.300791	1.848442	1.583236
104	1	0	-2.228501	1.581670	2.123265
105	6	0	-3.071239	3.811503	3.423013
106	1	0	-3.083883	4.398170	1.337455
107	1	0	-1.501551	3.902855	1.942047
108	6	0	-4.769030	1.973181	3.041028

109	1	0	-4.914616	2.512538	0.961756
110	1	0	-4.468487	0.828897	1.221829
111	6	0	-4.541359	3.395944	3.569858
112	1	0	-2.930431	4.845517	3.761869
113	1	0	-2.453689	3.177728	4.074975
114	1	0	-5.828942	1.700304	3.117207
115	1	0	-4.209595	1.258617	3.661006
116	1	0	-4.853381	3.469493	4.619002
117	1	0	-5.173177	4.094205	3.001748
118	6	0	-3.445000	2.146410	-1.431936
119	6	0	-3.830325	3.642606	-1.484560
120	6	0	-3.177488	1.606898	-2.849105
121	1	0	-4.305074	1.593462	-1.035870
122	6	0	-5.035704	3.875250	-2.409363
123	1	0	-2.980376	4.226194	-1.861442
124	1	0	-4.057917	4.021704	-0.484980
125	6	0	-4.378297	1.859771	-3.775233
126	1	0	-2.285178	2.092364	-3.268993
127	1	0	-2.960814	0.536781	-2.805557
128	6	0	-4.766505	3.342660	-3.821694
129	1	0	-5.274950	4.945375	-2.439507
130	1	0	-5.914512	3.364650	-1.989900
131	1	0	-4.149554	1.489498	-4.782330
132	1	0	-5.235711	1.276548	-3.411628
133	1	0	-5.646340	3.488038	-4.460477
134	1	0	-3.946543	3.918977	-4.274216
135	6	0	-0.213948	-0.036260	1.821960
136	8	0	0.091140	-1.136561	2.361958
137	8	0	-0.134490	1.100704	2.369029

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[1]HOOC-3-H E(opt) = -3189.16283262 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.716532	-0.078829	-0.216110
2	1	0	-0.913810	-0.089947	-1.857006
3	15	0	-1.968702	-2.032789	-0.173926
4	15	0	-2.060076	1.817657	-0.166174
5	6	0	2.139362	-0.751279	-0.316027
6	6	0	0.789122	-2.694345	-0.387956
7	6	0	3.296408	-1.520470	-0.258333
8	6	0	1.926668	-3.500247	-0.316210
9	6	0	3.196702	-2.918727	-0.245125
10	1	0	4.270416	-1.048057	-0.212808
11	1	0	1.817413	-4.579096	-0.322520
12	6	0	2.105454	0.728015	-0.316207
13	6	0	0.669765	2.609008	-0.417673
14	6	0	3.223535	1.552168	-0.251793
15	6	0	1.766282	3.467000	-0.344004
16	6	0	3.062072	2.944847	-0.248088
17	1	0	4.216221	1.124349	-0.187159
18	1	0	1.606627	4.539078	-0.367597
19	6	0	4.422125	-3.765725	-0.155713
20	6	0	5.177381	-4.027635	-1.315542
21	6	0	4.814248	-4.289966	1.092564
22	6	0	6.323051	-4.824313	-1.206192
23	6	0	5.968991	-5.077112	1.157787
24	6	0	6.734119	-5.359075	0.019768
25	1	0	6.907457	-5.030453	-2.100164

26	1	0	6.279036	-5.477545	2.120511
27	6	0	4.244874	3.846489	-0.142132
28	6	0	5.136963	3.966605	-1.227662
29	6	0	4.460442	4.574266	1.047685
30	6	0	6.235635	4.824946	-1.104137
31	6	0	5.576501	5.413352	1.129773
32	6	0	6.475724	5.552682	0.066162
33	1	0	6.918368	4.928030	-1.944507
34	1	0	5.748621	5.970279	2.048196
35	6	0	7.955271	-6.241566	0.110663
36	1	0	7.678812	-7.301051	0.032475
37	1	0	8.664658	-6.029726	-0.695341
38	1	0	8.472040	-6.112671	1.067204
39	6	0	4.760417	-3.464322	-2.653890
40	1	0	3.735434	-3.758200	-2.908861
41	1	0	4.782719	-2.368110	-2.651461
42	1	0	5.422146	-3.812899	-3.451305
43	6	0	4.013346	-3.998396	2.340003
44	1	0	3.915179	-2.919337	2.508290
45	1	0	2.995403	-4.398557	2.265772
46	1	0	4.485376	-4.438575	3.222396
47	6	0	4.914638	3.204318	-2.513896
48	1	0	5.069434	2.127866	-2.376357
49	1	0	3.892304	3.332681	-2.886919
50	1	0	5.605189	3.542461	-3.291166
51	6	0	3.519763	4.449442	2.224548
52	1	0	2.541967	4.895701	2.009261
53	1	0	3.339037	3.400432	2.485314
54	1	0	3.928492	4.952910	3.104767
55	6	0	7.687135	6.443737	0.192781

56	1	0	8.045069	6.776359	-0.786425
57	1	0	7.470889	7.328970	0.799694
58	1	0	8.514224	5.911667	0.680431
59	7	0	0.919520	-1.355205	-0.369737
60	7	0	0.859332	1.274666	-0.371746
61	6	0	-0.598277	-3.256055	-0.567513
62	6	0	-0.743212	3.088336	-0.620655
63	1	0	-0.700265	-3.524408	-1.625767
64	1	0	-0.721447	-4.179820	0.004347
65	1	0	-0.907305	4.054104	-0.140508
66	1	0	-0.868369	3.250068	-1.698526
67	6	0	-2.640801	-2.613495	1.458317
68	6	0	-3.472410	-1.536709	2.181782
69	6	0	-3.391224	-3.958317	1.439858
70	1	0	-1.713963	-2.737636	2.029934
71	6	0	-3.809364	-1.984434	3.612027
72	1	0	-4.404297	-1.353038	1.633958
73	1	0	-2.921131	-0.594707	2.207535
74	6	0	-3.708976	-4.406613	2.876500
75	1	0	-4.332548	-3.845494	0.889326
76	1	0	-2.806065	-4.729727	0.926533
77	6	0	-4.523728	-3.342949	3.625973
78	1	0	-4.427509	-1.221430	4.101025
79	1	0	-2.877407	-2.057721	4.189930
80	1	0	-4.252795	-5.358899	2.854511
81	1	0	-2.766973	-4.589456	3.412756
82	1	0	-4.712463	-3.664424	4.657494
83	1	0	-5.505593	-3.237810	3.142053
84	6	0	-3.208950	-2.272263	-1.540521
85	6	0	-3.518194	-3.721688	-1.974400

86	6	0	-4.515620	-1.504754	-1.256221
87	1	0	-2.702915	-1.776609	-2.380475
88	6	0	-4.427993	-3.719143	-3.214987
89	1	0	-4.024646	-4.257256	-1.166220
90	1	0	-2.598673	-4.272037	-2.197945
91	6	0	-5.425550	-1.510014	-2.493608
92	1	0	-5.041679	-1.984776	-0.421849
93	1	0	-4.297264	-0.477834	-0.949283
94	6	0	-5.725984	-2.940754	-2.960112
95	1	0	-4.651753	-4.752268	-3.507005
96	1	0	-3.888957	-3.260086	-4.055986
97	1	0	-6.355884	-0.972984	-2.272149
98	1	0	-4.927365	-0.963605	-3.304916
99	1	0	-6.343908	-2.924005	-3.866060
100	1	0	-6.310526	-3.458526	-2.186133
101	6	0	-2.778819	2.270100	1.511662
102	6	0	-2.462787	3.684513	2.037622
103	6	0	-4.289635	1.965790	1.611181
104	1	0	-2.275788	1.563377	2.177906
105	6	0	-2.964008	3.837806	3.484189
106	1	0	-2.936951	4.439536	1.398649
107	1	0	-1.383353	3.873864	2.009304
108	6	0	-4.760526	2.102443	3.066768
109	1	0	-4.855592	2.668872	0.989152
110	1	0	-4.505585	0.959608	1.239243
111	6	0	-4.456022	3.503174	3.615190
112	1	0	-2.767428	4.858247	3.834348
113	1	0	-2.385239	3.162909	4.130687
114	1	0	-5.834743	1.890755	3.128287
115	1	0	-4.250413	1.348226	3.682422

116	1	0	-4.769719	3.579642	4.663237
117	1	0	-5.043127	4.243508	3.053053
118	6	0	-3.398768	2.175142	-1.415614
119	6	0	-3.756930	3.678497	-1.483507
120	6	0	-3.086345	1.622826	-2.819237
121	1	0	-4.273319	1.633945	-1.036701
122	6	0	-4.925786	3.922365	-2.450867
123	1	0	-2.887468	4.247190	-1.836115
124	1	0	-4.010921	4.065562	-0.493136
125	6	0	-4.248236	1.895644	-3.788589
126	1	0	-2.172094	2.091894	-3.208347
127	1	0	-2.891798	0.549045	-2.762778
128	6	0	-4.608617	3.384809	-3.851219
129	1	0	-5.149266	4.995290	-2.489923
130	1	0	-5.825300	3.422997	-2.063652
131	1	0	-3.988052	1.518367	-4.785082
132	1	0	-5.128821	1.330250	-3.455951
133	1	0	-5.460354	3.542373	-4.523885
134	1	0	-3.762763	3.948025	-4.271072
135	6	0	-0.252257	-0.197696	1.901241
136	8	0	-0.097186	-1.229617	2.539544
137	8	0	0.095174	0.950136	2.616518
138	1	0	-0.002046	1.725274	2.044448

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^{3}HOOC-3-H E(opt) = -3189.08001324 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.729220	-0.073936	-0.150029

2	1	0	-0.715517	0.107100	-1.742249
3	15	0	-2.003700	-2.052057	-0.219203
4	15	0	-2.042068	1.875475	-0.133245
5	6	0	2.119507	-0.759155	-0.254488
6	6	0	0.748090	-2.730712	-0.361702
7	6	0	3.273844	-1.581975	-0.185759
8	6	0	1.864345	-3.549422	-0.296842
9	6	0	3.156728	-2.958532	-0.193025
10	1	0	4.254820	-1.124415	-0.122945
11	1	0	1.752424	-4.626225	-0.347171
12	6	0	2.109626	0.667471	-0.291119
13	6	0	0.694478	2.619916	-0.421159
14	6	0	3.246189	1.518008	-0.261855
15	6	0	1.793841	3.457488	-0.386922
16	6	0	3.104044	2.890999	-0.286833
17	1	0	4.236657	1.080869	-0.204382
18	1	0	1.660072	4.530936	-0.448183
19	6	0	4.367827	-3.828890	-0.111151
20	6	0	5.104817	-4.120166	-1.276623
21	6	0	4.765888	-4.358540	1.133403
22	6	0	6.235070	-4.940511	-1.176539
23	6	0	5.903322	-5.171850	1.191682
24	6	0	6.650045	-5.476668	0.047478
25	1	0	6.804393	-5.164832	-2.076152
26	1	0	6.214691	-5.574597	2.153258
27	6	0	4.293628	3.788117	-0.203527
28	6	0	5.153898	3.936332	-1.311822
29	6	0	4.546969	4.496507	0.990435
30	6	0	6.255072	4.793948	-1.205804
31	6	0	5.661274	5.341019	1.055896

32	6	0	6.528392	5.502615	-0.030315
33	1	0	6.913146	4.914174	-2.063871
34	1	0	5.857771	5.882681	1.978767
35	6	0	7.853326	-6.384933	0.128513
36	1	0	7.557474	-7.437972	0.034473
37	1	0	8.568770	-6.175927	-0.673106
38	1	0	8.371207	-6.279554	1.087368
39	6	0	4.686423	-3.557845	-2.615410
40	1	0	3.645448	-3.812130	-2.846699
41	1	0	4.752611	-2.463783	-2.627984
42	1	0	5.318013	-3.943832	-3.420397
43	6	0	3.985642	-4.042966	2.388064
44	1	0	3.944985	-2.962382	2.569552
45	1	0	2.947551	-4.386768	2.309970
46	1	0	4.435486	-4.518608	3.263907
47	6	0	4.893602	3.196703	-2.604291
48	1	0	5.051986	2.118296	-2.489848
49	1	0	3.859066	3.329169	-2.940642
50	1	0	5.558135	3.549758	-3.397948
51	6	0	3.643684	4.339623	2.192146
52	1	0	2.639691	4.733908	1.996921
53	1	0	3.519342	3.283973	2.460963
54	1	0	4.048827	4.866866	3.060253
55	6	0	7.742218	6.394517	0.070373
56	1	0	7.967648	6.874079	-0.887817
57	1	0	7.603880	7.177775	0.822296
58	1	0	8.630354	5.817669	0.359694
59	7	0	0.873837	-1.387041	-0.298680
60	7	0	0.851170	1.274920	-0.324184
61	6	0	-0.640893	-3.273521	-0.606365

62	6	0	-0.716587	3.115398	-0.618187
63	1	0	-0.714398	-3.502407	-1.675810
64	1	0	-0.802311	-4.213149	-0.070751
65	1	0	-0.868813	4.085628	-0.142853
66	1	0	-0.856143	3.269798	-1.694548
67	6	0	-2.693375	-2.620021	1.413933
68	6	0	-3.507599	-1.528348	2.134670
69	6	0	-3.470630	-3.949472	1.381674
70	1	0	-1.770622	-2.776058	1.986817
71	6	0	-3.863275	-1.975714	3.560446
72	1	0	-4.431305	-1.329661	1.579096
73	1	0	-2.940876	-0.596047	2.165467
74	6	0	-3.808658	-4.395907	2.814633
75	1	0	-4.404148	-3.812661	0.823878
76	1	0	-2.895642	-4.729306	0.870237
77	6	0	-4.606655	-3.318597	3.562431
78	1	0	-4.468228	-1.201295	4.047598
79	1	0	-2.937244	-2.071449	4.144309
80	1	0	-4.371877	-5.336322	2.782373
81	1	0	-2.874958	-4.601577	3.356892
82	1	0	-4.809093	-3.640701	4.591002
83	1	0	-5.582384	-3.190654	3.071989
84	6	0	-3.232531	-2.241597	-1.600808
85	6	0	-3.534848	-3.686178	-2.058067
86	6	0	-4.540202	-1.479796	-1.306958
87	1	0	-2.719892	-1.732146	-2.428951
88	6	0	-4.449340	-3.670271	-3.294650
89	1	0	-4.034584	-4.236260	-1.255509
90	1	0	-2.612901	-4.226561	-2.293633
91	6	0	-5.450720	-1.475720	-2.543942

92	1	0	-5.064045	-1.970417	-0.477794
93	1	0	-4.323381	-0.455680	-0.989228
94	6	0	-5.749624	-2.902103	-3.023479
95	1	0	-4.667887	-4.700822	-3.598970
96	1	0	-3.915937	-3.197141	-4.131335
97	1	0	-6.380576	-0.940763	-2.316344
98	1	0	-4.953551	-0.923307	-3.351259
99	1	0	-6.372278	-2.877233	-3.925871
100	1	0	-6.327614	-3.431016	-2.252222
101	6	0	-2.729882	2.329773	1.551638
102	6	0	-2.413993	3.750181	2.058704
103	6	0	-4.238529	2.021064	1.669198
104	1	0	-2.215490	1.629925	2.220054
105	6	0	-2.899468	3.913663	3.509615
106	1	0	-2.902411	4.493684	1.416822
107	1	0	-1.336409	3.942498	2.014165
108	6	0	-4.695601	2.167988	3.127924
109	1	0	-4.808177	2.721097	1.047052
110	1	0	-4.458081	1.013519	1.303795
111	6	0	-4.388469	3.573898	3.661913
112	1	0	-2.703273	4.937984	3.848126
113	1	0	-2.309550	3.247396	4.155167
114	1	0	-5.768747	1.955041	3.200844
115	1	0	-4.178892	1.419112	3.744759
116	1	0	-4.689037	3.656950	4.713242
117	1	0	-4.985507	4.307709	3.101864
118	6	0	-3.374892	2.200525	-1.387949
119	6	0	-3.745227	3.699047	-1.484698
120	6	0	-3.022808	1.625056	-2.774122
121	1	0	-4.248351	1.655352	-1.012448

122	6	0	-4.886900	3.918450	-2.489366
123	1	0	-2.871726	4.272730	-1.818277
124	1	0	-4.030617	4.092203	-0.504886
125	6	0	-4.159250	1.877161	-3.778542
126	1	0	-2.102256	2.092869	-3.148731
127	1	0	-2.824757	0.552241	-2.693406
128	6	0	-4.522554	3.364200	-3.871837
129	1	0	-5.118056	4.988617	-2.550340
130	1	0	-5.793377	3.416298	-2.122686
131	1	0	-3.870909	1.486021	-4.761679
132	1	0	-5.046989	1.315336	-3.460909
133	1	0	-5.353435	3.508201	-4.572894
134	1	0	-3.666430	3.925897	-4.272258
135	6	0	-0.150256	0.073075	1.973609
136	8	0	-0.413209	-0.898288	2.646966
137	8	0	0.503420	1.113124	2.492776
138	1	0	0.689838	1.758264	1.785735

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^{2}HOOC-2-H E(opt) = -3189.258567 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.727249	-0.091821	-0.260719
2	1	0	-0.944470	-0.125914	-1.907686
3	15	0	-1.967824	-2.050270	-0.162720
4	15	0	-2.046317	1.824196	-0.184320
5	6	0	2.131598	-0.739988	-0.383133
6	6	0	0.780476	-2.721825	-0.398977
7	6	0	3.296869	-1.549438	-0.298816

8	6	0	1.906094	-3.532438	-0.307646
9	6	0	3.193330	-2.926658	-0.251019
10	1	0	4.274256	-1.080696	-0.259764
11	1	0	1.801576	-4.611277	-0.292958
12	6	0	2.099247	0.686503	-0.409468
13	6	0	0.659484	2.606594	-0.545533
14	6	0	3.221897	1.555236	-0.337501
15	6	0	1.741802	3.470450	-0.480114
16	6	0	3.057248	2.926312	-0.352888
17	1	0	4.217668	1.134992	-0.248105
18	1	0	1.589083	4.541999	-0.533804
19	6	0	4.412646	-3.782931	-0.138683
20	6	0	5.151460	-4.115588	-1.292006
21	6	0	4.817415	-4.261549	1.124805
22	6	0	6.288059	-4.923251	-1.161863
23	6	0	5.960241	-5.064746	1.213477
24	6	0	6.708052	-5.409015	0.081264
25	1	0	6.857893	-5.178722	-2.052918
26	1	0	6.275229	-5.427859	2.189682
27	6	0	4.231475	3.839880	-0.228416
28	6	0	5.118376	4.012073	-1.311247
29	6	0	4.447152	4.539173	0.979570
30	6	0	6.207610	4.881172	-1.167648
31	6	0	5.548384	5.395812	1.082950
32	6	0	6.442381	5.579412	0.021199
33	1	0	6.886190	5.017831	-2.007090
34	1	0	5.714842	5.929942	2.016304
35	6	0	7.916961	-6.306352	0.196108
36	1	0	7.627806	-7.364191	0.143690
37	1	0	8.630581	-6.124547	-0.613784

38	1	0	8.435359	-6.160627	1.149465
39	6	0	4.727199	-3.610749	-2.651806
40	1	0	3.687054	-3.879908	-2.869456
41	1	0	4.786441	-2.517828	-2.709301
42	1	0	5.359089	-4.025775	-3.442134
43	6	0	4.038046	-3.902711	2.368520
44	1	0	3.983361	-2.816007	2.503321
45	1	0	3.003964	-4.261699	2.309604
46	1	0	4.497251	-4.334655	3.262092
47	6	0	4.901604	3.284918	-2.618943
48	1	0	5.076501	2.208087	-2.514733
49	1	0	3.872770	3.402919	-2.977156
50	1	0	5.577783	3.660080	-3.392578
51	6	0	3.516570	4.357118	2.156683
52	1	0	2.509451	4.729377	1.936697
53	1	0	3.407794	3.297462	2.416115
54	1	0	3.887646	4.887973	3.037866
55	6	0	7.640849	6.485611	0.169440
56	1	0	8.003338	6.834822	-0.802445
57	1	0	7.407118	7.361802	0.783428
58	1	0	8.471835	5.961544	0.659428
59	7	0	0.894889	-1.381423	-0.421656
60	7	0	0.832702	1.268632	-0.471287
61	6	0	-0.613129	-3.286876	-0.557861
62	6	0	-0.760523	3.071266	-0.759267
63	1	0	-0.735743	-3.565439	-1.611119
64	1	0	-0.736060	-4.203539	0.026219
65	1	0	-0.925323	4.067582	-0.346370
66	1	0	-0.920348	3.147830	-1.841923
67	6	0	-2.626891	-2.598691	1.487141

68	6	0	-3.441868	-1.498852	2.195046
69	6	0	-3.382701	-3.939470	1.513306
70	1	0	-1.694340	-2.708886	2.052225
71	6	0	-3.767165	-1.909077	3.639013
72	1	0	-4.378441	-1.317753	1.653542
73	1	0	-2.878686	-0.563608	2.192338
74	6	0	-3.688806	-4.349756	2.963899
75	1	0	-4.329349	-3.839018	0.969170
76	1	0	-2.805200	-4.726132	1.014232
77	6	0	-4.489867	-3.262315	3.694155
78	1	0	-4.374756	-1.130646	4.117441
79	1	0	-2.828917	-1.974922	4.207486
80	1	0	-4.238009	-5.299389	2.973039
81	1	0	-2.742473	-4.523750	3.495628
82	1	0	-4.671340	-3.556773	4.735170
83	1	0	-5.475708	-3.163226	3.216756
84	6	0	-3.237598	-2.325328	-1.500513
85	6	0	-3.550040	-3.783344	-1.902128
86	6	0	-4.542952	-1.557592	-1.211834
87	1	0	-2.750184	-1.844757	-2.360349
88	6	0	-4.479951	-3.809899	-3.127450
89	1	0	-4.041159	-4.305244	-1.075407
90	1	0	-2.632180	-4.335051	-2.129269
91	6	0	-5.473727	-1.589998	-2.433457
92	1	0	-5.054612	-2.022699	-0.360105
93	1	0	-4.323651	-0.523976	-0.927967
94	6	0	-5.776419	-3.030633	-2.867305
95	1	0	-4.705189	-4.849306	-3.395752
96	1	0	-3.956541	-3.365987	-3.986360
97	1	0	-6.402899	-1.052454	-2.207794

98	1	0	-4.991647	-1.057440	-3.263647
99	1	0	-6.409299	-3.033756	-3.763190
100	1	0	-6.346658	-3.535093	-2.073963
101	6	0	-2.642587	2.336646	1.526108
102	6	0	-2.251456	3.754263	1.987713
103	6	0	-4.148804	2.078317	1.745806
104	1	0	-2.107680	1.636364	2.173780
105	6	0	-2.639111	3.962368	3.461720
106	1	0	-2.750982	4.506874	1.364510
107	1	0	-1.172452	3.910262	1.873730
108	6	0	-4.507788	2.268459	3.227400
109	1	0	-4.742023	2.778507	1.145945
110	1	0	-4.418485	1.068401	1.421064
111	6	0	-4.125812	3.674146	3.711718
112	1	0	-2.390484	4.985931	3.767537
113	1	0	-2.032384	3.289124	4.083972
114	1	0	-5.579814	2.089704	3.375049
115	1	0	-3.973609	1.516960	3.826056
116	1	0	-4.359401	3.788008	4.777297
117	1	0	-4.733024	4.415743	3.172808
118	6	0	-3.470135	2.169145	-1.341086
119	6	0	-3.822722	3.672565	-1.423595
120	6	0	-3.263498	1.585505	-2.752055
121	1	0	-4.319943	1.643035	-0.889428
122	6	0	-5.061484	3.901824	-2.303685
123	1	0	-2.977788	4.221304	-1.858370
124	1	0	-3.994396	4.090356	-0.427866
125	6	0	-4.496829	1.834970	-3.635562
126	1	0	-2.384192	2.049048	-3.220120
127	1	0	-3.058852	0.514046	-2.689927

128	6	0	-4.858788	3.323489	-3.709418
129	1	0	-5.281045	4.975171	-2.356020
130	1	0	-5.931632	3.421275	-1.833908
131	1	0	-4.316493	1.431300	-4.639464
132	1	0	-5.349274	1.280668	-3.220669
133	1	0	-5.761167	3.466801	-4.316258
134	1	0	-4.047818	3.871025	-4.210960
135	6	0	-0.208836	-0.152714	1.840424
136	8	0	-0.157669	-1.138906	2.563865
137	8	0	0.276735	1.006897	2.456846
138	1	0	0.300631	1.712727	1.794079

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^{2}H-2-CO E(opt) = -3113.294156 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.724289	-0.051470	-0.116722
2	1	0	-0.876967	-0.060889	-1.727182
3	15	0	-1.960090	-2.044972	-0.152295
4	15	0	-2.064490	1.888535	-0.140418
5	6	0	2.134995	-0.701481	-0.285154
6	6	0	0.776061	-2.677819	-0.488946
7	6	0	3.294747	-1.522118	-0.263666
8	6	0	1.894947	-3.493116	-0.461976
9	6	0	3.186371	-2.897027	-0.334838
10	1	0	4.273708	-1.061623	-0.188755
11	1	0	1.788972	-4.567397	-0.556881
12	6	0	2.105312	0.724829	-0.251013
13	6	0	0.668772	2.652903	-0.349969

14	6	0	3.230233	1.587898	-0.161253
15	6	0	1.754027	3.509209	-0.258146
16	6	0	3.066662	2.958972	-0.152698
17	1	0	4.225184	1.162996	-0.088535
18	1	0	1.604540	4.582312	-0.281558
19	6	0	4.401177	-3.765044	-0.289741
20	6	0	4.930078	-4.298766	-1.482982
21	6	0	5.011128	-4.054447	0.948322
22	6	0	6.066275	-5.113818	-1.417681
23	6	0	6.144826	-4.875379	0.971066
24	6	0	6.686969	-5.416115	-0.200345
25	1	0	6.477734	-5.518915	-2.339845
26	1	0	6.614808	-5.098341	1.926688
27	6	0	4.245912	3.868796	-0.038021
28	6	0	4.803141	4.447122	-1.196468
29	6	0	4.788952	4.156498	1.231002
30	6	0	5.903435	5.302887	-1.066274
31	6	0	5.888205	5.018577	1.319061
32	6	0	6.462159	5.599093	0.182054
33	1	0	6.333655	5.747882	-1.961087
34	1	0	6.304331	5.244102	2.298782
35	6	0	7.890308	-6.326453	-0.148078
36	1	0	7.585661	-7.372494	-0.012706
37	1	0	8.472545	-6.275796	-1.073701
38	1	0	8.550254	-6.071357	0.687372
39	6	0	4.294440	-3.983407	-2.816882
40	1	0	3.262462	-4.349534	-2.866090
41	1	0	4.252073	-2.901736	-2.990500
42	1	0	4.854168	-4.438539	-3.638649
43	6	0	4.452911	-3.493288	2.235939

44	1	0	4.539279	-2.401123	2.268297
45	1	0	3.387356	-3.727439	2.343929
46	1	0	4.980332	-3.899058	3.103811
47	6	0	4.228487	4.144111	-2.560504
48	1	0	4.245111	3.067703	-2.767744
49	1	0	3.181655	4.461187	-2.633171
50	1	0	4.791585	4.651254	-3.348854
51	6	0	4.191929	3.551223	2.480448
52	1	0	3.118082	3.760650	2.551105
53	1	0	4.300056	2.460428	2.486923
54	1	0	4.675266	3.943815	3.379473
55	6	0	7.669654	6.497984	0.298231
56	1	0	7.721643	7.209706	-0.531769
57	1	0	7.660106	7.063580	1.235658
58	1	0	8.597981	5.912085	0.283401
59	7	0	0.897932	-1.338949	-0.366416
60	7	0	0.843542	1.315213	-0.321246
61	6	0	-0.617691	-3.199098	-0.750052
62	6	0	-0.741305	3.142032	-0.578466
63	1	0	-0.746304	-3.264241	-1.837719
64	1	0	-0.751476	-4.207890	-0.351830
65	1	0	-0.915883	4.100815	-0.087547
66	1	0	-0.855294	3.318878	-1.654791
67	6	0	-2.435856	-2.682567	1.528589
68	6	0	-3.280544	-1.688181	2.354005
69	6	0	-3.092120	-4.077577	1.551593
70	1	0	-1.448558	-2.768321	2.009527
71	6	0	-3.426412	-2.179495	3.802134
72	1	0	-4.276052	-1.595233	1.906036
73	1	0	-2.840698	-0.687790	2.339623

74	6	0	-3.234865	-4.574985	2.999859
75	1	0	-4.087129	-4.011465	1.096205
76	1	0	-2.512135	-4.796707	0.963761
77	6	0	-4.037267	-3.586576	3.857172
78	1	0	-4.042814	-1.471319	4.368786
79	1	0	-2.435928	-2.192845	4.278593
80	1	0	-3.714726	-5.560926	3.003132
81	1	0	-2.233638	-4.706371	3.433923
82	1	0	-4.090185	-3.938526	4.894358
83	1	0	-5.070114	-3.543676	3.482975
84	6	0	-3.329262	-2.213022	-1.389262
85	6	0	-3.651054	-3.644988	-1.868213
86	6	0	-4.611096	-1.496068	-0.922778
87	1	0	-2.921331	-1.659016	-2.246043
88	6	0	-4.690185	-3.596749	-3.001853
89	1	0	-4.053493	-4.234643	-1.038496
90	1	0	-2.748071	-4.154211	-2.219276
91	6	0	-5.644716	-1.450523	-2.057067
92	1	0	-5.037340	-2.042207	-0.072621
93	1	0	-4.379393	-0.486247	-0.571457
94	6	0	-5.966514	-2.860575	-2.570909
95	1	0	-4.927367	-4.617843	-3.323474
96	1	0	-4.250501	-3.083792	-3.868986
97	1	0	-6.555704	-0.949713	-1.707960
98	1	0	-5.244470	-0.847205	-2.882275
99	1	0	-6.674728	-2.808615	-3.406548
100	1	0	-6.459641	-3.431880	-1.771480
101	6	0	-2.800706	2.335863	1.522610
102	6	0	-2.665928	3.803579	1.973154
103	6	0	-4.260456	1.846606	1.645171

104	1	0	-2.201321	1.737501	2.217582
105	6	0	-3.188571	3.964241	3.411670
106	1	0	-3.230464	4.459706	1.300217
107	1	0	-1.618840	4.121380	1.934872
108	6	0	-4.755740	2.001535	3.090447
109	1	0	-4.902707	2.440957	0.984026
110	1	0	-4.347300	0.803859	1.325324
111	6	0	-4.628687	3.456229	3.563143
112	1	0	-3.119844	5.017272	3.709424
113	1	0	-2.533924	3.399116	4.090471
114	1	0	-5.796267	1.663068	3.161168
115	1	0	-4.162303	1.348869	3.746447
116	1	0	-4.954532	3.548619	4.606122
117	1	0	-5.299524	4.087727	2.963334
118	6	0	-3.375314	2.153377	-1.434291
119	6	0	-3.823264	3.631090	-1.523124
120	6	0	-2.957203	1.614096	-2.817025
121	1	0	-4.229128	1.558507	-1.090116
122	6	0	-4.938823	3.807372	-2.565406
123	1	0	-2.969687	4.258312	-1.809912
124	1	0	-4.170751	3.986488	-0.549442
125	6	0	-4.071035	1.823909	-3.855241
126	1	0	-2.047542	2.126965	-3.157450
127	1	0	-2.713019	0.551296	-2.743289
128	6	0	-4.504306	3.291974	-3.942154
129	1	0	-5.221230	4.865534	-2.619750
130	1	0	-5.830578	3.255770	-2.235438
131	1	0	-3.729222	1.462148	-4.832459
132	1	0	-4.939425	1.212407	-3.576209
133	1	0	-5.318676	3.406004	-4.667671

134	1	0	-3.664131	3.899785	-4.307562
135	6	0	-0.409455	-0.054785	1.840694
136	8	0	-0.112746	-0.053637	2.951504

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^{1}H-3-H E(opt) = -3000.56804260 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.763246	-0.091975	-0.277034
2	1	0	-0.944897	-0.189679	-1.948324
3	15	0	-1.954615	-2.049305	-0.046625
4	15	0	-2.083594	1.810280	-0.187682
5	6	0	2.102307	-0.741066	-0.272472
6	6	0	0.772590	-2.698320	-0.360216
7	6	0	3.265822	-1.502813	-0.205218
8	6	0	1.913563	-3.493403	-0.272348
9	6	0	3.180875	-2.901306	-0.190726
10	1	0	4.235189	-1.020267	-0.168182
11	1	0	1.812766	-4.572940	-0.278952
12	6	0	2.055415	0.736070	-0.306459
13	6	0	0.609743	2.596997	-0.531697
14	6	0	3.163813	1.574296	-0.224351
15	6	0	1.693796	3.468352	-0.447470
16	6	0	2.990054	2.963283	-0.278714
17	1	0	4.156866	1.158587	-0.105265
18	1	0	1.526561	4.537292	-0.519351
19	6	0	4.411691	-3.739979	-0.104570
20	6	0	4.845632	-4.465270	-1.234072
21	6	0	5.133879	-3.800624	1.105817

22	6	0	6.004316	-5.243076	-1.130842
23	6	0	6.282698	-4.597207	1.165867
24	6	0	6.733759	-5.326778	0.060255
25	1	0	6.346170	-5.794616	-2.003883
26	1	0	6.837728	-4.649558	2.099899
27	6	0	4.160906	3.880161	-0.160016
28	6	0	5.073196	3.997536	-1.229286
29	6	0	4.351126	4.616184	1.027965
30	6	0	6.165639	4.860800	-1.090992
31	6	0	5.461862	5.461792	1.125904
32	6	0	6.378053	5.601022	0.077535
33	1	0	6.867656	4.956432	-1.916403
34	1	0	5.616543	6.021475	2.045711
35	6	0	7.957902	-6.204129	0.158861
36	1	0	7.687349	-7.216712	0.485400
37	1	0	8.462213	-6.299219	-0.807973
38	1	0	8.676095	-5.810422	0.885075
39	6	0	4.094564	-4.398952	-2.544251
40	1	0	3.117584	-4.890812	-2.474179
41	1	0	3.906674	-3.363017	-2.848111
42	1	0	4.657825	-4.890479	-3.342093
43	6	0	4.679912	-3.034125	2.327015
44	1	0	4.788857	-1.952351	2.187350
45	1	0	3.622677	-3.220042	2.547570
46	1	0	5.265470	-3.316881	3.206009
47	6	0	4.880355	3.218503	-2.510003
48	1	0	5.012688	2.142067	-2.350886
49	1	0	3.871715	3.356733	-2.915737
50	1	0	5.599278	3.534096	-3.270857
51	6	0	3.391453	4.488146	2.188734

52	1	0	2.404247	4.895821	1.942236
53	1	0	3.239185	3.439811	2.469984
54	1	0	3.764894	5.024607	3.065169
55	6	0	7.548686	6.546745	0.191871
56	1	0	8.408916	6.191322	-0.384344
57	1	0	7.287570	7.540544	-0.194496
58	1	0	7.860616	6.674751	1.233187
59	7	0	0.887433	-1.354066	-0.332921
60	7	0	0.807880	1.266534	-0.428161
61	6	0	-0.613694	-3.253737	-0.565833
62	6	0	-0.802564	3.038356	-0.807039
63	1	0	-0.747828	-3.407249	-1.644487
64	1	0	-0.726825	-4.229098	-0.086184
65	1	0	-0.981361	4.055857	-0.457026
66	1	0	-0.935052	3.046760	-1.896988
67	6	0	-2.350530	-2.559659	1.700447
68	6	0	-3.129074	-1.487374	2.488010
69	6	0	-3.021070	-3.937326	1.863594
70	1	0	-1.339778	-2.616937	2.133786
71	6	0	-3.230731	-1.869058	3.972695
72	1	0	-4.138910	-1.386557	2.072353
73	1	0	-2.638808	-0.516985	2.384571
74	6	0	-3.108555	-4.320429	3.350530
75	1	0	-4.035264	-3.893139	1.449111
76	1	0	-2.477907	-4.709873	1.308164
77	6	0	-3.862363	-3.255363	4.158973
78	1	0	-3.810804	-1.107943	4.508938
79	1	0	-2.222290	-1.867539	4.411025
80	1	0	-3.599573	-5.295882	3.451689
81	1	0	-2.091838	-4.432479	3.753286

82	1	0	-3.882423	-3.526659	5.221466
83	1	0	-4.907909	-3.222194	3.820162
84	6	0	-3.362965	-2.386935	-1.208041
85	6	0	-3.687877	-3.861112	-1.527130
86	6	0	-4.635602	-1.626150	-0.785330
87	1	0	-2.987304	-1.922761	-2.130984
88	6	0	-4.756993	-3.936887	-2.631123
89	1	0	-4.064746	-4.365099	-0.631800
90	1	0	-2.789341	-4.399363	-1.846763
91	6	0	-5.702259	-1.707801	-1.887352
92	1	0	-5.033569	-2.072480	0.134718
93	1	0	-4.399577	-0.581309	-0.559993
94	6	0	-6.026316	-3.165714	-2.242388
95	1	0	-4.996125	-4.986666	-2.839707
96	1	0	-4.345611	-3.513936	-3.558710
97	1	0	-6.608411	-1.179246	-1.567150
98	1	0	-5.331107	-1.190223	-2.782005
99	1	0	-6.758976	-3.204882	-3.057584
100	1	0	-6.491788	-3.653265	-1.373748
101	6	0	-2.585558	2.344799	1.541321
102	6	0	-2.250229	3.796718	1.936499
103	6	0	-4.061326	2.015210	1.852440
104	1	0	-1.964470	1.691208	2.163560
105	6	0	-2.572292	4.033010	3.422451
106	1	0	-2.823702	4.500131	1.319997
107	1	0	-1.189040	4.004863	1.762478
108	6	0	-4.358198	2.239686	3.342772
109	1	0	-4.717257	2.664971	1.260045
110	1	0	-4.294772	0.982658	1.573028
111	6	0	-4.026900	3.679219	3.759926

112	1	0	-2.361652	5.077493	3.682305
113	1	0	-1.900359	3.412574	4.032601
114	1	0	-5.411337	2.013016	3.548364
115	1	0	-3.758479	1.537632	3.939292
116	1	0	-4.211686	3.818752	4.831970
117	1	0	-4.698707	4.369394	3.229637
118	6	0	-3.550075	2.123112	-1.291039
119	6	0	-3.906763	3.621438	-1.414471
120	6	0	-3.403072	1.474807	-2.680985
121	1	0	-4.378931	1.616986	-0.781251
122	6	0	-5.176420	3.816976	-2.258070
123	1	0	-3.077451	4.155912	-1.895171
124	1	0	-4.046848	4.069164	-0.426397
125	6	0	-4.669502	1.692856	-3.524487
126	1	0	-2.539126	1.909262	-3.202769
127	1	0	-3.204682	0.404906	-2.574447
128	6	0	-5.028787	3.179279	-3.644963
129	1	0	-5.396188	4.887757	-2.347263
130	1	0	-6.028918	3.359236	-1.736210
131	1	0	-4.529801	1.248097	-4.517364
132	1	0	-5.506151	1.158983	-3.053400
133	1	0	-5.953100	3.302288	-4.222368
134	1	0	-4.235498	3.701208	-4.199304
135	1	0	-0.584622	-0.018268	1.386608

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^{2}TS1 E(opt) =-3648.901609 hartree

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

1	77	0	-0.717521	-0.064244	-0.082700
2	1	0	-0.868013	-0.147148	-1.783309
3	15	0	-1.954137	-2.020186	0.053885
4	15	0	-2.040590	1.853830	-0.074584
5	6	0	2.128982	-0.731916	-0.187373
6	6	0	0.776431	-2.695775	-0.220949
7	6	0	3.287581	-1.523751	-0.092239
8	6	0	1.902849	-3.502895	-0.135420
9	6	0	3.185672	-2.909064	-0.063199
10	1	0	4.263635	-1.053690	-0.047349
11	1	0	1.796755	-4.581943	-0.145403
12	6	0	2.095546	0.717685	-0.235120
13	6	0	0.661204	2.611374	-0.427442
14	6	0	3.214295	1.565979	-0.158742
15	6	0	1.745878	3.473091	-0.361110
16	6	0	3.052073	2.945008	-0.209873
17	1	0	4.206496	1.143820	-0.048033
18	1	0	1.592108	4.543312	-0.441866
19	6	0	4.405993	-3.765659	0.018773
20	6	0	4.970235	-4.290609	-1.161336
21	6	0	4.978769	-4.055789	1.273364
22	6	0	6.107377	-5.101312	-1.065654
23	6	0	6.115044	-4.871445	1.326261
24	6	0	6.695554	-5.401785	0.168168
25	1	0	6.543059	-5.507288	-1.976187
26	1	0	6.555249	-5.099983	2.294618
27	6	0	4.228651	3.857679	-0.109903
28	6	0	5.103441	4.004731	-1.205519
29	6	0	4.462017	4.568843	1.086860
30	6	0	6.200646	4.867010	-1.086125

31	6	0	5.572351	5.415952	1.166244
32	6	0	6.452222	5.581494	0.089663
33	1	0	6.873906	4.982010	-1.932876
34	1	0	5.757986	5.955693	2.092603
35	6	0	7.940985	-6.251723	0.246675
36	1	0	8.007595	-6.945236	-0.597612
37	1	0	8.844055	-5.627733	0.227335
38	1	0	7.970746	-6.834336	1.173101
39	6	0	4.360373	-3.983003	-2.508979
40	1	0	3.333263	-4.360100	-2.578987
41	1	0	4.309474	-2.902168	-2.685330
42	1	0	4.941960	-4.433054	-3.318230
43	6	0	4.372255	-3.503430	2.542109
44	1	0	4.397203	-2.407522	2.552416
45	1	0	3.319485	-3.793716	2.639762
46	1	0	4.907596	-3.862627	3.425387
47	6	0	4.865911	3.254667	-2.496181
48	1	0	4.983374	2.173384	-2.361560
49	1	0	3.848342	3.415724	-2.870510
50	1	0	5.568538	3.574564	-3.270691
51	6	0	3.544320	4.404806	2.276385
52	1	0	2.532212	4.763904	2.057334
53	1	0	3.447594	3.350686	2.561853
54	1	0	3.918615	4.959208	3.141407
55	6	0	7.620532	6.532311	0.189356
56	1	0	8.393138	6.299504	-0.549717
57	1	0	7.299549	7.567429	0.013279
58	1	0	8.076531	6.503457	1.184617
59	7	0	0.898328	-1.350862	-0.227934
60	7	0	0.840566	1.274704	-0.341417

61	6	0	-0.614839	-3.242789	-0.417985
62	6	0	-0.749201	3.069148	-0.690991
63	1	0	-0.738921	-3.410903	-1.493903
64	1	0	-0.741554	-4.205649	0.083239
65	1	0	-0.918197	4.085152	-0.331484
66	1	0	-0.884838	3.087513	-1.779463
67	6	0	-2.485897	-2.531645	1.759134
68	6	0	-3.347185	-1.459523	2.457010
69	6	0	-3.146391	-3.917473	1.883422
70	1	0	-1.518948	-2.558567	2.282033
71	6	0	-3.567803	-1.820279	3.933785
72	1	0	-4.320717	-1.384383	1.958336
73	1	0	-2.859197	-0.487162	2.377996
74	6	0	-3.353613	-4.279873	3.363732
75	1	0	-4.122532	-3.897028	1.384249
76	1	0	-2.546912	-4.689302	1.388042
77	6	0	-4.189353	-3.215378	4.088928
78	1	0	-4.203981	-1.062583	4.408069
79	1	0	-2.600358	-1.793736	4.455167
80	1	0	-3.836206	-5.261935	3.440602
81	1	0	-2.372677	-4.368169	3.852152
82	1	0	-4.294008	-3.471597	5.150364
83	1	0	-5.203592	-3.206360	3.663896
84	6	0	-3.283521	-2.326440	-1.206897
85	6	0	-3.591399	-3.797871	-1.560286
86	6	0	-4.584986	-1.571417	-0.875184
87	1	0	-2.834245	-1.864442	-2.096704
88	6	0	-4.572323	-3.863786	-2.743615
89	1	0	-4.038211	-4.305409	-0.699142
90	1	0	-2.675892	-4.341591	-1.814409

91	6	0	-5.561237	-1.637613	-2.059193
92	1	0	-5.056901	-2.031544	0.001990
93	1	0	-4.369236	-0.530812	-0.613751
94	6	0	-5.865318	-3.090773	-2.448900
95	1	0	-4.797366	-4.911493	-2.977536
96	1	0	-4.089415	-3.435798	-3.633715
97	1	0	-6.486580	-1.103759	-1.810225
98	1	0	-5.115468	-1.120046	-2.918460
99	1	0	-6.533031	-3.120125	-3.318607
100	1	0	-6.398550	-3.582513	-1.622504
101	6	0	-2.606528	2.414514	1.620881
102	6	0	-2.245528	3.858592	2.019726
103	6	0	-4.102692	2.128172	1.872239
104	1	0	-2.033125	1.750299	2.275817
105	6	0	-2.618557	4.113594	3.490369
106	1	0	-2.772681	4.574982	1.376622
107	1	0	-1.172450	4.034204	1.886189
108	6	0	-4.449603	2.369393	3.349245
109	1	0	-4.719846	2.789872	1.251952
110	1	0	-4.352869	1.099892	1.591228
111	6	0	-4.094696	3.801714	3.772155
112	1	0	-2.389585	5.153359	3.754163
113	1	0	-1.988681	3.478215	4.129304
114	1	0	-5.515617	2.172816	3.516873
115	1	0	-3.891929	1.654961	3.971290
116	1	0	-4.317598	3.952747	4.835457
117	1	0	-4.725987	4.506976	3.212450
118	6	0	-3.465400	2.148165	-1.237922
119	6	0	-3.804682	3.646718	-1.402660
120	6	0	-3.256809	1.476406	-2.608354

121	1	0	-4.318898	1.655840	-0.756405
122	6	0	-5.028043	3.839672	-2.312125
123	1	0	-2.949656	4.166428	-1.853128
124	1	0	-3.985630	4.112388	-0.429387
125	6	0	-4.474078	1.695567	-3.520782
126	1	0	-2.360075	1.882247	-3.091863
127	1	0	-3.081245	0.405716	-2.475833
128	6	0	-4.809349	3.183687	-3.681162
129	1	0	-5.236027	4.910570	-2.425964
130	1	0	-5.910202	3.393108	-1.831324
131	1	0	-4.287442	1.233644	-4.498176
132	1	0	-5.342436	1.180776	-3.088196
133	1	0	-5.698110	3.308388	-4.311740
134	1	0	-3.980272	3.690769	-4.195564
135	6	0	-0.451102	-0.374926	-3.114227
136	8	0	0.016885	0.651661	-3.571988
137	8	0	-0.674292	-1.542417	-3.394720
138	17	0	-0.137519	0.018882	2.419248

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^{2}TS2 E(opt) = -3188.536360 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.762758	-0.049738	-0.188180
2	1	0	-0.976614	-0.159524	-1.805126
3	15	0	-1.950838	-2.006921	0.091818
4	15	0	-2.055463	1.857694	-0.055060
5	6	0	2.092705	-0.718394	-0.105731
6	6	0	0.748264	-2.674536	-0.248772

7	6	0	3.250571	-1.496689	-0.045235
8	6	0	1.879536	-3.476035	-0.170206
9	6	0	3.153833	-2.890300	-0.058710
10	1	0	4.224352	-1.023686	0.007232
11	1	0	1.775199	-4.554650	-0.211324
12	6	0	2.056375	0.749303	-0.133438
13	6	0	0.628326	2.631428	-0.382915
14	6	0	3.172812	1.583529	-0.064890
15	6	0	1.718242	3.488758	-0.311257
16	6	0	3.014507	2.970067	-0.135822
17	1	0	4.162781	1.158675	0.049457
18	1	0	1.564560	4.558087	-0.404643
19	6	0	4.376011	-3.743079	0.023474
20	6	0	4.922011	-4.297834	-1.151665
21	6	0	4.973958	-3.987994	1.276168
22	6	0	6.067777	-5.095262	-1.051544
23	6	0	6.116784	-4.793766	1.331975
24	6	0	6.677585	-5.357976	0.180461
25	1	0	6.494819	-5.518862	-1.957963
26	1	0	6.579196	-4.985219	2.297852
27	6	0	4.193981	3.878288	-0.042374
28	6	0	5.103128	3.963272	-1.117259
29	6	0	4.395052	4.643967	1.125663
30	6	0	6.202692	4.822170	-1.004880
31	6	0	5.511649	5.483720	1.198470
32	6	0	6.425027	5.590086	0.143251
33	1	0	6.901514	4.892369	-1.835552
34	1	0	5.673866	6.065554	2.103242
35	6	0	7.890797	-6.251822	0.269009
36	1	0	7.595286	-7.299104	0.414092

37	1	0	8.489315	-6.207822	-0.646428
38	1	0	8.531239	-5.976217	1.112919
39	6	0	4.294199	-4.027765	-2.499121
40	1	0	3.275138	-4.428021	-2.554774
41	1	0	4.220938	-2.951842	-2.696696
42	1	0	4.878611	-4.482057	-3.303753
43	6	0	4.391642	-3.399080	2.539920
44	1	0	4.423915	-2.303424	2.523882
45	1	0	3.339459	-3.681574	2.663591
46	1	0	4.940415	-3.739320	3.422255
47	6	0	4.900549	3.155303	-2.378640
48	1	0	5.041603	2.083346	-2.198434
49	1	0	3.886409	3.277949	-2.775453
50	1	0	5.608724	3.458732	-3.154484
51	6	0	3.438663	4.551990	2.292519
52	1	0	2.453234	4.959635	2.038876
53	1	0	3.280643	3.511972	2.600409
54	1	0	3.818302	5.107889	3.154098
55	6	0	7.601600	6.531312	0.231940
56	1	0	8.429608	6.199940	-0.402483
57	1	0	7.321359	7.540206	-0.097817
58	1	0	7.968666	6.617869	1.259741
59	7	0	0.866954	-1.324292	-0.175385
60	7	0	0.804858	1.292907	-0.249762
61	6	0	-0.640392	-3.208249	-0.496463
62	6	0	-0.777159	3.081674	-0.679611
63	1	0	-0.777441	-3.295145	-1.581920
64	1	0	-0.767752	-4.205910	-0.068660
65	1	0	-0.954803	4.103843	-0.342300
66	1	0	-0.902601	3.076934	-1.770395

67	6	0	-2.209320	-2.516643	1.865011
68	6	0	-2.849479	-1.406148	2.719775
69	6	0	-2.936430	-3.857915	2.077137
70	1	0	-1.168451	-2.634690	2.206336
71	6	0	-2.859182	-1.795224	4.205604
72	1	0	-3.879535	-1.233980	2.385050
73	1	0	-2.304966	-0.467364	2.578681
74	6	0	-2.932177	-4.244641	3.565438
75	1	0	-3.974675	-3.759491	1.737969
76	1	0	-2.474844	-4.651682	1.479424
77	6	0	-3.559010	-3.142667	4.431196
78	1	0	-3.348309	-1.006298	4.789999
79	1	0	-1.821898	-1.860927	4.564713
80	1	0	-3.469370	-5.190922	3.702521
81	1	0	-1.895854	-4.417188	3.889267
82	1	0	-3.517823	-3.421123	5.491168
83	1	0	-4.622550	-3.043286	4.170300
84	6	0	-3.429721	-2.326662	-0.973299
85	6	0	-3.783041	-3.794973	-1.283765
86	6	0	-4.660962	-1.553437	-0.460724
87	1	0	-3.107800	-1.860840	-1.914386
88	6	0	-4.927457	-3.852693	-2.310436
89	1	0	-4.096290	-4.310023	-0.370020
90	1	0	-2.909153	-4.328591	-1.673163
91	6	0	-5.801418	-1.621485	-1.487017
92	1	0	-4.998487	-1.991860	0.486950
93	1	0	-4.395668	-0.510967	-0.256295
94	6	0	-6.160036	-3.075115	-1.826631
95	1	0	-5.189813	-4.898366	-2.511769
96	1	0	-4.578838	-3.423535	-3.260587

97	1	0	-6.679794	-1.087855	-1.103868
98	1	0	-5.487123	-1.102343	-2.402591
99	1	0	-6.949582	-3.104132	-2.587308
100	1	0	-6.565510	-3.565060	-0.929637
101	6	0	-2.492559	2.363792	1.697162
102	6	0	-2.170693	3.818434	2.093620
103	6	0	-3.950447	2.004084	2.052964
104	1	0	-1.836488	1.715495	2.293326
105	6	0	-2.451981	4.039159	3.590111
106	1	0	-2.776716	4.513030	1.498534
107	1	0	-1.119854	4.047944	1.887701
108	6	0	-4.207272	2.214036	3.552468
109	1	0	-4.632472	2.647703	1.483355
110	1	0	-4.174652	0.970338	1.771478
111	6	0	-3.889245	3.656965	3.968608
112	1	0	-2.252271	5.085544	3.850790
113	1	0	-1.750841	3.427205	4.175620
114	1	0	-5.249690	1.967392	3.787385
115	1	0	-3.578012	1.519327	4.126725
116	1	0	-4.044345	3.786936	5.046504
117	1	0	-4.588823	4.337948	3.462991
118	6	0	-3.540094	2.175401	-1.125720
119	6	0	-3.906241	3.670035	-1.245319
120	6	0	-3.392819	1.520748	-2.513963
121	1	0	-4.360856	1.663732	-0.608004
122	6	0	-5.174017	3.858724	-2.093493
123	1	0	-3.078438	4.212561	-1.719940
124	1	0	-4.052259	4.109186	-0.253637
125	6	0	-4.658129	1.734204	-3.359078
126	1	0	-2.528889	1.951830	-3.038915

127	1	0	-3.192418	0.451862	-2.402611
128	6	0	-5.019472	3.220357	-3.479867
129	1	0	-5.399314	4.928157	-2.184799
130	1	0	-6.025961	3.396957	-1.574247
131	1	0	-4.515483	1.289459	-4.351600
132	1	0	-5.494414	1.198709	-2.888878
133	1	0	-5.941722	3.342132	-4.060787
134	1	0	-4.224800	3.743381	-4.031265
135	6	0	-0.593853	-0.610305	-3.383820
136	8	0	0.322751	0.098810	-3.685627
137	8	0	-1.382089	-1.480524	-3.630503

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^{2}TS3 E(opt) = -3188.512287 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.751759	-0.028440	-0.112505
2	1	0	-0.479472	-1.107499	-4.427613
3	15	0	-1.940231	-2.011851	0.127861
4	15	0	-2.039712	1.904219	-0.119434
5	6	0	2.105247	-0.715044	-0.009814
6	6	0	0.708080	-2.663364	-0.134246
7	6	0	3.256646	-1.482421	0.041737
8	6	0	1.876306	-3.469434	-0.062897
9	6	0	3.133145	-2.892997	0.029040
10	1	0	4.236752	-1.022977	0.077426
11	1	0	1.770684	-4.548910	-0.091245
12	6	0	2.075571	0.767043	-0.075245
13	6	0	0.665014	2.641562	-0.421016

14	6	0	3.195456	1.590720	-0.026101
15	6	0	1.763445	3.498447	-0.371817
16	6	0	3.047061	2.978070	-0.162133
17	1	0	4.181110	1.165398	0.118257
18	1	0	1.618977	4.563837	-0.512578
19	6	0	4.356024	-3.748537	0.100861
20	6	0	4.911468	-4.276591	-1.080687
21	6	0	4.947045	-4.020127	1.352212
22	6	0	6.056760	-5.077949	-0.989976
23	6	0	6.088725	-4.826659	1.399353
24	6	0	6.657631	-5.367243	0.239378
25	1	0	6.488638	-5.483486	-1.902315
26	1	0	6.544775	-5.038994	2.364117
27	6	0	4.237556	3.875273	-0.106009
28	6	0	5.135574	3.914207	-1.194730
29	6	0	4.459773	4.671457	1.034507
30	6	0	6.245438	4.760612	-1.120817
31	6	0	5.589242	5.499504	1.069134
32	6	0	6.490790	5.560799	0.002481
33	1	0	6.936395	4.796683	-1.960486
34	1	0	5.767608	6.107600	1.953057
35	6	0	7.874810	-6.256434	0.324053
36	1	0	7.600648	-7.266088	0.655729
37	1	0	8.371473	-6.352396	-0.646246
38	1	0	8.602834	-5.869018	1.045084
39	6	0	4.291721	-3.980566	-2.426637
40	1	0	3.276477	-4.387487	-2.498327
41	1	0	4.210383	-2.900912	-2.599399
42	1	0	4.886091	-4.410742	-3.237358
43	6	0	4.353620	-3.458115	2.622901

44	1	0	4.350444	-2.361891	2.612697
45	1	0	3.311269	-3.774300	2.748339
46	1	0	4.916469	-3.786623	3.500864
47	6	0	4.904660	3.069494	-2.426611
48	1	0	5.012324	2.000639	-2.208488
49	1	0	3.893598	3.210255	-2.825612
50	1	0	5.619511	3.323124	-3.213985
51	6	0	3.513661	4.628518	2.212322
52	1	0	2.527551	5.029774	1.951269
53	1	0	3.355088	3.601780	2.561913
54	1	0	3.902883	5.215629	3.048434
55	6	0	7.688841	6.478098	0.038946
56	1	0	8.600900	5.954252	-0.268042
57	1	0	7.557925	7.320990	-0.651528
58	1	0	7.849903	6.889900	1.039382
59	7	0	0.878119	-1.306275	-0.065197
60	7	0	0.837038	1.314898	-0.236503
61	6	0	-0.620937	-3.142267	-0.377149
62	6	0	-0.732678	3.093857	-0.756395
63	1	0	-0.633499	-2.752585	-1.955915
64	1	0	-0.778631	-4.214240	-0.268888
65	1	0	-0.905802	4.125636	-0.446767
66	1	0	-0.835036	3.069735	-1.848974
67	6	0	-2.359861	-2.413071	1.904001
68	6	0	-3.088904	-1.276820	2.645810
69	6	0	-3.068531	-3.762665	2.121737
70	1	0	-1.350543	-2.490092	2.337328
71	6	0	-3.225175	-1.596472	4.142500
72	1	0	-4.087343	-1.133007	2.216614
73	1	0	-2.543657	-0.338048	2.509360

74	6	0	-3.193605	-4.075249	3.622093
75	1	0	-4.073079	-3.717731	1.683723
76	1	0	-2.528035	-4.567791	1.610349
77	6	0	-3.918964	-2.946965	4.369309
78	1	0	-3.777634	-0.792084	4.643675
79	1	0	-2.223338	-1.624197	4.595126
80	1	0	-3.721761	-5.026628	3.760161
81	1	0	-2.188122	-4.204916	4.047457
82	1	0	-3.972707	-3.172643	5.441295
83	1	0	-4.955015	-2.884255	4.006090
84	6	0	-3.378167	-2.314843	-1.005878
85	6	0	-3.692012	-3.789043	-1.331045
86	6	0	-4.647507	-1.560184	-0.567636
87	1	0	-3.025246	-1.844652	-1.934735
88	6	0	-4.780171	-3.875083	-2.414157
89	1	0	-4.041590	-4.304297	-0.429797
90	1	0	-2.787574	-4.306095	-1.668361
91	6	0	-5.729812	-1.653294	-1.653858
92	1	0	-5.031642	-1.999695	0.361234
93	1	0	-4.412297	-0.511750	-0.354349
94	6	0	-6.048418	-3.114508	-2.001121
95	1	0	-5.014625	-4.926380	-2.621150
96	1	0	-4.389445	-3.446714	-3.348463
97	1	0	-6.635688	-1.129991	-1.323953
98	1	0	-5.374730	-1.136921	-2.555934
99	1	0	-6.797151	-3.160702	-2.801317
100	1	0	-6.492388	-3.605025	-1.122820
101	6	0	-2.494097	2.476614	1.608087
102	6	0	-2.130637	3.930398	1.969181
103	6	0	-3.972622	2.181533	1.939431

104	1	0	-1.877171	1.823937	2.240763
105	6	0	-2.437477	4.207081	3.451239
106	1	0	-2.699312	4.625796	1.338898
107	1	0	-1.068121	4.118239	1.781122
108	6	0	-4.254799	2.444077	3.425959
109	1	0	-4.616844	2.833506	1.336660
110	1	0	-4.230037	1.149809	1.681117
111	6	0	-3.895457	3.886701	3.807444
112	1	0	-2.206814	5.253539	3.684577
113	1	0	-1.771588	3.589730	4.071208
114	1	0	-5.310191	2.240517	3.643565
115	1	0	-3.663306	1.745403	4.034452
116	1	0	-4.069452	4.054202	4.877233
117	1	0	-4.559051	4.576144	3.266082
118	6	0	-3.498916	2.203521	-1.224598
119	6	0	-3.851135	3.694569	-1.407015
120	6	0	-3.325412	1.500749	-2.585774
121	1	0	-4.331883	1.713850	-0.704579
122	6	0	-5.106795	3.855676	-2.278816
123	1	0	-3.013048	4.210148	-1.893694
124	1	0	-4.004243	4.175926	-0.436081
125	6	0	-4.580767	1.679308	-3.453622
126	1	0	-2.458772	1.923092	-3.111187
127	1	0	-3.110859	0.438859	-2.436309
128	6	0	-4.938341	3.160500	-3.636393
129	1	0	-5.325179	4.921519	-2.416973
130	1	0	-5.967815	3.419812	-1.752263
131	1	0	-4.427846	1.197232	-4.427051
132	1	0	-5.423453	1.163429	-2.973270
133	1	0	-5.854029	3.260677	-4.231681

134	1	0	-4.136871	3.659834	-4.199782
135	6	0	-0.546482	-1.265252	-3.339011
136	8	0	-0.560113	-0.285241	-2.586559
137	8	0	-0.602394	-2.525740	-3.023916

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^{1}TS4 E(opt) = -3188.638938 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.759115	-0.064183	-0.393144
2	1	0	-1.239718	-0.352404	-1.949525
3	15	0	-1.889536	-1.989253	0.161570
4	15	0	-2.041979	1.834082	-0.132857
5	6	0	2.109918	-0.676347	-0.265278
6	6	0	0.772725	-2.669272	-0.269413
7	6	0	3.276407	-1.471395	-0.177469
8	6	0	1.898657	-3.453400	-0.167676
9	6	0	3.189926	-2.848815	-0.110809
10	1	0	4.248997	-0.990452	-0.168449
11	1	0	1.802923	-4.534012	-0.155666
12	6	0	2.060911	0.751559	-0.317229
13	6	0	0.600362	2.644104	-0.519776
14	6	0	3.165996	1.628077	-0.224030
15	6	0	1.665612	3.504966	-0.428645
16	6	0	2.991822	2.999012	-0.249720
17	1	0	4.161936	1.212890	-0.114036
18	1	0	1.499237	4.573530	-0.513956
19	6	0	4.412661	-3.699881	-0.006659
20	6	0	4.960715	-4.287863	-1.165745

21	6	0	5.014443	-3.919186	1.249491
22	6	0	6.106096	-5.084008	-1.048786
23	6	0	6.158311	-4.723173	1.325370
24	6	0	6.718582	-5.315872	0.188235
25	1	0	6.531388	-5.531313	-1.944921
26	1	0	6.622065	-4.890523	2.295355
27	6	0	4.141636	3.937280	-0.105505
28	6	0	5.132043	4.017932	-1.109000
29	6	0	4.238648	4.756950	1.043024
30	6	0	6.196178	4.914686	-0.947690
31	6	0	5.319553	5.636402	1.165831
32	6	0	6.307909	5.734594	0.179440
33	1	0	6.953871	4.976590	-1.726208
34	1	0	5.395140	6.256503	2.056913
35	6	0	7.932544	-6.207223	0.296305
36	1	0	7.639012	-7.255012	0.442511
37	1	0	8.542469	-6.166385	-0.611976
38	1	0	8.562807	-5.925904	1.146046
39	6	0	4.331130	-4.051566	-2.518830
40	1	0	3.298571	-4.418440	-2.549870
41	1	0	4.289696	-2.982150	-2.756500
42	1	0	4.893156	-4.555001	-3.310462
43	6	0	4.436357	-3.297616	2.499801
44	1	0	4.488271	-2.203333	2.463812
45	1	0	3.378047	-3.556804	2.621040
46	1	0	4.973250	-3.632083	3.392031
47	6	0	5.061231	3.164972	-2.355982
48	1	0	5.309728	2.118297	-2.146374
49	1	0	4.055458	3.168244	-2.789516
50	1	0	5.762353	3.525583	-3.114341

51	6	0	3.210499	4.677339	2.149028
52	1	0	2.244709	5.091184	1.836902
53	1	0	3.024659	3.639643	2.448274
54	1	0	3.541082	5.233561	3.030880
55	6	0	7.444656	6.718111	0.319792
56	1	0	8.311114	6.419386	-0.278484
57	1	0	7.143504	7.718515	-0.017685
58	1	0	7.764629	6.813954	1.362790
59	7	0	0.864697	-1.298343	-0.267821
60	7	0	0.773770	1.282744	-0.396188
61	6	0	-0.620712	-3.218087	-0.454129
62	6	0	-0.813423	3.073038	-0.811534
63	1	0	-0.812452	-3.317708	-1.532045
64	1	0	-0.727241	-4.209742	-0.006841
65	1	0	-1.002359	4.102155	-0.501378
66	1	0	-0.967902	3.024803	-1.898574
67	6	0	-2.001991	-2.423821	1.977015
68	6	0	-2.601661	-1.296822	2.836472
69	6	0	-2.662422	-3.772678	2.320230
70	1	0	-0.933253	-2.495083	2.235550
71	6	0	-2.453503	-1.608872	4.333192
72	1	0	-3.665464	-1.177598	2.596719
73	1	0	-2.110401	-0.349890	2.596046
74	6	0	-2.502355	-4.088578	3.817041
75	1	0	-3.731804	-3.719151	2.081868
76	1	0	-2.237720	-4.583674	1.718205
77	6	0	-3.078086	-2.964960	4.690520
78	1	0	-2.912055	-0.808326	4.926733
79	1	0	-1.384412	-1.622945	4.590599
80	1	0	-2.992028	-5.042286	4.049626

81	1	0	-1.434299	-4.215797	4.044786
82	1	0	-2.922433	-3.189774	5.752803
83	1	0	-4.165297	-2.911526	4.533958
84	6	0	-3.459900	-2.405512	-0.736295
85	6	0	-3.819629	-3.891515	-0.931219
86	6	0	-4.654322	-1.616887	-0.162953
87	1	0	-3.240275	-1.990969	-1.728460
88	6	0	-5.046873	-4.019362	-1.851143
89	1	0	-4.047405	-4.357570	0.032771
90	1	0	-2.973664	-4.438867	-1.362225
91	6	0	-5.877436	-1.748855	-1.082478
92	1	0	-4.906705	-2.006068	0.831965
93	1	0	-4.386590	-0.562296	-0.036689
94	6	0	-6.243986	-3.222533	-1.311474
95	1	0	-5.314525	-5.076780	-1.967656
96	1	0	-4.786358	-3.646064	-2.851655
97	1	0	-6.728301	-1.204575	-0.654226
98	1	0	-5.650134	-1.275329	-2.047942
99	1	0	-7.093685	-3.301154	-2.000719
100	1	0	-6.568251	-3.663400	-0.357633
101	6	0	-2.395068	2.356507	1.642718
102	6	0	-2.045754	3.810731	2.020167
103	6	0	-3.828758	2.004229	2.089353
104	1	0	-1.706542	1.711387	2.203070
105	6	0	-2.235026	4.034037	3.530978
106	1	0	-2.683102	4.509708	1.464031
107	1	0	-1.008492	4.036156	1.750972
108	6	0	-3.995166	2.215111	3.601395
109	1	0	-4.543518	2.649199	1.562643
110	1	0	-4.074141	0.971160	1.822812

111	6	0	-3.647986	3.657029	3.996925
112	1	0	-2.016108	5.079695	3.779958
113	1	0	-1.502099	3.419351	4.073210
114	1	0	-5.022026	1.971547	3.900702
115	1	0	-3.333926	1.519552	4.136967
116	1	0	-3.736913	3.788283	5.082334
117	1	0	-4.374818	4.340454	3.534538
118	6	0	-3.607950	2.171849	-1.088260
119	6	0	-3.984597	3.664363	-1.186687
120	6	0	-3.583857	1.515730	-2.481354
121	1	0	-4.387058	1.662630	-0.506346
122	6	0	-5.326438	3.847644	-1.914790
123	1	0	-3.202372	4.200719	-1.740304
124	1	0	-4.038686	4.115669	-0.191261
125	6	0	-4.923282	1.712801	-3.207432
126	1	0	-2.775858	1.955072	-3.083848
127	1	0	-3.359108	0.450669	-2.390828
128	6	0	-5.305974	3.195630	-3.303670
129	1	0	-5.561016	4.916220	-1.995466
130	1	0	-6.125566	3.391702	-1.312633
131	1	0	-4.870810	1.263184	-4.206910
132	1	0	-5.707926	1.172407	-2.658513
133	1	0	-6.281424	3.308646	-3.792623
134	1	0	-4.572186	3.717268	-3.935167
135	6	0	-1.078724	-1.049956	-3.618944
136	8	0	0.061673	-0.858502	-3.908161
137	8	0	-2.190205	-1.435254	-3.823387

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^{1}TS5 E(opt) = -3264.409039 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.868972	0.015761	-0.591282
2	15	0	-2.062581	-1.940067	-0.374534
3	15	0	-2.108323	1.907879	-0.148423
4	6	0	1.965611	-0.678843	-0.769736
5	6	0	0.598952	-2.601079	-0.940498
6	6	0	3.107153	-1.464787	-0.681285
7	6	0	1.719727	-3.423558	-0.844220
8	6	0	2.991757	-2.861919	-0.688443
9	1	0	4.082069	-1.005377	-0.573150
10	1	0	1.593329	-4.500285	-0.856734
11	6	0	1.953116	0.799366	-0.700771
12	6	0	0.542615	2.698852	-0.646883
13	6	0	3.083325	1.603130	-0.598277
14	6	0	1.649852	3.536954	-0.532620
15	6	0	2.941387	2.995243	-0.506684
16	1	0	4.071271	1.159864	-0.575693
17	1	0	1.503492	4.609568	-0.474126
18	6	0	4.193231	-3.717485	-0.472457
19	6	0	4.695361	-4.524098	-1.514728
20	6	0	4.819351	-3.709806	0.793434
21	6	0	5.826650	-5.311317	-1.272458
22	6	0	5.942693	-4.519926	0.992731
23	6	0	6.461759	-5.327106	-0.025567
24	1	0	6.222362	-5.925180	-2.078584
25	1	0	6.422584	-4.521211	1.969083
26	6	0	4.137205	3.876992	-0.383072
27	6	0	5.018962	4.022161	-1.475284

28	6	0	4.379310	4.560300	0.827763
29	6	0	6.130686	4.860446	-1.336915
30	6	0	5.508243	5.381478	0.923618
31	6	0	6.392816	5.549208	-0.147557
32	1	0	6.807705	4.978365	-2.180111
33	1	0	5.702746	5.899733	1.860012
34	6	0	7.656643	-6.214520	0.224828
35	1	0	7.342958	-7.191044	0.616184
36	1	0	8.219395	-6.399148	-0.695624
37	1	0	8.335901	-5.773873	0.961626
38	6	0	4.046380	-4.533239	-2.879904
39	1	0	3.060243	-5.010853	-2.854199
40	1	0	3.896793	-3.516792	-3.260971
41	1	0	4.660994	-5.079305	-3.600809
42	6	0	4.293774	-2.855512	1.926769
43	1	0	4.564608	-1.801298	1.790730
44	1	0	3.201656	-2.895492	1.991085
45	1	0	4.713925	-3.181497	2.882750
46	6	0	4.776393	3.304182	-2.783557
47	1	0	4.948081	2.225564	-2.690456
48	1	0	3.744668	3.432751	-3.129181
49	1	0	5.445032	3.679950	-3.562855
50	6	0	3.457655	4.403800	2.016124
51	1	0	2.489868	4.888464	1.843043
52	1	0	3.249724	3.349327	2.229387
53	1	0	3.897698	4.852072	2.911059
54	6	0	7.581053	6.472615	-0.034099
55	1	0	8.408002	6.142172	-0.670627
56	1	0	7.315787	7.490493	-0.348321
57	1	0	7.943282	6.535535	0.996872

58	7	0	0.737266	-1.259663	-0.877081
59	7	0	0.712383	1.360752	-0.716382
60	6	0	-0.804161	-3.119731	-1.118407
61	6	0	-0.873802	3.193112	-0.752377
62	1	0	-1.021979	-3.166607	-2.193001
63	1	0	-0.904089	-4.133458	-0.722955
64	1	0	-0.996169	4.166855	-0.276260
65	1	0	-1.103144	3.329029	-1.816777
66	6	0	-2.239144	-2.567416	1.365064
67	6	0	-2.861130	-1.537990	2.327782
68	6	0	-2.910642	-3.942998	1.532947
69	1	0	-1.180050	-2.654563	1.643824
70	6	0	-2.727783	-2.019538	3.780427
71	1	0	-3.921905	-1.390781	2.090101
72	1	0	-2.359545	-0.576461	2.213438
73	6	0	-2.774352	-4.425571	2.987607
74	1	0	-3.975672	-3.863199	1.281847
75	1	0	-2.473296	-4.682848	0.853030
76	6	0	-3.357740	-3.405470	3.975820
77	1	0	-3.190093	-1.289896	4.456947
78	1	0	-1.660158	-2.062836	4.038982
79	1	0	-3.270713	-5.396853	3.104117
80	1	0	-1.710192	-4.582905	3.213863
81	1	0	-3.213720	-3.750079	5.007238
82	1	0	-4.443240	-3.332005	3.815186
83	6	0	-3.601074	-2.197142	-1.384373
84	6	0	-3.959903	-3.647955	-1.766971
85	6	0	-4.807829	-1.483266	-0.742315
86	1	0	-3.351098	-1.662832	-2.313427
87	6	0	-5.174453	-3.663778	-2.710960

88	1	0	-4.200396	-4.223089	-0.867225
89	1	0	-3.110650	-4.143482	-2.249403
90	6	0	-6.018513	-1.506961	-1.686900
91	1	0	-5.070925	-1.993358	0.192955
92	1	0	-4.547272	-0.452115	-0.481911
93	6	0	-6.380384	-2.942702	-2.092182
94	1	0	-5.434263	-4.700035	-2.958974
95	1	0	-4.902364	-3.169601	-3.654643
96	1	0	-6.873626	-1.015104	-1.207411
97	1	0	-5.780724	-0.925366	-2.587985
98	1	0	-7.222586	-2.939335	-2.794703
99	1	0	-6.712137	-3.495580	-1.201571
100	6	0	-2.452088	2.264521	1.655796
101	6	0	-2.077395	3.673760	2.154617
102	6	0	-3.904567	1.912923	2.041725
103	1	0	-1.789264	1.556697	2.165726
104	6	0	-2.288057	3.773685	3.675410
105	1	0	-2.689143	4.429675	1.645394
106	1	0	-1.029726	3.894903	1.923375
107	6	0	-4.087587	1.995268	3.564160
108	1	0	-4.592627	2.621059	1.563419
109	1	0	-4.170629	0.914186	1.681672
110	6	0	-3.715768	3.389784	4.087126
111	1	0	-2.051898	4.790066	4.013242
112	1	0	-1.576608	3.100267	4.174364
113	1	0	-5.123765	1.750114	3.826952
114	1	0	-3.448928	1.240711	4.044559
115	1	0	-3.818366	3.428874	5.178379
116	1	0	-4.420939	4.126210	3.675516
117	6	0	-3.642322	2.297382	-1.120220

118	6	0	-4.043603	3.786171	-1.122000
119	6	0	-3.527869	1.747392	-2.557130
120	1	0	-4.433688	1.730231	-0.614873
121	6	0	-5.349538	3.997328	-1.905505
122	1	0	-3.247661	4.379192	-1.591166
123	1	0	-4.156396	4.154483	-0.097325
124	6	0	-4.834097	1.973243	-3.334229
125	1	0	-2.705353	2.251751	-3.083512
126	1	0	-3.282646	0.679563	-2.528669
127	6	0	-5.239804	3.453479	-3.336676
128	1	0	-5.603716	5.064071	-1.919001
129	1	0	-6.168278	3.481585	-1.383715
130	1	0	-4.723869	1.602422	-4.360607
131	1	0	-5.633267	1.382031	-2.866660
132	1	0	-6.190085	3.586006	-3.867906
133	1	0	-4.484967	4.034366	-3.886143
134	6	0	0.958839	-0.868155	2.526754
135	8	0	0.893498	-2.037838	2.128730
136	8	0	1.962356	-0.499334	3.385410
137	8	0	0.184942	0.120791	2.240493
138	1	0	-0.399737	-0.038871	1.050587
139	1	0	2.466562	-1.308390	3.569493

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^{1}TS6 E(opt) = -3453.72763485 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.882229	-0.007033	-0.024478
2	1	0	-2.550209	-0.908388	-4.151203

3	15	0	-2.104612	-1.921031	0.224189
4	15	0	-2.122023	1.913044	0.022415
5	6	0	1.941268	-0.731357	0.165628
6	6	0	0.569542	-2.652410	-0.028861
7	6	0	3.074919	-1.521990	0.317377
8	6	0	1.683283	-3.475999	0.126569
9	6	0	2.954890	-2.916512	0.305164
10	1	0	4.050533	-1.065530	0.431259
11	1	0	1.559334	-4.553104	0.092600
12	6	0	1.939249	0.743457	0.101084
13	6	0	0.564394	2.631025	-0.269707
14	6	0	3.067206	1.551536	0.201952
15	6	0	1.667612	3.472267	-0.165104
16	6	0	2.941408	2.941725	0.082944
17	1	0	4.041145	1.110043	0.375266
18	1	0	1.536221	4.540647	-0.295620
19	6	0	4.161987	-3.781665	0.453350
20	6	0	4.798011	-4.291987	-0.697456
21	6	0	4.656928	-4.078432	1.737716
22	6	0	5.930052	-5.097995	-0.537667
23	6	0	5.792097	-4.890573	1.852969
24	6	0	6.443333	-5.407524	0.728103
25	1	0	6.423640	-5.493799	-1.422884
26	1	0	6.173556	-5.124686	2.844451
27	6	0	4.126896	3.838001	0.199954
28	6	0	5.161961	3.775062	-0.757140
29	6	0	4.206727	4.755678	1.272703
30	6	0	6.254239	4.642629	-0.631434
31	6	0	5.321241	5.595256	1.363730
32	6	0	6.353157	5.560028	0.418350

33	1	0	7.046527	4.598696	-1.375758
34	1	0	5.387286	6.292520	2.196193
35	6	0	7.683540	-6.257339	0.865943
36	1	0	7.672467	-7.096993	0.162603
37	1	0	8.586574	-5.671376	0.651561
38	1	0	7.785405	-6.659794	1.878356
39	6	0	4.269726	-3.971960	-2.076324
40	1	0	3.258549	-4.372325	-2.217434
41	1	0	4.202779	-2.890846	-2.242207
42	1	0	4.911418	-4.400766	-2.851316
43	6	0	3.972766	-3.537448	2.971377
44	1	0	3.994708	-2.441434	2.992272
45	1	0	2.916860	-3.830985	3.003206
46	1	0	4.454694	-3.902119	3.882577
47	6	0	5.130479	2.795432	-1.909579
48	1	0	5.561106	1.832028	-1.603481
49	1	0	4.116396	2.606229	-2.274325
50	1	0	5.734628	3.161618	-2.744918
51	6	0	3.127941	4.832812	2.330363
52	1	0	2.223352	5.322377	1.951484
53	1	0	2.828348	3.838189	2.677651
54	1	0	3.474533	5.405324	3.195248
55	6	0	7.523933	6.507319	0.516285
56	1	0	8.414240	6.097196	0.029435
57	1	0	7.295446	7.463134	0.027010
58	1	0	7.772829	6.729751	1.558982
59	7	0	0.711429	-1.305331	0.017866
60	7	0	0.708579	1.294733	-0.104082
61	6	0	-0.814734	-3.165240	-0.324442
62	6	0	-0.818913	3.104070	-0.625061

63	1	0	-0.922564	-3.222447	-1.415633
64	1	0	-0.972808	-4.162597	0.094521
65	1	0	-0.980814	4.142224	-0.330426
66	1	0	-0.918801	3.058097	-1.717149
67	6	0	-2.374993	-2.395017	2.013845
68	6	0	-3.015872	-1.264905	2.842531
69	6	0	-3.095919	-3.731283	2.268915
70	1	0	-1.335042	-2.501549	2.361132
71	6	0	-3.021659	-1.612158	4.338915
72	1	0	-4.047272	-1.101901	2.505568
73	1	0	-2.471121	-0.331242	2.673060
74	6	0	-3.082491	-4.078220	3.767063
75	1	0	-4.137123	-3.647184	1.934541
76	1	0	-2.635632	-4.540314	1.690916
77	6	0	-3.712426	-2.956829	4.605276
78	1	0	-3.513344	-0.809991	4.903336
79	1	0	-1.983073	-1.662174	4.697268
80	1	0	-3.612465	-5.024075	3.933831
81	1	0	-2.043385	-4.234667	4.090682
82	1	0	-3.665867	-3.205649	5.672580
83	1	0	-4.777708	-2.871344	4.345976
84	6	0	-3.595636	-2.291569	-0.818993
85	6	0	-3.956628	-3.771557	-1.057042
86	6	0	-4.825744	-1.491458	-0.348898
87	1	0	-3.275248	-1.882935	-1.785800
88	6	0	-5.094972	-3.876552	-2.086584
89	1	0	-4.281409	-4.237980	-0.121509
90	1	0	-3.083284	-4.329714	-1.409986
91	6	0	-5.963445	-1.604512	-1.375006
92	1	0	-5.169077	-1.882265	0.617887

93	1	0	-4.559657	-0.440537	-0.193437
94	6	0	-6.326687	-3.071279	-1.647598
95	1	0	-5.361764	-4.929718	-2.238592
96	1	0	-4.739488	-3.495940	-3.054574
97	1	0	-6.842264	-1.050031	-1.023046
98	1	0	-5.642777	-1.131225	-2.313211
99	1	0	-7.113191	-3.133273	-2.409737
100	1	0	-6.738887	-3.516219	-0.730233
101	6	0	-2.564969	2.504198	1.751959
102	6	0	-2.227013	3.967806	2.095921
103	6	0	-4.031506	2.181990	2.106905
104	1	0	-1.927094	1.870409	2.381829
105	6	0	-2.520098	4.252257	3.579606
106	1	0	-2.816394	4.647725	1.467637
107	1	0	-1.170829	4.175340	1.892612
108	6	0	-4.301942	2.452316	3.594279
109	1	0	-4.698283	2.813740	1.506299
110	1	0	-4.268712	1.142006	1.861087
111	6	0	-3.966524	3.905424	3.958106
112	1	0	-2.308015	5.305162	3.802306
113	1	0	-1.834029	3.653704	4.196092
114	1	0	-5.350421	2.230425	3.827894
115	1	0	-3.689043	1.771406	4.201994
116	1	0	-4.130493	4.079810	5.028542
117	1	0	-4.651029	4.576235	3.419120
118	6	0	-3.598112	2.238676	-1.060537
119	6	0	-3.941447	3.728452	-1.256533
120	6	0	-3.445366	1.515239	-2.412223
121	1	0	-4.432037	1.763175	-0.528622
122	6	0	-5.197946	3.891623	-2.127576

123	1	0	-3.100470	4.235678	-1.747544
124	1	0	-4.090876	4.218407	-0.289015
125	6	0	-4.700608	1.694761	-3.278722
126	1	0	-2.573730	1.911078	-2.949884
127	1	0	-3.248230	0.452843	-2.241411
128	6	0	-5.041942	3.177971	-3.477465
129	1	0	-5.407946	4.957575	-2.278916
130	1	0	-6.061751	3.470263	-1.593408
131	1	0	-4.556592	1.199813	-4.247260
132	1	0	-5.547422	1.193422	-2.789476
133	1	0	-5.958087	3.282721	-4.071586
134	1	0	-4.235931	3.660783	-4.048840
135	6	0	-1.542456	-1.251846	-3.828809
136	8	0	-0.642880	-0.336491	-3.939190
137	8	0	-1.398596	-2.416868	-3.438201
138	6	0	2.400319	-0.020491	-3.053814
139	8	0	2.182799	1.191573	-3.112140
140	8	0	3.650727	-0.480724	-2.720638
141	8	0	1.592983	-0.997789	-3.281502
142	1	0	0.496543	-0.666911	-3.570864
143	1	0	4.189091	0.306699	-2.548749

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^{1}TS7 E(opt) = -3188.64523298 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.728821	0.020869	-0.149894
2	1	0	-0.773727	-1.052361	-2.502283
3	15	0	-1.911068	-1.908025	0.273469

4	15	0	-1.996257	1.912494	-0.177661
5	6	0	2.115373	-0.699793	-0.134420
6	6	0	0.703380	-2.630688	-0.104677
7	6	0	3.262539	-1.479548	-0.074616
8	6	0	1.856632	-3.443986	-0.019195
9	6	0	3.128506	-2.881112	-0.004395
10	1	0	4.246570	-1.026503	-0.085543
11	1	0	1.737715	-4.521935	0.022673
12	6	0	2.095748	0.776083	-0.226650
13	6	0	0.687987	2.656307	-0.538979
14	6	0	3.216202	1.598973	-0.152652
15	6	0	1.785352	3.509347	-0.459766
16	6	0	3.070169	2.988594	-0.249039
17	1	0	4.198781	1.168824	0.001025
18	1	0	1.639324	4.578774	-0.566697
19	6	0	4.343825	-3.746176	0.078315
20	6	0	4.893299	-4.296769	-1.096782
21	6	0	4.938019	-3.999793	1.330775
22	6	0	6.035503	-5.099926	-0.997551
23	6	0	6.078426	-4.809443	1.387280
24	6	0	6.640902	-5.370527	0.235006
25	1	0	6.463130	-5.521976	-1.904591
26	1	0	6.538200	-5.005471	2.353657
27	6	0	4.251661	3.890856	-0.121954
28	6	0	5.183747	3.986203	-1.175488
29	6	0	4.431962	4.638465	1.061060
30	6	0	6.284606	4.838370	-1.028609
31	6	0	5.549905	5.472806	1.168638
32	6	0	6.485512	5.589930	0.134256
33	1	0	7.001758	4.915881	-1.842892

34	1	0	5.695442	6.041635	2.084490
35	6	0	7.851358	-6.268646	0.322835
36	1	0	7.553189	-7.317043	0.454092
37	1	0	8.457110	-6.216013	-0.587502
38	1	0	8.486531	-6.003706	1.174199
39	6	0	4.267140	-4.018953	-2.443444
40	1	0	3.237884	-4.393088	-2.490467
41	1	0	4.218446	-2.942439	-2.645624
42	1	0	4.836530	-4.490742	-3.248964
43	6	0	4.354244	-3.409975	2.593339
44	1	0	4.356878	-2.314117	2.560720
45	1	0	3.310644	-3.716851	2.730159
46	1	0	4.919528	-3.724120	3.475074
47	6	0	5.002325	3.193744	-2.449509
48	1	0	5.106074	2.117023	-2.272435
49	1	0	4.005728	3.348028	-2.878691
50	1	0	5.744215	3.482331	-3.199084
51	6	0	3.451190	4.533787	2.206528
52	1	0	2.471651	4.945419	1.937080
53	1	0	3.285137	3.490297	2.497962
54	1	0	3.813371	5.078419	3.082770
55	6	0	7.663647	6.524935	0.261381
56	1	0	8.501767	6.202472	-0.364282
57	1	0	7.392962	7.541068	-0.053852
58	1	0	8.012647	6.590644	1.297046
59	7	0	0.877377	-1.272191	-0.132346
60	7	0	0.850661	1.318301	-0.382611
61	6	0	-0.652261	-3.120626	-0.265388
62	6	0	-0.711337	3.117739	-0.848439
63	1	0	-0.819237	-3.093267	-1.715153

64	1	0	-0.798314	-4.156954	0.047005
65	1	0	-0.871357	4.152891	-0.542555
66	1	0	-0.837317	3.085707	-1.938366
67	6	0	-2.200413	-2.259740	2.091747
68	6	0	-2.875969	-1.103615	2.853537
69	6	0	-2.887099	-3.600169	2.411324
70	1	0	-1.161738	-2.320558	2.452210
71	6	0	-2.888070	-1.372534	4.366370
72	1	0	-3.907969	-0.981325	2.503719
73	1	0	-2.351927	-0.167253	2.638924
74	6	0	-2.888412	-3.866861	3.925841
75	1	0	-3.924833	-3.567151	2.057439
76	1	0	-2.392372	-4.423565	1.883231
77	6	0	-3.553976	-2.716350	4.694562
78	1	0	-3.401856	-0.553603	4.885477
79	1	0	-1.852385	-1.382736	4.736252
80	1	0	-3.400213	-4.814036	4.137113
81	1	0	-1.851051	-3.982270	4.271612
82	1	0	-3.518378	-2.907511	5.774185
83	1	0	-4.616952	-2.667686	4.416491
84	6	0	-3.442231	-2.288857	-0.719269
85	6	0	-3.778598	-3.774921	-0.952014
86	6	0	-4.677340	-1.514634	-0.222644
87	1	0	-3.169515	-1.869300	-1.697187
88	6	0	-4.942070	-3.905904	-1.949665
89	1	0	-4.061524	-4.251195	-0.006866
90	1	0	-2.901195	-4.304805	-1.334889
91	6	0	-5.837492	-1.649528	-1.220651
92	1	0	-4.992905	-1.911778	0.750492
93	1	0	-4.428938	-0.458704	-0.071357

94	6	0	-6.178518	-3.123463	-1.483676
95	1	0	-5.192233	-4.964383	-2.093881
96	1	0	-4.617640	-3.521020	-2.927331
97	1	0	-6.718493	-1.112674	-0.847103
98	1	0	-5.550607	-1.170268	-2.167037
99	1	0	-6.981486	-3.202075	-2.227036
100	1	0	-6.560638	-3.574508	-0.556280
101	6	0	-2.522942	2.575664	1.502273
102	6	0	-2.247199	4.064233	1.789065
103	6	0	-3.989569	2.218094	1.821833
104	1	0	-1.887466	1.995367	2.183885
105	6	0	-2.605153	4.406620	3.246078
106	1	0	-2.833336	4.694501	1.108322
107	1	0	-1.191287	4.298761	1.616644
108	6	0	-4.323961	2.547969	3.283865
109	1	0	-4.656096	2.795183	1.168398
110	1	0	-4.181082	1.159901	1.619290
111	6	0	-4.052124	4.027515	3.589444
112	1	0	-2.436198	5.475384	3.426264
113	1	0	-1.923149	3.861249	3.914247
114	1	0	-5.372138	2.299475	3.490781
115	1	0	-3.710909	1.918636	3.944629
116	1	0	-4.261244	4.245628	4.643887
117	1	0	-4.738477	4.647838	2.995107
118	6	0	-3.440126	2.142160	-1.332780
119	6	0	-3.845685	3.606762	-1.589966
120	6	0	-3.194742	1.393221	-2.658411
121	1	0	-4.272990	1.639276	-0.824689
122	6	0	-5.070949	3.684593	-2.515878
123	1	0	-3.009259	4.139416	-2.061851

124	1	0	-4.058867	4.118395	-0.646097
125	6	0	-4.419166	1.484942	-3.581324
126	1	0	-2.325468	1.827849	-3.172000
127	1	0	-2.948393	0.345999	-2.455435
128	6	0	-4.825555	2.942676	-3.836900
129	1	0	-5.325079	4.734465	-2.706993
130	1	0	-5.935145	3.236481	-2.004647
131	1	0	-4.208353	0.971967	-4.527845
132	1	0	-5.259586	0.953869	-3.112717
133	1	0	-5.720816	2.984233	-4.469368
134	1	0	-4.022003	3.449673	-4.390629
135	6	0	-0.943486	-1.802125	-3.312492
136	8	0	-1.101742	-1.440041	-4.475867
137	8	0	-0.957572	-3.042493	-2.901091

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^{1}TS8 E(opt) = -3263.89301507 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.722345	0.221694	-0.221078
2	15	0	1.925908	2.160219	-0.232269
3	15	0	2.011534	-1.711490	-0.243882
4	6	0	-2.135656	0.878353	-0.176432
5	6	0	-0.810374	2.831504	-0.314785
6	6	0	-3.295071	1.643665	-0.089226
7	6	0	-1.948794	3.628022	-0.211178
8	6	0	-3.213722	3.041042	-0.086534
9	1	0	-4.262222	1.161410	-0.012039
10	1	0	-1.846361	4.707680	-0.236527

11	6	0	-2.101475	-0.597744	-0.180609
12	6	0	-0.634748	-2.480705	-0.148357
13	6	0	-3.225084	-1.411652	-0.195480
14	6	0	-1.765794	-3.331717	-0.201554
15	6	0	-3.052205	-2.811009	-0.219210
16	1	0	-4.221713	-0.987762	-0.196257
17	1	0	-1.612206	-4.406050	-0.197806
18	6	0	-4.442404	3.878761	0.039775
19	6	0	-5.002549	4.481153	-1.105096
20	6	0	-5.037285	4.057745	1.305401
21	6	0	-6.157410	5.258665	-0.962273
22	6	0	-6.189079	4.846684	1.404595
23	6	0	-6.763339	5.456766	0.283674
24	1	0	-6.595286	5.717846	-1.845980
25	1	0	-6.648084	4.987576	2.380785
26	6	0	-4.242329	-3.713316	-0.236872
27	6	0	-4.892496	-3.996903	-1.454850
28	6	0	-4.708687	-4.275448	0.968469
29	6	0	-6.005014	-4.845883	-1.446702
30	6	0	-5.826245	-5.118168	0.933920
31	6	0	-6.489316	-5.413747	-0.262401
32	1	0	-6.503906	-5.069902	-2.387337
33	1	0	-6.187160	-5.552758	1.863703
34	6	0	-7.986975	6.330363	0.418982
35	1	0	-7.703836	7.377474	0.588143
36	1	0	-8.601151	6.303410	-0.486804
37	1	0	-8.608547	6.021778	1.265525
38	6	0	-4.380652	4.281864	-2.467710
39	1	0	-3.374161	4.713256	-2.516730
40	1	0	-4.278687	3.217141	-2.707938

41	1	0	-4.985735	4.750362	-3.248676
42	6	0	-4.442766	3.417452	2.538288
43	1	0	-4.476516	2.323407	2.478836
44	1	0	-3.388966	3.692959	2.662611
45	1	0	-4.982375	3.722067	3.439165
46	6	0	-4.390620	-3.405029	-2.751199
47	1	0	-4.429870	-2.309660	-2.732205
48	1	0	-3.344690	-3.678004	-2.934511
49	1	0	-4.986359	-3.750562	-3.600554
50	6	0	-4.021788	-3.970138	2.279573
51	1	0	-2.979516	-4.308722	2.277629
52	1	0	-3.998503	-2.891129	2.473426
53	1	0	-4.534351	-4.454387	3.115340
54	6	0	-7.712894	-6.298174	-0.273685
55	1	0	-7.779786	-6.878109	-1.199994
56	1	0	-7.711324	-6.996439	0.569230
57	1	0	-8.630437	-5.699934	-0.199802
58	7	0	-0.908490	1.479081	-0.260168
59	7	0	-0.842864	-1.126847	-0.181945
60	6	0	0.558196	3.406150	-0.568453
61	6	0	0.712387	-2.945715	0.071463
62	1	0	0.613402	3.662603	-1.633689
63	1	0	0.701635	4.338040	-0.014335
64	1	0	0.904396	-3.972507	-0.245402
65	6	0	2.572839	2.726856	1.431148
66	6	0	3.433269	1.656051	2.127894
67	6	0	3.275762	4.095165	1.495190
68	1	0	1.629600	2.804112	1.995009
69	6	0	3.722864	2.046336	3.585069
70	1	0	4.382792	1.547000	1.589178

71	1	0	2.928121	0.687235	2.088762
72	6	0	3.548145	4.494291	2.955634
73	1	0	4.233277	4.029469	0.964644
74	1	0	2.684240	4.871325	0.997144
75	6	0	4.383854	3.428577	3.679101
76	1	0	4.359345	1.285066	4.053373
77	1	0	2.776822	2.057336	4.145659
78	1	0	4.058658	5.464830	2.986103
79	1	0	2.589465	4.622835	3.478260
80	1	0	4.535620	3.709958	4.728436
81	1	0	5.380513	3.381445	3.216647
82	6	0	3.125091	2.529939	-1.619626
83	6	0	3.493272	4.002448	-1.895506
84	6	0	4.392970	1.662803	-1.534889
85	1	0	2.541295	2.171023	-2.481787
86	6	0	4.312675	4.111975	-3.193186
87	1	0	4.092287	4.397178	-1.069280
88	1	0	2.596910	4.627381	-1.968688
89	6	0	5.233431	1.783230	-2.815230
90	1	0	4.994159	1.977429	-0.671115
91	1	0	4.117051	0.618798	-1.370614
92	6	0	5.578339	3.245313	-3.130134
93	1	0	4.577015	5.160778	-3.376150
94	1	0	3.691788	3.788301	-4.040898
95	1	0	6.148142	1.185579	-2.716815
96	1	0	4.664220	1.356315	-3.653577
97	1	0	6.133955	3.311581	-4.073604
98	1	0	6.241044	3.635852	-2.344294
99	6	0	3.332919	-2.040941	1.037950
100	6	0	3.577269	-3.509907	1.448056

101	6	0	4.673002	-1.359107	0.709985
102	1	0	2.899718	-1.539248	1.911924
103	6	0	4.506773	-3.562787	2.672935
104	1	0	4.044575	-4.062564	0.625035
105	1	0	2.635970	-4.009391	1.683435
106	6	0	5.618475	-1.411534	1.920296
107	1	0	5.145183	-1.866906	-0.142264
108	1	0	4.513200	-0.322054	0.412391
109	6	0	5.840843	-2.852909	2.400215
110	1	0	4.683469	-4.606471	2.962235
111	1	0	4.002227	-3.080542	3.522940
112	1	0	6.577023	-0.940308	1.668590
113	1	0	5.179425	-0.820550	2.736616
114	1	0	6.471082	-2.863409	3.298297
115	1	0	6.387491	-3.408127	1.624050
116	6	0	2.772940	-2.076007	-1.919565
117	6	0	3.365826	-3.486865	-2.092425
118	6	0	1.748744	-1.777190	-3.034894
119	1	0	3.591881	-1.349485	-2.012344
120	6	0	3.964006	-3.677743	-3.496964
121	1	0	2.578383	-4.235830	-1.929235
122	1	0	4.141421	-3.669425	-1.344205
123	6	0	2.355806	-1.970197	-4.431966
124	1	0	0.886808	-2.450530	-2.919424
125	1	0	1.364997	-0.756055	-2.918591
126	6	0	2.939744	-3.379121	-4.598786
127	1	0	4.350834	-4.699421	-3.598788
128	1	0	4.823415	-3.001295	-3.612455
129	1	0	1.595190	-1.776644	-5.198886
130	1	0	3.153678	-1.228174	-4.581846

131	1	0	3.399595	-3.490026	-5.588672
132	1	0	2.124555	-4.115284	-4.543225
133	6	0	0.786206	-2.596264	3.533678
134	8	0	0.981288	-1.392859	3.363133
135	8	0	0.881667	-3.149025	4.777499
136	8	0	0.475374	-3.493974	2.650940
137	1	0	0.611893	-3.136082	1.548678
138	1	0	1.099372	-2.415726	5.375925

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^{1}TS9 E(opt) = -3265.09024945 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.904880	-0.067505	-0.779236
2	15	0	-1.981070	-2.037361	-0.282580
3	15	0	-2.188411	1.783655	-0.278159
4	6	0	1.971864	-0.648090	-0.830900
5	6	0	0.676365	-2.640131	-0.876803
6	6	0	3.148662	-1.403096	-0.735121
7	6	0	1.821134	-3.407292	-0.771611
8	6	0	3.088801	-2.791078	-0.681436
9	1	0	4.107578	-0.900966	-0.678897
10	1	0	1.737040	-4.488150	-0.737306
11	6	0	1.898759	0.804170	-0.808605
12	6	0	0.409499	2.657889	-0.821601
13	6	0	2.993592	1.672136	-0.685208
14	6	0	1.469538	3.534052	-0.683859
15	6	0	2.794003	3.045296	-0.602017
16	1	0	3.997800	1.268010	-0.630988

17	1	0	1.278894	4.601174	-0.644381
18	6	0	4.322427	-3.607195	-0.487460
19	6	0	4.799453	-4.437589	-1.524705
20	6	0	5.007275	-3.549976	0.746287
21	6	0	5.955199	-5.196731	-1.309902
22	6	0	6.156319	-4.330909	0.920302
23	6	0	6.645691	-5.161715	-0.093041
24	1	0	6.327138	-5.828317	-2.113952
25	1	0	6.679924	-4.290483	1.873231
26	6	0	3.940726	3.982045	-0.419802
27	6	0	4.805783	4.261108	-1.497264
28	6	0	4.150490	4.591068	0.836680
29	6	0	5.869979	5.150108	-1.300078
30	6	0	5.227235	5.470436	0.991847
31	6	0	6.099083	5.763072	-0.064104
32	1	0	6.532196	5.371270	-2.134403
33	1	0	5.390905	5.937081	1.961101
34	6	0	7.866950	-6.020678	0.129484
35	1	0	7.585559	-7.010406	0.512402
36	1	0	8.420398	-6.179872	-0.801608
37	1	0	8.546272	-5.571271	0.860818
38	6	0	4.095211	-4.499988	-2.860948
39	1	0	3.119152	-4.992005	-2.780997
40	1	0	3.911180	-3.497755	-3.263925
41	1	0	4.689278	-5.056931	-3.590979
42	6	0	4.519768	-2.670744	1.877358
43	1	0	4.752661	-1.615408	1.690015
44	1	0	3.433956	-2.736432	2.000795
45	1	0	4.998906	-2.951236	2.820125
46	6	0	4.590206	3.628222	-2.852927

47	1	0	4.762971	2.546271	-2.824621
48	1	0	3.562163	3.773333	-3.203963
49	1	0	5.267927	4.055585	-3.597289
50	6	0	3.239847	4.292187	2.005787
51	1	0	2.222743	4.661453	1.830531
52	1	0	3.154998	3.213471	2.181138
53	1	0	3.612210	4.758401	2.922209
54	6	0	7.269204	6.695055	0.139332
55	1	0	7.644483	7.082416	-0.812842
56	1	0	6.997504	7.546212	0.772844
57	1	0	8.101264	6.178394	0.635017
58	7	0	0.754137	-1.278788	-0.882069
59	7	0	0.622738	1.309660	-0.849967
60	6	0	-0.711298	-3.212060	-1.003562
61	6	0	-1.024934	3.079626	-0.978061
62	1	0	-0.962573	-3.286246	-2.070758
63	1	0	-0.768295	-4.217815	-0.580067
64	1	0	-1.196679	4.084739	-0.590429
65	1	0	-1.263826	3.093589	-2.050551
66	6	0	-2.061242	-2.555812	1.502460
67	6	0	-2.714038	-1.507443	2.421404
68	6	0	-2.632196	-3.955289	1.798053
69	1	0	-0.989603	-2.557117	1.746627
70	6	0	-2.481214	-1.870099	3.895913
71	1	0	-3.792792	-1.452813	2.227224
72	1	0	-2.292808	-0.523682	2.212511
73	6	0	-2.396596	-4.325970	3.272864
74	1	0	-3.711416	-3.959443	1.599565
75	1	0	-2.183083	-4.714085	1.147188
76	6	0	-3.001203	-3.278095	4.218579

77	1	0	-2.963569	-1.127703	4.544041
78	1	0	-1.402574	-1.821500	4.102104
79	1	0	-2.820237	-5.316503	3.480738
80	1	0	-1.314903	-4.398299	3.455115
81	1	0	-2.784643	-3.537176	5.262439
82	1	0	-4.095738	-3.288816	4.110752
83	6	0	-3.559926	-2.444517	-1.178726
84	6	0	-3.904655	-3.928397	-1.413431
85	6	0	-4.757664	-1.695604	-0.560073
86	1	0	-3.361373	-1.993497	-2.161673
87	6	0	-5.143053	-4.044390	-2.319785
88	1	0	-4.113849	-4.423015	-0.459497
89	1	0	-3.059305	-4.454299	-1.871057
90	6	0	-5.994904	-1.813517	-1.462423
91	1	0	-4.986370	-2.128040	0.422613
92	1	0	-4.506250	-0.642231	-0.396409
93	6	0	-6.343714	-3.283635	-1.737636
94	1	0	-5.397168	-5.101235	-2.467492
95	1	0	-4.901098	-3.634460	-3.310808
96	1	0	-6.845860	-1.298499	-0.999573
97	1	0	-5.792590	-1.301533	-2.413723
98	1	0	-7.201687	-3.350922	-2.417774
99	1	0	-6.648575	-3.761727	-0.795428
100	6	0	-2.414899	2.203089	1.545473
101	6	0	-1.958344	3.610986	1.981418
102	6	0	-3.834745	1.900977	2.068901
103	1	0	-1.732409	1.495831	2.025609
104	6	0	-2.032951	3.750366	3.511945
105	1	0	-2.587454	4.378613	1.512884
106	1	0	-0.929049	3.794831	1.654764

107	6	0	-3.882466	2.024987	3.599175
108	1	0	-4.550146	2.611219	1.636156
109	1	0	-4.154405	0.899037	1.763784
110	6	0	-3.430705	3.419820	4.052661
111	1	0	-1.738826	4.765815	3.805005
112	1	0	-1.301597	3.065633	3.964739
113	1	0	-4.897375	1.814287	3.958357
114	1	0	-3.223208	1.265704	4.042534
115	1	0	-3.440067	3.488450	5.147422
116	1	0	-4.147364	4.166995	3.681931
117	6	0	-3.827442	2.189781	-1.078622
118	6	0	-4.182597	3.691568	-1.044857
119	6	0	-3.956926	1.634232	-2.508456
120	1	0	-4.559149	1.653882	-0.460752
121	6	0	-5.593808	3.935639	-1.603380
122	1	0	-3.458076	4.248837	-1.653355
123	1	0	-4.113675	4.085648	-0.026760
124	6	0	-5.365041	1.888149	-3.069747
125	1	0	-3.211496	2.111184	-3.160196
126	1	0	-3.738524	0.562862	-2.513365
127	6	0	-5.737859	3.376085	-3.024709
128	1	0	-5.817196	5.009554	-1.589218
129	1	0	-6.328612	3.449607	-0.945486
130	1	0	-5.427645	1.507891	-4.096940
131	1	0	-6.091955	1.315341	-2.476127
132	1	0	-6.760527	3.525291	-3.392423
133	1	0	-5.073431	3.934791	-3.699702
134	6	0	1.159211	-0.659955	2.422585
135	8	0	1.106125	-1.871559	2.202909
136	8	0	2.229622	-0.122139	3.084487

137	8	0	0.296520	0.252799	2.105419
138	1	0	-0.314948	-0.000984	1.067517
139	1	0	2.807426	-0.868993	3.311262
140	1	0	-1.453971	-0.201204	-2.419319

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^{1}TS10 E(opt) = -3189.15692023 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.798427	-0.092151	-0.443120
2	1	0	-1.048635	-0.176502	-2.069919
3	15	0	-1.966848	-2.058771	-0.166150
4	15	0	-2.124574	1.803651	-0.309822
5	6	0	2.064465	-0.726324	-0.489647
6	6	0	0.744104	-2.690560	-0.565440
7	6	0	3.231103	-1.480884	-0.418182
8	6	0	1.889210	-3.479828	-0.472057
9	6	0	3.152777	-2.880374	-0.393744
10	1	0	4.197973	-0.993612	-0.380738
11	1	0	1.793616	-4.559762	-0.466964
12	6	0	2.009290	0.752075	-0.512469
13	6	0	0.549683	2.607021	-0.701887
14	6	0	3.111313	1.595734	-0.415279
15	6	0	1.627812	3.484629	-0.602525
16	6	0	2.926730	2.984811	-0.443151
17	1	0	4.107347	1.185920	-0.301108
18	1	0	1.452901	4.553559	-0.651314
19	6	0	4.388409	-3.710106	-0.295701
20	6	0	4.823675	-4.453283	-1.413089

21	6	0	5.114790	-3.743059	0.913499
22	6	0	5.987723	-5.221368	-1.299129
23	6	0	6.268847	-4.531146	0.984333
24	6	0	6.721285	-5.278161	-0.108943
25	1	0	6.330803	-5.786413	-2.162979
26	1	0	6.827174	-4.562556	1.917302
27	6	0	4.090284	3.906906	-0.300478
28	6	0	5.003822	4.056143	-1.364095
29	6	0	4.271638	4.614789	0.906154
30	6	0	6.089181	4.924591	-1.202320
31	6	0	5.375082	5.466468	1.026852
32	6	0	6.292488	5.638281	-0.016105
33	1	0	6.792537	5.045239	-2.023244
34	1	0	5.523581	6.005041	1.960209
35	6	0	7.951476	-6.145463	0.001801
36	1	0	7.687148	-7.156833	0.337071
37	1	0	8.459318	-6.246235	-0.962631
38	1	0	8.664561	-5.739601	0.726301
39	6	0	4.069078	-4.415400	-2.722413
40	1	0	3.097584	-4.916499	-2.642473
41	1	0	3.869746	-3.386439	-3.042251
42	1	0	4.635854	-4.913611	-3.513580
43	6	0	4.659763	-2.958915	2.123150
44	1	0	4.751441	-1.878529	1.962297
45	1	0	3.607458	-3.155804	2.356623
46	1	0	5.256530	-3.216253	3.002379
47	6	0	4.820113	3.305238	-2.662792
48	1	0	4.961339	2.226582	-2.527725
49	1	0	3.811171	3.444204	-3.067565
50	1	0	5.537855	3.644051	-3.414721

51	6	0	3.311171	4.448507	2.061483
52	1	0	2.318342	4.846166	1.821264
53	1	0	3.173470	3.392420	2.320627
54	1	0	3.674702	4.971980	2.949831
55	6	0	7.454190	6.591305	0.125378
56	1	0	8.299090	6.289920	-0.501752
57	1	0	7.166977	7.605753	-0.180436
58	1	0	7.799014	6.651483	1.162597
59	7	0	0.853383	-1.346563	-0.547938
60	7	0	0.758531	1.277183	-0.623775
61	6	0	-0.642769	-3.251254	-0.748692
62	6	0	-0.868512	3.041136	-0.955696
63	1	0	-0.808616	-3.387965	-1.825183
64	1	0	-0.738702	-4.233290	-0.279266
65	1	0	-1.048201	4.056475	-0.600019
66	1	0	-1.021122	3.049367	-2.042976
67	6	0	-2.243331	-2.558196	1.603058
68	6	0	-2.969772	-1.490752	2.444323
69	6	0	-2.887325	-3.940896	1.820635
70	1	0	-1.205320	-2.600210	1.963251
71	6	0	-2.932715	-1.864310	3.933751
72	1	0	-4.013332	-1.408315	2.117279
73	1	0	-2.505584	-0.514191	2.295380
74	6	0	-2.842461	-4.319399	3.310892
75	1	0	-3.933176	-3.906195	1.492129
76	1	0	-2.385853	-4.710079	1.223014
77	6	0	-3.528619	-3.257022	4.181309
78	1	0	-3.472033	-1.107653	4.516787
79	1	0	-1.888286	-1.845783	4.276342
80	1	0	-3.316303	-5.297532	3.457843

81	1	0	-1.793352	-4.423789	3.622185
82	1	0	-3.448127	-3.524418	5.241936
83	1	0	-4.601261	-3.235473	3.940344
84	6	0	-3.431230	-2.401387	-1.247887
85	6	0	-3.769945	-3.878581	-1.534429
86	6	0	-4.676423	-1.636674	-0.756856
87	1	0	-3.108323	-1.943563	-2.194045
88	6	0	-4.904828	-3.966188	-2.569605
89	1	0	-4.088510	-4.375769	-0.612795
90	1	0	-2.889743	-4.415196	-1.904342
91	6	0	-5.808164	-1.731075	-1.790562
92	1	0	-5.015638	-2.072062	0.191498
93	1	0	-4.427051	-0.589437	-0.559045
94	6	0	-6.149579	-3.193140	-2.110781
95	1	0	-5.154234	-5.018175	-2.753276
96	1	0	-4.552071	-3.551497	-3.524654
97	1	0	-6.694265	-1.201161	-1.420510
98	1	0	-5.493514	-1.221306	-2.711144
99	1	0	-6.930934	-3.241860	-2.878808
100	1	0	-6.559375	-3.672776	-1.210283
101	6	0	-2.573977	2.315583	1.435417
102	6	0	-2.273033	3.777373	1.822585
103	6	0	-4.028258	1.939383	1.790826
104	1	0	-1.908738	1.685266	2.034275
105	6	0	-2.558198	4.002288	3.318070
106	1	0	-2.886218	4.463083	1.224738
107	1	0	-1.224674	4.018804	1.617890
108	6	0	-4.282944	2.148961	3.290809
109	1	0	-4.721392	2.572583	1.223183
110	1	0	-4.240218	0.901892	1.513211

111	6	0	-3.988478	3.598656	3.700315
112	1	0	-2.375891	5.053642	3.571608
113	1	0	-1.847544	3.406404	3.907681
114	1	0	-5.319983	1.884923	3.530705
115	1	0	-3.638863	1.467242	3.864218
116	1	0	-4.143736	3.730782	4.777954
117	1	0	-4.700426	4.265467	3.192970
118	6	0	-3.620978	2.096563	-1.374735
119	6	0	-4.002286	3.589323	-1.486380
120	6	0	-3.493074	1.449738	-2.767581
121	1	0	-4.430431	1.578128	-0.846491
122	6	0	-5.288900	3.768106	-2.307699
123	1	0	-3.188915	4.138778	-1.977521
124	1	0	-4.133366	4.028558	-0.493172
125	6	0	-4.777968	1.652165	-3.586397
126	1	0	-2.644652	1.894205	-3.306287
127	1	0	-3.280262	0.382090	-2.663871
128	6	0	-5.157462	3.134263	-3.698031
129	1	0	-5.524908	4.835832	-2.391217
130	1	0	-6.125657	3.297884	-1.771696
131	1	0	-4.651441	1.210132	-4.582203
132	1	0	-5.598690	1.107431	-3.099833
133	1	0	-6.093198	3.246659	-4.258888
134	1	0	-4.380425	3.666561	-4.265408
135	1	0	-0.575876	-0.037543	1.253698
136	6	0	0.418106	-0.017235	2.575735
137	8	0	0.447745	1.140478	2.862813
138	8	0	0.708267	-1.163838	2.732686

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^{1}TS11 E(opt) = -3188.643889 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.787672	-0.099713	-0.615410
2	1	0	-1.288314	-0.321783	-2.154198
3	15	0	-1.863035	-2.090425	-0.180559
4	15	0	-2.175260	1.724689	-0.322391
5	6	0	2.099823	-0.637066	-0.621638
6	6	0	0.822187	-2.656840	-0.671182
7	6	0	3.287359	-1.395729	-0.547919
8	6	0	1.969588	-3.412243	-0.569977
9	6	0	3.242615	-2.777997	-0.502583
10	1	0	4.243139	-0.885329	-0.503569
11	1	0	1.899408	-4.494597	-0.562885
12	6	0	2.009788	0.791405	-0.564994
13	6	0	0.484256	2.639441	-0.531930
14	6	0	3.086493	1.685032	-0.396067
15	6	0	1.525409	3.519535	-0.362376
16	6	0	2.868684	3.046008	-0.263561
17	1	0	4.097122	1.294454	-0.349507
18	1	0	1.322634	4.584684	-0.325241
19	6	0	4.487223	-3.592542	-0.386060
20	6	0	5.387866	-3.674624	-1.469857
21	6	0	4.764066	-4.284826	0.814013
22	6	0	6.547343	-4.448379	-1.335042
23	6	0	5.935648	-5.044290	0.907916
24	6	0	6.839100	-5.142661	-0.156387
25	1	0	7.237421	-4.512258	-2.173875
26	1	0	6.150707	-5.567512	1.837456

27	6	0	3.994361	3.996558	-0.037991
28	6	0	4.972892	4.198077	-1.037046
29	6	0	4.082127	4.706087	1.182407
30	6	0	6.017147	5.100298	-0.798019
31	6	0	5.144085	5.595247	1.380899
32	6	0	6.124117	5.806259	0.404292
33	1	0	6.762394	5.259351	-1.574804
34	1	0	5.210532	6.133342	2.324424
35	6	0	8.077533	-5.998705	-0.043943
36	1	0	7.863697	-7.038099	-0.325629
37	1	0	8.874558	-5.641031	-0.703530
38	1	0	8.461693	-6.015092	0.981240
39	6	0	5.117611	-2.950670	-2.769691
40	1	0	4.094630	-3.124732	-3.121084
41	1	0	5.232258	-1.866199	-2.660350
42	1	0	5.808037	-3.280877	-3.551175
43	6	0	3.830900	-4.193655	1.999843
44	1	0	3.605024	-3.150934	2.250393
45	1	0	2.870900	-4.682830	1.798982
46	1	0	4.270184	-4.669130	2.881363
47	6	0	4.907140	3.474933	-2.364026
48	1	0	5.200269	2.423054	-2.268236
49	1	0	3.893318	3.482597	-2.778012
50	1	0	5.578421	3.938452	-3.092929
51	6	0	3.062503	4.505335	2.281054
52	1	0	2.093379	4.947412	2.022544
53	1	0	2.880359	3.441524	2.470040
54	1	0	3.398667	4.966067	3.214387
55	6	0	7.277859	6.747079	0.655250
56	1	0	7.690923	7.134607	-0.281469

57	1	0	6.974828	7.597834	1.274493
58	1	0	8.093297	6.236905	1.184602
59	7	0	0.876628	-1.288734	-0.670347
60	7	0	0.706007	1.281695	-0.563443
61	6	0	-0.552667	-3.251200	-0.836954
62	6	0	-0.941549	3.064891	-0.769303
63	1	0	-0.764801	-3.344354	-1.911022
64	1	0	-0.612107	-4.252234	-0.402759
65	1	0	-1.159046	4.029874	-0.308500
66	1	0	-1.072680	3.191607	-1.852755
67	6	0	-2.021512	-2.601169	1.607589
68	6	0	-2.754004	-1.559656	2.472152
69	6	0	-2.570069	-4.010507	1.897173
70	1	0	-0.963533	-2.579227	1.907380
71	6	0	-2.599302	-1.887049	3.964317
72	1	0	-3.819855	-1.545163	2.211807
73	1	0	-2.361143	-0.561954	2.263545
74	6	0	-2.402919	-4.349629	3.388811
75	1	0	-3.636867	-4.042586	1.643991
76	1	0	-2.069556	-4.766451	1.281921
77	6	0	-3.090768	-3.306587	4.281849
78	1	0	-3.145401	-1.150074	4.566329
79	1	0	-1.538031	-1.797138	4.237597
80	1	0	-2.806671	-5.349466	3.590844
81	1	0	-1.330755	-4.384960	3.629484
82	1	0	-2.923708	-3.541724	5.340188
83	1	0	-4.176662	-3.354178	4.114642
84	6	0	-3.378236	-2.534800	-1.165628
85	6	0	-3.712351	-4.029077	-1.344379
86	6	0	-4.616810	-1.748220	-0.696211

87	1	0	-3.095082	-2.141048	-2.153090
88	6	0	-4.871115	-4.195975	-2.343012
89	1	0	-4.006549	-4.465650	-0.384675
90	1	0	-2.835473	-4.584027	-1.695868
91	6	0	-5.779901	-1.922110	-1.684578
92	1	0	-4.924771	-2.110403	0.293447
93	1	0	-4.372141	-0.687261	-0.588898
94	6	0	-6.111999	-3.405220	-1.903279
95	1	0	-5.115929	-5.259635	-2.452167
96	1	0	-4.546922	-3.841571	-3.331994
97	1	0	-6.662389	-1.381380	-1.320766
98	1	0	-5.501651	-1.465592	-2.645265
99	1	0	-6.913135	-3.511144	-2.644988
100	1	0	-6.492966	-3.829618	-0.963055
101	6	0	-2.821965	2.093201	1.407934
102	6	0	-2.626844	3.530660	1.931665
103	6	0	-4.274619	1.617851	1.617873
104	1	0	-2.179925	1.458105	2.020256
105	6	0	-3.044744	3.626394	3.409618
106	1	0	-3.218851	4.240023	1.340201
107	1	0	-1.578141	3.829262	1.836575
108	6	0	-4.663249	1.707529	3.101477
109	1	0	-4.962674	2.243892	1.036214
110	1	0	-4.397599	0.589725	1.262657
111	6	0	-4.480809	3.134868	3.634461
112	1	0	-2.934608	4.660820	3.758131
113	1	0	-2.358365	3.014296	4.011507
114	1	0	-5.700853	1.376932	3.234449
115	1	0	-4.032502	1.018839	3.681000
116	1	0	-4.735494	3.181134	4.700472

117	1	0	-5.178788	3.805347	3.112308
118	6	0	-3.625221	2.078585	-1.453669
119	6	0	-4.079336	3.554144	-1.443440
120	6	0	-3.405066	1.591180	-2.897799
121	1	0	-4.437127	1.472317	-1.032519
122	6	0	-5.340300	3.753459	-2.300412
123	1	0	-3.273852	4.185555	-1.841611
124	1	0	-4.275015	3.892938	-0.422554
125	6	0	-4.665762	1.800023	-3.751570
126	1	0	-2.564404	2.136571	-3.349965
127	1	0	-3.127365	0.533624	-2.894840
128	6	0	-5.127551	3.262719	-3.737738
129	1	0	-5.627603	4.812144	-2.293909
130	1	0	-6.172406	3.195989	-1.846643
131	1	0	-4.474663	1.467246	-4.779364
132	1	0	-5.470873	1.162936	-3.357236
133	1	0	-6.048477	3.379542	-4.322200
134	1	0	-4.362716	3.886998	-4.222100
135	6	0	0.319527	0.187336	2.195898
136	8	0	0.870313	-0.864113	2.318246
137	8	0	0.033173	1.287639	2.560294

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^{1}TS12 E(opt) =-3453.719307 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.940006	0.072398	-0.520785
2	1	0	1.340978	0.014423	-2.170572
3	15	0	2.192426	2.004494	-0.325048

4	15	0	2.196370	-1.836834	-0.122734
5	6	0	-1.881850	0.778579	-0.877672
6	6	0	-0.504632	2.701272	-0.825789
7	6	0	-3.028165	1.564147	-0.827919
8	6	0	-1.629582	3.521250	-0.755403
9	6	0	-2.911527	2.956638	-0.739358
10	1	0	-4.006816	1.102412	-0.812084
11	1	0	-1.503857	4.596826	-0.696741
12	6	0	-1.871207	-0.697751	-0.868876
13	6	0	-0.470365	-2.594164	-0.717144
14	6	0	-3.006356	-1.502738	-0.890963
15	6	0	-1.582097	-3.433437	-0.709116
16	6	0	-2.870592	-2.890702	-0.792055
17	1	0	-3.991779	-1.058483	-0.944336
18	1	0	-1.442210	-4.506730	-0.638599
19	6	0	-4.126494	3.811946	-0.600396
20	6	0	-4.569207	4.591086	-1.689771
21	6	0	-4.824623	3.831980	0.625719
22	6	0	-5.712589	5.381740	-1.533967
23	6	0	-5.960885	4.642738	0.738278
24	6	0	-6.420111	5.424607	-0.326722
25	1	0	-6.061435	5.974962	-2.376571
26	1	0	-6.499781	4.662987	1.682998
27	6	0	-4.072847	-3.774843	-0.748559
28	6	0	-4.646184	-4.242397	-1.947401
29	6	0	-4.614649	-4.143367	0.499207
30	6	0	-5.765737	-5.079106	-1.878127
31	6	0	-5.736199	-4.980916	0.523511
32	6	0	-6.326665	-5.457339	-0.652554
33	1	0	-6.207786	-5.445358	-2.802255

34	1	0	-6.156518	-5.268980	1.484722
35	6	0	-7.633464	6.309989	-0.176226
36	1	0	-7.339187	7.348725	0.021929
37	1	0	-8.239518	6.316012	-1.088417
38	1	0	-8.267347	5.984875	0.654474
39	6	0	-3.840286	4.561505	-3.013403
40	1	0	-2.831838	4.982037	-2.927826
41	1	0	-3.724015	3.536028	-3.382834
42	1	0	-4.379560	5.136585	-3.771054
43	6	0	-4.354915	3.014743	1.807463
44	1	0	-4.295772	1.947563	1.574347
45	1	0	-3.346645	3.313698	2.120366
46	1	0	-5.024147	3.146102	2.662606
47	6	0	-4.057440	-3.855461	-3.283558
48	1	0	-4.068543	-2.768392	-3.425328
49	1	0	-3.010670	-4.171787	-3.364346
50	1	0	-4.614020	-4.310327	-4.107448
51	6	0	-3.993540	-3.649726	1.785041
52	1	0	-2.973407	-4.034921	1.905390
53	1	0	-3.918734	-2.556827	1.801303
54	1	0	-4.577646	-3.971156	2.652162
55	6	0	-7.559506	-6.327300	-0.603463
56	1	0	-7.603483	-7.009566	-1.458363
57	1	0	-7.595304	-6.921868	0.314809
58	1	0	-8.471170	-5.715883	-0.629968
59	7	0	-0.652857	1.362473	-0.863503
60	7	0	-0.636848	-1.258909	-0.783008
61	6	0	0.902225	3.233593	-0.920094
62	6	0	0.945135	-3.100462	-0.731930
63	1	0	1.111455	3.415862	-1.981712

64	1	0	0.994833	4.194521	-0.407527
65	1	0	1.029485	-4.062205	-0.224040
66	1	0	1.214747	-3.273569	-1.781763
67	6	0	2.647950	2.621007	1.368828
68	6	0	3.363380	1.555576	2.219575
69	6	0	3.401318	3.962106	1.425848
70	1	0	1.650169	2.748220	1.804498
71	6	0	3.512692	2.031463	3.672485
72	1	0	4.357756	1.347088	1.806007
73	1	0	2.796082	0.623486	2.191427
74	6	0	3.529473	4.438199	2.883021
75	1	0	4.407163	3.838453	1.006748
76	1	0	2.893318	4.725782	0.825854
77	6	0	4.230297	3.385891	3.754000
78	1	0	4.053371	1.275745	4.255839
79	1	0	2.512770	2.122781	4.119646
80	1	0	4.077525	5.387977	2.916348
81	1	0	2.525968	4.634659	3.286555
82	1	0	4.285403	3.727727	4.794900
83	1	0	5.266319	3.265639	3.404903
84	6	0	3.610273	2.219473	-1.514030
85	6	0	3.987704	3.654931	-1.937387
86	6	0	4.860594	1.449885	-1.042727
87	1	0	3.219755	1.706762	-2.403951
88	6	0	5.050352	3.614942	-3.049475
89	1	0	4.390221	4.207674	-1.083224
90	1	0	3.108531	4.204173	-2.290059
91	6	0	5.923909	1.414514	-2.150657
92	1	0	5.279488	1.947618	-0.159262
93	1	0	4.592980	0.432746	-0.740790

94	6	0	6.295562	2.830569	-2.612077
95	1	0	5.323887	4.638151	-3.334617
96	1	0	4.618434	3.140744	-3.942406
97	1	0	6.813732	0.880184	-1.795797
98	1	0	5.531101	0.846152	-3.004273
99	1	0	7.023799	2.785633	-3.431084
100	1	0	6.783274	3.363368	-1.783032
101	6	0	2.625318	-2.237611	1.661059
102	6	0	2.183879	-3.622613	2.173218
103	6	0	4.106957	-1.970971	2.001019
104	1	0	2.016544	-1.508003	2.198511
105	6	0	2.434599	-3.735593	3.687326
106	1	0	2.729632	-4.418992	1.650939
107	1	0	1.118271	-3.775590	1.975228
108	6	0	4.325964	-2.061405	3.518929
109	1	0	4.747895	-2.713408	1.510268
110	1	0	4.419783	-0.987911	1.635940
111	6	0	3.893405	-3.432875	4.055410
112	1	0	2.152000	-4.737136	4.034520
113	1	0	1.778335	-3.023179	4.207032
114	1	0	5.380507	-1.871993	3.754386
115	1	0	3.741444	-1.273454	4.014471
116	1	0	4.027348	-3.478210	5.143194
117	1	0	4.543703	-4.207356	3.623360
118	6	0	3.721830	-2.286692	-1.107788
119	6	0	4.045389	-3.797947	-1.058088
120	6	0	3.690764	-1.789911	-2.565140
121	1	0	4.533079	-1.750958	-0.600287
122	6	0	5.370032	-4.103140	-1.775287
123	1	0	3.241929	-4.359260	-1.552085

124	1	0	4.094188	-4.154732	-0.025892
125	6	0	5.009820	-2.113735	-3.285405
126	1	0	2.857596	-2.265141	-3.101473
127	1	0	3.506956	-0.713324	-2.589963
128	6	0	5.343648	-3.609590	-3.226934
129	1	0	5.568369	-5.181307	-1.738362
130	1	0	6.192588	-3.609704	-1.237930
131	1	0	4.953532	-1.771553	-4.326203
132	1	0	5.821984	-1.546697	-2.810249
133	1	0	6.305830	-3.805565	-3.715806
134	1	0	4.582643	-4.173750	-3.785298
135	6	0	0.197332	0.221824	1.509752
136	8	0	-0.039080	1.332512	2.029234
137	8	0	-0.162767	-0.897428	2.086973
138	6	0	-3.055979	-0.173755	3.108379
139	8	0	-3.353696	-0.230902	1.911616
140	8	0	-3.960358	0.304057	4.017885
141	8	0	-1.956366	-0.524926	3.682387
142	1	0	-1.110517	-0.689484	2.926021
143	1	0	-4.753963	0.523532	3.504418

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^{1}TS13 E(opt) =-3454.284134 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.941284	0.086178	-0.426946
2	1	0	1.348365	0.123986	-1.996225
3	15	0	2.189155	2.050581	-0.245509
4	15	0	2.216384	-1.860680	-0.219855

5	6	0	-1.875432	0.773459	-0.870363
6	6	0	-0.505272	2.743395	-0.770283
7	6	0	-3.032159	1.595293	-0.854261
8	6	0	-1.622437	3.563119	-0.746006
9	6	0	-2.920318	2.968518	-0.769343
10	1	0	-4.012186	1.133688	-0.867468
11	1	0	-1.508021	4.640448	-0.712664
12	6	0	-1.858072	-0.651197	-0.902290
13	6	0	-0.441169	-2.594500	-0.862393
14	6	0	-2.995489	-1.501669	-0.908523
15	6	0	-1.538007	-3.438568	-0.864095
16	6	0	-2.851132	-2.872264	-0.866310
17	1	0	-3.985632	-1.062854	-0.890997
18	1	0	-1.399160	-4.513495	-0.857734
19	6	0	-4.137006	3.829708	-0.674468
20	6	0	-4.591007	4.542343	-1.803275
21	6	0	-4.827386	3.930396	0.552783
22	6	0	-5.733401	5.343549	-1.688942
23	6	0	-5.965136	4.743149	0.624993
24	6	0	-6.433000	5.459505	-0.482602
25	1	0	-6.087245	5.885440	-2.563665
26	1	0	-6.498244	4.820007	1.570499
27	6	0	-4.040399	-3.770141	-0.766297
28	6	0	-4.640004	-4.293284	-1.928560
29	6	0	-4.549609	-4.099990	0.507732
30	6	0	-5.749460	-5.138161	-1.800095
31	6	0	-5.660401	-4.947374	0.593673
32	6	0	-6.272991	-5.478492	-0.547799
33	1	0	-6.215167	-5.538086	-2.698520
34	1	0	-6.056997	-5.198873	1.575352

35	6	0	-7.642933	6.355847	-0.369991
36	1	0	-8.159608	6.455767	-1.329950
37	1	0	-8.357759	5.974190	0.366288
38	1	0	-7.355657	7.365764	-0.049055
39	6	0	-3.870651	4.428518	-3.126729
40	1	0	-2.841910	4.800245	-3.057218
41	1	0	-3.804588	3.384121	-3.453621
42	1	0	-4.383805	4.997665	-3.906962
43	6	0	-4.344047	3.184736	1.775723
44	1	0	-4.282999	2.106759	1.597416
45	1	0	-3.332268	3.503384	2.057218
46	1	0	-5.002334	3.365526	2.631075
47	6	0	-4.099755	-3.940833	-3.294790
48	1	0	-4.157087	-2.861687	-3.479156
49	1	0	-3.043474	-4.218820	-3.389381
50	1	0	-4.657273	-4.450445	-4.085738
51	6	0	-3.908078	-3.542132	1.757112
52	1	0	-2.857130	-3.847459	1.831771
53	1	0	-3.912958	-2.447290	1.754688
54	1	0	-4.424688	-3.891311	2.656084
55	6	0	-7.448412	-6.418754	-0.426973
56	1	0	-8.078157	-6.392191	-1.321938
57	1	0	-7.111023	-7.455428	-0.296948
58	1	0	-8.071863	-6.171917	0.438680
59	7	0	-0.634199	1.400046	-0.797383
60	7	0	-0.599818	-1.250401	-0.842178
61	6	0	0.906257	3.276479	-0.848238
62	6	0	0.981260	-3.088766	-0.915619
63	1	0	1.130541	3.457384	-1.906470
64	1	0	1.001867	4.236375	-0.333974

65	1	0	1.080586	-4.077527	-0.465051
66	1	0	1.255211	-3.194198	-1.972543
67	6	0	2.625327	2.636388	1.465284
68	6	0	3.364207	1.566329	2.294540
69	6	0	3.358597	3.988222	1.558980
70	1	0	1.629836	2.763435	1.910344
71	6	0	3.486855	2.007137	3.760587
72	1	0	4.367723	1.408976	1.881851
73	1	0	2.840711	0.610498	2.234248
74	6	0	3.466467	4.432780	3.027582
75	1	0	4.368593	3.883281	1.145975
76	1	0	2.845347	4.756759	0.970499
77	6	0	4.176237	3.373332	3.882600
78	1	0	4.037719	1.247690	4.329135
79	1	0	2.480830	2.065836	4.198759
80	1	0	3.999236	5.389791	3.085506
81	1	0	2.456467	4.605685	3.425570
82	1	0	4.210520	3.691435	4.931704
83	1	0	5.218709	3.281144	3.544959
84	6	0	3.619272	2.269494	-1.415059
85	6	0	3.987668	3.716103	-1.811194
86	6	0	4.870244	1.505586	-0.938433
87	1	0	3.240376	1.767219	-2.316021
88	6	0	5.071302	3.707843	-2.903037
89	1	0	4.367399	4.259038	-0.940576
90	1	0	3.109204	4.260564	-2.171682
91	6	0	5.951505	1.504269	-2.029350
92	1	0	5.269105	1.993413	-0.040612
93	1	0	4.609440	0.480698	-0.657603
94	6	0	6.317631	2.932630	-2.454262

95	1	0	5.335206	4.739525	-3.165333
96	1	0	4.663003	3.243033	-3.811829
97	1	0	6.839189	0.968367	-1.671806
98	1	0	5.577379	0.954505	-2.902488
99	1	0	7.062683	2.911233	-3.258865
100	1	0	6.781559	3.455486	-1.605545
101	6	0	2.638575	-2.355635	1.539206
102	6	0	2.285068	-3.796912	1.953399
103	6	0	4.099035	-2.016849	1.906734
104	1	0	1.988769	-1.697769	2.122898
105	6	0	2.536706	-3.992842	3.458911
106	1	0	2.886735	-4.516027	1.383556
107	1	0	1.233466	-4.007974	1.734804
108	6	0	4.319916	-2.194443	3.416347
109	1	0	4.783313	-2.684434	1.369163
110	1	0	4.347813	-0.994091	1.607272
111	6	0	3.971859	-3.622933	3.857726
112	1	0	2.317754	-5.031161	3.736346
113	1	0	1.833869	-3.360143	4.019147
114	1	0	5.360176	-1.956613	3.669745
115	1	0	3.686861	-1.478147	3.959200
116	1	0	4.103450	-3.731080	4.941239
117	1	0	4.671760	-4.324724	3.381604
118	6	0	3.738639	-2.192429	-1.245249
119	6	0	4.109614	-3.693225	-1.289887
120	6	0	3.640692	-1.608265	-2.668214
121	1	0	4.542860	-1.658504	-0.725450
122	6	0	5.404424	-3.922198	-2.085102
123	1	0	3.299899	-4.256586	-1.770552
124	1	0	4.222004	-4.094949	-0.279145

125	6	0	4.931590	-1.865837	-3.462469
126	1	0	2.793947	-2.062940	-3.200580
127	1	0	3.442530	-0.534712	-2.617538
128	6	0	5.292200	-3.355438	-3.505352
129	1	0	5.631184	-4.994868	-2.113421
130	1	0	6.239872	-3.433482	-1.563673
131	1	0	4.822713	-1.464190	-4.477371
132	1	0	5.755980	-1.315068	-2.990687
133	1	0	6.230927	-3.504617	-4.052594
134	1	0	4.513029	-3.904666	-4.053337
135	6	0	0.301026	0.167815	1.590360
136	8	0	0.205706	0.899937	2.499895
137	8	0	-0.486365	-1.421560	2.161722
138	6	0	-3.184810	-0.152134	3.141821
139	8	0	-3.447704	-0.107453	1.933583
140	8	0	-4.002200	0.478029	4.043219
141	8	0	-2.201280	-0.744484	3.719085
142	1	0	-1.368028	-1.098127	2.913190
143	1	0	-4.717209	0.870590	3.517939
144	1	0	-0.907513	-1.804031	1.378972

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^{1}TS14 E(opt) = -3454.18761834 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.904921	0.087678	-0.315131
2	1	0	1.223487	0.131503	-1.897920
3	15	0	2.175152	2.041203	-0.219597
4	15	0	2.224228	-1.836030	-0.213610

5	6	0	-1.914198	0.798382	-0.723152
6	6	0	-0.542431	2.727764	-0.688440
7	6	0	-3.059735	1.580313	-0.794556
8	6	0	-1.670887	3.546841	-0.723032
9	6	0	-2.948350	2.975586	-0.758119
10	1	0	-4.037708	1.118718	-0.840010
11	1	0	-1.549533	4.624320	-0.723322
12	6	0	-1.900882	-0.679518	-0.698728
13	6	0	-0.498840	-2.585881	-0.626980
14	6	0	-3.035299	-1.482257	-0.706658
15	6	0	-1.613509	-3.422022	-0.604484
16	6	0	-2.903885	-2.874380	-0.630968
17	1	0	-4.020016	-1.034857	-0.738803
18	1	0	-1.472234	-4.495721	-0.558519
19	6	0	-4.175376	3.823758	-0.732529
20	6	0	-4.635981	4.435815	-1.915057
21	6	0	-4.865281	3.995687	0.485145
22	6	0	-5.794809	5.217705	-1.859869
23	6	0	-6.019076	4.788348	0.494632
24	6	0	-6.501220	5.404255	-0.665687
25	1	0	-6.155058	5.690198	-2.771115
26	1	0	-6.551706	4.929272	1.432613
27	6	0	-4.109604	-3.748061	-0.566311
28	6	0	-4.414736	-4.608451	-1.640603
29	6	0	-4.938238	-3.706873	0.578638
30	6	0	-5.554569	-5.417874	-1.553423
31	6	0	-6.058524	-4.541441	0.624842
32	6	0	-6.386616	-5.401619	-0.430634
33	1	0	-5.796451	-6.074965	-2.385630
34	1	0	-6.691956	-4.521692	1.509142

35	6	0	-7.768115	6.224541	-0.638520
36	1	0	-7.733835	7.038860	-1.369416
37	1	0	-8.640587	5.605189	-0.884071
38	1	0	-7.944668	6.657433	0.351095
39	6	0	-3.900623	4.244882	-3.220770
40	1	0	-2.881338	4.645008	-3.169636
41	1	0	-3.809932	3.182088	-3.474786
42	1	0	-4.419130	4.746734	-4.042028
43	6	0	-4.354507	3.371114	1.763196
44	1	0	-4.150453	2.300977	1.652266
45	1	0	-3.406198	3.831088	2.070323
46	1	0	-5.070066	3.507437	2.579178
47	6	0	-3.551076	-4.661647	-2.880590
48	1	0	-3.312466	-3.658736	-3.251061
49	1	0	-2.596819	-5.165080	-2.686702
50	1	0	-4.055710	-5.208323	-3.681822
51	6	0	-4.627512	-2.801061	1.748417
52	1	0	-3.591401	-2.906546	2.086154
53	1	0	-4.763071	-1.745307	1.493533
54	1	0	-5.282000	-3.023921	2.595309
55	6	0	-7.615540	-6.274043	-0.351076
56	1	0	-7.666601	-6.975567	-1.188867
57	1	0	-7.631064	-6.852167	0.579930
58	1	0	-8.529638	-5.667612	-0.364894
59	7	0	-0.693067	1.390140	-0.645741
60	7	0	-0.667318	-1.247254	-0.636346
61	6	0	0.864426	3.260515	-0.782510
62	6	0	0.914350	-3.103480	-0.684567
63	1	0	1.057734	3.462553	-1.842867
64	1	0	0.960546	4.213808	-0.256845

65	1	0	1.017207	-4.026702	-0.111871
66	1	0	1.113529	-3.365041	-1.730496
67	6	0	2.679575	2.657749	1.459658
68	6	0	3.463883	1.615621	2.283093
69	6	0	3.411179	4.014671	1.479673
70	1	0	1.703480	2.794332	1.943899
71	6	0	3.641817	2.098834	3.730055
72	1	0	4.451412	1.460825	1.834480
73	1	0	2.953059	0.651157	2.270750
74	6	0	3.581644	4.502015	2.928545
75	1	0	4.401206	3.897988	1.023987
76	1	0	2.870417	4.765451	0.893344
77	6	0	4.330122	3.469847	3.783592
78	1	0	4.219424	1.357679	4.295750
79	1	0	2.654514	2.166266	4.207715
80	1	0	4.114432	5.460548	2.933278
81	1	0	2.589472	4.686452	3.364168
82	1	0	4.406077	3.818606	4.820546
83	1	0	5.357960	3.370254	3.405967
84	6	0	3.551689	2.205905	-1.455200
85	6	0	3.914951	3.630674	-1.925564
86	6	0	4.813931	1.453880	-0.988930
87	1	0	3.135530	1.668316	-2.317993
88	6	0	4.952573	3.557582	-3.059686
89	1	0	4.334370	4.205861	-1.094538
90	1	0	3.028583	4.168841	-2.276270
91	6	0	5.846617	1.382468	-2.122643
92	1	0	5.253769	1.986078	-0.136927
93	1	0	4.556046	0.450225	-0.639276
94	6	0	6.208004	2.784458	-2.631938

95	1	0	5.218199	4.572856	-3.377598
96	1	0	4.498847	3.060313	-3.928805
97	1	0	6.743165	0.855222	-1.774904
98	1	0	5.429838	0.793036	-2.949680
99	1	0	6.914235	2.715663	-3.468085
100	1	0	6.717108	3.338957	-1.830717
101	6	0	2.903338	-2.256958	1.480654
102	6	0	2.692586	-3.699242	1.980412
103	6	0	4.381530	-1.832561	1.621859
104	1	0	2.308362	-1.610895	2.132400
105	6	0	3.169299	-3.827228	3.438304
106	1	0	3.243853	-4.406129	1.348581
107	1	0	1.633841	-3.972363	1.926425
108	6	0	4.824760	-1.944250	3.087865
109	1	0	5.016195	-2.484878	1.010142
110	1	0	4.528971	-0.811392	1.259400
111	6	0	4.624408	-3.372093	3.613627
112	1	0	3.049032	-4.864724	3.772550
113	1	0	2.520761	-3.210782	4.076513
114	1	0	5.875351	-1.643694	3.179923
115	1	0	4.236550	-1.242711	3.696107
116	1	0	4.915449	-3.435335	4.669084
117	1	0	5.286133	-4.053622	3.060057
118	6	0	3.578567	-2.171700	-1.451191
119	6	0	3.992180	-3.662218	-1.481321
120	6	0	3.236144	-1.661453	-2.865109
121	1	0	4.434070	-1.591149	-1.088019
122	6	0	5.148023	-3.895056	-2.466979
123	1	0	3.138746	-4.277899	-1.791795
124	1	0	4.285846	-4.001969	-0.484844

125	6	0	4.385770	-1.931977	-3.849194
126	1	0	2.325696	-2.156643	-3.229795
127	1	0	3.022479	-0.590075	-2.831614
128	6	0	4.784717	-3.411956	-3.875501
129	1	0	5.406969	-4.960544	-2.477692
130	1	0	6.037629	-3.353894	-2.114723
131	1	0	4.094356	-1.591175	-4.850086
132	1	0	5.257691	-1.334346	-3.551868
133	1	0	5.625189	-3.567327	-4.562567
134	1	0	3.945284	-4.010345	-4.257951
135	6	0	0.411424	0.171006	1.743465
136	8	0	0.309258	0.898999	2.649026
137	8	0	-0.139349	-1.507247	2.437905
138	6	0	-2.963943	-0.292907	3.100571
139	8	0	-2.836918	0.233362	1.987051
140	8	0	-4.083149	-0.043474	3.846847
141	8	0	-2.155173	-1.091441	3.697729
142	1	0	-1.141265	-1.282383	3.041525
143	1	0	-4.626855	0.557785	3.313335
144	1	0	-0.393534	-2.094014	1.711935

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^{1}TS15 E(opt) = -3377.72450017 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.791515	0.095238	-0.152097
2	1	0	0.905982	-0.026438	-1.761236
3	15	0	2.102178	2.009745	-0.385687
4	15	0	2.077439	-1.844557	-0.029470

5	6	0	-2.043221	0.851002	-0.333602
6	6	0	-0.637980	2.739307	-0.584794
7	6	0	-3.173980	1.658547	-0.324647
8	6	0	-1.748362	3.584110	-0.569901
9	6	0	-3.032767	3.050347	-0.419917
10	1	0	-4.160655	1.221585	-0.232142
11	1	0	-1.606442	4.653649	-0.677482
12	6	0	-2.057138	-0.626339	-0.270021
13	6	0	-0.692889	-2.554986	-0.192225
14	6	0	-3.205236	-1.405353	-0.316391
15	6	0	-1.824363	-3.370155	-0.223264
16	6	0	-3.101499	-2.804478	-0.290737
17	1	0	-4.179309	-0.938525	-0.389276
18	1	0	-1.700663	-4.446615	-0.198627
19	6	0	-4.230717	3.936981	-0.365675
20	6	0	-4.721972	4.528183	-1.547204
21	6	0	-4.864171	4.168573	0.872517
22	6	0	-5.851763	5.349840	-1.467665
23	6	0	-5.987165	5.002564	0.906502
24	6	0	-6.495707	5.602675	-0.251016
25	1	0	-6.239328	5.800212	-2.378801
26	1	0	-6.476095	5.187024	1.860490
27	6	0	-4.321411	-3.658038	-0.366830
28	6	0	-4.521888	-4.488958	-1.492027
29	6	0	-5.272576	-3.628311	0.677300
30	6	0	-5.673496	-5.281298	-1.548973
31	6	0	-6.402465	-4.448562	0.580781
32	6	0	-6.624244	-5.278690	-0.522830
33	1	0	-5.831776	-5.915150	-2.418760
34	1	0	-7.127065	-4.438547	1.391990

35	6	0	-7.690118	6.522984	-0.184583
36	1	0	-7.373993	7.562427	-0.027361
37	1	0	-8.268366	6.497215	-1.113665
38	1	0	-8.355354	6.257482	0.643085
39	6	0	-4.059779	4.269481	-2.880612
40	1	0	-3.043812	4.679715	-2.911977
41	1	0	-3.973594	3.195544	-3.082988
42	1	0	-4.629620	4.723893	-3.695453
43	6	0	-4.340859	3.541545	2.144217
44	1	0	-4.431902	2.449358	2.123224
45	1	0	-3.278154	3.765865	2.293303
46	1	0	-4.890419	3.906557	3.015984
47	6	0	-3.536654	-4.528972	-2.639294
48	1	0	-3.217468	-3.524355	-2.936659
49	1	0	-2.630689	-5.087152	-2.376613
50	1	0	-3.981052	-5.015831	-3.511721
51	6	0	-5.088209	-2.753675	1.896617
52	1	0	-4.080292	-2.840178	2.313193
53	1	0	-5.244037	-1.694613	1.660063
54	1	0	-5.808095	-3.023472	2.674600
55	6	0	-7.870976	-6.123131	-0.621004
56	1	0	-7.685802	-7.048239	-1.176190
57	1	0	-8.255973	-6.386337	0.369148
58	1	0	-8.668208	-5.582668	-1.147738
59	7	0	-0.807335	1.413921	-0.423395
60	7	0	-0.830617	-1.217186	-0.203681
61	6	0	0.759018	3.229425	-0.864836
62	6	0	0.703497	-3.123036	-0.200801
63	1	0	0.829902	3.380641	-1.948495
64	1	0	0.933392	4.203581	-0.400869

65	1	0	0.796771	-3.909749	0.551672
66	1	0	0.849266	-3.615484	-1.168080
67	6	0	2.832888	2.751926	1.155376
68	6	0	3.669094	1.753641	1.979561
69	6	0	3.611210	4.067921	0.956251
70	1	0	1.928354	2.980392	1.733973
71	6	0	4.044485	2.359727	3.339974
72	1	0	4.585823	1.503848	1.434000
73	1	0	3.119228	0.821500	2.123995
74	6	0	3.977668	4.677462	2.320013
75	1	0	4.532278	3.862398	0.398669
76	1	0	3.029601	4.787065	0.369243
77	6	0	4.786872	3.693035	3.175710
78	1	0	4.658323	1.646056	3.902674
79	1	0	3.127820	2.521976	3.924066
80	1	0	4.541986	5.605346	2.167613
81	1	0	3.054556	4.949324	2.851196
82	1	0	5.004610	4.131846	4.156879
83	1	0	5.755117	3.507244	2.688954
84	6	0	3.305534	2.030422	-1.802178
85	6	0	3.631172	3.401211	-2.433330
86	6	0	4.602813	1.279619	-1.442864
87	1	0	2.767524	1.437161	-2.554352
88	6	0	4.513287	3.209339	-3.679566
89	1	0	4.164354	4.029621	-1.713622
90	1	0	2.717373	3.934816	-2.712846
91	6	0	5.482640	1.094014	-2.687309
92	1	0	5.157594	1.857645	-0.693994
93	1	0	4.371202	0.310879	-0.992667
94	6	0	5.800508	2.441090	-3.349756

95	1	0	4.751561	4.188446	-4.111935
96	1	0	3.944729	2.655336	-4.440050
97	1	0	6.406418	0.570703	-2.412547
98	1	0	4.954476	0.453594	-3.405843
99	1	0	6.394598	2.287729	-4.258690
100	1	0	6.415204	3.043999	-2.666167
101	6	0	2.969498	-2.115882	1.600892
102	6	0	2.812863	-3.491558	2.280192
103	6	0	4.459933	-1.721897	1.501265
104	1	0	2.495002	-1.376216	2.254749
105	6	0	3.468578	-3.468904	3.672067
106	1	0	3.276143	-4.271069	1.663967
107	1	0	1.756344	-3.759835	2.389644
108	6	0	5.090691	-1.684332	2.900765
109	1	0	4.996676	-2.455819	0.889029
110	1	0	4.570834	-0.751045	1.011673
111	6	0	4.939839	-3.037232	3.609276
112	1	0	3.378052	-4.459176	4.133894
113	1	0	2.912859	-2.767990	4.310981
114	1	0	6.148679	-1.407749	2.820159
115	1	0	4.599737	-0.901300	3.495343
116	1	0	5.362178	-2.988287	4.620077
117	1	0	5.515692	-3.795883	3.060271
118	6	0	3.268121	-2.327306	-1.380655
119	6	0	3.682931	-3.815768	-1.304084
120	6	0	2.747486	-1.967656	-2.786146
121	1	0	4.159065	-1.718936	-1.188654
122	6	0	4.710586	-4.157041	-2.394681
123	1	0	2.802853	-4.456114	-1.442090
124	1	0	4.098554	-4.052137	-0.321424

125	6	0	3.766392	-2.348385	-3.872423
126	1	0	1.801057	-2.492762	-2.976859
127	1	0	2.532862	-0.897116	-2.839691
128	6	0	4.171831	-3.824545	-3.790615
129	1	0	4.975191	-5.218824	-2.324452
130	1	0	5.632087	-3.585671	-2.213910
131	1	0	3.348738	-2.115201	-4.859302
132	1	0	4.663557	-1.726648	-3.752474
133	1	0	4.922556	-4.055549	-4.555870
134	1	0	3.297078	-4.456610	-4.000935
135	6	0	0.505521	0.425344	1.921812
136	8	0	0.411979	1.316735	2.676297
137	8	0	0.016485	-1.053784	2.864039
138	1	0	0.355153	-1.862750	2.449991
139	6	0	-1.714492	-1.393394	2.967533
140	8	0	-2.303713	-0.345628	2.998112
141	8	0	-1.813408	-2.598389	2.991061

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^{1}TS16 E(opt) = -3187.960285 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.755894	-0.045089	-0.320990
2	15	0	-1.965464	-1.987387	-0.173731
3	15	0	-2.074457	1.839229	-0.251550
4	6	0	2.090197	-0.725379	-0.379452
5	6	0	0.739138	-2.660757	-0.537805
6	6	0	3.244062	-1.500279	-0.337528
7	6	0	1.872064	-3.470626	-0.482992

8	6	0	3.145658	-2.897734	-0.377339
9	1	0	4.217716	-1.030767	-0.265294
10	1	0	1.759617	-4.547915	-0.535492
11	6	0	2.059973	0.752075	-0.338332
12	6	0	0.632573	2.636900	-0.435459
13	6	0	3.177212	1.570108	-0.208673
14	6	0	1.727785	3.488018	-0.299357
15	6	0	3.019745	2.962369	-0.174068
16	1	0	4.166230	1.137753	-0.117439
17	1	0	1.571194	4.561069	-0.297730
18	6	0	4.368254	-3.749497	-0.313797
19	6	0	5.244376	-3.803483	-1.417926
20	6	0	4.642936	-4.491138	0.854523
21	6	0	6.384964	-4.610067	-1.334671
22	6	0	5.799073	-5.278231	0.897118
23	6	0	6.680018	-5.354998	-0.187606
24	1	0	7.058724	-4.656987	-2.187444
25	1	0	6.018250	-5.841878	1.801386
26	6	0	4.199976	3.858333	-0.006265
27	6	0	5.118141	4.017639	-1.065975
28	6	0	4.388403	4.542450	1.212488
29	6	0	6.213059	4.869378	-0.886478
30	6	0	5.502423	5.378780	1.350930
31	6	0	6.425677	5.555497	0.314986
32	1	0	6.915849	5.002210	-1.706148
33	1	0	5.652145	5.902714	2.292352
34	6	0	7.900355	-6.241328	-0.132194
35	1	0	7.661777	-7.256809	-0.474285
36	1	0	8.701264	-5.862119	-0.774716
37	1	0	8.288042	-6.326287	0.887994

38	6	0	4.963850	-3.018751	-2.679106
39	1	0	3.942283	-3.186976	-3.038267
40	1	0	5.068017	-1.939960	-2.514750
41	1	0	5.655709	-3.302112	-3.476894
42	6	0	3.723254	-4.430916	2.052735
43	1	0	3.507504	-3.396220	2.342488
44	1	0	2.758802	-4.908587	1.844630
45	1	0	4.168315	-4.939368	2.912295
46	6	0	4.924293	3.301434	-2.382959
47	1	0	5.065183	2.219433	-2.277737
48	1	0	3.913123	3.452009	-2.777680
49	1	0	5.637971	3.658970	-3.130180
50	6	0	3.420887	4.375330	2.362005
51	1	0	2.444362	4.818928	2.135926
52	1	0	3.242700	3.317457	2.586569
53	1	0	3.803615	4.855331	3.266778
54	6	0	7.635743	6.439798	0.493025
55	1	0	7.885681	6.966539	-0.433857
56	1	0	7.477825	7.183821	1.279779
57	1	0	8.515656	5.846843	0.774354
58	7	0	0.862298	-1.315512	-0.462479
59	7	0	0.810506	1.296015	-0.426323
60	6	0	-0.651697	-3.202519	-0.744947
61	6	0	-0.770185	3.133920	-0.663790
62	1	0	-0.800763	-3.333777	-1.824016
63	1	0	-0.766314	-4.187416	-0.284456
64	1	0	-0.937814	4.087150	-0.160040
65	1	0	-0.875629	3.328861	-1.738105
66	6	0	-2.351479	-2.569304	1.554661
67	6	0	-3.072953	-1.500175	2.399040

68	6	0	-3.061070	-3.929155	1.689506
69	1	0	-1.337911	-2.674820	1.964049
70	6	0	-3.134646	-1.923927	3.873713
71	1	0	-4.092728	-1.359138	2.021507
72	1	0	-2.566233	-0.536065	2.302627
73	6	0	-3.114409	-4.358049	3.166021
74	1	0	-4.084833	-3.843879	1.305778
75	1	0	-2.555378	-4.697556	1.094223
76	6	0	-3.803419	-3.296319	4.035332
77	1	0	-3.672468	-1.164924	4.455250
78	1	0	-2.111767	-1.966469	4.274450
79	1	0	-3.635006	-5.319473	3.254061
80	1	0	-2.089279	-4.516867	3.530108
81	1	0	-3.796116	-3.603385	5.088242
82	1	0	-4.858393	-3.217901	3.735300
83	6	0	-3.390603	-2.289442	-1.334156
84	6	0	-3.718040	-3.752580	-1.698894
85	6	0	-4.659787	-1.549525	-0.867846
86	1	0	-3.032772	-1.793147	-2.248784
87	6	0	-4.807181	-3.797879	-2.784656
88	1	0	-4.076826	-4.286791	-0.813624
89	1	0	-2.824522	-4.278010	-2.051691
90	6	0	-5.750841	-1.602065	-1.947374
91	1	0	-5.036280	-2.022151	0.048168
92	1	0	-4.424350	-0.510917	-0.618376
93	6	0	-6.073382	-3.048933	-2.345698
94	1	0	-5.044373	-4.841395	-3.024977
95	1	0	-4.416310	-3.340733	-3.705015
96	1	0	-6.653046	-1.091601	-1.588689
97	1	0	-5.404449	-1.051229	-2.832681

98	1	0	-6.822249	-3.065710	-3.146865
99	1	0	-6.518227	-3.568602	-1.484848
100	6	0	-2.852993	2.311795	1.387728
101	6	0	-2.728875	3.783662	1.826405
102	6	0	-4.316827	1.830739	1.480207
103	1	0	-2.268108	1.718161	2.096396
104	6	0	-3.289468	3.967378	3.247682
105	1	0	-3.271341	4.434175	1.128902
106	1	0	-1.680788	4.100640	1.815185
107	6	0	-4.850389	2.004057	2.909944
108	1	0	-4.942976	2.415881	0.795170
109	1	0	-4.398313	0.783796	1.174209
110	6	0	-4.734093	3.464154	3.368225
111	1	0	-3.226498	5.024202	3.534350
112	1	0	-2.655094	3.409815	3.951668
113	1	0	-5.893014	1.667235	2.959727
114	1	0	-4.274353	1.359825	3.589517
115	1	0	-5.087817	3.570695	4.400961
116	1	0	-5.387777	4.089105	2.742814
117	6	0	-3.361705	2.101331	-1.570567
118	6	0	-3.845005	3.557485	-1.725762
119	6	0	-2.885559	1.522842	-2.919475
120	1	0	-4.212957	1.494514	-1.238391
121	6	0	-4.939071	3.659965	-2.801190
122	1	0	-3.001098	4.197664	-2.015144
123	1	0	-4.223169	3.938998	-0.772576
124	6	0	-3.980301	1.644424	-3.990665
125	1	0	-1.990566	2.062892	-3.258609
126	1	0	-2.592749	0.474364	-2.790593
127	6	0	-4.461313	3.093599	-4.144890

128	1	0	-5.249442	4.705870	-2.913878
129	1	0	-5.824051	3.100031	-2.466466
130	1	0	-3.606617	1.259415	-4.947411
131	1	0	-4.831819	1.011753	-3.704219
132	1	0	-5.264436	3.150764	-4.889649
133	1	0	-3.633485	3.711173	-4.522409
134	6	0	0.124775	0.022945	2.364555
135	8	0	0.430158	-1.110836	2.523608
136	8	0	-0.009593	1.175652	2.606600

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^{1}TS17 E(opt) = -3453.678896 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.927662	0.053036	-0.583548
2	15	0	-2.182809	1.914599	-0.021333
3	15	0	-2.089796	-1.891464	0.022251
4	6	0	1.893662	0.779339	-0.126039
5	6	0	0.486933	2.704192	-0.120828
6	6	0	3.021016	1.606283	0.057184
7	6	0	1.570261	3.519819	0.095988
8	6	0	2.883754	2.975575	0.192199
9	1	0	4.005852	1.155967	0.103249
10	1	0	1.420960	4.592432	0.159269
11	6	0	1.916206	-0.649571	-0.206783
12	6	0	0.566470	-2.605845	-0.370207
13	6	0	3.061240	-1.456626	-0.049928
14	6	0	1.669312	-3.410483	-0.195968
15	6	0	2.960167	-2.834990	-0.042381

16	1	0	4.028635	-0.986640	0.083230
17	1	0	1.546745	-4.488108	-0.179754
18	6	0	4.056809	3.869186	0.409971
19	6	0	4.183163	4.579994	1.626973
20	6	0	5.041193	4.018326	-0.590937
21	6	0	5.284269	5.420982	1.816242
22	6	0	6.125534	4.875589	-0.362469
23	6	0	6.265590	5.587867	0.831602
24	1	0	5.382267	5.955479	2.759023
25	1	0	6.877251	4.990232	-1.140775
26	6	0	4.160564	-3.697359	0.158824
27	6	0	4.356924	-4.342752	1.398788
28	6	0	5.100014	-3.860159	-0.881344
29	6	0	5.493268	-5.139655	1.578512
30	6	0	6.223188	-4.666661	-0.659983
31	6	0	6.437514	-5.316262	0.560611
32	1	0	5.647851	-5.628628	2.538202
33	1	0	6.946671	-4.792765	-1.462834
34	6	0	7.424141	6.531456	1.046432
35	1	0	7.139625	7.564295	0.806494
36	1	0	7.758331	6.524198	2.089290
37	1	0	8.276783	6.272098	0.411130
38	6	0	3.164762	4.425160	2.734120
39	1	0	2.216373	4.915327	2.485666
40	1	0	2.934274	3.370814	2.922634
41	1	0	3.531435	4.866683	3.665193
42	6	0	4.962789	3.272060	-1.904739
43	1	0	5.363472	2.255759	-1.794660
44	1	0	3.933237	3.190695	-2.267472
45	1	0	5.559685	3.771455	-2.673333

46	6	0	3.370830	-4.163795	2.530731
47	1	0	3.184761	-3.102877	2.733929
48	1	0	2.398754	-4.612020	2.294309
49	1	0	3.738941	-4.628094	3.449917
50	6	0	4.893518	-3.202179	-2.226426
51	1	0	3.947968	-3.523886	-2.679152
52	1	0	4.840232	-2.111238	-2.155497
53	1	0	5.702341	-3.460726	-2.916017
54	6	0	7.638515	-6.207957	0.765383
55	1	0	7.973884	-6.195971	1.807578
56	1	0	7.401550	-7.250043	0.513798
57	1	0	8.477375	-5.903895	0.131275
58	7	0	0.623925	1.335397	-0.196300
59	7	0	0.676850	-1.237908	-0.389042
60	6	0	-0.900754	3.220996	-0.376673
61	6	0	-0.826095	-3.144217	-0.552914
62	1	0	-1.085924	4.168667	0.132218
63	1	0	-1.001227	3.407778	-1.454795
64	1	0	-1.024035	-3.308833	-1.619632
65	1	0	-0.944302	-4.117207	-0.071135
66	6	0	-3.611858	2.502696	-1.055890
67	6	0	-4.694902	1.431123	-1.275758
68	6	0	-4.235749	3.843130	-0.621891
69	1	0	-3.120239	2.652593	-2.026087
70	6	0	-5.728402	1.909161	-2.306933
71	1	0	-5.209647	1.221423	-0.331984
72	1	0	-4.230460	0.499189	-1.608734
73	6	0	-5.270260	4.314674	-1.657609
74	1	0	-4.733391	3.718260	0.347169
75	1	0	-3.461695	4.607830	-0.490240

76	6	0	-6.351354	3.250840	-1.896029
77	1	0	-6.507613	1.146725	-2.429684
78	1	0	-5.236782	2.021812	-3.283557
79	1	0	-5.725922	5.255237	-1.324450
80	1	0	-4.756521	4.528287	-2.605766
81	1	0	-7.059783	3.593204	-2.660254
82	1	0	-6.927483	3.110947	-0.969752
83	6	0	-2.572179	2.044236	1.805726
84	6	0	-2.514087	3.449888	2.439359
85	6	0	-3.890346	1.333592	2.168007
86	1	0	-1.750351	1.457342	2.239328
87	6	0	-2.702830	3.357341	3.963808
88	1	0	-3.296720	4.088534	2.014842
89	1	0	-1.553796	3.929563	2.225022
90	6	0	-4.065346	1.243676	3.690565
91	1	0	-4.733175	1.893516	1.745266
92	1	0	-3.917154	0.333726	1.725493
93	6	0	-4.003627	2.633816	4.337614
94	1	0	-2.686208	4.364584	4.397729
95	1	0	-1.850842	2.812139	4.394860
96	1	0	-5.016260	0.750414	3.926828
97	1	0	-3.267486	0.613455	4.106971
98	1	0	-4.093351	2.552738	5.427767
99	1	0	-4.860493	3.229982	3.992044
100	6	0	-3.683560	-2.369609	-0.830878
101	6	0	-3.846858	-3.846740	-1.247830
102	6	0	-4.920105	-1.896251	-0.038496
103	1	0	-3.628006	-1.773748	-1.752650
104	6	0	-5.133891	-4.027114	-2.072119
105	1	0	-3.891686	-4.486146	-0.358312

106	1	0	-2.990572	-4.181640	-1.841351
107	6	0	-6.197304	-2.066420	-0.873070
108	1	0	-5.013614	-2.488443	0.880379
109	1	0	-4.806870	-0.854282	0.266345
110	6	0	-6.373771	-3.524183	-1.319968
111	1	0	-5.252518	-5.083638	-2.341681
112	1	0	-5.032382	-3.469020	-3.013960
113	1	0	-7.066768	-1.734610	-0.292549
114	1	0	-6.137650	-1.416144	-1.757237
115	1	0	-7.266297	-3.626262	-1.949247
116	1	0	-6.537284	-4.153364	-0.433178
117	6	0	-2.298601	-2.238596	1.852251
118	6	0	-2.674968	-3.690680	2.211384
119	6	0	-1.045221	-1.798083	2.639309
120	1	0	-3.128225	-1.586110	2.154505
121	6	0	-2.880496	-3.846610	3.727867
122	1	0	-1.871992	-4.367612	1.892097
123	1	0	-3.581916	-3.999222	1.684579
124	6	0	-1.247577	-1.966591	4.152121
125	1	0	-0.184919	-2.404368	2.323747
126	1	0	-0.801631	-0.756809	2.400328
127	6	0	-1.638590	-3.405682	4.512675
128	1	0	-3.131320	-4.889015	3.959616
129	1	0	-3.741099	-3.236330	4.037273
130	1	0	-0.332625	-1.672722	4.681383
131	1	0	-2.041038	-1.283520	4.485993
132	1	0	-1.816424	-3.494905	5.591351
133	1	0	-0.802419	-4.078043	4.271564
134	6	0	-1.461497	0.137624	-2.527366
135	8	0	-2.072017	0.768560	-3.318870

136	8	0	-0.568999	-1.157594	-3.518732
137	6	0	2.381865	0.271847	-3.360679
138	8	0	1.842053	1.372473	-3.447758
139	8	0	3.718477	0.162263	-3.100104
140	8	0	1.849781	-0.899263	-3.517764
141	1	0	0.727278	-0.901538	-3.540298
142	1	0	4.043220	1.069950	-3.001536
143	1	0	-0.577858	-1.902051	-2.901306

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^{1}TS18 E(opt) = -3453.568269 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.974685	0.009905	-0.541002
2	15	0	-2.190241	1.939561	-0.075105
3	15	0	-2.124004	-1.950027	0.042267
4	6	0	1.865814	0.758000	-0.307757
5	6	0	0.477371	2.680398	-0.409760
6	6	0	2.983962	1.558790	-0.073438
7	6	0	1.567174	3.501570	-0.166143
8	6	0	2.845960	2.946518	0.029406
9	1	0	3.955076	1.102471	0.073130
10	1	0	1.421993	4.574438	-0.115183
11	6	0	1.876537	-0.709574	-0.337298
12	6	0	0.513527	-2.649109	-0.492222
13	6	0	3.008252	-1.500951	-0.155458
14	6	0	1.620309	-3.465423	-0.306988
15	6	0	2.892029	-2.891787	-0.135031
16	1	0	3.979849	-1.041331	-0.022749

17	1	0	1.494703	-4.542053	-0.287766
18	6	0	4.002727	3.816459	0.386245
19	6	0	3.984183	4.524759	1.609223
20	6	0	5.111535	3.928424	-0.481659
21	6	0	5.076145	5.336958	1.936444
22	6	0	6.175534	4.759915	-0.116936
23	6	0	6.177104	5.475401	1.085412
24	1	0	5.066256	5.872516	2.883133
25	1	0	7.023681	4.852914	-0.791738
26	6	0	4.097657	-3.737143	0.096015
27	6	0	4.319589	-4.292431	1.372847
28	6	0	5.017518	-3.947502	-0.951357
29	6	0	5.474374	-5.054060	1.583046
30	6	0	6.158350	-4.717489	-0.696959
31	6	0	6.404742	-5.278393	0.561643
32	1	0	5.654442	-5.475364	2.569702
33	1	0	6.871367	-4.882755	-1.501777
34	6	0	7.322905	6.391926	1.437724
35	1	0	7.399773	6.541967	2.519053
36	1	0	8.277831	5.997523	1.075384
37	1	0	7.186734	7.380055	0.979269
38	6	0	2.830727	4.409896	2.581957
39	1	0	1.959794	4.986165	2.248812
40	1	0	2.499793	3.372771	2.700981
41	1	0	3.117601	4.790029	3.566410
42	6	0	5.163325	3.183026	-1.794904
43	1	0	5.352892	2.113726	-1.640167
44	1	0	4.221386	3.262869	-2.343835
45	1	0	5.964778	3.570084	-2.430358
46	6	0	3.344938	-4.055100	2.503849

47	1	0	3.169094	-2.984696	2.663256
48	1	0	2.367882	-4.506697	2.295499
49	1	0	3.718315	-4.480535	3.439203
50	6	0	4.763534	-3.387166	-2.331929
51	1	0	3.872973	-3.846066	-2.779719
52	1	0	4.576722	-2.308325	-2.320934
53	1	0	5.610301	-3.583305	-2.995472
54	6	0	7.628978	-6.127496	0.804481
55	1	0	7.950450	-6.077406	1.849641
56	1	0	7.425734	-7.182034	0.577037
57	1	0	8.465768	-5.815077	0.171653
58	7	0	0.631629	1.331488	-0.449639
59	7	0	0.656163	-1.298522	-0.507083
60	6	0	-0.917356	3.182748	-0.651410
61	6	0	-0.890129	-3.154194	-0.685140
62	1	0	-1.067861	4.176876	-0.227780
63	1	0	-1.076038	3.261052	-1.735309
64	1	0	-1.115571	-3.182051	-1.758923
65	1	0	-1.009594	-4.168161	-0.299993
66	6	0	-3.694996	2.427760	-1.039764
67	6	0	-4.783257	1.339644	-1.070103
68	6	0	-4.289208	3.798572	-0.661422
69	1	0	-3.284700	2.499816	-2.056548
70	6	0	-5.906257	1.729418	-2.043195
71	1	0	-5.207434	1.210386	-0.068389
72	1	0	-4.343412	0.385768	-1.366992
73	6	0	-5.411343	4.180910	-1.641114
74	1	0	-4.702436	3.744838	0.352929
75	1	0	-3.512916	4.571824	-0.656597
76	6	0	-6.501074	3.100996	-1.695561

77	1	0	-6.686318	0.958713	-2.030625
78	1	0	-5.502165	1.756901	-3.064968
79	1	0	-5.842431	5.145795	-1.348320
80	1	0	-4.981518	4.314920	-2.643874
81	1	0	-7.273153	3.376998	-2.423839
82	1	0	-6.996136	3.040592	-0.715632
83	6	0	-2.373208	2.179236	1.762182
84	6	0	-2.346974	3.629054	2.286698
85	6	0	-3.592354	1.410026	2.307884
86	1	0	-1.468390	1.678468	2.137537
87	6	0	-2.362723	3.632621	3.825260
88	1	0	-3.217027	4.179906	1.913911
89	1	0	-1.453567	4.152276	1.930576
90	6	0	-3.596506	1.421579	3.843094
91	1	0	-4.510864	1.885234	1.941957
92	1	0	-3.591471	0.381017	1.934304
93	6	0	-3.562556	2.856772	4.386133
94	1	0	-2.371943	4.667400	4.187964
95	1	0	-1.432638	3.175414	4.192093
96	1	0	-4.480765	0.889764	4.214422
97	1	0	-2.717254	0.872761	4.208277
98	1	0	-3.530040	2.849056	5.482229
99	1	0	-4.490632	3.371707	4.099352
100	6	0	-3.775207	-2.399968	-0.679947
101	6	0	-3.957238	-3.871396	-1.109967
102	6	0	-4.931740	-1.959830	0.242897
103	1	0	-3.809165	-1.785617	-1.589716
104	6	0	-5.313670	-4.047070	-1.814724
105	1	0	-3.914562	-4.525207	-0.230885
106	1	0	-3.153880	-4.182303	-1.785001

107	6	0	-6.278510	-2.123795	-0.475365
108	1	0	-4.929134	-2.584520	1.144945
109	1	0	-4.797158	-0.925832	0.569836
110	6	0	-6.482003	-3.573018	-0.939223
111	1	0	-5.447190	-5.099138	-2.093566
112	1	0	-5.304491	-3.469336	-2.749939
113	1	0	-7.092879	-1.816113	0.191390
114	1	0	-6.306193	-1.452014	-1.344455
115	1	0	-7.427587	-3.669476	-1.486163
116	1	0	-6.557835	-4.224044	-0.056565
117	6	0	-2.152475	-2.277443	1.875770
118	6	0	-2.387192	-3.753150	2.257544
119	6	0	-0.885881	-1.726644	2.567150
120	1	0	-3.007548	-1.689112	2.232324
121	6	0	-2.473206	-3.910436	3.785047
122	1	0	-1.556068	-4.364677	1.883510
123	1	0	-3.302204	-4.131896	1.792998
124	6	0	-0.976426	-1.895956	4.090430
125	1	0	-0.001513	-2.262331	2.197292
126	1	0	-0.748355	-0.669489	2.310416
127	6	0	-1.220778	-3.359942	4.479594
128	1	0	-2.618725	-4.967878	4.036244
129	1	0	-3.358395	-3.371314	4.151220
130	1	0	-0.056995	-1.521785	4.556905
131	1	0	-1.801548	-1.277445	4.470140
132	1	0	-1.316362	-3.453805	5.567990
133	1	0	-0.349453	-3.961919	4.183445
134	6	0	-1.552924	-0.032140	-2.453135
135	8	0	-2.371630	0.353641	-3.204265
136	8	0	-0.288877	-0.897476	-3.514235

137	6	0	2.335283	0.553583	-3.691173
138	8	0	2.640393	-0.541090	-3.203023
139	8	0	3.285795	1.512197	-3.889780
140	8	0	1.166584	0.940828	-4.076002
141	1	0	0.399138	0.031062	-3.847546
142	1	0	4.115995	1.141015	-3.550357
143	1	0	0.345538	-1.335303	-2.922816

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^{1}TS19 E(opt) = -3453.434347 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.920616	-0.000900	-0.197960
2	15	0	-2.245561	1.959807	-0.176548
3	15	0	-2.109477	-2.043332	0.109855
4	6	0	1.892642	0.841016	0.098037
5	6	0	0.478785	2.721737	-0.173680
6	6	0	2.997504	1.665723	0.252191
7	6	0	1.565673	3.581551	-0.024966
8	6	0	2.845145	3.059806	0.192411
9	1	0	3.979354	1.241992	0.419471
10	1	0	1.410789	4.651627	-0.099146
11	6	0	1.948204	-0.638570	0.108370
12	6	0	0.664916	-2.624030	0.013529
13	6	0	3.120893	-1.373605	0.205435
14	6	0	1.822088	-3.394446	0.100715
15	6	0	3.074083	-2.777014	0.186841
16	1	0	4.076026	-0.872213	0.289663
17	1	0	1.739026	-4.474840	0.088089

18	6	0	4.026122	3.955319	0.340352
19	6	0	4.133204	4.798041	1.468749
20	6	0	5.027528	3.957362	-0.653114
21	6	0	5.252296	5.627982	1.582398
22	6	0	6.124106	4.813926	-0.502413
23	6	0	6.257552	5.652945	0.608007
24	1	0	5.341861	6.271969	2.454457
25	1	0	6.889286	4.826549	-1.275013
26	6	0	4.321277	-3.586363	0.252121
27	6	0	4.530055	-4.473151	1.332656
28	6	0	5.285119	-3.468589	-0.775898
29	6	0	5.703796	-5.233547	1.361380
30	6	0	6.434819	-4.263042	-0.709075
31	6	0	6.663298	-5.151753	0.346506
32	1	0	5.872784	-5.905734	2.199648
33	1	0	7.171088	-4.184689	-1.506050
34	6	0	7.459562	6.550531	0.769449
35	1	0	8.027097	6.633712	-0.162028
36	1	0	7.164578	7.557748	1.083436
37	1	0	8.138099	6.160868	1.538792
38	6	0	3.077071	4.807765	2.550678
39	1	0	2.161080	5.307748	2.214780
40	1	0	2.795137	3.792782	2.851375
41	1	0	3.436081	5.337426	3.437176
42	6	0	4.923627	3.083085	-1.882824
43	1	0	5.060469	2.023941	-1.636078
44	1	0	3.942847	3.187849	-2.360945
45	1	0	5.688281	3.352124	-2.615982
46	6	0	3.537170	-4.603071	2.466950
47	1	0	3.150080	-3.629857	2.786276

48	1	0	2.673217	-5.214259	2.181257
49	1	0	4.003697	-5.082233	3.332029
50	6	0	5.103605	-2.521400	-1.939831
51	1	0	4.074286	-2.484234	-2.305837
52	1	0	5.363031	-1.493044	-1.664548
53	1	0	5.755920	-2.806907	-2.770507
54	6	0	7.897757	-6.018668	0.373849
55	1	0	8.183608	-6.278487	1.397835
56	1	0	7.724077	-6.959250	-0.164934
57	1	0	8.746693	-5.522415	-0.107052
58	7	0	0.662408	1.390952	-0.090539
59	7	0	0.751490	-1.280299	-0.005611
60	6	0	-0.901445	3.210309	-0.518648
61	6	0	-0.701512	-3.260781	-0.074071
62	1	0	-1.115766	4.164992	-0.034886
63	1	0	-0.930969	3.399396	-1.599157
64	1	0	-0.795443	-3.821647	-1.009065
65	1	0	-0.796869	-4.019614	0.708808
66	6	0	-3.505142	2.354159	-1.472278
67	6	0	-4.528647	1.233356	-1.723225
68	6	0	-4.193659	3.718627	-1.246913
69	1	0	-2.885170	2.440133	-2.373231
70	6	0	-5.423694	1.590549	-2.919408
71	1	0	-5.155425	1.097630	-0.836246
72	1	0	-4.014758	0.285336	-1.907669
73	6	0	-5.092619	4.056507	-2.447561
74	1	0	-4.804436	3.675694	-0.338323
75	1	0	-3.448547	4.508536	-1.101390
76	6	0	-6.116304	2.945012	-2.716086
77	1	0	-6.165667	0.797110	-3.066672

78	1	0	-4.809038	1.627306	-3.829739
79	1	0	-5.600469	5.010391	-2.263063
80	1	0	-4.463871	4.195737	-3.337971
81	1	0	-6.725602	3.195451	-3.592423
82	1	0	-6.803192	2.873515	-1.860654
83	6	0	-2.833801	2.203856	1.572342
84	6	0	-2.829157	3.656732	2.091452
85	6	0	-4.203702	1.529397	1.801040
86	1	0	-2.082920	1.643646	2.148930
87	6	0	-3.231395	3.687233	3.576093
88	1	0	-3.530206	4.263026	1.507107
89	1	0	-1.836368	4.103399	1.979795
90	6	0	-4.586310	1.572944	3.287337
91	1	0	-4.968495	2.057401	1.220519
92	1	0	-4.187295	0.495848	1.443781
93	6	0	-4.587346	3.011968	3.818342
94	1	0	-3.251345	4.726988	3.922695
95	1	0	-2.459371	3.170342	4.163778
96	1	0	-5.570520	1.109603	3.423244
97	1	0	-3.869109	0.972519	3.863020
98	1	0	-4.829498	3.022764	4.887560
99	1	0	-5.373866	3.584934	3.307288
100	6	0	-3.535745	-2.541930	-0.957121
101	6	0	-3.642467	-4.050469	-1.262277
102	6	0	-4.859653	-2.008679	-0.364187
103	1	0	-3.346470	-2.012649	-1.900779
104	6	0	-4.816853	-4.304599	-2.223983
105	1	0	-3.797028	-4.605454	-0.329058
106	1	0	-2.720074	-4.422495	-1.718649
107	6	0	-6.011566	-2.250104	-1.349291

108	1	0	-5.076313	-2.534686	0.572478
109	1	0	-4.781266	-0.946893	-0.124568
110	6	0	-6.139604	-3.741715	-1.686807
111	1	0	-4.904859	-5.381359	-2.409243
112	1	0	-4.588504	-3.832655	-3.189887
113	1	0	-6.945187	-1.870501	-0.918168
114	1	0	-5.826479	-1.676941	-2.268224
115	1	0	-6.940683	-3.899783	-2.418392
116	1	0	-6.424661	-4.291346	-0.778614
117	6	0	-2.542546	-2.095065	1.909160
118	6	0	-2.997151	-3.467705	2.442679
119	6	0	-1.352181	-1.547147	2.730667
120	1	0	-3.376018	-1.388553	2.000562
121	6	0	-3.358238	-3.358824	3.933943
122	1	0	-2.186792	-4.197917	2.323890
123	1	0	-3.853750	-3.839969	1.873730
124	6	0	-1.711992	-1.454517	4.219779
125	1	0	-0.485859	-2.210263	2.611301
126	1	0	-1.045654	-0.558417	2.354966
127	6	0	-2.186805	-2.810521	4.760395
128	1	0	-3.662556	-4.343371	4.307268
129	1	0	-4.225412	-2.692828	4.044200
130	1	0	-0.843028	-1.097401	4.784683
131	1	0	-2.508676	-0.710705	4.350540
132	1	0	-2.476631	-2.715088	5.813257
133	1	0	-1.352829	-3.525583	4.722875
134	6	0	-1.086937	0.021502	-2.079970
135	8	0	-1.447816	0.550013	-3.047622
136	8	0	-0.412893	-1.699212	-2.906186
137	6	0	2.310875	-0.186435	-3.046116

138	8	0	1.539826	0.764151	-2.818956
139	8	0	3.636506	0.079078	-3.289830
140	8	0	2.028013	-1.428717	-3.086927
141	1	0	0.660252	-1.572854	-2.974457
142	1	0	3.722052	1.043777	-3.242687
143	1	0	-0.555037	-2.528793	-2.431316

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^{1}TS20 E(opt) = -3265.072905 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.817076	0.063242	-0.132376
2	15	0	-2.035825	-1.873928	-0.334257
3	15	0	-2.160674	1.921674	-0.058947
4	6	0	2.015156	-0.548868	-0.547889
5	6	0	0.669827	-2.484211	-0.828567
6	6	0	3.175590	-1.326737	-0.625042
7	6	0	1.799980	-3.281124	-0.895961
8	6	0	3.083780	-2.706568	-0.776735
9	1	0	4.149314	-0.857263	-0.546606
10	1	0	1.692924	-4.349437	-1.052223
11	6	0	1.978000	0.899062	-0.399861
12	6	0	0.534247	2.779542	-0.258384
13	6	0	3.098056	1.734357	-0.321047
14	6	0	1.625085	3.628169	-0.166951
15	6	0	2.937899	3.110237	-0.183236
16	1	0	4.093977	1.308156	-0.352175
17	1	0	1.462335	4.697547	-0.084653
18	6	0	4.311394	-3.554451	-0.806986

19	6	0	4.811564	-4.035354	-2.033867
20	6	0	4.970590	-3.862012	0.401440
21	6	0	5.971314	-4.819378	-2.031689
22	6	0	6.126733	-4.649638	0.360107
23	6	0	6.642197	-5.138985	-0.845801
24	1	0	6.362285	-5.184315	-2.979120
25	1	0	6.635539	-4.887795	1.291879
26	6	0	4.119666	4.011214	-0.050235
27	6	0	4.475745	4.873662	-1.109252
28	6	0	4.875569	4.001138	1.141561
29	6	0	5.587042	5.710407	-0.958151
30	6	0	5.976816	4.858526	1.252695
31	6	0	6.351602	5.717489	0.214193
32	1	0	5.863513	6.371287	-1.777026
33	1	0	6.553255	4.857453	2.175332
34	6	0	7.872495	-6.013874	-0.863345
35	1	0	7.602975	-7.072339	-0.752361
36	1	0	8.420872	-5.916227	-1.805744
37	1	0	8.552929	-5.765756	-0.042383
38	6	0	4.121621	-3.697290	-3.334903
39	1	0	3.106370	-4.108966	-3.370549
40	1	0	4.025202	-2.612892	-3.464185
41	1	0	4.675934	-4.093950	-4.189986
42	6	0	4.424576	-3.369676	1.721240
43	1	0	4.374320	-2.276320	1.760935
44	1	0	3.402557	-3.727029	1.886027
45	1	0	5.042092	-3.714365	2.555912
46	6	0	3.685212	4.893226	-2.397485
47	1	0	3.554499	3.883105	-2.801851
48	1	0	2.680565	5.305436	-2.248693

49	1	0	4.186376	5.501581	-3.155493
50	6	0	4.504673	3.098233	2.296410
51	1	0	3.443086	3.188863	2.552403
52	1	0	4.680378	2.043111	2.058166
53	1	0	5.091919	3.341141	3.186492
54	6	0	7.564015	6.607894	0.341329
55	1	0	7.423816	7.554483	-0.190875
56	1	0	7.788771	6.832636	1.388681
57	1	0	8.452093	6.124902	-0.086765
58	7	0	0.779670	-1.141728	-0.620105
59	7	0	0.712480	1.431575	-0.346260
60	6	0	-0.724820	-2.997675	-1.070368
61	6	0	-0.886284	3.279960	-0.332713
62	1	0	-0.888519	-2.992037	-2.155912
63	1	0	-0.832297	-4.033113	-0.736728
64	1	0	-1.033216	4.122069	0.346411
65	1	0	-1.049237	3.672714	-1.343465
66	6	0	-2.450134	-2.741453	1.270657
67	6	0	-3.250898	-1.866641	2.256036
68	6	0	-3.090744	-4.138198	1.162141
69	1	0	-1.444316	-2.857010	1.698930
70	6	0	-3.312931	-2.532088	3.639431
71	1	0	-4.271521	-1.722259	1.881087
72	1	0	-2.793756	-0.877243	2.337389
73	6	0	-3.151632	-4.811564	2.544103
74	1	0	-4.110093	-4.040093	0.768961
75	1	0	-2.538015	-4.775483	0.462821
76	6	0	-3.910437	-3.944015	3.558364
77	1	0	-3.899819	-1.909162	4.326431
78	1	0	-2.294316	-2.587667	4.047406

79	1	0	-3.623627	-5.798218	2.456961
80	1	0	-2.126977	-4.980304	2.905016
81	1	0	-3.904403	-4.420411	4.546630
82	1	0	-4.963352	-3.870847	3.248930
83	6	0	-3.464729	-2.018281	-1.532050
84	6	0	-3.744793	-3.402464	-2.155333
85	6	0	-4.761139	-1.425735	-0.946084
86	1	0	-3.134539	-1.354932	-2.344094
87	6	0	-4.831263	-3.286668	-3.239102
88	1	0	-4.084721	-4.100360	-1.383317
89	1	0	-2.836421	-3.827381	-2.594613
90	6	0	-5.850612	-1.313738	-2.022433
91	1	0	-5.121833	-2.074720	-0.138352
92	1	0	-4.566742	-0.444901	-0.503772
93	6	0	-6.123362	-2.672201	-2.682644
94	1	0	-5.032702	-4.276245	-3.667422
95	1	0	-4.454476	-2.657075	-4.057992
96	1	0	-6.770054	-0.909623	-1.580971
97	1	0	-5.523921	-0.596772	-2.788192
98	1	0	-6.869036	-2.566563	-3.480196
99	1	0	-6.552946	-3.355133	-1.935512
100	6	0	-2.993887	2.283419	1.590194
101	6	0	-3.039050	3.736705	2.101608
102	6	0	-4.394973	1.639158	1.646533
103	1	0	-2.349183	1.720714	2.278666
104	6	0	-3.630547	3.789152	3.522064
105	1	0	-3.644660	4.359359	1.432495
106	1	0	-2.033209	4.169391	2.120499
107	6	0	-4.968284	1.689902	3.069904
108	1	0	-5.074014	2.175774	0.971464

109	1	0	-4.350801	0.603615	1.299277
110	6	0	-5.015219	3.131303	3.594215
111	1	0	-3.683514	4.831121	3.860945
112	1	0	-2.948971	3.267006	4.208856
113	1	0	-5.970096	1.242971	3.083464
114	1	0	-4.338355	1.080069	3.733068
115	1	0	-5.392357	3.152854	4.624059
116	1	0	-5.723061	3.711879	2.984976
117	6	0	-3.433178	2.248859	-1.389139
118	6	0	-4.033170	3.669400	-1.391900
119	6	0	-2.876731	1.884752	-2.781471
120	1	0	-4.239787	1.540237	-1.162719
121	6	0	-5.096397	3.821436	-2.493004
122	1	0	-3.235792	4.406178	-1.559765
123	1	0	-4.480997	3.898872	-0.421326
124	6	0	-3.944424	2.048029	-3.873612
125	1	0	-2.023742	2.536421	-3.019144
126	1	0	-2.489977	0.859673	-2.767822
127	6	0	-4.536599	3.463394	-3.875271
128	1	0	-5.486788	4.846610	-2.489823
129	1	0	-5.943389	3.158653	-2.264069
130	1	0	-3.510273	1.811608	-4.853032
131	1	0	-4.750069	1.321047	-3.700032
132	1	0	-5.319740	3.550021	-4.638480
133	1	0	-3.750316	4.183816	-4.143938
134	6	0	1.553318	-1.467204	3.095729
135	8	0	2.234890	-0.518338	2.695467
136	8	0	2.145624	-2.461911	3.843597
137	8	0	0.296561	-1.688229	2.931335
138	1	0	-0.266738	-0.704669	2.218001

139	1	0	3.082426	-2.215905	3.903135
140	1	0	-0.758162	0.000234	1.765373

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