Supplementary information

Theoretical prediction of the synthesis of 2,3-dihydropyridines through Ir(III)-catalysed reaction of unsaturated oximes with alkenes

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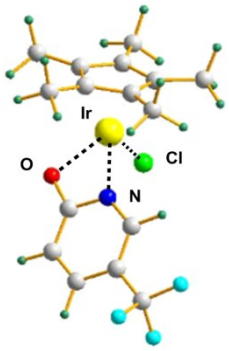
S1. The B3LY/BS1 calculated main bond parameters for Cp*Ir catalyst **M**



M

Table 1. Calculated main bond parameters by the B3LYP/BS1 method and corresponding experimental data

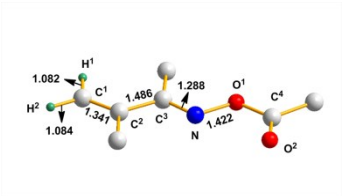
Bond Parameters	B3LYP/BS1	Experimental Data[1]
Ir - N	2.138	2.108
Ir - O	2.211	2.229
Ir - Cl	2.417	2.380
N - Ir - O	60.8	60.6

N - Ir - Cl	85.1	85.3
O - Ir - Cl	87.1	85.2

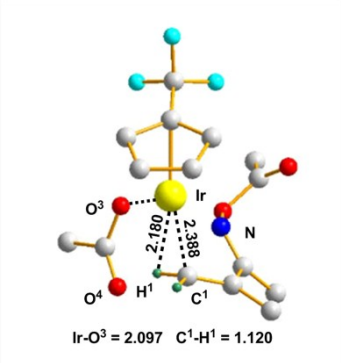
Reference

1 R. Yamaguchi, C. Ikeda, Y. Takahashi and K. Fujita, *J. Am. Chem. Soc.*, 2009, **131**, 8410-8412.

S2. Figure S1. (a) Optimised structures of selective species in the catalytic cycle. For clarity, H atoms that are not involved in the reaction and the methyls on Cp* and pivaloyls are omitted. **(b)** Transition states **TS5a-6a**, **TS5b-6b**, **TS5c-6c**, and **TS5d-6d** that are involved in the reaction catalysed by **1-CF$_3$**. The distances are given in Å, the angles and dihedral angles are given in degrees.



a$_1$



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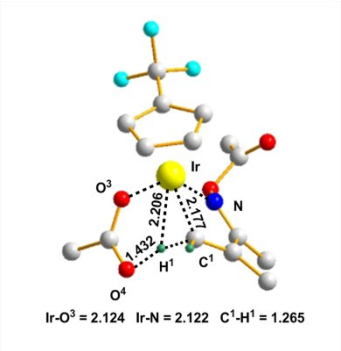

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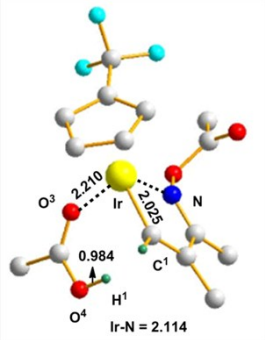

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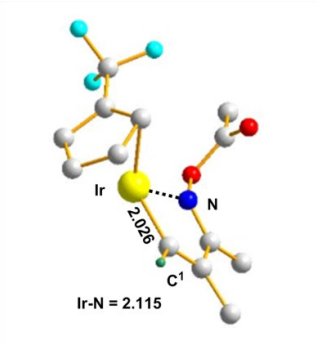

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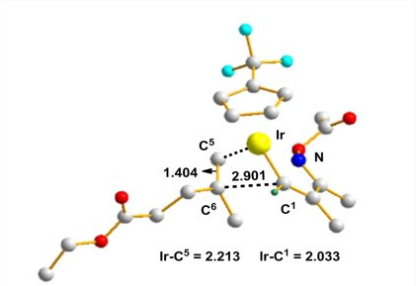

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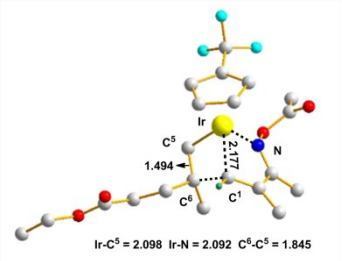

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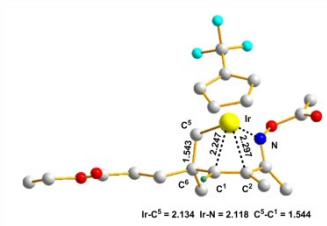

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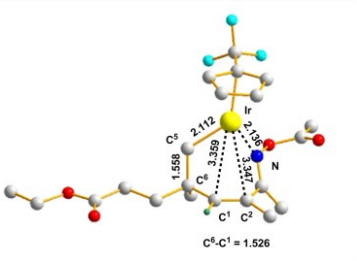

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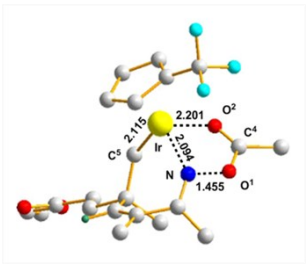

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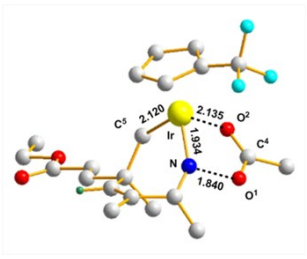

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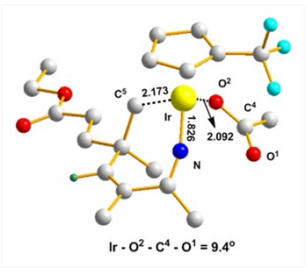

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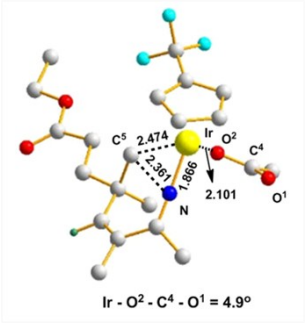

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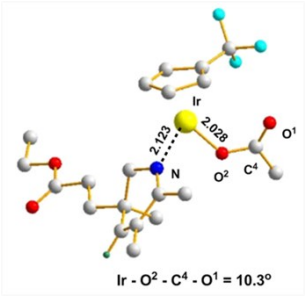

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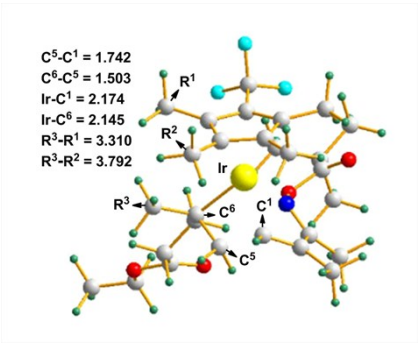

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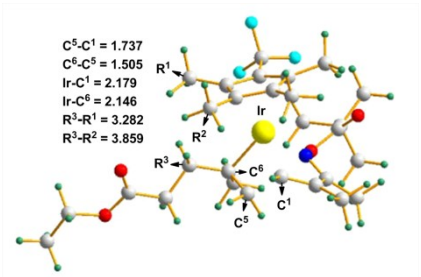

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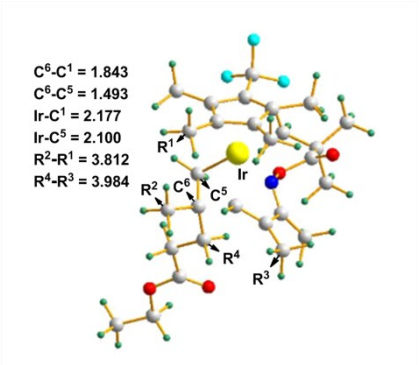

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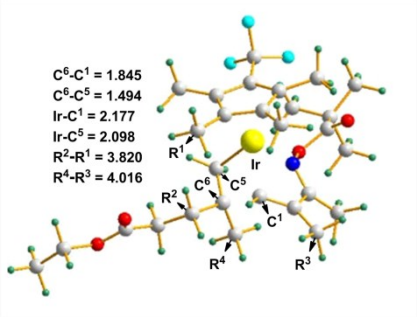
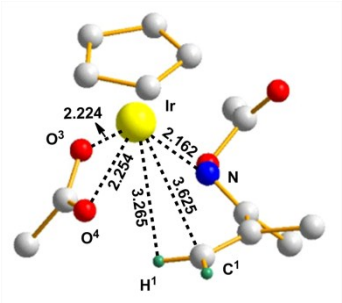


TS5d-6d

(b)

S3. Figure S2. Optimised structures for selected species in the reactions catalysed by **1-CH_3**, **1-NH_2**, and **1-$N(CH_3)_2$**. For clarity, H atoms that are not involved in the reactions and the methyls on Cp* and pivaloyls are omitted. The distances are given in Å, and angles are given in degrees.



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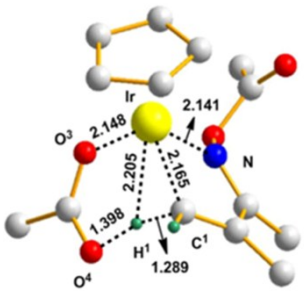

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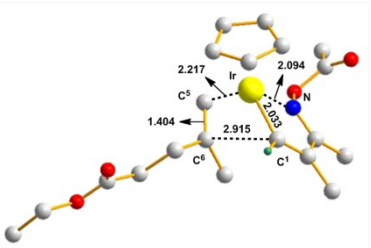

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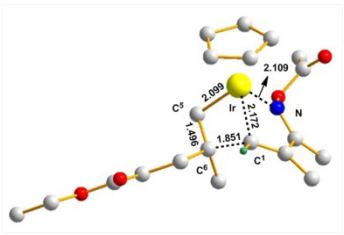

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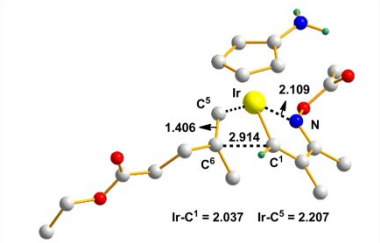

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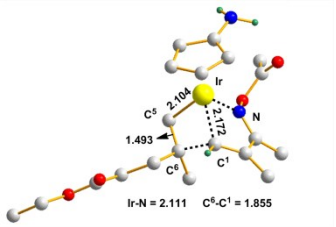

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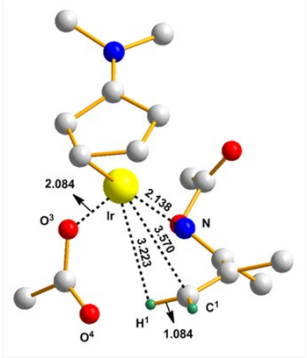

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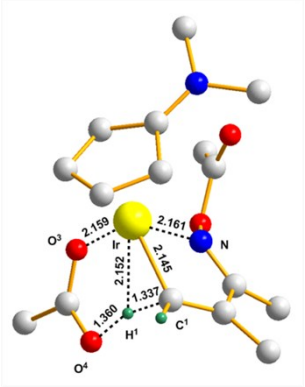

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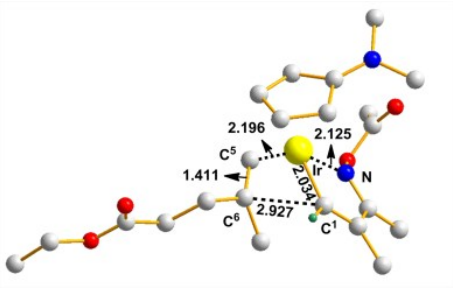

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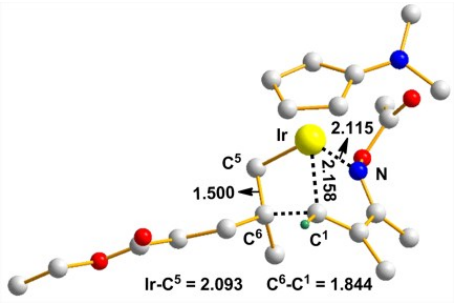
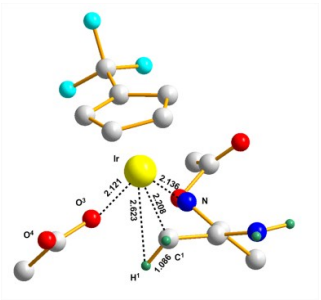


TS27-28

S4. Figure S3. Optimised structures of selected species in the reactions of NH_2-, phenyl-, and p-CF_3-phenyl-substituted α,β-unsaturated oxime pivalates with alkene $\mathbf{b_1}$, and the reactions of α,β-unsaturated oxime pivalates $\mathbf{a_1}$ with alkenes $\mathbf{b_2}$-$\mathbf{b_5}$. For clarity, H atoms that are not involved in the reactions and the methyls on Cp* and pivaloyls are omitted. The distances are given in Å, and the angles in degrees.



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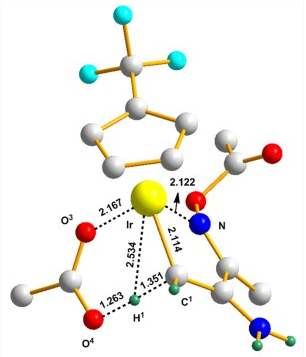

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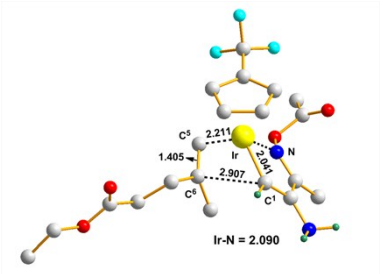

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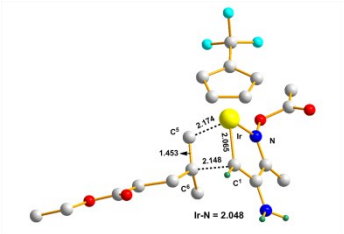

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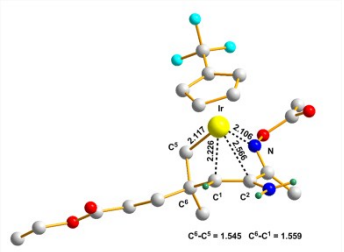

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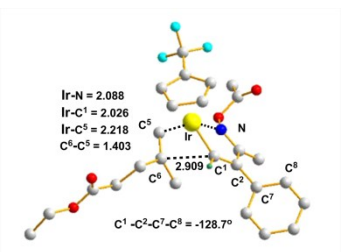

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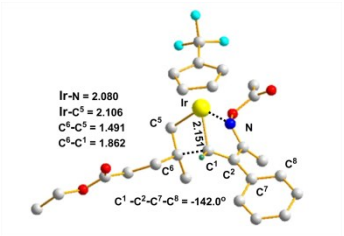

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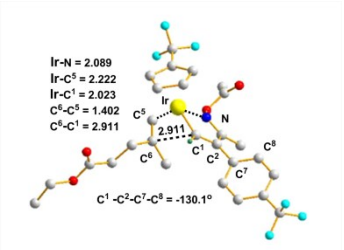

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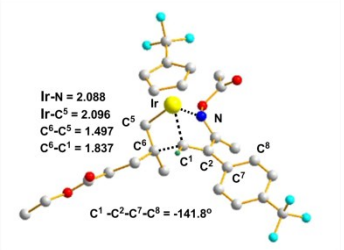

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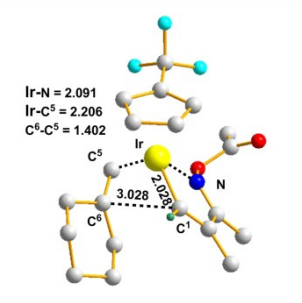

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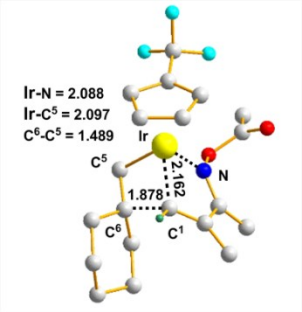

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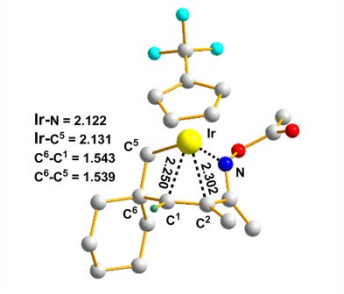

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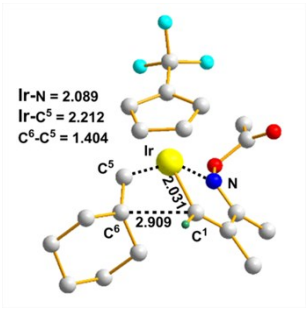

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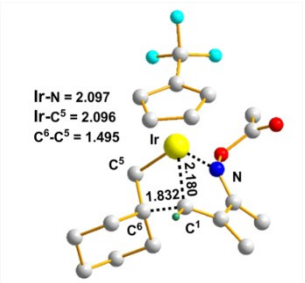

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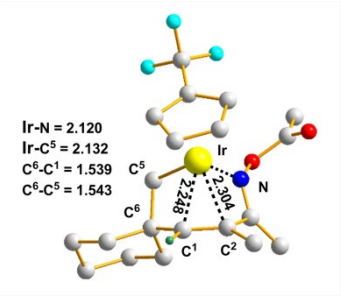

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S5. Optimised Cartesian coordinates and electronic energies (E) for species involved in the study

In Gas:
M (E = -1615.0489385 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	1.014327	-0.171824	-0.065012
2	17	0.549885	-2.540794	0.056163
3	8	-0.526448	-0.066263	-1.647710
4	7	-1.036397	0.073132	0.489443
5	6	2.098277	1.730704	-0.085539
6	6	2.193379	1.122793	1.224777
7	6	2.843723	-0.158706	1.094841
8	6	3.175059	-0.344414	-0.313034
9	6	2.710146	0.811587	-1.027082
10	6	1.596645	3.113328	-0.401213
11	6	1.739821	1.752625	2.512244
12	6	3.223277	-1.099681	2.203572
13	6	3.918596	-1.523454	-0.875105
14	6	2.822321	1.050039	-2.506425
15	6	-1.504881	0.000342	-0.792525
16	6	-2.895503	-0.003761	-1.052324
17	6	-3.750215	0.062875	0.037545
18	6	-3.250296	0.114136	1.359416
19	6	-1.875345	0.102141	1.542834
20	1	1.150565	3.154316	-1.398859
21	1	2.420458	3.840273	-0.368625
22	1	0.836031	3.436242	0.315322
23	1	0.867146	2.393567	2.359012
24	1	2.544676	2.373607	2.928583

25	1	1.480751	0.996210	3.257980
26	1	2.627074	-0.921236	3.102494
27	1	4.282667	-0.973163	2.466096
28	1	3.061792	-2.138361	1.902734
29	1	3.540123	-2.458467	-0.452668
30	1	4.989522	-1.442862	-0.644343
31	1	3.807882	-1.586461	-1.960519
32	1	2.976102	0.115719	-3.051122
33	1	3.671279	1.714456	-2.717087
34	1	1.915185	1.517328	-2.899806
35	1	-3.252759	-0.071752	-2.070201
36	1	-1.426255	0.114801	2.528886
37	1	-3.919694	0.150628	2.208430
38	6	-5.241721	0.096269	-0.160020
39	9	-5.619268	-0.098256	-1.460131
40	9	-5.776057	1.308585	0.230730
41	9	-5.884327	-0.859569	0.593257

In 2-Propanol:
1-CF_3 (E = -1020.9239473 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.112827	-0.698918	-0.424039
2	6	0.837119	0.996921	0.323229
3	6	1.825283	0.340222	-0.524992
4	6	2.069162	-0.950733	0.031202
5	6	1.261555	-1.101009	1.216522
6	6	0.513558	0.126878	1.444348
7	6	0.431952	2.437799	0.143949
8	9	-0.041192	2.697784	-1.116078
9	9	1.531872	3.246626	0.329339
10	9	-0.518279	2.851423	1.024670
11	6	2.468082	0.914390	-1.750035
12	1	2.759809	0.128430	-2.449335
13	1	1.810393	1.614256	-2.267726
14	1	3.375926	1.456362	-1.454352
15	6	2.996399	-1.988668	-0.526471
16	1	3.970427	-1.906927	-0.027153
17	1	2.617705	-2.999357	-0.357813
18	1	3.155809	-1.856127	-1.598248
19	6	1.240640	-2.298572	2.112441
20	1	0.268669	-2.431020	2.592059
21	1	1.488165	-3.213082	1.570158
22	1	1.991633	-2.160418	2.902320
23	6	-0.320557	0.437709	2.647473
24	1	-0.545248	-0.470457	3.209140
25	1	0.240368	1.115451	3.303991
26	1	-1.257520	0.919464	2.366944
27	8	-2.074786	-0.818930	-0.753651
28	6	-3.102635	-0.191619	-0.169708
29	8	-2.966352	0.710309	0.631372
30	6	-4.439834	-0.731266	-0.626057
31	1	-5.252247	-0.169859	-0.162780
32	1	-4.519035	-0.666423	-1.716203
33	1	-4.523993	-1.789468	-0.354589

2 (E = -1617.4515724 au)

Center Number	Atomic	Coordinates (Angstroms)

	Number	X	Y	Z
1	77	-0.910238	0.224463	0.171685
2	6	-1.080814	-1.774597	-0.509621
3	6	-1.291415	-0.944830	-1.699511
4	6	-2.440403	-0.150425	-1.440451
5	6	-2.983477	-0.519681	-0.130754
6	6	-2.187469	-1.565908	0.416603
7	6	-0.096724	-2.902223	-0.414757
8	9	1.071508	-2.655243	-1.082949
9	9	-0.631961	-4.046360	-0.971113
10	9	0.241134	-3.214907	0.872948
11	6	-0.509965	-0.981346	-2.979188
12	1	-0.747166	-0.120043	-3.605807
13	1	0.565432	-0.996426	-2.804816
14	1	-0.782646	-1.888507	-3.534166
15	6	-3.090596	0.802328	-2.399594
16	1	-3.840234	0.256156	-2.986904
17	1	-3.605946	1.613836	-1.881987
18	1	-2.371878	1.240523	-3.094406
19	6	-4.249285	0.028517	0.459503
20	1	-4.253472	-0.040326	1.548778
21	1	-4.406027	1.073324	0.183169
22	1	-5.101978	-0.547752	0.077311
23	6	-2.429611	-2.291219	1.707215
24	1	-3.265267	-1.849442	2.251837
25	1	-2.674882	-3.339026	1.497345
26	1	-1.546318	-2.269415	2.348410
27	8	-0.155390	-0.002134	2.115519
28	6	0.012583	0.945438	2.993778
29	8	-0.245114	2.135944	2.804848
30	6	0.538949	0.446108	4.329466
31	1	1.236008	-0.384122	4.193355
32	1	1.023168	1.261677	4.870690
33	1	-0.305006	0.084076	4.929412
34	6	0.930328	2.516445	-0.541178
35	7	0.922501	1.266967	-0.193796
36	6	-0.421975	3.058477	-0.755751
37	6	-0.643893	4.090722	-1.825086
38	1	-1.699359	4.364204	-1.883225
39	1	-0.064470	4.998266	-1.614960
40	1	-0.319534	3.720983	-2.805852
41	6	2.155135	3.358111	-0.712187
42	1	1.978053	4.363662	-0.321074
43	1	3.017613	2.925509	-0.207724
44	1	2.386659	3.455003	-1.780807
45	6	-1.396312	2.559603	0.050068
46	1	-2.423573	2.882745	-0.059180
47	1	-1.108411	2.200805	1.070800
48	8	2.152946	0.735024	0.236609
49	6	2.883664	0.067286	-0.741402
50	8	2.536687	0.049717	-1.888372
51	6	4.146601	-0.546799	-0.132008
52	6	3.781069	-1.430416	1.089516
53	1	3.100416	-2.239634	0.806036
54	1	4.697668	-1.879171	1.486223
55	1	3.313438	-0.843562	1.884683
56	6	4.844668	-1.396349	-1.215757
57	1	5.756473	-1.831958	-0.795125
58	1	4.200609	-2.212317	-1.558736
59	1	5.120489	-0.788958	-2.083077
60	6	5.083972	0.610814	0.316996
61	1	6.012424	0.180346	0.706226

62	1	5.340464	1.265253	-0.523756
63	1	4.628716	1.211752	1.109932

TS2-3 (E = -1617.4475218 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.943997	0.258620	0.275652
2	6	-1.144839	-1.781533	-0.455996
3	6	-1.310254	-0.899401	-1.605747
4	6	-2.450059	-0.080533	-1.342122
5	6	-3.019773	-0.472688	-0.057499
6	6	-2.238822	-1.547558	0.469549
7	6	-0.206385	-2.942710	-0.390176
8	9	0.967431	-2.730563	-1.065024
9	9	-0.778186	-4.066590	-0.958829
10	9	0.134065	-3.293802	0.890161
11	6	-0.527461	-0.913280	-2.885689
12	1	-0.712719	-0.007611	-3.465748
13	1	0.544392	-1.000280	-2.715316
14	1	-0.853840	-1.771828	-3.487396
15	6	-3.057540	0.910506	-2.292234
16	1	-3.755863	0.386337	-2.957355
17	1	-3.619888	1.684883	-1.766453
18	1	-2.302433	1.398328	-2.911862
19	6	-4.292617	0.070442	0.525560
20	1	-4.331399	-0.058124	1.608861
21	1	-4.414759	1.133707	0.306536
22	1	-5.148376	-0.460058	0.088580
23	6	-2.511617	-2.289517	1.745519
24	1	-3.276210	-1.783860	2.336904
25	1	-2.877089	-3.296020	1.507211
26	1	-1.612449	-2.391888	2.354698
27	8	-0.253514	0.052765	2.273954
28	6	-0.355257	1.005717	3.123456
29	8	-0.790777	2.147621	2.838946
30	6	0.074737	0.702178	4.540308
31	1	0.793327	1.456517	4.874819
32	1	-0.799251	0.761484	5.198274
33	1	0.516668	-0.291965	4.611807
34	6	0.992258	2.492743	-0.235188
35	7	0.930268	1.209442	-0.018025
36	6	-0.333750	3.106976	-0.359855
37	6	-0.495525	4.418618	-1.076278
38	1	-1.543713	4.725453	-1.080098
39	1	0.093178	5.209953	-0.595609
40	1	-0.149693	4.346243	-2.115575
41	6	2.254065	3.290446	-0.330171
42	1	2.188407	4.170181	0.318518
43	1	3.133232	2.713022	-0.052624
44	1	2.378247	3.652956	-1.358117
45	6	-1.344917	2.398157	0.229442
46	1	-2.357510	2.782006	0.148890
47	1	-1.091062	2.127302	1.438391
48	8	2.132911	0.584879	0.367543
49	6	2.830280	-0.049753	-0.653219
50	8	2.489133	0.030765	-1.799487
51	6	4.062353	-0.764411	-0.090170
52	6	3.675033	-1.656335	1.117674
53	1	2.934647	-2.410957	0.834470
54	1	4.571103	-2.174951	1.474144

55	1	3.270851	-1.063191	1.942431
56	6	4.680601	-1.624957	-1.213353
57	1	5.572215	-2.128829	-0.826969
58	1	3.978394	-2.389001	-1.562034
59	1	4.974481	-1.011836	-2.070492
60	6	5.080860	0.320935	0.363934
61	1	5.987903	-0.176161	0.723154
62	1	5.360870	0.977623	-0.467282
63	1	4.680755	0.930261	1.180066

3 (E = -1617.4746871 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.957597	0.102480	-0.120496
2	6	-0.514585	-2.161986	-0.123860
3	6	-0.756728	-1.608605	-1.463071
4	6	-2.131425	-1.161026	-1.480519
5	6	-2.674430	-1.306461	-0.155308
6	6	-1.679465	-1.982998	0.660163
7	6	0.690039	-2.933080	0.297668
8	9	1.802498	-2.658509	-0.454520
9	9	0.477746	-4.297055	0.178118
10	9	1.049268	-2.726306	1.609422
11	6	0.117930	-1.749412	-2.679064
12	1	-0.255681	-1.126288	-3.494134
13	1	1.150438	-1.465654	-2.477622
14	1	0.104892	-2.793361	-3.018495
15	6	-2.889611	-0.707961	-2.694507
16	1	-3.284738	-1.589095	-3.216120
17	1	-3.736733	-0.072322	-2.427425
18	1	-2.254993	-0.158455	-3.393318
19	6	-4.098512	-1.059012	0.264411
20	1	-4.161618	-0.783783	1.320319
21	1	-4.555475	-0.257646	-0.320756
22	1	-4.696685	-1.967775	0.117095
23	6	-1.925434	-2.382753	2.085303
24	1	-2.712300	-3.146933	2.107992
25	1	-1.036705	-2.783524	2.569422
26	1	-2.282100	-1.529376	2.670532
27	8	-0.979213	0.913920	1.935527
28	6	-1.384012	1.961879	2.451505
29	8	-1.849271	2.983930	1.766055
30	6	-1.383289	2.158532	3.936634
31	1	-0.963607	1.284661	4.432767
32	1	-0.800699	3.049690	4.191395
33	1	-2.408965	2.325553	4.282986
34	6	0.694856	2.473033	-0.802578
35	7	0.798004	1.261668	-0.324797
36	6	-0.647141	2.775287	-1.298824
37	6	-0.920175	4.053178	-2.062043
38	1	-1.969240	4.086278	-2.369597
39	1	-0.716373	4.945341	-1.457300
40	1	-0.299688	4.119934	-2.964358
41	6	1.807189	3.473029	-0.846873
42	1	1.465283	4.426744	-0.431461
43	1	2.688808	3.146905	-0.299559
44	1	2.087094	3.658879	-1.891332
45	6	-1.564863	1.808587	-1.027670
46	1	-2.590781	1.945978	-1.365358
47	1	-1.787312	2.805205	0.800415

48	8	2.004980	0.941647	0.338210
49	6	2.980143	0.362953	-0.457330
50	8	2.829338	0.198056	-1.636469
51	6	4.243987	0.066552	0.359560
52	6	3.908371	-0.479642	1.768565
53	1	3.333893	-1.408753	1.710169
54	1	4.844026	-0.690144	2.297178
55	1	3.339111	0.244643	2.357645
56	6	5.098733	-0.957459	-0.420545
57	1	6.019780	-1.152973	0.137943
58	1	4.566174	-1.905778	-0.546314
59	1	5.368130	-0.579837	-1.411020
60	6	5.026479	1.406857	0.491802
61	1	5.973133	1.212387	1.006740
62	1	5.254874	1.834990	-0.490430
63	1	4.466341	2.141336	1.079454

4 (E = -1388.306768 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	1.019165	0.455660	-0.230537
2	6	0.983981	-1.814055	0.160596
3	6	1.323338	-0.983450	1.319731
4	6	2.604916	-0.342623	1.013575
5	6	2.937083	-0.648431	-0.340181
6	6	1.948594	-1.599047	-0.846082
7	6	0.117639	-2.817584	0.075595
8	9	1.065740	-2.667769	1.050406
9	9	0.374135	-4.104490	0.210065
10	9	0.786542	-2.799060	-1.127291
11	6	0.673813	-0.993154	2.672373
12	1	1.050719	-0.172443	3.285454
13	1	0.410434	-0.903527	2.601484
14	1	0.909997	-1.936246	3.182930
15	6	3.438704	0.440425	1.983249
16	1	4.023802	-0.256542	2.596918
17	1	4.138492	1.101602	1.467602
18	1	2.824410	1.045708	2.654155
19	6	4.180340	-0.240746	-1.080761
20	1	3.984376	-0.108824	-2.148107
21	1	4.587287	0.696215	-0.693730
22	1	4.950283	-1.015764	-0.973100
23	6	2.017972	-2.199936	-2.216513
24	1	2.881724	-2.875992	-2.263786
25	1	1.122511	-2.762173	-2.476608
26	1	2.174845	-1.424019	-2.972770
27	6	0.924711	2.656036	-0.331799
28	7	0.895319	1.352556	-0.281143
29	6	0.372883	3.287381	-0.020633
30	6	0.463990	4.785994	0.157092
31	1	1.485628	5.064000	0.430611
32	1	0.203892	5.321873	-0.764351
33	1	0.209208	5.144447	0.945888
34	6	2.142808	3.463258	-0.639480
35	1	1.900377	4.224793	-1.387914
36	1	2.968588	2.854828	-1.001217
37	1	2.461668	3.996710	0.265377
38	6	1.398888	2.416200	0.110328
39	1	2.391485	2.785140	0.357435
40	8	2.081658	0.683866	-0.659488

41	6	2.825388	0.202942	0.407761
42	8	2.489951	0.373360	1.547330
43	6	4.118190	-0.468489	-0.070492
44	6	3.980984	-1.099086	-1.475570
45	1	3.199401	-1.864513	-1.495375
46	1	4.930495	-1.574959	-1.742129
47	1	3.751829	-0.348472	-2.237116
48	6	4.514371	-1.548666	0.963786
49	1	5.468480	-1.995277	0.665973
50	1	3.764143	-2.344251	1.013317
51	1	4.629807	-1.118836	1.962718
52	6	5.206124	0.646817	-0.097817
53	1	6.167003	0.195652	-0.366435
54	1	5.311886	1.121764	0.883266
55	1	4.974172	1.416753	-0.841074

5a (E = -1852.0597123 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.518781	-0.926970	0.036287
2	6	-2.660428	-0.742886	-0.899270
3	6	-2.741346	-0.868097	0.558930
4	6	-2.257452	-2.172012	0.894515
5	6	-1.779494	-2.797867	-0.303416
6	6	-2.113450	-1.935070	-1.428765
7	6	-3.299101	0.343310	-1.698875
8	9	-3.355089	1.543649	-1.035737
9	9	-4.609020	0.025818	-2.016112
10	9	-2.672844	0.592613	-2.895472
11	6	-3.455096	0.049566	1.513450
12	1	-3.205659	-0.198186	2.547042
13	1	-3.211297	1.097070	1.348058
14	1	-4.538543	-0.077961	1.389119
15	6	-2.307954	-2.811441	2.252500
16	1	-3.277273	-3.312130	2.374000
17	1	-1.528128	-3.566475	2.373989
18	1	-2.204628	-2.080203	3.056653
19	6	-1.321774	-4.226543	-0.420291
20	1	-0.702333	-4.388369	-1.305184
21	1	-0.748060	-4.540294	0.454956
22	1	-2.195744	-4.885473	-0.504378
23	6	-2.025206	-2.371293	-2.863086
24	1	-2.841902	-3.080665	-3.053142
25	1	-2.125540	-1.544415	-3.564077
26	1	-1.092684	-2.900704	-3.075265
27	6	0.721344	1.031711	1.870814
28	7	0.001943	0.961437	0.776697
29	6	0.987103	-0.270346	2.455462
30	6	1.709678	-0.408217	3.779232
31	1	1.769174	-1.463485	4.061305
32	1	2.733076	-0.015975	3.730275
33	1	1.187986	0.128375	4.580930
34	6	1.256690	2.304842	2.448759
35	1	2.227742	2.125321	2.915412
36	1	1.367097	3.086020	1.697095
37	1	0.576446	2.670492	3.228463
38	6	0.560828	-1.308683	1.694606
39	1	0.749291	-2.332459	2.009373
40	8	-0.129474	2.139285	0.004571
41	6	-1.069031	3.063014	0.433972

42	8	-1.718962	2.903102	1.429905
43	6	-1.077932	4.298019	-0.476032
44	6	-0.869484	3.931799	-1.964934
45	1	-1.641717	3.242525	-2.319553
46	1	-0.928115	4.846519	-2.563999
47	1	0.109953	3.476932	-2.135198
48	6	-2.428841	5.025743	-0.289479
49	1	-2.431558	5.935476	-0.898400
50	1	-3.266591	4.397301	-0.609497
51	1	-2.588911	5.307674	0.754928
52	6	0.082782	5.221187	0.001206
53	1	0.065072	6.142580	-0.590266
54	1	-0.030156	5.491169	1.056795
55	1	1.058285	4.745278	-0.142706
56	6	1.147938	-1.871365	-1.083422
57	1	1.843568	-2.328856	-0.389610
58	1	0.713923	-2.554301	-1.802523
59	6	1.298057	-0.518727	-1.425917
60	6	0.782022	0.029202	-2.743028
61	1	0.021580	-0.610409	-3.191417
62	1	0.369457	1.033514	-2.614811
63	1	1.614159	0.104218	-3.456531
64	6	2.443986	0.273311	-0.806060
65	1	2.217314	1.343663	-0.823405
66	1	2.592407	-0.019065	0.235645
67	6	3.760961	0.021673	-1.571601
68	1	3.692074	0.339553	-2.617914
69	1	3.997682	-1.050574	-1.591474
70	6	4.939661	0.742189	-0.946525
71	8	4.914344	1.374646	0.101673
72	8	6.054386	0.593147	-1.700206
73	6	7.294962	1.228519	-1.204620
74	1	7.520079	0.809507	-0.219965
75	1	7.106323	2.299962	-1.095293
76	6	8.383512	0.934086	-2.220427
77	1	9.323576	1.389074	-1.890974
78	1	8.543583	-0.143571	-2.325328
79	1	8.128803	1.347580	-3.201308

5b (E = -1852.0594236 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	1.304668	-1.093336	-0.640134
2	6	1.085212	-1.321589	1.682856
3	6	2.410680	-0.800548	1.334470
4	6	3.088853	-1.833168	0.612037
5	6	2.174799	-2.919593	0.411531
6	6	0.957165	-2.627821	1.155000
7	6	0.134194	-0.699058	2.650329
8	9	0.268420	0.662151	2.746673
9	9	0.332832	-1.190804	3.929560
10	9	-1.186438	-0.939635	2.356948
11	6	3.069862	0.442575	1.867044
12	1	3.988015	0.660029	1.317271
13	1	2.424433	1.316866	1.809520
14	1	3.338657	0.280914	2.919275
15	6	4.531261	-1.815875	0.193681
16	1	5.147148	-2.188068	1.022530
17	1	4.710005	-2.461885	-0.668571
18	1	4.875709	-0.810184	-0.055952

19	6	2.524020	-4.261330	-0.173870
20	1	1.643265	-4.787771	-0.548749
21	1	3.238013	-4.169577	-0.995828
22	1	2.980667	-4.891473	0.600331
23	6	-0.119429	-3.640306	1.420195
24	1	0.266381	-4.362370	2.152273
25	1	-1.025773	-3.195601	1.828104
26	1	-0.380794	-4.209768	0.524203
27	6	1.670049	1.464293	-2.079883
28	7	0.989142	0.926169	-1.096964
29	6	2.631503	0.549233	-2.666792
30	6	3.594809	0.998756	-3.745325
31	1	4.264267	0.175403	-4.011059
32	1	3.071623	1.312387	-4.657375
33	1	4.211319	1.842033	-3.411174
34	6	1.464203	2.860523	-2.580478
35	1	1.655002	2.907753	-3.654913
36	1	0.455185	3.223326	-2.385275
37	1	2.173946	3.536835	-2.087422
38	6	2.549184	-0.713998	-2.181353
39	1	3.189684	-1.495528	-2.583802
40	8	-0.121691	1.648760	-0.604241
41	6	0.144961	2.667374	0.296094
42	8	1.262273	2.966053	0.616224
43	6	-1.149814	3.368592	0.726473
44	6	-2.320505	2.373670	0.910678
45	1	-2.084335	1.610807	1.658360
46	1	-3.201650	2.925662	1.253890
47	1	-2.576933	1.874750	-0.027619
48	6	-0.875883	4.120078	2.049138
49	1	-1.781337	4.657798	2.348144
50	1	-0.609469	3.425267	2.852428
51	1	-0.064088	4.844130	1.936620
52	6	-1.507543	4.392207	-0.392058
53	1	-2.395041	4.954498	-0.083303
54	1	-0.693017	5.105785	-0.557804
55	1	-1.737705	3.888725	-1.336711
56	6	0.244544	-2.445278	-2.048091
57	1	0.043175	-3.367741	-1.517627
58	1	0.827263	-2.561061	-2.954301
59	6	-0.662387	-1.380333	-1.937651
60	6	-0.804133	-0.404101	-3.089736
61	1	0.136503	-0.254994	-3.622449
62	1	-1.521676	-0.822448	-3.808244
63	1	-1.194741	0.562657	-2.760800
64	6	-1.876043	-1.485745	-1.022533
65	1	-1.661610	-2.146624	-0.181774
66	1	-2.110004	-0.501969	-0.603918
67	6	-3.112361	-2.031396	-1.769952
68	1	-2.872360	-2.972225	-2.282820
69	1	-3.455835	-1.336932	-2.545550
70	6	-4.279000	-2.292051	-0.836422
71	8	-4.280529	-2.098649	0.372479
72	8	-5.346070	-2.777942	-1.514030
73	6	-6.561206	-3.082599	-0.726762
74	1	-6.884813	-2.161824	-0.233798
75	1	-6.293563	-3.815218	0.039524
76	6	-7.600688	-3.614846	-1.696036
77	1	-8.520128	-3.852707	-1.150678
78	1	-7.840636	-2.872271	-2.463406
79	1	-7.249528	-4.527136	-2.188330

5c (E = -1852.0610187 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	1.187152	-0.561754	-0.011759
2	6	2.778788	0.494902	1.236024
3	6	3.215911	0.453783	-0.152422
4	6	3.396872	-0.928412	-0.486258
5	6	3.040281	-1.736524	0.652077
6	6	2.712803	-0.845853	1.736547
7	6	2.680897	1.715527	2.087620
8	9	2.475900	2.864053	1.370111
9	9	3.846068	1.918813	2.808010
10	9	1.671762	1.653100	3.021095
11	6	3.615352	1.610618	-1.026397
12	1	3.757326	1.283069	-2.058024
13	1	2.876500	2.410560	-1.020048
14	1	4.569334	2.018895	-0.668759
15	6	3.974988	-1.453087	-1.769175
16	1	5.070410	-1.433669	-1.699618
17	1	3.673030	-2.486145	-1.954669
18	1	3.681232	-0.850217	-2.631089
19	6	3.282873	-3.217290	0.766569
20	1	2.769882	-3.652413	1.625563
21	1	2.959137	-3.755049	-0.128049
22	1	4.357695	-3.398886	0.895102
23	6	2.504863	-1.273763	3.161337
24	1	3.489563	-1.356465	3.640259
25	1	1.914534	-0.559845	3.735094
26	1	2.031353	-2.255427	3.227513
27	6	-0.440645	0.644891	-2.169475
28	7	-0.021848	0.864767	-0.946626
29	6	0.068211	-0.595328	-2.725785
30	6	-0.220874	-0.993437	-4.158036
31	1	0.277801	-1.939736	-4.387583
32	1	-1.294832	-1.128360	-4.337627
33	1	0.140994	-0.239427	-4.867703
34	6	-1.377671	1.547563	-2.910731
35	1	-2.040583	0.959628	-3.549795
36	1	-1.983156	2.155170	-2.238748
37	1	-0.802867	2.219528	-3.560884
38	6	0.754423	-1.350960	-1.834347
39	1	1.123952	-2.331186	-2.125959
40	8	-0.612775	1.933663	-0.238173
41	6	-0.103903	3.198944	-0.487256
42	8	0.756531	3.395720	-1.299614
43	6	-0.844761	4.251423	0.346222
44	6	-1.087706	3.767270	1.796999
45	1	-0.145815	3.537262	2.304123
46	1	-1.589841	4.564207	2.355391
47	1	-1.723814	2.878384	1.825470
48	6	-0.003124	5.546972	0.350020
49	1	-0.535876	6.317534	0.916275
50	1	0.971448	5.385971	0.822447
51	1	0.163764	5.917230	-0.665502
52	6	-2.211156	4.516596	-0.352405
53	1	-2.736961	5.307933	0.192053
54	1	-2.072999	4.850082	-1.386778
55	1	-2.843762	3.623268	-0.347839
56	6	-0.467575	-0.784183	1.440936
57	1	-1.113030	0.082568	1.361647
58	1	-0.016485	-0.928751	2.414512
59	6	-0.706911	-1.902122	0.625586

60	6	-0.244556	-3.286670	1.032780
61	1	0.501058	-3.256076	1.828325
62	1	-1.103589	-3.857505	1.410058
63	1	0.162950	-3.843209	0.183150
64	6	-1.882334	-1.881121	-0.343199
65	1	-1.999669	-0.892083	-0.787766
66	1	-1.715219	-2.588122	-1.161684
67	6	-3.198958	-2.238730	0.380911
68	1	-3.373525	-1.557680	1.224681
69	1	-3.174029	-3.249788	0.802238
70	6	-4.400268	-2.151027	-0.541077
71	8	-4.382594	-1.745234	-1.696228
72	8	-5.523757	-2.577384	0.081799
73	6	-6.782962	-2.532652	-0.693891
74	1	-6.657447	-3.163460	-1.578159
75	1	-6.944675	-1.501196	-1.018707
76	6	-7.888345	-3.030776	0.218871
77	1	-8.841602	-3.014834	-0.320033
78	1	-7.697202	-4.057895	0.545089
79	1	-7.985079	-2.394033	1.103801

5d (E = -1852.0610561 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.120721	0.267508	0.725311
2	6	1.047721	2.155427	-0.161838
3	6	1.490206	2.023888	1.217332
4	6	0.321976	2.133665	2.038856
5	6	-0.833723	2.296149	1.192034
6	6	-0.372510	2.362837	-0.170085
7	6	1.933332	2.319820	-1.350668
8	9	3.173463	1.758969	-1.187747
9	9	2.154221	3.657581	-1.632847
10	9	1.410703	1.777622	-2.502304
11	6	2.901410	1.993550	1.733957
12	1	2.921931	1.690955	2.782638
13	1	3.537277	1.314334	1.169482
14	1	3.327228	3.003305	1.666613
15	6	0.308296	2.201928	3.538886
16	1	0.476809	3.242047	3.847307
17	1	-0.653191	1.886720	3.949910
18	1	1.091502	1.587027	3.987113
19	6	-2.215133	2.639422	1.680417
20	1	-2.969734	2.523418	0.901157
21	1	-2.511942	2.019395	2.530187
22	1	-2.233741	3.686891	2.008181
23	6	-1.226004	2.753372	-1.342986
24	1	-1.250509	3.849946	-1.395937
25	1	-0.837674	2.383495	-2.291599
26	1	-2.257320	2.413838	-1.228468
27	6	1.537806	-2.140758	1.697046
28	7	1.503525	-1.298179	0.693583
29	6	0.587735	-1.810498	2.744726
30	6	0.529709	-2.604218	4.033328
31	1	-0.227625	-2.177558	4.697455
32	1	0.267562	-3.655157	3.857915
33	1	1.490890	-2.587641	4.561422
34	6	2.429018	-3.342813	1.753255
35	1	1.915698	-4.170282	2.249038
36	1	2.749867	-3.667527	0.763924

37	1	3.322281	-3.107151	2.346032
38	6	-0.243266	-0.789203	2.423650
39	1	-1.040979	-0.498781	3.103139
40	8	2.218298	-1.644252	-0.474648
41	6	3.568345	-1.333778	-0.493690
42	8	4.131765	-0.861120	0.454028
43	6	4.198202	-1.752029	-1.828008
44	6	3.268429	-1.442719	-3.027021
45	1	3.030415	-0.376143	-3.083300
46	1	3.780399	-1.726602	-3.952456
47	1	2.332755	-2.005696	-2.969278
48	6	5.540463	-1.002962	-1.987498
49	1	6.018220	-1.321854	-2.919391
50	1	5.387715	0.080303	-2.033849
51	1	6.219731	-1.219964	-1.158247
52	6	4.459944	-3.285454	-1.751071
53	1	4.963992	-3.603054	-2.669882
54	1	5.106391	-3.538100	-0.903499
55	1	3.524423	-3.847645	-1.666396
56	6	-0.761039	-0.659314	-1.080181
57	1	-1.098005	0.152222	-1.712556
58	1	-0.022713	-1.311612	-1.530244
59	6	-1.625177	-1.170689	-0.098572
60	6	-1.518192	-2.628931	0.298843
61	1	-0.497699	-3.005595	0.224999
62	1	-1.897232	-2.812445	1.307557
63	1	-2.128891	-3.215967	-0.400297
64	6	-2.974364	-0.520548	0.173537
65	1	-3.172803	-0.514256	1.251489
66	1	-2.964202	0.518135	-0.158940
67	6	-4.130022	-1.250220	-0.545062
68	1	-4.266445	-2.268635	-0.167842
69	1	-3.919443	-1.341408	-1.619928
70	6	-5.447936	-0.514208	-0.395852
71	8	-5.581629	0.622917	0.038695
72	8	-6.482348	-1.275499	-0.821915
73	6	-7.832359	-0.672256	-0.764521
74	1	-7.825573	0.231473	-1.380123
75	1	-8.032321	-0.389004	0.272430
76	6	-8.809560	-1.713921	-1.277400
77	1	-9.825264	-1.305302	-1.251500
78	1	-8.580325	-1.995074	-2.310018
79	1	-8.787487	-2.614434	-0.655665

TS5a-6a (E = -1852.0144399 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.517421	-0.906790	0.053775
2	6	-2.271275	-0.454542	-1.125078
3	6	-2.864539	-0.702941	0.205275
4	6	-2.576017	-2.035527	0.528927
5	6	-1.840566	-2.645743	-0.577638
6	6	-1.767482	-1.701683	-1.650752
7	6	-2.555525	0.745301	-1.966872
8	9	-2.707981	1.896706	-1.236999
9	9	-3.734628	0.586491	-2.676044
10	9	-1.583546	1.001883	-2.901200
11	6	-3.677663	0.262832	1.020305
12	1	-3.887286	-0.147257	2.010422
13	1	-3.175933	1.222864	1.146795

14	1	-4.638653	0.446552	0.522593
15	6	-2.973157	-2.769603	1.777313
16	1	-3.867427	-3.374577	1.577806
17	1	-2.187533	-3.452708	2.111245
18	1	-3.204462	-2.088380	2.598591
19	6	-1.524924	-4.114303	-0.656210
20	1	-0.850799	-4.348206	-1.482012
21	1	-1.070445	-4.479925	0.268727
22	1	-2.453268	-4.678727	-0.814189
23	6	-1.414662	-2.000159	-3.081094
24	1	-2.347299	-2.103358	-3.651262
25	1	-0.826487	-1.207129	-3.543678
26	1	-0.868909	-2.939525	-3.171850
27	6	0.492888	0.692034	2.363783
28	7	0.109185	0.803028	1.110839
29	6	0.419271	-0.668993	2.847205
30	6	0.313336	-0.969468	4.320452
31	1	0.095037	-2.029308	4.476674
32	1	1.254503	-0.742749	4.840469
33	1	-0.474441	-0.377640	4.800964
34	6	0.960090	1.837127	3.210721
35	1	1.646079	1.484192	3.983259
36	1	1.464832	2.596822	2.611220
37	1	0.104400	2.310329	3.708065
38	6	0.437379	-1.636235	1.865538
39	1	0.295943	-2.668007	2.162907
40	8	0.308011	2.063167	0.498568
41	6	-0.643030	3.036207	0.762575
42	8	-1.555595	2.852347	1.519681
43	6	-0.300834	4.336222	0.025145
44	6	0.143673	4.066441	-1.433768
45	1	-0.641828	3.558639	-2.001750
46	1	0.351282	5.024900	-1.920960
47	1	1.051749	3.459347	-1.474110
48	6	-1.548818	5.246487	0.042736
49	1	-1.307510	6.192812	-0.451761
50	1	-2.385686	4.784422	-0.491263
51	1	-1.870943	5.462697	1.065416
52	6	0.859120	5.019525	0.807758
53	1	1.087709	5.978610	0.331444
54	1	0.577971	5.214697	1.848544
55	1	1.766311	4.407557	0.792639
56	6	1.704048	-1.579036	0.671528
57	1	2.401805	-0.918955	1.175485
58	1	2.000635	-2.622314	0.743835
59	6	1.457250	-1.150470	-0.748044
60	6	1.607289	-2.285377	-1.761947
61	1	1.024339	-3.165460	-1.482456
62	1	1.313100	-1.964795	-2.764730
63	1	2.658871	-2.600203	-1.815506
64	6	2.185408	0.125578	-1.197208
65	1	1.679534	0.521146	-2.087290
66	1	2.121757	0.896516	-0.428845
67	6	3.682764	-0.097095	-1.530290
68	1	3.818205	-0.701860	-2.429174
69	1	4.175289	-0.632136	-0.704271
70	6	4.424197	1.212377	-1.711962
71	8	4.245380	2.222992	-1.041803
72	8	5.344210	1.134763	-2.702816
73	6	6.172078	2.335470	-2.949227
74	1	6.708989	2.572031	-2.026371
75	1	5.501587	3.165822	-3.186897
76	6	7.110459	2.004310	-4.095246

77	1	7.744376	2.870982	-4.310658
78	1	7.759749	1.160457	-3.841646
79	1	6.551332	1.755884	-5.002817

TS5b-6b (E = -1852.0140106 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.646079	-0.763827	-0.287839
2	6	0.910579	-0.806325	1.853790
3	6	2.311287	-0.747551	1.386542
4	6	2.532347	-1.910762	0.636620
5	6	1.314302	-2.720840	0.645574
6	6	0.360839	-2.098289	1.511628
7	6	0.309824	0.094164	2.882589
8	9	0.834700	1.360788	2.871063
9	9	0.523771	-0.395011	4.160735
10	9	-1.050927	0.235318	2.755579
11	6	3.324221	0.311639	1.717047
12	1	4.242888	0.161783	1.146217
13	1	2.955530	1.317422	1.514560
14	1	3.577877	0.253643	2.783632
15	6	3.808148	-2.315856	-0.044649
16	1	4.347922	-3.035348	0.584861
17	1	3.617910	-2.803391	-1.004546
18	1	4.466517	-1.463188	-0.221610
19	6	1.231385	-4.115329	0.088264
20	1	0.200682	-4.464832	0.003760
21	1	1.695656	-4.183386	-0.899468
22	1	1.766114	-4.806616	0.752998
23	6	-0.852217	-2.748753	2.114432
24	1	-0.567651	-3.146177	3.097902
25	1	-1.675491	-2.049443	2.263521
26	1	-1.205439	-3.586312	1.512474
27	6	1.448972	1.423753	-2.156964
28	7	0.797939	1.202612	-1.036698
29	6	2.001686	0.213885	-2.726507
30	6	3.179043	0.262083	-3.666862
31	1	3.554281	-0.747137	-3.856822
32	1	2.896358	0.700224	-4.634146
33	1	3.999143	0.867454	-3.263497
34	6	1.614678	2.772137	-2.789907
35	1	1.723018	2.673039	-3.871954
36	1	0.763392	3.420981	-2.578732
37	1	2.518450	3.259481	-2.403460
38	6	1.385918	-0.952224	-2.328420
39	1	1.817139	-1.891507	-2.651708
40	8	0.081147	2.297962	-0.499184
41	6	0.809097	3.199990	0.259954
42	8	1.997965	3.111245	0.396008
43	6	-0.102922	4.307858	0.800715
44	6	-1.439365	3.736310	1.335165
45	1	-1.269868	3.012183	2.137822
46	1	-2.037745	4.559607	1.739261
47	1	-2.015986	3.250264	0.543744
48	6	0.649257	5.048050	1.929031
49	1	0.020236	5.862837	2.301684
50	1	0.871997	4.377117	2.765137
51	1	1.590202	5.474287	1.569513
52	6	-0.385175	5.290819	-0.373481

53	1	-0.989097	6.123196	0.002483
54	1	0.544577	5.702241	-0.781792
55	1	-0.942894	4.803009	-1.179197
56	6	-0.341378	-1.079527	-2.457535
57	1	-0.373499	-2.068646	-2.906375
58	1	-0.528062	-0.296744	-3.185051
59	6	-1.254147	-0.959852	-1.266463
60	6	-2.191188	0.249029	-1.262683
61	1	-1.692771	1.174855	-1.546529
62	1	-3.019924	0.090744	-1.967090
63	1	-2.625345	0.388236	-0.266230
64	6	-1.997052	-2.258000	-0.921904
65	1	-1.291250	-3.091060	-0.880567
66	1	-2.449261	-2.159263	0.069616
67	6	-3.110447	-2.631542	-1.928015
68	1	-2.729532	-2.597132	-2.959733
69	1	-3.953516	-1.936784	-1.885775
70	6	-3.639567	-4.034384	-1.697205
71	8	-3.036794	-4.935803	-1.126660
72	8	-4.875875	-4.189642	-2.227231
73	6	-5.492026	-5.530126	-2.117074
74	1	-5.547096	-5.790973	-1.056709
75	1	-4.836844	-6.246473	-2.620504
76	6	-6.862948	-5.447750	-2.762930
77	1	-7.354539	-6.424462	-2.701453
78	1	-7.495152	-4.714344	-2.252615
79	1	-6.785747	-5.169753	-3.818730

TS5c-6c (E = -1852.0210572 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	1.292075	-0.436370	0.140376
2	6	2.740294	0.557119	1.419413
3	6	3.368841	0.612587	0.085873
4	6	3.587040	-0.715342	-0.325048
5	6	3.126880	-1.609544	0.730681
6	6	2.681336	-0.823864	1.842606
7	6	2.559954	1.733161	2.316085
8	9	2.241837	2.887180	1.640766
9	9	3.724016	2.016853	3.014711
10	9	1.585074	1.561052	3.267831
11	6	3.798217	1.849241	-0.651932
12	1	4.077021	1.610647	-1.680359
13	1	3.019794	2.611443	-0.677687
14	1	4.678208	2.280037	-0.155936
15	6	4.239875	-1.169811	-1.600555
16	1	5.303636	-1.374885	-1.421855
17	1	3.787148	-2.090341	-1.979259
18	1	4.171105	-0.412699	-2.384691
19	6	3.353868	-3.095385	0.732353
20	1	2.764828	-3.602107	1.499205
21	1	3.122453	-3.545820	-0.236750
22	1	4.413161	-3.295750	0.941300
23	6	2.322391	-1.355546	3.202949
24	1	3.211435	-1.326898	3.845918
25	1	1.540089	-0.767660	3.683346
26	1	1.987914	-2.393868	3.145968
27	6	-0.425473	0.484514	-2.105608
28	7	0.020876	0.832035	-0.924826
29	6	0.075504	-0.820736	-2.509654

30	6	0.160166	-1.191838	-3.964770
31	1	0.691083	-2.138716	-4.088186
32	1	-0.842625	-1.308144	-4.398933
33	1	0.675839	-0.419558	-4.547746
34	6	-1.351292	1.308652	-2.947265
35	1	-1.948204	0.670369	-3.601564
36	1	-2.022532	1.911067	-2.333941
37	1	-0.767026	1.987694	-3.581622
38	6	0.465201	-1.641111	-1.473013
39	1	0.918201	-2.587080	-1.744997
40	8	-0.608561	1.947676	-0.327673
41	6	-0.065285	3.187380	-0.627159
42	8	0.833935	3.315312	-1.410894
43	6	-0.820712	4.300257	0.107420
44	6	-1.161196	3.900549	1.564268
45	1	-0.256433	3.680458	2.138984
46	1	-1.677152	4.737098	2.046910
47	1	-1.818537	3.027591	1.601079
48	6	0.057293	5.571547	0.092974
49	1	-0.484578	6.385110	0.585594
50	1	0.997540	5.410766	0.630620
51	1	0.293234	5.881637	-0.928990
52	6	-2.136005	4.562336	-0.684815
53	1	-2.664867	5.400833	-0.219830
54	1	-1.928262	4.826379	-1.727532
55	1	-2.797632	3.690471	-0.663291
56	6	-0.455476	-1.147231	1.062828
57	1	-1.203083	-0.374329	1.228701
58	1	-0.211689	-1.671360	1.983475
59	6	-0.714498	-2.031105	-0.112179
60	6	-0.387057	-3.508856	0.128958
61	1	0.644074	-3.645949	0.458042
62	1	-1.040983	-3.887430	0.922584
63	1	-0.555497	-4.110377	-0.769822
64	6	-2.107597	-1.826915	-0.751766
65	1	-2.281239	-0.764812	-0.937017
66	1	-2.148222	-2.345674	-1.715707
67	6	-3.236882	-2.340511	0.162280
68	1	-3.118102	-1.955565	1.184511
69	1	-3.234366	-3.432021	0.239727
70	6	-4.606790	-1.906609	-0.326251
71	8	-4.821796	-1.040319	-1.164735
72	8	-5.587031	-2.594357	0.302955
73	6	-6.983600	-2.248167	-0.043294
74	1	-7.115534	-2.411011	-1.116373
75	1	-7.132305	-1.186496	0.171790
76	6	-7.884776	-3.139228	0.791523
77	1	-8.932173	-2.915373	0.563141
78	1	-7.705587	-4.196513	0.572515
79	1	-7.724425	-2.970641	1.860995

TS5d-6d (E = -1852.0202435 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.201235	0.408490	0.554309
2	6	1.094957	2.220368	-0.241417
3	6	1.572397	2.198100	1.155398
4	6	0.436711	2.276127	1.979925
5	6	-0.748960	2.366966	1.133592
6	6	-0.336254	2.421523	-0.237084

7	6	1.973778	2.393085	-1.433230
8	9	3.198193	1.785178	-1.298203
9	9	2.242634	3.732887	-1.669236
10	9	1.429487	1.910229	-2.598394
11	6	3.003815	2.196229	1.611671
12	1	3.066673	2.040700	2.690657
13	1	3.595000	1.424452	1.118777
14	1	3.459627	3.168873	1.384390
15	6	0.412915	2.321072	3.482380
16	1	0.356784	3.363359	3.822824
17	1	-0.457873	1.797617	3.886339
18	1	1.308724	1.872717	3.917618
19	6	-2.134033	2.638025	1.651343
20	1	-2.901634	2.447585	0.898690
21	1	-2.363711	2.038125	2.536264
22	1	-2.208630	3.694118	1.943192
23	6	-1.227196	2.725403	-1.409841
24	1	-1.216234	3.806508	-1.598783
25	1	-0.899449	2.220169	-2.318589
26	1	-2.260296	2.435140	-1.206427
27	6	1.347148	-2.156719	1.524826
28	7	1.452034	-1.268163	0.569743
29	6	0.298062	-1.809431	2.473461
30	6	0.341807	-2.331161	3.883260
31	1	-0.481617	-1.919434	4.471226
32	1	0.258168	-3.426509	3.900500
33	1	1.287637	-2.074525	4.376364
34	6	2.177764	-3.396976	1.646127
35	1	1.561908	-4.241488	1.967636
36	1	2.669678	-3.655403	0.709792
37	1	2.949518	-3.242795	2.411419
38	6	-0.684202	-0.978362	1.979174
39	1	-1.432421	-0.639250	2.686024
40	8	2.224628	-1.649325	-0.551071
41	6	3.566053	-1.300178	-0.518646
42	8	4.069939	-0.795931	0.445881
43	6	4.259279	-1.720256	-1.819532
44	6	3.404831	-1.355834	-3.059569
45	1	3.214425	-0.279446	-3.110219
46	1	3.951112	-1.648728	-3.962247
47	1	2.445179	-1.879877	-3.055927
48	6	5.631138	-1.013640	-1.889215
49	1	6.150106	-1.330765	-2.799424
50	1	5.516682	0.074791	-1.921050
51	1	6.255797	-1.268579	-1.028172
52	6	4.464847	-3.262655	-1.760614
53	1	5.009674	-3.579188	-2.656113
54	1	5.053674	-3.554444	-0.883948
55	1	3.508017	-3.794004	-1.740380
56	6	-1.014532	-0.720972	-0.729128
57	1	-1.703083	-0.067737	-1.259019
58	1	-0.462418	-1.355311	-1.419175
59	6	-1.598295	-1.439193	0.443865
60	6	-1.468321	-2.966124	0.354935
61	1	-0.450237	-3.281762	0.122020
62	1	-1.798446	-3.452839	1.277799
63	1	-2.100623	-3.308897	-0.473237
64	6	-3.021586	-0.984936	0.828297
65	1	-3.299284	-1.417506	1.795926
66	1	-3.038367	0.101588	0.941232
67	6	-4.074808	-1.395397	-0.218407
68	1	-4.234081	-2.478651	-0.230695
69	1	-3.754749	-1.119986	-1.232091

70	6	-5.416719	-0.731436	0.029404
71	8	-5.629782	0.166898	0.833747
72	8	-6.371218	-1.253565	-0.774837
73	6	-7.730516	-0.677753	-0.670746
74	1	-7.663022	0.390871	-0.892438
75	1	-8.072115	-0.801523	0.360451
76	6	-8.607359	-1.419241	-1.662884
77	1	-9.626268	-1.020302	-1.618286
78	1	-8.236587	-1.296351	-2.685312
79	1	-8.648316	-2.488039	-1.430750

6a (E = -1852.0406558 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.391203	-0.977699	0.212620
2	6	-1.770847	-0.733969	-1.453302
3	6	-2.648531	-0.437505	-0.310308
4	6	-2.724051	-1.597438	0.474595
5	6	-1.903599	-2.628075	-0.152072
6	6	-1.436251	-2.144211	-1.415074
7	6	-1.659465	0.163793	-2.639922
8	9	-1.386566	1.470388	-2.305081
9	9	-2.843633	0.199770	-3.358868
10	9	-0.687752	-0.212555	-3.531763
11	6	-3.413282	0.833509	-0.070834
12	1	-3.561885	1.016057	0.995346
13	1	-2.919468	1.704568	-0.499979
14	1	-4.402624	0.745673	-0.539911
15	6	-3.587123	-1.790877	1.688058
16	1	-4.570595	-2.168015	1.376749
17	1	-3.165167	-2.521841	2.381359
18	1	-3.749263	-0.855119	2.228996
19	6	-1.829079	-4.060705	0.300927
20	1	-0.916974	-4.548552	-0.050124
21	1	-1.860473	-4.142761	1.390018
22	1	-2.686569	-4.617936	-0.099048
23	6	-0.968657	-3.026670	-2.539078
24	1	-1.861262	-3.418370	-3.046169
25	1	-0.371839	-2.496865	-3.278466
26	1	-0.397785	-3.881126	-2.172397
27	6	0.480734	0.472047	2.395024
28	7	0.235406	0.815247	1.182570
29	6	0.273853	-1.012961	2.425458
30	6	-0.605239	-1.575625	3.517950
31	1	-0.801506	-2.637006	3.348868
32	1	-0.084718	-1.483253	4.480547
33	1	-1.555321	-1.041992	3.600036
34	6	0.894035	1.316402	3.548923
35	1	1.663081	0.797752	4.129744
36	1	1.279510	2.283434	3.222137
37	1	0.036337	1.488882	4.210928
38	6	1.142340	-1.802525	1.659517
39	1	1.056909	-2.875255	1.793682
40	8	0.418950	2.140741	0.769073
41	6	-0.557416	3.052559	1.181874
42	8	-1.460549	2.728984	1.897940
43	6	-0.251150	4.441694	0.617020
44	6	-0.141697	4.374310	-0.929339
45	1	-1.072868	4.013499	-1.378473
46	1	0.052518	5.381630	-1.312172

47	1	0.675914	3.722327	-1.247131
48	6	-1.393826	5.394855	1.028253
49	1	-1.179290	6.395899	0.640990
50	1	-2.354023	5.066145	0.617909
51	1	-1.489573	5.459150	2.116470
52	6	1.095194	4.934285	1.219397
53	1	1.297927	5.943372	0.846298
54	1	1.049976	4.980758	2.313399
55	1	1.926711	4.287279	0.926290
56	6	2.332722	-1.278044	0.880229
57	1	2.689943	-0.329996	1.287028
58	1	3.170792	-1.980431	0.909430
59	6	1.705893	-1.116851	-0.516408
60	6	1.965351	-2.383167	-1.338469
61	1	1.551611	-3.277433	-0.861727
62	1	1.559957	-2.304760	-2.349163
63	1	3.050331	-2.543557	-1.429533
64	6	2.136023	0.149151	-1.278484
65	1	1.543356	0.229668	-2.197575
66	1	1.928810	1.042668	-0.686641
67	6	3.640027	0.159461	-1.648638
68	1	3.886408	-0.611623	-2.382204
69	1	4.249791	-0.044172	-0.755326
70	6	4.091137	1.500821	-2.190543
71	8	3.664535	2.591471	-1.829735
72	8	5.063318	1.360598	-3.125049
73	6	5.631305	2.600593	-3.695977
74	1	6.051963	3.189947	-2.876318
75	1	4.815662	3.168407	-4.151997
76	6	6.683250	2.186572	-4.708776
77	1	7.131370	3.079896	-5.156638
78	1	7.480373	1.605603	-4.234260
79	1	6.242643	1.586459	-5.511150

6b (E = -1852.0398991 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.683984	-0.800043	-0.395495
2	6	0.505287	-1.207199	1.739592
3	6	1.835047	-0.591498	1.672225
4	6	2.647461	-1.414756	0.871995
5	6	1.849115	-2.550667	0.437411
6	6	0.568304	-2.497547	1.076132
7	6	-0.559816	-0.776004	2.690206
8	9	-0.731753	0.587917	2.736053
9	9	-0.270368	-1.162603	3.989024
10	9	-1.794286	-1.305613	2.405243
11	6	2.292986	0.645081	2.390289
12	1	3.100195	1.143520	1.850487
13	1	1.486893	1.361436	2.544123
14	1	2.674631	0.356626	3.379371
15	6	4.114493	-1.218189	0.611694
16	1	4.691829	-1.617425	1.456190
17	1	4.444402	-1.746167	-0.285363
18	1	4.375124	-0.161475	0.505602
19	6	2.370578	-3.737384	-0.324273
20	1	1.568123	-4.267336	-0.842371
21	1	3.121011	-3.448292	-1.063400
22	1	2.845018	-4.439890	0.373673
23	6	-0.321590	-3.697075	1.260568

24	1	0.127272	-4.326164	2.041492
25	1	-1.328573	-3.438304	1.580980
26	1	-0.388201	-4.298825	0.352458
27	6	1.355023	1.203547	-2.177370
28	7	0.698388	1.226257	-1.075347
29	6	1.678600	-0.242436	-2.402515
30	6	3.114093	-0.587292	-2.728921
31	1	3.262969	-1.669228	-2.757545
32	1	3.353442	-0.195403	-3.726542
33	1	3.818976	-0.143053	-2.022062
34	6	1.731350	2.329834	-3.074121
35	1	1.599155	2.030173	-4.118586
36	1	1.133321	3.220302	-2.874302
37	1	2.789728	2.581304	-2.931609
38	6	0.607227	-1.120484	-2.625585
39	1	0.871124	-2.131283	-2.917647
40	8	0.152595	2.428183	-0.603904
41	6	1.047696	3.308012	0.009966
42	8	2.223080	3.084717	0.055594
43	6	0.293743	4.525693	0.549378
44	6	-0.771344	4.061034	1.579708
45	1	-0.311271	3.523839	2.416367
46	1	-1.280173	4.942840	1.982401
47	1	-1.520943	3.412549	1.118099
48	6	1.311713	5.468536	1.226100
49	1	0.782336	6.344599	1.613979
50	1	1.819100	4.975351	2.061219
51	1	2.071937	5.811514	0.517317
52	6	-0.401030	5.254244	-0.634682
53	1	-0.912897	6.142142	-0.249791
54	1	0.328716	5.581589	-1.383626
55	1	-1.142745	4.614376	-1.120776
56	6	-0.843970	-0.700086	-2.759124
57	1	-1.364353	-1.310769	-3.501280
58	1	-0.932566	0.337937	-3.084713
59	6	-1.340424	-0.891544	-1.313921
60	6	-2.274781	0.216414	-0.815224
61	1	-1.829186	1.209912	-0.880797
62	1	-3.191975	0.232496	-1.424064
63	1	-2.567327	0.041096	0.225654
64	6	-1.982267	-2.278516	-1.133729
65	1	-1.289002	-3.060048	-1.461638
66	1	-2.184483	-2.444672	-0.073332
67	6	-3.316265	-2.463659	-1.897791
68	1	-3.225267	-2.121368	-2.938890
69	1	-4.123743	-1.879791	-1.448985
70	6	-3.749452	-3.915291	-1.955129
71	8	-2.996291	-4.882275	-1.962723
72	8	-5.097744	-4.029185	-2.029128
73	6	-5.652662	-5.394457	-2.151273
74	1	-5.330213	-5.970261	-1.279402
75	1	-5.230448	-5.853628	-3.049501
76	6	-7.162477	-5.258861	-2.227275
77	1	-7.614695	-6.252411	-2.315395
78	1	-7.560671	-4.780746	-1.326803
79	1	-7.461878	-4.668388	-3.098924

6c (E = -1852.0512633 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	77	1.384582	-0.512667	-0.068673
2	6	2.683252	0.276164	1.474839
3	6	3.370763	0.777280	0.274346
4	6	3.770510	-0.340055	-0.476255
5	6	3.366145	-1.543708	0.241665
6	6	2.802147	-1.170731	1.505080
7	6	2.311829	1.138589	2.633557
8	9	1.754704	2.338168	2.255875
9	9	3.419576	1.463642	3.400179
10	9	1.417065	0.551854	3.492255
11	6	3.670484	2.214934	-0.041057
12	1	4.034581	2.324582	-1.064108
13	1	2.798347	2.857143	0.079184
14	1	4.453486	2.578323	0.637477
15	6	4.556720	-0.330233	-1.757040
16	1	5.626804	-0.438528	-1.536206
17	1	4.274694	-1.158518	-2.411828
18	1	4.422051	0.600707	-2.312375
19	6	3.742914	-2.941445	-0.166155
20	1	3.101106	-3.691459	0.300254
21	1	3.692923	-3.076286	-1.249371
22	1	4.776547	-3.142445	0.144738
23	6	2.538342	-2.101182	2.656869
24	1	3.416999	-2.108924	3.315041
25	1	1.678591	-1.798099	3.254637
26	1	2.374378	-3.123267	2.309360
27	6	-0.375385	0.221705	-2.053203
28	7	-0.049086	0.782582	-0.947484
29	6	0.464255	-1.022175	-2.108177
30	6	1.324023	-1.196719	-3.343545
31	1	1.991235	-2.054973	-3.234460
32	1	0.679958	-1.383202	-4.213228
33	1	1.921993	-0.305273	-3.554431
34	6	-1.322006	0.697441	-3.100718
35	1	-1.871971	-0.145363	-3.528066
36	1	-2.026190	1.429220	-2.701864
37	1	-0.753807	1.167628	-3.914285
38	6	0.239737	-2.077565	-1.202920
39	1	0.830776	-2.964747	-1.413430
40	8	-0.781556	1.884954	-0.486168
41	6	-0.216034	3.129091	-0.754134
42	8	0.784613	3.239680	-1.403459
43	6	-1.077896	4.241968	-0.154207
44	6	-1.403225	3.938763	1.331442
45	1	-0.489775	3.827305	1.925051
46	1	-1.978305	4.774076	1.744091
47	1	-1.999144	3.027901	1.435469
48	6	-0.304380	5.573284	-0.269662
49	1	-0.920631	6.380512	0.138742
50	1	0.633447	5.539096	0.294440
51	1	-0.069975	5.811017	-1.311496
52	6	-2.395115	4.321205	-0.979249
53	1	-3.004590	5.144491	-0.592747
54	1	-2.189995	4.516788	-2.037701
55	1	-2.975640	3.397609	-0.895620
56	6	-0.365047	-1.239134	0.908513
57	1	-1.049638	-0.409945	1.089493
58	1	-0.097729	-1.699783	1.856837
59	6	-0.863213	-2.257604	-0.138236
60	6	-0.771092	-3.703034	0.396008
61	1	0.252349	-3.938371	0.707982
62	1	-1.421098	-3.834907	1.266496
63	1	-1.070342	-4.424761	-0.374483

64	6	-2.282126	-1.975249	-0.696301
65	1	-2.341485	-0.943413	-1.054584
66	1	-2.454079	-2.624363	-1.565944
67	6	-3.406057	-2.181917	0.331585
68	1	-3.157286	-1.681023	1.278982
69	1	-3.550447	-3.239338	0.571764
70	6	-4.735306	-1.619044	-0.132703
71	8	-4.887114	-0.789219	-1.021278
72	8	-5.763299	-2.136001	0.581642
73	6	-7.120245	-1.639149	0.267216
74	1	-7.319654	-1.843860	-0.788213
75	1	-7.129863	-0.556632	0.421943
76	6	-8.086126	-2.362403	1.187860
77	1	-9.107431	-2.022948	0.985184
78	1	-8.047522	-3.444450	1.027599
79	1	-7.859167	-2.155461	2.238403

6d (E = -1852.0512412 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.229343	0.443395	0.843353
2	6	0.730083	2.289935	-0.167705
3	6	1.716964	2.289525	0.923562
4	6	1.003770	2.332644	2.134808
5	6	-0.420889	2.368363	1.827335
6	6	-0.592604	2.457743	0.407828
7	6	1.066243	2.495554	-1.606536
8	9	2.238162	1.885478	-1.982443
9	9	1.227945	3.839733	-1.902038
10	9	0.100024	2.034876	-2.466811
11	6	3.211999	2.324189	0.777889
12	1	3.703318	2.095257	1.725123
13	1	3.572138	1.621224	0.027175
14	1	3.523195	3.331060	0.469559
15	6	1.584504	2.415147	3.518465
16	1	1.686161	3.467652	3.814438
17	1	0.939843	1.930963	4.255960
18	1	2.573650	1.955188	3.577191
19	6	-1.509877	2.552763	2.847938
20	1	-2.483913	2.239839	2.466704
21	1	-1.307015	1.994643	3.765257
22	1	-1.578714	3.615340	3.115584
23	6	-1.873404	2.804438	-0.299920
24	1	-1.932819	3.894979	-0.411651
25	1	-1.935351	2.363844	-1.295172
26	1	-2.743797	2.481893	0.275319
27	6	1.203465	-2.054118	1.466339
28	7	1.435692	-1.260646	0.486824
29	6	0.214205	-1.316549	2.320194
30	6	0.596949	-1.136395	3.775456
31	1	-0.107386	-0.476120	4.287026
32	1	0.567483	-2.110403	4.281988
33	1	1.608125	-0.733219	3.882743
34	6	1.806980	-3.384017	1.759517
35	1	1.056014	-4.056735	2.182804
36	1	2.238111	-3.834815	0.864006
37	1	2.603244	-3.264978	2.505899
38	6	-1.090111	-1.068773	1.854150
39	1	-1.741231	-0.624575	2.602055
40	8	2.216748	-1.683101	-0.596330

41	6	3.591363	-1.491816	-0.450690
42	8	4.062516	-1.057823	0.561201
43	6	4.324713	-1.946978	-1.713876
44	6	3.741778	-1.228205	-2.959177
45	1	3.826936	-0.140307	-2.868115
46	1	4.306997	-1.541423	-3.843053
47	1	2.690234	-1.483708	-3.116298
48	6	5.822452	-1.607133	-1.555460
49	1	6.359193	-1.938360	-2.450025
50	1	5.976980	-0.529411	-1.441258
51	1	6.256805	-2.110240	-0.686239
52	6	4.142862	-3.485033	-1.858081
53	1	4.703530	-3.824702	-2.735018
54	1	4.530472	-4.015890	-0.981237
55	1	3.091894	-3.753744	-1.998929
56	6	-1.103018	-0.610729	-0.448631
57	1	-1.788338	0.096393	-0.910753
58	1	-0.537033	-1.126757	-1.224391
59	6	-1.790526	-1.549051	0.564884
60	6	-1.592454	-3.050012	0.273978
61	1	-0.537089	-3.312927	0.165183
62	1	-2.021941	-3.663255	1.075694
63	1	-2.083000	-3.319170	-0.667553
64	6	-3.299892	-1.221839	0.728487
65	1	-3.684637	-1.771433	1.599113
66	1	-3.401011	-0.154310	0.959399
67	6	-4.158954	-1.546878	-0.500880
68	1	-4.256722	-2.626173	-0.656003
69	1	-3.698103	-1.147521	-1.416095
70	6	-5.556157	-0.964090	-0.413656
71	8	-5.928292	-0.115086	0.387223
72	8	-6.366661	-1.493852	-1.361508
73	6	-7.755679	-0.990579	-1.418978
74	1	-7.719001	0.089658	-1.584893
75	1	-8.225118	-1.180347	-0.449782
76	6	-8.451093	-1.725343	-2.550531
77	1	-9.488043	-1.381511	-2.626849
78	1	-7.956044	-1.533884	-3.507760
79	1	-8.461174	-2.805046	-2.371181

TS6c-7c (E = -1852.0356901 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.229343	0.443395	0.843353
2	6	0.730083	2.289935	-0.167705
3	6	1.716964	2.289525	0.923562
4	6	1.003770	2.332644	2.134808
5	6	-0.420889	2.368363	1.827335
6	6	-0.592604	2.457743	0.407828
7	6	1.066243	2.495554	-1.606536
8	9	2.238162	1.885478	-1.982443
9	9	1.227945	3.839733	-1.902038
10	9	0.100024	2.034876	-2.466811
11	6	3.211999	2.324189	0.777889
12	1	3.703318	2.095257	1.725123
13	1	3.572138	1.621224	0.027175
14	1	3.523195	3.331060	0.469559
15	6	1.584504	2.415147	3.518465
16	1	1.686161	3.467652	3.814438
17	1	0.939843	1.930963	4.255960

18	1	2.573650	1.955188	3.577191
19	6	-1.509877	2.552763	2.847938
20	1	-2.483913	2.239839	2.466704
21	1	-1.307015	1.994643	3.765257
22	1	-1.578714	3.615340	3.115584
23	6	-1.873404	2.804438	-0.299920
24	1	-1.932819	3.894979	-0.411651
25	1	-1.935351	2.363844	-1.295172
26	1	-2.743797	2.481893	0.275319
27	6	1.203465	-2.054118	1.466339
28	7	1.435692	-1.260646	0.486824
29	6	0.214205	-1.316549	2.320194
30	6	0.596949	-1.136395	3.775456
31	1	-0.107386	-0.476120	4.287026
32	1	0.567483	-2.110403	4.281988
33	1	1.608125	-0.733219	3.882743
34	6	1.806980	-3.384017	1.759517
35	1	1.056014	-4.056735	2.182804
36	1	2.238111	-3.834815	0.864006
37	1	2.603244	-3.264978	2.505899
38	6	-1.090111	-1.068773	1.854150
39	1	-1.741231	-0.624575	2.602055
40	8	2.216748	-1.683101	-0.596330
41	6	3.591363	-1.491816	-0.450690
42	8	4.062516	-1.057823	0.561201
43	6	4.324713	-1.946978	-1.713876
44	6	3.741778	-1.228205	-2.959177
45	1	3.826936	-0.140307	-2.868115
46	1	4.306997	-1.541423	-3.843053
47	1	2.690234	-1.483708	-3.116298
48	6	5.822452	-1.607133	-1.555460
49	1	6.359193	-1.938360	-2.450025
50	1	5.976980	-0.529411	-1.441258
51	1	6.256805	-2.110240	-0.686239
52	6	4.142862	-3.485033	-1.858081
53	1	4.703530	-3.824702	-2.735018
54	1	4.530472	-4.015890	-0.981237
55	1	3.091894	-3.753744	-1.998929
56	6	-1.103018	-0.610729	-0.448631
57	1	-1.788338	0.096393	-0.910753
58	1	-0.537033	-1.126757	-1.224391
59	6	-1.790526	-1.549051	0.564884
60	6	-1.592454	-3.050012	0.273978
61	1	-0.537089	-3.312927	0.165183
62	1	-2.021941	-3.663255	1.075694
63	1	-2.083000	-3.319170	-0.667553
64	6	-3.299892	-1.221839	0.728487
65	1	-3.684637	-1.771433	1.599113
66	1	-3.401011	-0.154310	0.959399
67	6	-4.158954	-1.546878	-0.500880
68	1	-4.256722	-2.626173	-0.656003
69	1	-3.698103	-1.147521	-1.416095
70	6	-5.556157	-0.964090	-0.413656
71	8	-5.928292	-0.115086	0.387223
72	8	-6.366661	-1.493852	-1.361508
73	6	-7.755679	-0.990579	-1.418978
74	1	-7.719001	0.089658	-1.584893
75	1	-8.225118	-1.180347	-0.449782
76	6	-8.451093	-1.725343	-2.550531
77	1	-9.488043	-1.381511	-2.626849
78	1	-7.956044	-1.533884	-3.507760
79	1	-8.461174	-2.805046	-2.371181

7c (E = -1852.0360042 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.426449	0.263439	0.028012
2	6	0.566854	-0.106436	1.886871
3	6	1.474076	0.643365	1.018199
4	6	1.006854	2.012929	0.910138
5	6	-0.246950	2.088653	1.534059
6	6	-0.558430	0.764819	2.106791
7	6	0.888392	-1.435214	2.507626
8	1	1.485170	-2.047955	1.828057
9	1	1.482731	-1.262598	3.414816
10	1	-0.002171	-1.995088	2.788535
11	6	2.820081	0.164020	0.563721
12	1	3.102823	0.620263	-0.387863
13	1	2.849864	-0.921185	0.452744
14	1	3.573918	0.448968	1.310524
15	6	1.777424	3.137850	0.278944
16	1	2.503188	3.532025	1.002635
17	1	1.126454	3.960847	-0.023952
18	1	2.327207	2.805977	-0.603398
19	6	-1.123816	3.300494	1.638438
20	1	-2.152244	3.084197	1.338421
21	1	-0.745047	4.117699	1.023007
22	1	-1.153579	3.645709	2.680195
23	6	-1.698056	0.528986	3.042203
24	9	-2.881857	1.071007	2.596026
25	9	-1.460341	1.107055	4.276983
26	9	-1.949556	-0.796701	3.282057
27	6	0.575176	-0.670480	-2.808709
28	7	-0.013283	0.189146	-2.043484
29	6	1.093947	-1.909393	-2.191657
30	6	0.311018	-2.738749	-1.483748
31	1	0.802402	-3.638990	-1.120592
32	6	-1.451323	-1.550245	-0.081653
33	1	-2.488153	-1.187506	-0.195539
34	1	-1.400508	-2.013018	0.903919
35	6	-1.175960	-2.648724	-1.156195
36	8	-0.653438	1.273920	-2.730976
37	6	0.148053	2.360841	-3.041430
38	8	1.331927	2.357592	-2.848612
39	6	-0.692832	3.478714	-3.669540
40	6	-1.859212	3.862058	-2.720297
41	1	-1.486779	4.197084	-1.745909
42	1	-2.543775	3.023394	-2.566111
43	1	-2.422441	4.687117	-3.168410
44	6	0.219851	4.700572	-3.908508
45	1	-0.369168	5.501993	-4.366019
46	1	1.048244	4.455256	-4.579991
47	1	0.639575	5.075513	-2.969558
48	6	-1.262967	2.971785	-5.024185
49	1	-0.459539	2.688961	-5.713573
50	1	-1.838140	3.779291	-5.488885
51	1	-1.927995	2.114508	-4.884895
52	6	0.762694	-0.468276	-4.288434
53	1	0.898736	-1.430885	-4.783492
54	1	1.654974	0.142293	-4.473360
55	1	-0.094933	0.041265	-4.730371
56	6	2.546743	-2.232855	-2.500651
57	1	2.706512	-2.403007	-3.572061

58	1	2.848317	-3.138612	-1.967295
59	1	3.213007	-1.416394	-2.198404
60	6	-1.578269	-4.019898	-0.543825
61	1	-2.608737	-4.003075	-0.175555
62	1	-0.925953	-4.263483	0.302776
63	1	-1.489755	-4.822198	-1.287761
64	6	-2.002211	-2.407161	-2.464538
65	1	-1.860406	-1.380935	-2.809938
66	1	-1.604001	-3.066164	-3.247149
67	6	-3.515687	-2.654896	-2.338456
68	1	-3.924021	-2.152697	-1.449099
69	1	-3.748373	-3.717017	-2.226128
70	6	-4.288100	-2.123807	-3.530890
71	8	-3.924120	-1.215285	-4.268518
72	8	-5.471928	-2.765919	-3.678618
73	6	-6.353637	-2.308256	-4.773917
74	1	-5.802611	-2.401434	-5.713660
75	1	-6.583328	-1.252259	-4.606077
76	6	-7.595137	-3.180993	-4.743868
77	1	-8.276872	-2.874259	-5.544195
78	1	-7.339636	-4.234147	-4.897436
79	1	-8.122373	-3.083903	-3.789629

TS6d-7d (E = -1852.0292493 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.068537	0.305481	0.118465
2	6	-0.160900	0.756998	2.229064
3	6	1.190413	0.389782	1.984321
4	6	1.785715	1.393013	1.087662
5	6	0.843629	2.425866	0.836488
6	6	-0.392920	1.958671	1.410449
7	6	-1.110805	0.121657	3.204993
8	1	-0.784757	-0.887210	3.465445
9	1	-1.138891	0.714480	4.127825
10	1	-2.125824	0.062056	2.809550
11	6	1.950370	-0.736035	2.622143
12	1	2.653911	-1.194028	1.922117
13	1	1.285916	-1.516424	2.997928
14	1	2.527643	-0.346086	3.470719
15	6	3.213741	1.373343	0.636361
16	1	3.847926	1.804931	1.423007
17	1	3.360250	1.957769	-0.274089
18	1	3.560893	0.353446	0.453971
19	6	1.140874	3.721496	0.134792
20	1	0.258677	4.164689	-0.322230
21	1	1.893553	3.584795	-0.644087
22	1	1.537626	4.438446	0.865795
23	6	-1.688284	2.719839	1.451222
24	9	-1.842093	3.608105	0.422729
25	9	-1.765041	3.450141	2.618404
26	9	-2.789820	1.904820	1.425576
27	6	0.406151	-0.327460	-2.916708
28	7	-0.114871	0.425796	-2.005997
29	6	1.261064	-1.452394	-2.467833
30	6	0.799281	-2.435719	-1.679782
31	1	1.519112	-3.219780	-1.452775
32	6	-0.712836	-1.656170	0.174263
33	1	-1.775951	-1.521638	0.413414
34	1	-0.253027	-2.123384	1.049859

35	6	-0.573882	-2.620673	-1.041153
36	8	-1.046332	1.397321	-2.486700
37	6	-0.507111	2.574257	-2.974262
38	8	0.676542	2.770684	-3.011312
39	6	-1.599649	3.513577	-3.505055
40	6	-3.005699	3.189591	-2.951840
41	1	-3.037177	3.264532	-1.860934
42	1	-3.334803	2.187125	-3.239824
43	1	-3.718809	3.911866	-3.362547
44	6	-1.203491	4.966241	-3.141775
45	1	-1.925592	5.654567	-3.592595
46	1	-0.207068	5.212151	-3.518966
47	1	-1.216731	5.125905	-2.058447
48	6	-1.595883	3.352711	-5.054874
49	1	-0.606690	3.565688	-5.472605
50	1	-2.311400	4.062204	-5.483123
51	1	-1.899125	2.344467	-5.355853
52	6	0.204453	-0.119551	-4.392074
53	1	0.415148	-1.044057	-4.931745
54	1	0.885482	0.656617	-4.761923
55	1	-0.818204	0.195345	-4.609186
56	6	2.677057	-1.439799	-3.017556
57	1	2.690803	-1.463188	-4.113661
58	1	3.228143	-2.310658	-2.652237
59	1	3.212758	-0.535371	-2.703154
60	6	-0.602214	-4.103253	-0.533113
61	1	0.265317	-4.256230	0.121602
62	1	-0.461039	-4.765716	-1.398798
63	6	-1.730986	-2.419010	-2.055157
64	1	-1.826370	-1.384400	-2.387379
65	1	-1.587134	-3.056062	-2.935588
66	1	-2.685968	-2.687220	-1.592504
67	6	-1.869500	-4.523527	0.222591
68	1	-2.758822	-4.485221	-0.415895
69	1	-2.069159	-3.845550	1.063350
70	6	-1.777944	-5.926146	0.790311
71	8	-0.773114	-6.626333	0.814714
72	8	-2.971595	-6.326456	1.294516
73	6	-3.029986	-7.670893	1.905677
74	1	-2.301037	-7.706565	2.720104
75	1	-2.741735	-8.402493	1.145732
76	6	-4.451879	-7.878286	2.395048
77	1	-4.538758	-8.867006	2.857921
78	1	-4.725136	-7.125953	3.141647
79	1	-5.165285	-7.824736	1.566647

7d (E = -1852.0356901 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.188654	0.423418	0.133937
2	6	-0.353321	1.597060	2.020424
3	6	0.402603	0.405326	2.254074
4	6	1.555940	0.452991	1.380243
5	6	1.556522	1.749514	0.685483
6	6	0.399594	2.449560	1.109149
7	6	-1.638541	1.960299	2.703189
8	1	-2.201599	1.067395	2.982615
9	1	-1.414147	2.517747	3.622196
10	1	-2.270696	2.589310	2.073303
11	6	0.109540	-0.639137	3.294261

12	1	0.554021	-1.603498	3.037336
13	1	-0.965172	-0.786067	3.429560
14	1	0.531136	-0.324590	4.257280
15	6	2.685322	-0.532584	1.366217
16	1	3.435789	-0.230670	2.109465
17	1	3.174871	-0.577546	0.391485
18	1	2.342618	-1.537681	1.621255
19	6	2.650729	2.224576	-0.226450
20	1	2.256000	2.749763	-1.096714
21	1	3.265342	1.389849	-0.567988
22	1	3.302303	2.915744	0.323372
23	6	0.027930	3.865108	0.831632
24	9	0.896243	4.512329	0.000997
25	9	-0.005704	4.601359	2.005911
26	9	-1.231364	4.008701	0.281360
27	6	0.370173	-0.093040	-2.904905
28	7	-0.268840	0.532303	-1.972401
29	6	1.327369	-1.140180	-2.494363
30	6	0.955931	-2.177232	-1.727390
31	1	1.741000	-2.902839	-1.523833
32	6	-0.769183	-1.582418	0.056944
33	1	-1.866941	-1.501369	0.130804
34	1	-0.426211	-2.042747	0.984482
35	6	-0.407606	-2.526602	-1.134830
36	8	-1.329304	1.377239	-2.433362
37	6	-0.979125	2.682261	-2.741678
38	8	0.154154	3.069343	-2.676979
39	6	-2.206867	3.471108	-3.214745
40	6	-3.438046	3.197569	-2.314732
41	1	-3.239748	3.470189	-1.273394
42	1	-3.738119	2.146652	-2.350734
43	1	-4.276647	3.804701	-2.671097
44	6	-1.854935	4.975158	-3.198253
45	1	-2.714531	5.545990	-3.563952
46	1	-0.997529	5.191171	-3.842253
47	1	-1.620166	5.317368	-2.185611
48	6	-2.516690	3.021687	-4.673025
49	1	-1.655451	3.179720	-5.331385
50	1	-3.350592	3.619781	-5.055034
51	1	-2.808152	1.967642	-4.714224
52	6	0.183216	0.196714	-4.369815
53	1	0.561107	-0.632133	-4.969427
54	1	0.734340	1.103348	-4.649039
55	1	-0.870350	0.356939	-4.606599
56	6	2.731198	-1.004613	-3.058835
57	1	2.736231	-1.033166	-4.154868
58	1	3.361096	-1.821694	-2.696566
59	1	3.189980	-0.055036	-2.756656
60	6	-0.252419	-3.988735	-0.594703
61	1	0.563816	-3.993630	0.138639
62	1	0.070686	-4.628620	-1.428049
63	6	-1.518348	-2.508757	-2.219840
64	1	-1.688833	-1.511863	-2.630694
65	1	-1.260747	-3.182657	-3.045292
66	1	-2.468920	-2.841249	-1.789984
67	6	-1.501251	-4.603140	0.051528
68	1	-2.300658	-4.769953	-0.677087
69	1	-1.917471	-3.932257	0.816471
70	6	-1.212301	-5.926337	0.734126
71	8	-0.103545	-6.340903	1.050409
72	8	-2.355619	-6.611333	0.982053
73	6	-2.226396	-7.904277	1.687230
74	1	-1.745741	-7.718484	2.651838

75	1	-1.577225	-8.552164	1.091847
76	6	-3.625282	-8.473199	1.839562
77	1	-3.573753	-9.435527	2.359831
78	1	-4.262399	-7.802133	2.424198
79	1	-4.092001	-8.637085	0.863168

8 (E = -1852.0507585 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.228168	0.607405	0.214202
2	6	-0.134407	1.885274	2.061977
3	6	0.350166	0.564658	2.347656
4	6	1.513235	0.330176	1.513894
5	6	1.748014	1.523595	0.729229
6	6	0.743194	2.492126	1.089683
7	6	-1.302415	2.539643	2.743785
8	1	-2.031450	1.798080	3.077106
9	1	-0.942124	3.077010	3.630748
10	1	-1.808662	3.256485	2.096402
11	6	-0.152684	-0.339944	3.438506
12	1	0.004722	-1.393559	3.195007
13	1	-1.219131	-0.193458	3.626741
14	1	0.387512	-0.129388	4.370565
15	6	2.436719	-0.850859	1.616310
16	1	3.184295	-0.665240	2.398613
17	1	2.966860	-1.035413	0.679943
18	1	1.894829	-1.761471	1.882681
19	6	2.929554	1.729157	-0.176861
20	1	2.657120	2.210534	-1.116724
21	1	3.421890	0.780856	-0.394992
22	1	3.657937	2.376074	0.328245
23	6	0.663225	3.913227	0.660601
24	9	1.478529	4.214427	-0.400049
25	9	1.031853	4.778730	1.681634
26	9	-0.607706	4.311870	0.293589
27	6	0.441746	0.139212	-2.834441
28	7	-0.247888	0.670533	-1.879183
29	6	1.376237	-0.934152	-2.449962
30	6	0.976142	-1.972452	-1.691648
31	1	1.746108	-2.720141	-1.510619
32	6	-0.792820	-1.428050	0.101301
33	1	-1.882471	-1.457428	0.209235
34	1	-0.373495	-1.880922	1.001333
35	6	-0.393294	-2.327959	-1.115218
36	8	-1.296189	1.544437	-2.383631
37	6	-2.325126	1.640657	-1.534968
38	8	-2.266541	1.161119	-0.404049
39	6	-3.533728	2.371337	-2.102542
40	6	-4.164435	1.465754	-3.200735
41	1	-4.470947	0.497317	-2.791282
42	1	-3.470873	1.296717	-4.029466
43	1	-5.054089	1.966858	-3.594717
44	6	-4.551861	2.617466	-0.968291
45	1	-5.420428	3.138494	-1.381665
46	1	-4.124381	3.239016	-0.175218
47	1	-4.892836	1.677530	-0.524588
48	6	-3.078575	3.720067	-2.723400
49	1	-2.608857	4.365026	-1.973393
50	1	-3.960014	4.237350	-3.114586
51	1	-2.376216	3.568834	-3.547695

52	6	0.336408	0.561591	-4.275363
53	1	1.047336	1.377686	-4.463224
54	1	-0.660002	0.923787	-4.525408
55	1	0.598159	-0.269937	-4.931977
56	6	2.769947	-0.864388	-3.051609
57	1	2.743947	-0.968114	-4.143134
58	1	3.389605	-1.672557	-2.653568
59	1	3.262317	0.088906	-2.827548
60	6	-0.246088	-3.809199	-0.617317
61	1	0.566404	-3.840713	0.119165
62	1	0.076148	-4.426327	-1.468139
63	6	-1.487582	-2.296432	-2.219715
64	1	-1.628343	-1.306605	-2.656496
65	1	-1.233151	-2.990637	-3.029361
66	1	-2.452244	-2.599473	-1.799622
67	6	-1.501283	-4.437080	0.004156
68	1	-2.312132	-4.538963	-0.723815
69	1	-1.893316	-3.807824	0.815260
70	6	-1.235217	-5.807491	0.595671
71	8	-0.133422	-6.264716	0.875556
72	8	-2.391237	-6.484337	0.805737
73	6	-2.285737	-7.824429	1.420438
74	1	-1.800169	-7.714771	2.394246
75	1	-1.650218	-8.442407	0.780235
76	6	-3.695229	-8.375608	1.537522
77	1	-3.661488	-9.372436	1.989822
78	1	-4.318143	-7.734446	2.169136
79	1	-4.166837	-8.462400	0.553604

TS8-9 (E = -1852.0411624 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.153615	0.636659	0.120424
2	6	-0.140273	1.869823	2.085363
3	6	0.346360	0.545169	2.314675
4	6	1.540755	0.359793	1.505825
5	6	1.782925	1.587244	0.782352
6	6	0.745386	2.517581	1.154162
7	6	-1.333409	2.485525	2.757965
8	1	-2.073561	1.727742	3.022975
9	1	-1.007354	2.973395	3.685675
10	1	-1.816322	3.237261	2.132417
11	6	-0.172278	-0.409716	3.353970
12	1	-0.001776	-1.451052	3.071334
13	1	-1.242958	-0.277691	3.527231
14	1	0.348405	-0.234796	4.304152
15	6	2.480133	-0.810798	1.590889
16	1	3.219828	-0.629667	2.381335
17	1	3.017832	-0.971572	0.653975
18	1	1.950402	-1.734148	1.837087
19	6	2.984649	1.853693	-0.081547
20	1	2.722852	2.349747	-1.017489
21	1	3.510727	0.925831	-0.310524
22	1	3.678861	2.508255	0.459258
23	6	0.632871	3.954036	0.770127
24	9	1.532315	4.337432	-0.187937
25	9	0.850911	4.783591	1.858296
26	9	-0.615238	4.298883	0.292440
27	6	0.711214	0.204922	-2.806557
28	7	0.069207	0.649951	-1.800987

29	6	1.571240	-0.970156	-2.494312
30	6	1.086825	-2.014006	-1.795525
31	1	1.794749	-2.829234	-1.660346
32	6	-0.659935	-1.419056	0.011506
33	1	-1.740322	-1.461350	0.172947
34	1	-0.181167	-1.867781	0.881742
35	6	-0.305949	-2.291239	-1.234758
36	8	-1.351368	1.610371	-2.468572
37	6	-2.294357	1.546577	-1.613048
38	8	-2.165425	1.053152	-0.459300
39	6	-3.661623	2.108680	-2.057771
40	6	-4.177288	1.226909	-3.227123
41	1	-4.302791	0.184172	-2.914978
42	1	-3.494238	1.258774	-4.080893
43	1	-5.153094	1.603799	-3.550681
44	6	-4.658428	2.069196	-0.881050
45	1	-5.620118	2.466893	-1.221359
46	1	-4.312610	2.680359	-0.041617
47	1	-4.816152	1.048213	-0.521552
48	6	-3.458058	3.568605	-2.540463
49	1	-3.059852	4.200540	-1.738958
50	1	-4.425600	3.978536	-2.847883
51	1	-2.775766	3.615058	-3.393984
52	6	0.660537	0.762658	-4.203127
53	1	1.681337	0.984832	-4.530454
54	1	0.057971	1.665411	-4.258797
55	1	0.254603	0.006914	-4.885300
56	6	2.976430	-0.956640	-3.068062
57	1	2.962191	-1.027905	-4.162195
58	1	3.542378	-1.809428	-2.683405
59	1	3.517107	-0.040237	-2.804939
60	6	-0.261443	-3.794255	-0.779431
61	1	0.556622	-3.903967	-0.055309
62	1	0.009067	-4.404260	-1.651649
63	6	-1.387324	-2.146492	-2.343515
64	1	-1.438042	-1.140520	-2.761272
65	1	-1.184690	-2.845207	-3.163289
66	1	-2.376933	-2.375386	-1.934780
67	6	-1.548614	-4.353970	-0.160564
68	1	-2.385662	-4.318414	-0.868859
69	1	-1.864271	-3.770379	0.712337
70	6	-1.399195	-5.796129	0.283797
71	8	-0.404968	-6.494333	0.127366
72	8	-2.527634	-6.240355	0.890080
73	6	-2.528828	-7.638818	1.369505
74	1	-1.695286	-7.759897	2.066779
75	1	-2.362892	-8.292991	0.509006
76	6	-3.873191	-7.884548	2.030007
77	1	-3.916085	-8.914705	2.399193
78	1	-4.023489	-7.210450	2.879146
79	1	-4.693407	-7.741438	1.319538

9 (E = -1852.0570464 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.276032	0.778626	-0.145370
2	6	-0.204031	1.767594	1.949277
3	6	0.618883	0.626803	2.159654
4	6	1.877657	0.813577	1.449687
5	6	1.837572	2.093467	0.801727

6	6	0.519605	2.652310	1.073436
7	6	-1.564905	1.985460	2.542936
8	1	-1.830677	1.164822	3.210703
9	1	-1.576385	2.916128	3.120375
10	1	-2.330199	2.064570	1.766659
11	6	0.304084	-0.505450	3.092453
12	1	0.978241	-1.351491	2.951204
13	1	-0.724074	-0.858856	2.983440
14	1	0.428962	-0.153837	4.124572
15	6	3.069678	-0.091632	1.556971
16	1	3.557467	0.068896	2.526944
17	1	3.802325	0.107638	0.773352
18	1	2.787685	-1.145634	1.497760
19	6	2.986536	2.764223	0.104681
20	1	2.660146	3.361899	-0.746284
21	1	3.716530	2.031440	-0.242987
22	1	3.491463	3.430728	0.815565
23	6	0.078973	4.035318	0.693736
24	9	0.530363	4.425473	-0.539552
25	9	0.562994	4.959543	1.597000
26	9	-1.281440	4.174663	0.681373
27	6	1.432215	-0.034865	-2.844149
28	7	0.938505	0.502343	-1.823982
29	6	1.969782	-1.413815	-2.643099
30	6	1.300718	-2.321637	-1.912925
31	1	1.798308	-3.283550	-1.811823
32	6	-0.135653	-1.351348	-0.016335
33	1	-1.135612	-1.346367	0.411855
34	1	0.582382	-1.730620	0.706701
35	6	-0.088119	-2.254086	-1.275063
36	8	-1.573366	1.783781	-2.619710
37	6	-2.244098	1.346721	-1.694495
38	8	-1.763018	0.780441	-0.611435
39	6	-3.795991	1.449596	-1.711264
40	6	-4.299508	0.963458	-3.092780
41	1	-4.075129	-0.098583	-3.246663
42	1	-3.838391	1.535497	-3.902651
43	1	-5.386531	1.091005	-3.150378
44	6	-4.467138	0.625200	-0.593340
45	1	-5.555649	0.729017	-0.670781
46	1	-4.162079	0.969551	0.399143
47	1	-4.219898	-0.438603	-0.675531
48	6	-4.141563	2.953062	-1.531379
49	1	-3.791588	3.328975	-0.563038
50	1	-5.228785	3.085413	-1.573952
51	1	-3.687543	3.556396	-2.323873
52	6	1.512528	0.695885	-4.165985
53	1	2.557614	0.930451	-4.396074
54	1	0.934938	1.619845	-4.124184
55	1	1.122573	0.053440	-4.962092
56	6	3.315339	-1.693114	-3.281178
57	1	3.262017	-1.607802	-4.373009
58	1	3.645560	-2.705847	-3.033552
59	1	4.079514	-0.987463	-2.932736
60	6	-0.363119	-3.719457	-0.759252
61	1	0.428018	-3.992285	-0.049415
62	1	-0.248872	-4.385849	-1.623959
63	6	-1.164310	-1.886640	-2.328038
64	1	-0.978937	-0.920491	-2.796420
65	1	-1.185674	-2.650880	-3.112743
66	1	-2.154085	-1.838216	-1.865633
67	6	-1.731365	-3.978566	-0.114606
68	1	-2.552645	-3.722876	-0.793683

69	1	-1.880010	-3.370463	0.786006
70	6	-1.915825	-5.428918	0.289737
71	8	-1.076716	-6.314332	0.182135
72	8	-3.153479	-5.636427	0.800583
73	6	-3.481720	-7.010209	1.238111
74	1	-2.763510	-7.301809	2.009396
75	1	-3.363440	-7.676774	0.379391
76	6	-4.907952	-6.985381	1.756835
77	1	-5.192490	-7.988538	2.091584
78	1	-5.007041	-6.300955	2.605245
79	1	-5.606534	-6.675495	0.973281

TS9-10 (E = -1852.0423927 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.306279	0.861738	-0.002915
2	6	1.126188	0.730873	2.068945
3	6	2.007958	1.545565	1.292393
4	6	1.267659	2.715527	0.850096
5	6	-0.080033	2.626125	1.340101
6	6	-0.183402	1.380900	2.057372
7	6	1.523902	-0.487930	2.848419
8	1	2.371587	-0.997227	2.385384
9	1	1.833928	-0.171199	3.852949
10	1	0.705082	-1.198404	2.964527
11	6	3.474784	1.309484	1.075786
12	1	3.800243	1.682961	0.102265
13	1	3.726622	0.248641	1.133494
14	1	4.047562	1.836571	1.849045
15	6	1.818760	3.854789	0.050460
16	1	2.010488	4.704986	0.718465
17	1	1.111248	4.174718	-0.717866
18	1	2.758477	3.586576	-0.435495
19	6	-1.134858	3.678663	1.155653
20	1	-2.111869	3.246807	0.939366
21	1	-0.866287	4.354001	0.343201
22	1	-1.221231	4.265441	2.078633
23	6	-1.344242	0.927237	2.887098
24	9	-2.527852	1.516192	2.544220
25	9	-1.132744	1.211744	4.220231
26	9	-1.548941	-0.432616	2.815108
27	6	1.704884	-0.723440	-2.296319
28	7	1.062932	-0.102762	-1.409414
29	6	1.816271	-2.205040	-2.344088
30	6	0.840445	-2.978333	-1.854959
31	1	0.956668	-4.051994	-1.972842
32	6	-0.259798	-1.544772	-0.087487
33	1	-1.186741	-1.179957	0.340774
34	1	0.486625	-1.852041	0.635114
35	6	-0.465545	-2.528936	-1.214264
36	8	-0.745133	2.836636	-2.222372
37	6	-1.623338	2.024099	-1.943758
38	8	-1.478574	1.036371	-1.098233
39	6	-3.018098	2.093411	-2.620182
40	6	-2.838576	1.584716	-4.076759
41	1	-2.516888	0.537160	-4.095294
42	1	-2.097374	2.186957	-4.612366
43	1	-3.793008	1.656227	-4.611195
44	6	-4.074379	1.234286	-1.893169
45	1	-5.041216	1.338735	-2.399447

46	1	-4.198981	1.553077	-0.852328
47	1	-3.800747	0.175725	-1.892798
48	6	-3.479835	3.571027	-2.644401
49	1	-3.618805	3.959851	-1.628496
50	1	-4.438862	3.647136	-3.169686
51	1	-2.749635	4.202353	-3.157913
52	6	2.371896	0.118548	-3.378454
53	1	3.457150	-0.018808	-3.331782
54	1	2.136979	1.174276	-3.241713
55	1	2.023844	-0.207967	-4.364239
56	6	3.042650	-2.780647	-3.023576
57	1	3.095201	-2.493868	-4.080074
58	1	3.017767	-3.872429	-2.970761
59	1	3.965597	-2.436698	-2.541375
60	6	-1.056347	-3.815393	-0.503893
61	1	-0.323676	-4.185900	0.223549
62	1	-1.125302	-4.577113	-1.290521
63	6	-1.445680	-2.036047	-2.307421
64	1	-1.011548	-1.216126	-2.882148
65	1	-1.674792	-2.859263	-2.992148
66	1	-2.378426	-1.673530	-1.868577
67	6	-2.427385	-3.670850	0.170012
68	1	-3.171524	-3.250579	-0.516976
69	1	-2.395496	-2.998814	1.035378
70	6	-2.965482	-5.005872	0.651728
71	8	-2.421752	-6.091247	0.491976
72	8	-4.149554	-4.851903	1.287784
73	6	-4.805121	-6.076602	1.797072
74	1	-4.120958	-6.559617	2.500056
75	1	-4.970205	-6.748573	0.950381
76	6	-6.103207	-5.647952	2.456020
77	1	-6.622956	-6.529566	2.845768
78	1	-5.914964	-4.965239	3.290575
79	1	-6.763847	-5.151029	1.738699

10 (E = -1852.1372748 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.090890	1.160497	0.129840
2	6	-0.117864	1.205385	2.313437
3	6	1.183055	0.743003	1.908307
4	6	1.776194	1.761955	1.096190
5	6	0.868743	2.911502	1.044507
6	6	-0.297896	2.553531	1.795269
7	6	-1.075838	0.456966	3.188537
8	1	-0.986614	-0.621413	3.040546
9	1	-0.840967	0.673212	4.239183
10	1	-2.110987	0.750250	3.005683
11	6	1.825802	-0.549809	2.321627
12	1	2.539318	-0.904010	1.574321
13	1	1.087138	-1.335579	2.493968
14	1	2.373303	-0.394535	3.260093
15	6	3.159892	1.725205	0.519554
16	1	3.865933	2.109433	1.267642
17	1	3.250443	2.345460	-0.373842
18	1	3.462032	0.706989	0.264943
19	6	1.172589	4.218220	0.381255
20	1	0.286519	4.625069	-0.105147
21	1	1.966429	4.107038	-0.359571
22	1	1.516785	4.931613	1.141642

23	6	-1.434123	3.436675	2.219113
24	9	-1.361540	4.706680	1.735261
25	9	-1.437925	3.550687	3.600365
26	9	-2.668448	2.936376	1.884721
27	6	1.045375	-0.525660	-2.192153
28	7	0.349814	-0.513463	-1.098877
29	6	1.280069	-1.782765	-2.939161
30	6	0.461585	-2.821651	-2.709533
31	1	0.553287	-3.721786	-3.311998
32	6	-0.178487	-1.803706	-0.583336
33	1	-1.000401	-1.581385	0.095339
34	1	0.623666	-2.265348	0.004459
35	6	-0.640292	-2.773286	-1.680817
36	8	-1.736756	3.703185	-1.047531
37	6	-2.049400	2.653633	-1.582588
38	8	-1.438461	1.497633	-1.347543
39	6	-3.181354	2.536474	-2.624994
40	6	-2.584018	2.015419	-3.958674
41	1	-2.136833	1.025769	-3.830257
42	1	-1.815833	2.698001	-4.341762
43	1	-3.377382	1.942520	-4.711365
44	6	-4.241688	1.532993	-2.099728
45	1	-5.059009	1.450750	-2.825364
46	1	-4.667963	1.870159	-1.147104
47	1	-3.806708	0.539947	-1.955136
48	6	-3.833076	3.916042	-2.849966
49	1	-4.260592	4.310305	-1.922315
50	1	-4.637568	3.825024	-3.588496
51	1	-3.104771	4.643623	-3.222719
52	6	1.627231	0.741115	-2.754047
53	1	2.722013	0.684308	-2.759594
54	1	1.322808	1.617125	-2.183126
55	1	1.306991	0.873209	-3.793436
56	6	2.370287	-1.827893	-3.989662
57	1	2.191070	-1.111435	-4.799600
58	1	2.419345	-2.827624	-4.430206
59	1	3.353057	-1.598922	-3.560376
60	6	-0.819705	-4.199718	-1.081618
61	1	0.153529	-4.555281	-0.719375
62	1	-1.109014	-4.868933	-1.901551
63	6	-1.943577	-2.289411	-2.369679
64	1	-1.807696	-1.297878	-2.811672
65	1	-2.230043	-2.985240	-3.166324
66	1	-2.769738	-2.228350	-1.652908
67	6	-1.852347	-4.313117	0.049355
68	1	-2.833242	-3.933542	-0.260897
69	1	-1.560148	-3.720876	0.925747
70	6	-2.051626	-5.741702	0.518874
71	8	-1.473373	-6.726348	0.077186
72	8	-2.972183	-5.801849	1.511136
73	6	-3.281380	-7.137139	2.066495
74	1	-2.356576	-7.559863	2.468691
75	1	-3.630239	-7.772336	1.247708
76	6	-4.340105	-6.941905	3.136420
77	1	-4.599542	-7.911318	3.574848
78	1	-3.975813	-6.291005	3.937479
79	1	-5.249810	-6.503053	2.714693

11 (E = -1852.1476112 au)

Center Number	Atomic Number	Coordinates (Angstroms)		

		X	Y	Z
1	77	1.258692	-0.062546	-0.367314
2	6	1.454778	-2.134659	-1.074774
3	6	0.959136	-1.325412	-2.153768
4	6	1.948706	-0.305939	-2.451950
5	6	3.059470	-0.476560	-1.557090
6	6	2.741014	-1.592933	-0.679242
7	6	0.762863	-3.336436	-0.503114
8	1	-0.297136	-3.339170	-0.762127
9	1	1.216235	-4.242523	-0.926060
10	1	0.858188	-3.387985	0.581844
11	6	-0.287331	-1.589465	-2.949110
12	1	-0.668566	-0.678426	-3.415364
13	1	-1.081716	-2.019560	-2.335450
14	1	-0.058010	-2.303023	-3.751236
15	6	1.868186	0.657833	-3.600957
16	1	2.194156	0.149983	-4.517824
17	1	2.509017	1.528609	-3.454339
18	1	0.845879	1.008564	-3.761070
19	6	4.330696	0.322293	-1.568449
20	1	4.606790	0.664227	-0.569614
21	1	4.246112	1.190153	-2.223849
22	1	5.147411	-0.306588	-1.944433
23	6	3.681796	-2.230652	0.292343
24	9	4.592929	-1.352948	0.818934
25	9	4.416838	-3.229770	-0.319102
26	9	3.046962	-2.819923	1.356049
27	6	-0.182084	2.613716	-0.923132
28	7	-0.302577	1.368050	-0.581552
29	6	-1.369389	3.463034	-1.178417
30	6	-2.563523	3.052846	-0.724443
31	1	-3.430551	3.699314	-0.834885
32	6	-1.662201	0.784210	-0.476166
33	1	-1.588218	-0.072201	0.190964
34	1	-1.923397	0.414835	-1.474468
35	6	-2.750778	1.752706	0.013088
36	8	1.971846	1.184942	1.290138
37	6	1.202630	0.614606	2.132353
38	8	0.435569	-0.287276	1.663781
39	6	1.252189	0.968014	3.612414
40	6	0.089513	0.297391	4.374326
41	1	0.126371	-0.792235	4.280435
42	1	-0.882591	0.640571	4.006328
43	1	0.161452	0.552904	5.436805
44	6	2.613162	0.442989	4.156517
45	1	2.687659	0.682692	5.222590
46	1	3.453397	0.912748	3.636153
47	1	2.693314	-0.643988	4.044217
48	6	1.190324	2.508540	3.772088
49	1	2.009259	2.994679	3.234060
50	1	1.272847	2.764163	4.833775
51	1	0.241456	2.910444	3.399614
52	6	1.171820	3.251755	-1.066142
53	1	1.325195	3.588378	-2.097741
54	1	1.973107	2.571542	-0.786486
55	1	1.232791	4.140737	-0.428110
56	6	-1.189886	4.794032	-1.880023
57	1	-0.542860	5.473728	-1.313604
58	1	-2.161388	5.280715	-2.003709
59	1	-0.744826	4.670662	-2.874484
60	6	-4.154787	1.180599	-0.343907
61	1	-4.235795	1.109058	-1.436377

62	1	-4.906341	1.913175	-0.023987
63	6	-2.636975	2.036557	1.534057
64	1	-1.670177	2.489055	1.775968
65	1	-3.424852	2.730231	1.849361
66	1	-2.735949	1.114137	2.115783
67	6	-4.485592	-0.184579	0.276634
68	1	-4.425118	-0.152099	1.371761
69	1	-3.778994	-0.959607	-0.043780
70	6	-5.879300	-0.664469	-0.080998
71	8	-6.714379	-0.027037	-0.710076
72	8	-6.101502	-1.913179	0.395572
73	6	-7.431566	-2.506639	0.139627
74	1	-7.586196	-2.539342	-0.942370
75	1	-8.186457	-1.850641	0.581876
76	6	-7.431765	-3.889922	0.764349
77	1	-8.403934	-4.365801	0.597755
78	1	-6.659711	-4.524242	0.317530
79	1	-7.258539	-3.834721	1.843652

12 (E = -1138.84453 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	1.604204	-0.381215	-0.261411
2	6	1.774440	-2.296700	-1.298273
3	6	1.080665	-1.390207	-2.153544
4	6	1.944425	-0.249110	-2.431619
5	6	3.190176	-0.431295	-1.757157
6	6	3.058536	-1.666910	-0.986951
7	6	1.279724	-3.631701	-0.829480
8	1	0.202827	-3.723035	-0.977891
9	1	1.771486	-4.419661	-1.414304
10	1	1.502636	-3.805872	0.223617
11	6	-0.291520	-1.583723	-2.724023
12	1	-0.813970	-0.631545	-2.841951
13	1	-0.904216	-2.236583	-2.099637
14	1	-0.205880	-2.044013	-3.717125
15	6	1.575838	0.901495	-3.316899
16	1	1.745905	0.617068	-4.363683
17	1	2.174831	1.788576	-3.104264
18	1	0.520544	1.164879	-3.210587
19	6	4.390646	0.462659	-1.843925
20	1	4.849870	0.629189	-0.868956
21	1	4.127520	1.429569	-2.274914
22	1	5.138974	-0.007432	-2.494619
23	6	4.167322	-2.317804	-0.203535
24	9	5.023068	-1.414982	0.362119
25	9	4.916071	-3.115030	-1.037992
26	9	3.709550	-3.115272	0.807841
27	8	2.147348	0.972652	1.333450
28	6	1.403070	0.375172	2.187797
29	8	0.771156	-0.645826	1.755258
30	6	1.338536	0.822653	3.634873
31	6	0.035712	0.321375	4.296125
32	1	-0.041791	-0.768653	4.251654
33	1	-0.847181	0.750667	3.810359
34	1	0.027730	0.625083	5.347912
35	6	2.573635	0.182593	4.341434
36	1	2.570769	0.482075	5.394607
37	1	3.509873	0.523912	3.888373
38	1	2.535591	-0.910932	4.295450

39	6	1.434234	2.365259	3.712343
40	1	2.354646	2.730487	3.248458
41	1	1.430690	2.672168	4.763250
42	1	0.581691	2.840992	3.215103

13 (E = -713.2563588 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.103534	2.637228	-0.812030
2	7	-0.208527	1.391560	-0.527005
3	6	-1.281561	3.525086	-1.030061
4	6	-2.474624	3.094625	-0.594059
5	1	-3.346503	3.741354	-0.672620
6	6	-1.556706	0.817253	-0.467795
7	1	-1.497305	-0.094086	0.132669
8	1	-1.821382	0.504705	-1.489411
9	6	-2.657429	1.749413	0.076119
10	6	1.282673	3.235000	-0.917911
11	1	1.462050	3.643166	-1.920367
12	1	2.030214	2.465937	-0.710194
13	1	1.412397	4.060468	-0.206336
14	6	-1.093067	4.880334	-1.678336
15	1	-0.411103	5.516450	-1.100765
16	1	-2.053160	5.399808	-1.760225
17	1	-0.670967	4.786714	-2.687055
18	6	-4.068410	1.209526	-0.295380
19	1	-4.160608	1.204522	-1.389588
20	1	-4.815195	1.924446	0.075717
21	6	-2.522233	1.940011	1.610317
22	1	-1.539606	2.352692	1.862880
23	1	-3.289521	2.630789	1.980676
24	1	-2.633296	0.986409	2.139769
25	6	-4.401694	-0.190219	0.240640
26	1	-4.327887	-0.230017	1.334527
27	1	-3.698971	-0.943231	-0.137504
28	6	-5.798067	-0.646342	-0.133861
29	8	-6.616777	0.002237	-0.773701
30	8	-6.047508	-1.894337	0.335874
31	6	-7.377362	-2.469770	0.045822
32	1	-7.504842	-2.501146	-1.039860
33	1	-8.135568	-1.804106	0.467649
34	6	-7.412833	-3.852821	0.670455
35	1	-8.386156	-4.316356	0.477568
36	1	-6.636891	-4.497036	0.245069
37	1	-7.268174	-3.799347	1.754102

1-CH_3 (E = -723.2269077 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.215495	-0.081518	0.629544
2	6	2.084743	-0.403990	-0.333950
3	6	1.269401	-1.594470	-0.536269
4	6	0.969755	-2.165136	0.743550
5	6	1.572480	-1.334374	1.754076
6	6	2.284035	-0.247955	1.095580
7	6	2.705533	0.438967	-1.402976
8	1	2.123341	0.411135	-2.326937

9	1	3.710805	0.054596	-1.623250
10	1	2.794129	1.477990	-1.079575
11	6	0.854234	-2.140261	-1.867486
12	1	-0.065667	-2.724651	-1.797498
13	1	0.705721	-1.344687	-2.601545
14	1	1.646191	-2.801283	-2.244881
15	6	0.165907	-3.407596	0.993318
16	1	0.836248	-4.276617	1.018928
17	1	-0.358858	-3.362727	1.950647
18	1	-0.571929	-3.576447	0.205510
19	6	1.520704	-1.567407	3.232253
20	1	1.599701	-0.631796	3.790644
21	1	0.598526	-2.071963	3.529640
22	1	2.364833	-2.206663	3.524411
23	6	3.151242	0.776621	1.756505
24	1	2.846618	0.955548	2.790100
25	1	4.188058	0.413909	1.765667
26	1	3.117488	1.724774	1.216942
27	8	-0.576894	1.761273	0.703644
28	6	-0.002015	2.949402	0.529697
29	8	1.178386	3.099989	0.272313
30	6	-0.982318	4.094415	0.676988
31	1	-1.446606	4.064846	1.668550
32	1	-0.475370	5.050169	0.536824
33	1	-1.784818	3.992905	-0.061882

14 (E = -1319.7612098 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.903234	0.045946	0.493128
2	6	-1.087884	-1.695530	-0.797907
3	6	-1.521505	-0.538378	-1.544648
4	6	-2.630197	0.057727	-0.852369
5	6	-2.921127	-0.767908	0.318911
6	6	-1.985931	-1.847441	0.340278
7	6	-0.049567	-2.689624	-1.229870
8	1	0.737030	-2.215504	-1.819685
9	1	-0.522800	-3.464413	-1.848272
10	1	0.414043	-3.184449	-0.372779
11	6	-0.940667	-0.095523	-2.855014
12	1	-1.209637	0.935833	-3.090059
13	1	0.148238	-0.182209	-2.859305
14	1	-1.337721	-0.735423	-3.653887
15	6	-3.468566	1.213358	-1.313521
16	1	-4.351931	0.830607	-1.842218
17	1	-3.818317	1.816086	-0.471471
18	1	-2.922461	1.866811	-1.995924
19	6	-4.059378	-0.542480	1.271172
20	1	-3.884777	-1.030749	2.232443
21	1	-4.223602	0.522657	1.453612
22	1	-4.981303	-0.956574	0.842420
23	6	-1.931958	-2.966948	1.336769
24	1	-2.406510	-2.692340	2.281190
25	1	-2.462267	-3.837897	0.929894
26	1	-0.902437	-3.268991	1.545123
27	8	0.114167	-0.317685	2.436481
28	6	-0.390934	0.714701	2.976541
29	8	-1.175699	1.414944	2.262584
30	6	-0.049403	1.107625	4.385522
31	1	0.811013	1.787625	4.367783

32	1	-0.887394	1.631450	4.850991
33	1	0.221052	0.228844	4.974920
34	6	0.997302	2.475358	-0.413646
35	7	0.813347	1.284867	0.055344
36	6	-0.155062	3.293820	-0.872627
37	6	-0.059932	3.821291	-2.292703
38	1	-0.961992	4.388382	-2.537671
39	1	0.803815	4.482920	-2.425470
40	1	0.044370	3.005133	-3.017040
41	6	2.369415	3.090092	-0.536831
42	1	2.289826	4.169290	-0.670259
43	1	2.967308	2.881627	0.352411
44	1	2.897070	2.673728	-1.403784
45	6	-1.137833	3.624956	-0.031639
46	1	-1.930385	4.290030	-0.356886
47	1	-1.171391	3.262126	0.986613
48	8	2.026237	0.685797	0.531743
49	6	2.695985	-0.103247	-0.377797
50	8	2.355085	-0.195990	-1.526900
51	6	3.876275	-0.811926	0.297746
52	6	3.301088	-1.914072	1.232151
53	1	2.735168	-2.659127	0.662133
54	1	4.132587	-2.426729	1.727466
55	1	2.647389	-1.486981	1.997815
56	6	4.755343	-1.453166	-0.797303
57	1	5.590050	-1.979807	-0.323470
58	1	4.187756	-2.172991	-1.394370
59	1	5.166760	-0.695872	-1.472997
60	6	4.714089	0.194544	1.129186
61	1	5.566080	-0.334408	1.568899
62	1	5.106098	1.002873	0.501699
63	1	4.128447	0.633612	1.941331

TS14-15 (E = -1319.7421682 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.969613	0.333763	0.198891
2	6	-1.044649	-1.671418	-0.795517
3	6	-1.479145	-0.622622	-1.716086
4	6	-2.671506	-0.035709	-1.173664
5	6	-2.934946	-0.640167	0.116681
6	6	-1.947275	-1.682803	0.311571
7	6	0.048774	-2.665862	-1.060287
8	1	0.839385	-2.240697	-1.680290
9	1	-0.373335	-3.528604	-1.593382
10	1	0.496888	-3.033478	-0.134051
11	6	-0.887402	-0.357475	-3.071207
12	1	-1.142995	0.641656	-3.432007
13	1	0.201309	-0.447057	-3.051971
14	1	-1.278338	-1.087320	-3.792500
15	6	-3.544348	0.976200	-1.853999
16	1	-4.292930	0.444499	-2.456192
17	1	-4.081929	1.601492	-1.137202
18	1	-2.975104	1.624466	-2.523954
19	6	-4.140865	-0.398398	0.981985
20	1	-3.924016	-0.602118	2.033667
21	1	-4.491601	0.633566	0.902804
22	1	-4.961791	-1.059037	0.673208
23	6	-1.899093	-2.611285	1.488033
24	1	-2.155892	-2.095076	2.416595

25	1	-2.627955	-3.419052	1.340042
26	1	-0.912448	-3.063359	1.607946
27	8	-0.405465	0.269871	2.270371
28	6	-0.525043	1.295466	3.019195
29	8	-0.897456	2.423150	2.600118
30	6	-0.204533	1.124531	4.486546
31	1	0.537811	1.869457	4.789552
32	1	-1.111322	1.302681	5.074915
33	1	0.170902	0.121317	4.690707
34	6	1.098730	2.450678	-0.364282
35	7	0.976723	1.186692	-0.065915
36	6	-0.189063	3.101383	-0.604369
37	6	-0.257607	4.375764	-1.403534
38	1	-1.292876	4.713783	-1.491614
39	1	0.324800	5.176200	-0.930074
40	1	0.148464	4.235322	-2.413686
41	6	2.393869	3.198085	-0.444086
42	1	2.362882	4.065718	0.224765
43	1	3.249909	2.581885	-0.178352
44	1	2.531687	3.580100	-1.462519
45	6	-1.262580	2.465618	-0.041415
46	1	-2.248661	2.888014	-0.211780
47	1	-1.100773	2.281184	1.224283
48	8	2.147622	0.567000	0.429954
49	6	2.805686	-0.245930	-0.474451
50	8	2.469660	-0.325566	-1.624409
51	6	3.991088	-0.944385	0.200282
52	6	3.510500	-1.715303	1.458060
53	1	2.766095	-2.476120	1.198969
54	1	4.368359	-2.222585	1.911835
55	1	3.076912	-1.040997	2.201558
56	6	4.624363	-1.921459	-0.813033
57	1	5.477720	-2.421082	-0.343490
58	1	3.908566	-2.687313	-1.128618
59	1	4.979815	-1.396766	-1.705074
60	6	5.030200	0.136769	0.612337
61	1	5.902721	-0.360049	1.049191
62	1	5.368948	0.714853	-0.254921
63	1	4.620134	0.824196	1.358169

15 (E = -1319.7671807 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.977402	0.421975	0.027286
2	6	-0.992367	-1.766334	-0.830667
3	6	-1.492445	-0.722664	-1.736214
4	6	-2.711500	-0.188912	-1.154762
5	6	-2.838947	-0.742373	0.159909
6	6	-1.792114	-1.762999	0.321638
7	6	0.134337	-2.705244	-1.153209
8	1	0.918363	-2.212123	-1.731416
9	1	-0.250288	-3.537303	-1.758573
10	1	0.582937	-3.129898	-0.252005
11	6	-1.021271	-0.515755	-3.149724
12	1	-1.327469	0.460561	-3.533495
13	1	0.067702	-0.580649	-3.217623
14	1	-1.450264	-1.287032	-3.803570
15	6	-3.682988	0.732060	-1.834247
16	1	-4.409395	0.134634	-2.400253
17	1	-4.238374	1.340331	-1.115666

18	1	-3.182092	1.402344	-2.537686
19	6	-3.979943	-0.530927	1.117658
20	1	-3.642100	-0.572489	2.156974
21	1	-4.465573	0.434730	0.956676
22	1	-4.734584	-1.316914	0.980163
23	6	-1.651290	-2.635547	1.535649
24	1	-1.721429	-2.049355	2.457590
25	1	-2.457714	-3.380267	1.556775
26	1	-0.698009	-3.168969	1.542966
27	8	-0.657842	0.680823	2.212955
28	6	-0.794360	1.643018	2.974487
29	8	-1.074051	2.863227	2.564848
30	6	-0.652889	1.504574	4.460218
31	1	0.145919	2.162474	4.818034
32	1	-1.581459	1.818700	4.948603
33	1	-0.427722	0.471750	4.722508
34	6	1.172180	2.458701	-0.292546
35	7	1.003736	1.174929	-0.108422
36	6	-0.074979	3.158003	-0.584299
37	6	-0.063885	4.605571	-1.027530
38	1	-1.087926	4.949322	-1.200589
39	1	0.390892	5.262773	-0.275832
40	1	0.499389	4.736826	-1.960309
41	6	2.488306	3.168920	-0.212151
42	1	2.420298	3.994644	0.505168
43	1	3.303635	2.512792	0.084789
44	1	2.723581	3.611432	-1.187608
45	6	-1.187339	2.383565	-0.437808
46	1	-2.159483	2.830456	-0.644481
47	1	-1.113500	2.886625	1.580949
48	8	2.131592	0.467593	0.378451
49	6	2.829719	-0.247418	-0.571921
50	8	2.554039	-0.207772	-1.740772
51	6	3.984446	-1.019390	0.079586
52	6	3.475524	-1.843168	1.290793
53	1	2.708931	-2.564932	0.988511
54	1	4.315050	-2.401428	1.718392
55	1	3.059490	-1.198496	2.069774
56	6	4.606349	-1.956730	-0.977650
57	1	5.441847	-2.501816	-0.526726
58	1	3.876370	-2.687182	-1.341524
59	1	4.984380	-1.393965	-1.836372
60	6	5.046330	0.012116	0.557215
61	1	5.900292	-0.528076	0.979333
62	1	5.410748	0.623582	-0.275979
63	1	4.644037	0.671959	1.331911

16 (E = -1090.600618 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.952582	0.179344	-0.222441
2	6	0.856368	-2.020538	0.571521
3	6	1.593434	-1.047323	1.391940
4	6	2.772012	-0.622879	0.637368
5	6	2.633335	-1.159468	-0.674723
6	6	1.468066	-2.066216	-0.686017
7	6	-0.303214	-2.839127	1.060639
8	1	-0.962729	-2.258252	1.709195
9	1	0.072844	-3.690448	1.643796
10	1	-0.896606	-3.238079	0.234756

11	6	1.346481	-0.795147	2.849187
12	1	1.778639	0.155458	3.170285
13	1	0.277065	-0.781167	3.074112
14	1	1.808171	-1.596754	3.442540
15	6	3.918553	0.182810	1.175581
16	1	4.643096	-0.488793	1.653989
17	1	4.437787	0.727468	0.383117
18	1	3.586638	0.905010	1.926212
19	6	3.598406	-1.005493	-1.815423
20	1	3.076926	-0.932953	-2.774295
21	1	4.220631	-0.115398	-1.697038
22	1	4.261648	-1.879795	-1.862023
23	6	1.057788	-2.886903	-1.873194
24	1	1.737767	-3.741878	-1.986879
25	1	0.042566	-3.275224	-1.767093
26	1	1.108113	-2.306088	-2.799526
27	6	-0.962650	2.423534	-0.237410
28	7	-0.954397	1.119693	-0.166040
29	6	0.362285	3.033968	-0.033288
30	6	0.488114	4.532186	0.135200
31	1	1.540831	4.803113	0.256336
32	1	0.095958	5.076829	-0.732751
33	1	-0.056736	4.889514	1.018660
34	6	-2.180928	3.249840	-0.495393
35	1	-2.044247	3.820514	-1.422340
36	1	-3.085962	2.652788	-0.579987
37	1	-2.302110	3.981332	0.311665
38	6	1.386406	2.146812	-0.002225
39	1	2.400370	2.517529	0.136675
40	8	-2.155420	0.480047	-0.561299
41	6	-2.830228	-0.161156	0.458383
42	8	-2.471368	-0.104795	1.603123
43	6	-4.069887	-0.879109	-0.089991
44	6	-3.689688	-1.780864	-1.293019
45	1	-2.952397	-2.538652	-1.006486
46	1	-4.587273	-2.299987	-1.645140
47	1	-3.284394	-1.195494	-2.122887
48	6	-4.683042	-1.732804	1.040620
49	1	-5.577362	-2.238775	0.662950
50	1	-3.979403	-2.495109	1.390658
51	1	-4.971394	-1.114475	1.895905
52	6	-5.091526	0.200722	-0.547942
53	1	-6.006657	-0.297455	-0.884835
54	1	-5.354800	0.874346	0.275267
55	1	-4.701227	0.794455	-1.380043

17 (E = -1554.3531079 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.264907	0.634099	0.151406
2	6	1.609580	2.138061	-1.064439
3	6	1.332019	2.572272	0.297381
4	6	-0.090798	2.831646	0.388270
5	6	-0.686700	2.442252	-0.852205
6	6	0.385075	2.042313	-1.759715
7	6	2.979134	1.960468	-1.653310
8	1	3.704566	1.628383	-0.909347
9	1	3.323387	2.925735	-2.049315
10	1	2.978631	1.247564	-2.481437
11	6	2.375635	2.961065	1.309880

12	1	1.973819	2.947031	2.325764
13	1	3.233428	2.284309	1.277039
14	1	2.737476	3.976845	1.102421
15	6	-0.795843	3.506107	1.530226
16	1	-0.805147	4.590264	1.357500
17	1	-1.832989	3.173487	1.622414
18	1	-0.291351	3.326980	2.482856
19	6	-2.100813	2.730666	-1.274521
20	1	-2.470179	2.010965	-2.009779
21	1	-2.788259	2.741337	-0.425985
22	1	-2.136064	3.722994	-1.744523
23	6	0.216433	1.738082	-3.221802
24	1	0.271281	2.671785	-3.797804
25	1	0.999148	1.071049	-3.591913
26	1	-0.752901	1.281623	-3.439425
27	6	1.738071	-1.174840	1.981630
28	7	1.663492	-0.815540	0.722896
29	6	0.814105	-0.446593	2.830993
30	6	0.787195	-0.661330	4.330845
31	1	0.049768	0.006338	4.786664
32	1	0.514579	-1.691064	4.595726
33	1	1.761781	-0.450782	4.788521
34	6	2.646776	-2.249409	2.496660
35	1	2.168001	-2.784355	3.320137
36	1	2.920370	-2.965798	1.721610
37	1	3.567133	-1.797304	2.887769
38	6	-0.020562	0.376613	2.148088
39	1	-0.795063	0.921939	2.683303
40	8	2.394547	-1.582560	-0.213598
41	6	3.737425	-1.279488	-0.342361
42	8	4.281785	-0.458848	0.344545
43	6	4.382329	-2.161978	-1.418859
44	6	3.560481	-2.111577	-2.732952
45	1	3.492708	-1.090233	-3.123446
46	1	4.060545	-2.727975	-3.487351
47	1	2.548016	-2.498724	-2.590144
48	6	5.818650	-1.654867	-1.670679
49	1	6.295709	-2.289252	-2.424654
50	1	5.818212	-0.623978	-2.039573
51	1	6.420347	-1.691364	-0.757690
52	6	4.424890	-3.622957	-0.885655
53	1	4.922024	-4.255934	-1.628193
54	1	4.991491	-3.690081	0.049840
55	1	3.418140	-4.018103	-0.719494
56	6	-0.692241	-0.900330	-1.131694
57	1	-1.139138	-0.374046	-1.966390
58	1	0.046647	-1.646454	-1.401401
59	6	-1.436573	-1.064573	0.047248
60	6	-1.193522	-2.286342	0.913034
61	1	-0.169551	-2.653173	0.837910
62	1	-1.432573	-2.102949	1.964093
63	1	-1.849330	-3.092749	0.558488
64	6	-2.816529	-0.437843	0.204138
65	1	-2.964551	-0.124408	1.243996
66	1	-2.896798	0.454382	-0.415774
67	6	-3.944213	-1.414828	-0.194093
68	1	-3.983879	-2.281975	0.475096
69	1	-3.774647	-1.812559	-1.203698
70	6	-5.311904	-0.760893	-0.174548
71	8	-5.540317	0.408142	0.109819
72	8	-6.278538	-1.645442	-0.518182
73	6	-7.670931	-1.147246	-0.544799
74	1	-7.720426	-0.316743	-1.254365

75	1	-7.915526	-0.771481	0.452522
76	6	-8.554424	-2.310903	-0.955712
77	1	-9.598792	-1.982872	-0.987953
78	1	-8.281521	-2.681222	-1.948872
79	1	-8.477106	-3.135915	-0.240633

TS17-18 (E = -1554.3101312 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.204551	0.408929	0.539627
2	6	1.317603	2.213608	-0.085813
3	6	1.465876	2.162497	1.375013
4	6	0.179726	2.265959	1.940889
5	6	-0.796293	2.368770	0.857923
6	6	-0.071224	2.412993	-0.386445
7	6	2.454142	2.328994	-1.062888
8	1	3.330141	1.768672	-0.730549
9	1	2.746886	3.384300	-1.156399
10	1	2.171562	1.972438	-2.056765
11	6	2.779812	2.103190	2.102709
12	1	2.654965	1.757199	3.132159
13	1	3.483790	1.434217	1.601831
14	1	3.231461	3.104133	2.137647
15	6	-0.162168	2.306912	3.403616
16	1	-0.301091	3.348758	3.721581
17	1	-1.092661	1.773618	3.618672
18	1	0.630009	1.871712	4.017600
19	6	-2.251583	2.702578	1.041573
20	1	-2.850157	2.408247	0.175622
21	1	-2.671085	2.220516	1.928812
22	1	-2.366866	3.787461	1.170995
23	6	-0.653845	2.702996	-1.741693
24	1	-0.669396	3.788250	-1.909268
25	1	-0.063085	2.248008	-2.540798
26	1	-1.681502	2.340625	-1.829058
27	6	1.408229	-2.135700	1.531782
28	7	1.488076	-1.264036	0.555216
29	6	0.383664	-1.783747	2.495389
30	6	0.456611	-2.290004	3.912961
31	1	-0.362407	-1.879224	4.508672
32	1	0.383491	-3.385641	3.946246
33	1	1.405689	-2.016321	4.390751
34	6	2.253961	-3.366678	1.663387
35	1	1.631425	-4.234067	1.904686
36	1	2.820699	-3.580576	0.759081
37	1	2.958280	-3.231727	2.494200
38	6	-0.612766	-0.962017	2.012526
39	1	-1.348672	-0.615316	2.728948
40	8	2.221871	-1.702370	-0.580434
41	6	3.509930	-1.220496	-0.683548
42	8	4.024688	-0.568723	0.184443
43	6	4.146121	-1.677124	-2.002394
44	6	3.246846	-1.271014	-3.199672
45	1	3.105262	-0.185529	-3.241893
46	1	3.731765	-1.584945	-4.130000
47	1	2.265194	-1.749712	-3.145319
48	6	5.534778	-1.015672	-2.131993
49	1	6.002677	-1.344703	-3.065416
50	1	5.456180	0.076071	-2.153348
51	1	6.189121	-1.295344	-1.300779

52	6	4.300383	-3.224080	-1.963427
53	1	4.794913	-3.553866	-2.883058
54	1	4.917171	-3.541780	-1.115080
55	1	3.328583	-3.722723	-1.900973
56	6	-1.033305	-0.729350	-0.716821
57	1	-1.747576	-0.087156	-1.226102
58	1	-0.510314	-1.376419	-1.418123
59	6	-1.560707	-1.432472	0.493679
60	6	-1.408244	-2.958759	0.414158
61	1	-0.393077	-3.258514	0.149816
62	1	-1.696346	-3.443120	1.352237
63	1	-2.062322	-3.320160	-0.388962
64	6	-2.979490	-1.003072	0.925448
65	1	-3.218497	-1.451546	1.896193
66	1	-3.005365	0.081248	1.055861
67	6	-4.065159	-1.411940	-0.086992
68	1	-4.162629	-2.501446	-0.157141
69	1	-3.822784	-1.060302	-1.097577
70	6	-5.427619	-0.855860	0.281404
71	8	-5.669538	-0.142603	1.246941
72	8	-6.369940	-1.249525	-0.607439
73	6	-7.752547	-0.776029	-0.377431
74	1	-7.739081	0.317323	-0.367445
75	1	-8.072904	-1.131718	0.605695
76	6	-8.608536	-1.332678	-1.500245
77	1	-9.644612	-1.004030	-1.366616
78	1	-8.259989	-0.976786	-2.474840
79	1	-8.594470	-2.427079	-1.501158

18 (E = -1554.3393378 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.213802	0.440480	0.875441
2	6	0.715087	2.299551	-0.201178
3	6	1.684681	2.254119	0.893646
4	6	0.986999	2.300935	2.121053
5	6	-0.436696	2.357165	1.816406
6	6	-0.593417	2.448614	0.390066
7	6	1.051788	2.469281	-1.659106
8	1	1.946847	1.904224	-1.932825
9	1	1.240638	3.527500	-1.885184
10	1	0.232865	2.130786	-2.299587
11	6	3.176596	2.256138	0.718613
12	1	3.688614	1.794340	1.565738
13	1	3.479944	1.730700	-0.189390
14	1	3.529528	3.293070	0.633988
15	6	1.589024	2.381323	3.496143
16	1	1.690120	3.432712	3.797930
17	1	0.964249	1.886735	4.244646
18	1	2.583827	1.929089	3.530517
19	6	-1.527617	2.555404	2.833877
20	1	-2.500476	2.234219	2.454112
21	1	-1.325717	2.009243	3.759211
22	1	-1.601518	3.621144	3.088475
23	6	-1.866702	2.761642	-0.344283
24	1	-1.978496	3.850842	-0.428179
25	1	-1.863789	2.350741	-1.357167
26	1	-2.745630	2.375652	0.178209
27	6	1.199316	-2.054117	1.514319
28	7	1.431656	-1.267864	0.529016

29	6	0.209408	-1.311860	2.362885
30	6	0.585114	-1.126841	3.819882
31	1	-0.107868	-0.441858	4.314593
32	1	0.528396	-2.092532	4.340242
33	1	1.603571	-0.743797	3.933941
34	6	1.801677	-3.383797	1.816258
35	1	1.048663	-4.052870	2.241929
36	1	2.234441	-3.840962	0.924575
37	1	2.596292	-3.261401	2.563670
38	6	-1.098287	-1.072629	1.896345
39	1	-1.751125	-0.630046	2.643790
40	8	2.214756	-1.702547	-0.554119
41	6	3.587346	-1.524921	-0.409236
42	8	4.071309	-1.130957	0.613918
43	6	4.308321	-1.914972	-1.702395
44	6	3.815040	-1.002755	-2.858808
45	1	4.010648	0.053828	-2.644222
46	1	4.356111	-1.267660	-3.773153
47	1	2.744866	-1.131893	-3.043191
48	6	5.825876	-1.728962	-1.490580
49	1	6.352060	-2.010013	-2.408426
50	1	6.071749	-0.688167	-1.257799
51	1	6.195188	-2.358978	-0.675275
52	6	3.996454	-3.400532	-2.033904
53	1	4.541563	-3.681321	-2.940989
54	1	4.320194	-4.065130	-1.225035
55	1	2.929109	-3.557594	-2.213032
56	6	-1.104678	-0.640736	-0.414532
57	1	-1.792450	0.048128	-0.901977
58	1	-0.535632	-1.176895	-1.175422
59	6	-1.797526	-1.564567	0.611303
60	6	-1.609293	-3.071022	0.340448
61	1	-0.555176	-3.342865	0.239821
62	1	-2.045921	-3.671410	1.148509
63	1	-2.097753	-3.349990	-0.599578
64	6	-3.306524	-1.229806	0.767507
65	1	-3.695578	-1.765039	1.645425
66	1	-3.403963	-0.158574	0.982709
67	6	-4.163824	-1.570519	-0.458779
68	1	-4.263519	-2.651890	-0.598492
69	1	-3.697881	-1.186179	-1.377789
70	6	-5.559616	-0.983084	-0.387358
71	8	-5.935116	-0.122148	0.399176
72	8	-6.366272	-1.523122	-1.333523
73	6	-7.752690	-1.015435	-1.407497
74	1	-7.710907	0.062834	-1.584900
75	1	-8.230902	-1.192700	-0.440219
76	6	-8.441941	-1.759836	-2.536578
77	1	-9.476868	-1.412835	-2.625192
78	1	-7.938287	-1.580806	-3.491734
79	1	-8.457793	-2.837480	-2.345613

19 (E = -1554.4416438 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	1.526273	-0.519855	-0.014325
2	6	2.095469	-2.464040	0.848521
3	6	1.098150	-2.644419	-0.204801
4	6	1.680392	-2.185277	-1.440788
5	6	2.989560	-1.659942	-1.153976

6	6	3.248991	-1.860769	0.271093
7	6	1.919623	-2.885404	2.278189
8	1	0.892836	-2.728823	2.619437
9	1	2.144185	-3.955949	2.372614
10	1	2.589299	-2.339437	2.946364
11	6	-0.210976	-3.363343	-0.042527
12	1	-0.914693	-3.106246	-0.837685
13	1	-0.680426	-3.131180	0.917093
14	1	-0.043060	-4.447961	-0.080477
15	6	1.050318	-2.283806	-2.800076
16	1	1.324991	-3.245331	-3.253050
17	1	1.394263	-1.490323	-3.467397
18	1	-0.040169	-2.240819	-2.747806
19	6	4.000459	-1.177570	-2.154338
20	1	4.616119	-0.369917	-1.749255
21	1	3.525980	-0.819862	-3.070608
22	1	4.670044	-2.005502	-2.422960
23	6	4.538324	-1.528575	0.964978
24	1	4.972517	-0.601346	0.581552
25	1	5.264215	-2.334271	0.794227
26	1	4.400838	-1.420708	2.043183
27	6	0.411950	1.532374	-2.053414
28	7	0.142153	0.692051	-1.103777
29	6	-0.661816	2.184665	-2.840453
30	6	-1.910677	2.180745	-2.350654
31	1	-2.695724	2.719753	-2.875209
32	6	-1.278113	0.359611	-0.833567
33	1	-1.329902	-0.004771	0.190286
34	1	-1.538913	-0.471479	-1.500494
35	6	-2.269167	1.515144	-1.046712
36	8	2.345986	1.378192	0.794616
37	6	1.486958	1.423645	1.733252
38	8	0.628078	0.486470	1.764279
39	6	1.536331	2.522761	2.790659
40	6	0.234631	2.544505	3.619715
41	1	0.064527	1.586420	4.119982
42	1	-0.635564	2.761907	2.991814
43	1	0.306160	3.324684	4.385264
44	6	2.744828	2.199733	3.717163
45	1	2.819290	2.969452	4.493040
46	1	3.682234	2.186860	3.152138
47	1	2.618143	1.229296	4.210440
48	6	1.762747	3.892126	2.103358
49	1	2.683718	3.890108	1.513396
50	1	1.841699	4.672936	2.867501
51	1	0.927673	4.148788	1.441701
52	6	1.834720	1.882327	-2.392783
53	1	2.070423	1.555977	-3.412852
54	1	2.536156	1.423629	-1.699289
55	1	1.971100	2.969350	-2.365038
56	6	-0.306847	2.888232	-4.134559
57	1	0.391953	3.717318	-3.973605
58	1	-1.211231	3.295356	-4.595669
59	1	0.159372	2.202437	-4.852140
60	6	-3.715518	0.950406	-1.166193
61	1	-3.764342	0.295870	-2.045976
62	1	-4.387407	1.794159	-1.369329
63	6	-2.178354	2.574274	0.083407
64	1	-1.176464	3.012345	0.128164
65	1	-2.895514	3.383270	-0.097930
66	1	-2.398599	2.129732	1.059781
67	6	-4.228301	0.184181	0.061714
68	1	-4.194186	0.802669	0.966386

69	1	-3.612153	-0.698980	0.273995
70	6	-5.657564	-0.294514	-0.107049
71	8	-6.346960	-0.145889	-1.108191
72	8	-6.095758	-0.924916	1.009476
73	6	-7.478734	-1.447895	0.989709
74	1	-7.558459	-2.165431	0.168338
75	1	-8.154837	-0.611732	0.791202
76	6	-7.734314	-2.087883	2.342034
77	1	-8.752809	-2.489415	2.369540
78	1	-7.037062	-2.911183	2.526594
79	1	-7.633512	-1.355749	3.149394

20 (E = -841.1469366 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.220916	-0.520693	0.004024
2	6	1.919692	0.117344	1.200901
3	6	2.175410	-1.193455	0.689923
4	6	2.164082	-1.127755	-0.768784
5	6	1.900681	0.224123	-1.153416
6	6	1.712389	1.002728	0.063879
7	6	1.892345	0.527379	2.642531
8	1	1.618501	-0.305997	3.293182
9	1	2.890795	0.875438	2.938031
10	1	1.187264	1.343884	2.815452
11	6	2.457237	-2.425036	1.495534
12	1	2.066808	-3.322442	1.008733
13	1	2.026802	-2.359942	2.497121
14	1	3.543654	-2.547015	1.600412
15	6	2.433672	-2.281322	-1.686431
16	1	3.518525	-2.406600	-1.801956
17	1	2.004805	-2.117832	-2.677303
18	1	2.030835	-3.215114	-1.285747
19	6	1.851820	0.765309	-2.550491
20	1	1.148612	1.597110	-2.635974
21	1	1.563907	-0.003141	-3.271202
22	1	2.847373	1.135731	-2.828190
23	6	1.476411	2.478382	0.133360
24	1	0.907177	2.836104	-0.727521
25	1	2.445949	2.995410	0.136920
26	1	0.941787	2.758083	1.043820
27	8	-1.675587	-0.375557	-1.074053
28	6	-2.348679	-0.367744	0.014778
29	8	-1.673820	-0.413552	1.097777
30	6	-3.864877	-0.285767	0.000052
31	6	-4.431571	-0.400300	1.430571
32	1	-4.056592	0.400800	2.074939
33	1	-4.169133	-1.359485	1.888373
34	1	-5.523333	-0.326981	1.391881
35	6	-4.250240	1.087102	-0.622587
36	1	-5.341696	1.167318	-0.659453
37	1	-3.861028	1.181089	-1.640672
38	1	-3.866961	1.918391	-0.020345
39	6	-4.410314	-1.433283	-0.892255
40	1	-4.017924	-1.362064	-1.910661
41	1	-5.502312	-1.364675	-0.935054
42	1	-4.146270	-2.414487	-0.481905

1-NH_2 (E = -739.2849561 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.113560	-1.042191	-0.434517
2	6	0.571386	1.003752	0.384190
3	6	1.513653	0.586875	-0.646468
4	6	2.236320	-0.561993	-0.161444
5	6	1.634584	-0.966331	1.080264
6	6	0.541238	-0.047792	1.385461
7	7	-0.151818	2.131294	0.392251
8	1	-0.980749	2.173720	0.974563
9	1	-0.198008	2.695485	-0.448056
10	6	1.791714	1.359337	-1.900846
11	1	2.246064	0.726065	-2.665759
12	1	0.878561	1.791940	-2.320602
13	1	2.488868	2.179033	-1.681452
14	6	3.411535	-1.212162	-0.831463
15	1	4.341876	-0.757047	-0.467306
16	1	3.455166	-2.282582	-0.615476
17	1	3.378123	-1.084181	-1.916225
18	6	2.073264	-2.105469	1.948186
19	1	1.237472	-2.524749	2.513500
20	1	2.528837	-2.905952	1.360531
21	1	2.820837	-1.746080	2.668063
22	6	-0.294674	-0.025181	2.629511
23	1	-0.365671	-1.018741	3.077625
24	1	0.161086	0.649577	3.366458
25	1	-1.308967	0.320549	2.414140
26	8	-1.825631	-1.551849	-0.706122
27	6	-2.894682	-0.907043	-0.258661
28	8	-2.847635	0.116920	0.404680
29	6	-4.193682	-1.571573	-0.668816
30	1	-4.216498	-2.604957	-0.306500
31	1	-5.047505	-1.022706	-0.268802
32	1	-4.261641	-1.608372	-1.761787

21 (E = -1106.6613836 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.882538	0.175975	-0.154405
2	6	-1.794354	-1.969192	-0.788570
3	6	-2.748247	-0.905203	-0.496934
4	6	-2.572458	-0.557941	0.888152
5	6	-1.399316	-1.298099	1.381421
6	6	-0.913407	-2.138195	0.332901
7	7	-1.705259	-2.615444	-1.952903
8	1	-0.946700	-3.257670	-2.143013
9	1	-2.325004	-2.401185	-2.723250
10	6	-3.885187	-0.511815	-1.402369
11	1	-4.318164	0.443366	-1.095650
12	1	-3.553148	-0.400458	-2.440200
13	1	-4.682245	-1.266564	-1.376483
14	6	-3.517583	0.246884	1.732148
15	1	-4.267027	-0.417598	2.182754
16	1	-2.992402	0.762319	2.540359
17	1	-4.046233	0.996022	1.137347
18	6	-0.914575	-1.291644	2.800306
19	1	0.149254	-1.533137	2.863471
20	1	-1.075368	-0.319326	3.272373

21	1	-1.467532	-2.043537	3.380030
22	6	0.188895	-3.159640	0.407213
23	1	-0.227397	-4.169327	0.523859
24	1	0.812839	-3.154041	-0.493191
25	1	0.842776	-2.971581	1.261738
26	6	0.972443	2.464388	0.067174
27	7	0.954611	1.163000	0.165680
28	6	-0.347008	3.052270	-0.217212
29	6	-0.502043	4.555694	-0.311707
30	1	-1.547095	4.804637	-0.518713
31	1	-0.213646	5.058802	0.620299
32	1	0.110868	4.982674	-1.115962
33	6	2.195338	3.308585	0.240450
34	1	2.044821	3.998095	1.080220
35	1	3.090261	2.718700	0.425041
36	1	2.345735	3.925970	-0.652678
37	6	-1.344046	2.144261	-0.361505
38	1	-2.350574	2.506813	-0.567807
39	8	2.188237	0.556737	0.506768
40	6	2.708530	-0.257326	-0.471951
41	8	2.180690	-0.390987	-1.545079
42	6	4.028328	-0.888928	-0.011005
43	6	3.901362	-1.470622	1.419628
44	1	3.136770	-2.253367	1.464812
45	1	4.858720	-1.917881	1.707202
46	1	3.651823	-0.696511	2.150237
47	6	4.414010	-2.004881	-1.005739
48	1	5.365784	-2.448453	-0.696056
49	1	3.657918	-2.796776	-1.027876
50	1	4.529356	-1.612785	-2.020466
51	6	5.112916	0.227153	-0.027093
52	1	6.080197	-0.214410	0.234821
53	1	5.202887	0.681076	-1.020243
54	1	4.889450	1.012704	0.701377

22 (E = -1570.4093811 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.097068	0.236318	0.711541
2	6	1.642254	2.103022	0.359399
3	6	1.191391	1.879629	1.722876
4	6	-0.240562	2.148500	1.750860
5	6	-0.667793	2.330154	0.396161
6	6	0.499319	2.246061	-0.473430
7	7	2.939784	2.180335	-0.028293
8	1	3.141082	2.103252	-1.018068
9	1	3.632246	1.719973	0.550751
10	6	2.115201	1.787279	2.908126
11	1	1.586527	1.436081	3.796928
12	1	2.941556	1.093556	2.722751
13	1	2.542291	2.773700	3.133106
14	6	-1.068430	2.363689	2.986748
15	1	-1.025650	3.420755	3.280104
16	1	-2.116043	2.099824	2.821709
17	1	-0.698570	1.771814	3.828196
18	6	-2.011773	2.837945	-0.047521
19	1	-2.351654	2.371907	-0.976760
20	1	-2.777909	2.686474	0.715289
21	1	-1.935807	3.917523	-0.234687
22	6	0.530188	2.543675	-1.948080

23	1	0.719498	3.612230	-2.119791
24	1	1.312843	1.977572	-2.463995
25	1	-0.420381	2.298236	-2.428584
26	6	1.590161	-2.206173	1.523893
27	7	1.460849	-1.362647	0.530370
28	6	0.730235	-1.888093	2.651020
29	6	0.764597	-2.717060	3.919605
30	1	0.077975	-2.290859	4.657548
31	1	0.461338	-3.757098	3.742725
32	1	1.767158	-2.738466	4.364943
33	6	2.503884	-3.394547	1.509549
34	1	2.023461	-4.243696	2.002768
35	1	2.788546	-3.688183	0.499545
36	1	3.416375	-3.162957	2.074059
37	6	-0.098870	-0.836707	2.431537
38	1	-0.818157	-0.556794	3.199232
39	8	2.152386	-1.671038	-0.667527
40	6	3.459161	-1.238683	-0.741352
41	8	4.013542	-0.691437	0.174661
42	6	4.065917	-1.599655	-2.103267
43	6	3.141838	-1.122351	-3.253518
44	1	2.990735	-0.037564	-3.219143
45	1	3.612130	-1.366654	-4.211815
46	1	2.165365	-1.612609	-3.215545
47	6	5.448886	-0.923685	-2.219454
48	1	5.897538	-1.189029	-3.182096
49	1	5.363795	0.166843	-2.168965
50	1	6.122467	-1.251844	-1.422232
51	6	4.228051	-3.145301	-2.168110
52	1	4.705692	-3.411593	-3.116872
53	1	4.862772	-3.514070	-1.354546
54	1	3.259703	-3.652605	-2.119937
55	6	-0.990930	-0.566296	-1.033412
56	1	-1.416769	0.279546	-1.560137
57	1	-0.321467	-1.181451	-1.624594
58	6	-1.710358	-1.150912	0.023995
59	6	-1.533813	-2.633373	0.302047
60	1	-0.527745	-2.982042	0.065392
61	1	-1.763288	-2.887959	1.340445
62	1	-2.228832	-3.191300	-0.339987
63	6	-3.035692	-0.568440	0.500857
64	1	-3.116460	-0.683521	1.588426
65	1	-3.078124	0.498915	0.286341
66	6	-4.247358	-1.254192	-0.167755
67	1	-4.319957	-2.311541	0.106203
68	1	-4.147703	-1.224055	-1.262320
69	6	-5.561792	-0.588977	0.190396
70	8	-5.685229	0.498776	0.739648
71	8	-6.614143	-1.352799	-0.189952
72	6	-7.967446	-0.815513	0.068714
73	1	-8.063067	0.134082	-0.465191
74	1	-8.057108	-0.625204	1.141663
75	6	-8.961094	-1.854393	-0.418234
76	1	-9.980723	-1.494176	-0.245259
77	1	-8.841912	-2.042055	-1.489936
78	1	-8.836794	-2.799900	0.118972

TS22-23 (E = -1570.3646453 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	77	0.221336	0.347021	0.553782
2	6	1.579996	2.190588	0.154770
3	6	1.349575	2.076227	1.586473
4	6	-0.051556	2.218707	1.792567
5	6	-0.711675	2.335620	0.501827
6	6	0.317013	2.311220	-0.517842
7	7	2.809176	2.291372	-0.430222
8	1	2.838311	2.172510	-1.436598
9	1	3.568924	1.799021	0.028350
10	6	2.434164	2.017892	2.627562
11	1	2.039971	1.689501	3.592565
12	1	3.233094	1.326043	2.342557
13	1	2.883539	3.010365	2.769301
14	6	-0.738496	2.302307	3.126351
15	1	-0.799322	3.351726	3.443290
16	1	-1.758309	1.911117	3.082636
17	1	-0.193778	1.750761	3.896962
18	6	-2.148151	2.723707	0.274441
19	1	-2.538061	2.302675	-0.656761
20	1	-2.793270	2.392173	1.092337
21	1	-2.234814	3.816528	0.206376
22	6	0.130255	2.581635	-1.985765
23	1	0.215758	3.658275	-2.187950
24	1	0.877174	2.063289	-2.595177
25	1	-0.855559	2.256188	-2.328083
26	6	1.441121	-2.222659	1.489975
27	7	1.507671	-1.326815	0.531619
28	6	0.438122	-1.890966	2.477053
29	6	0.521449	-2.451752	3.874037
30	1	-0.267872	-2.031185	4.502452
31	1	0.403006	-3.544229	3.868949
32	1	1.490271	-2.235422	4.341316
33	6	2.295189	-3.452550	1.584006
34	1	1.673980	-4.336923	1.760975
35	1	2.891900	-3.614812	0.688334
36	1	2.971231	-3.356137	2.443056
37	6	-0.553190	-1.034631	2.039363
38	1	-1.261452	-0.697440	2.787917
39	8	2.244248	-1.742433	-0.614570
40	6	3.477197	-1.154908	-0.761844
41	8	3.967341	-0.460779	0.090468
42	6	4.102140	-1.546220	-2.106067
43	6	3.120916	-1.213873	-3.261284
44	1	2.872841	-0.146582	-3.279268
45	1	3.595737	-1.466825	-4.215050
46	1	2.192658	-1.785484	-3.176296
47	6	5.418602	-0.760601	-2.285192
48	1	5.877047	-1.042174	-3.238570
49	1	5.239052	0.319478	-2.296613
50	1	6.128597	-0.981515	-1.482476
51	6	4.395958	-3.072985	-2.088546
52	1	4.880526	-3.351457	-3.030275
53	1	5.072113	-3.338538	-1.267968
54	1	3.475842	-3.657053	-1.992244
55	6	-1.073771	-0.775614	-0.666121
56	1	-1.790561	-0.116849	-1.150683
57	1	-0.582081	-1.425328	-1.387688
58	6	-1.571805	-1.477544	0.553741
59	6	-1.454210	-3.005750	0.459647
60	1	-0.451720	-3.320855	0.165001
61	1	-1.723448	-3.490730	1.403093
62	1	-2.138122	-3.351059	-0.325934
63	6	-2.962186	-1.015650	1.041100

64	1	-3.172964	-1.454509	2.022719
65	1	-2.955279	0.070303	1.166786
66	6	-4.095977	-1.402131	0.074314
67	1	-4.219761	-2.489311	0.011314
68	1	-3.883756	-1.058380	-0.945941
69	6	-5.430242	-0.813503	0.491231
70	8	-5.614644	-0.068077	1.445169
71	8	-6.420653	-1.216422	-0.339701
72	6	-7.782454	-0.711687	-0.058466
73	1	-7.751492	0.381037	-0.085230
74	1	-8.059567	-1.029694	0.950403
75	6	-8.701746	-1.289345	-1.118889
76	1	-9.725045	-0.940592	-0.944028
77	1	-8.397948	-0.969404	-2.120556
78	1	-8.703102	-2.383337	-1.085655

23 (E = -1570.395955 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.319432	0.353440	0.895401
2	6	1.712370	2.282536	0.415790
3	6	1.571166	2.126080	1.833861
4	6	0.162009	2.198375	2.126659
5	6	-0.574146	2.326123	0.887039
6	6	0.397132	2.279450	-0.193487
7	7	2.881333	2.416241	-0.253478
8	1	2.861732	2.311478	-1.260558
9	1	3.718896	2.034659	0.170529
10	6	2.714944	2.127980	2.813227
11	1	2.396507	1.785281	3.800871
12	1	3.531467	1.475008	2.485795
13	1	3.123200	3.141434	2.929486
14	6	-0.436746	2.315120	3.500670
15	1	-0.502894	3.375172	3.779555
16	1	-1.446267	1.897901	3.538403
17	1	0.173129	1.812116	4.254539
18	6	-2.026492	2.694541	0.747765
19	1	-2.458274	2.298341	-0.175330
20	1	-2.620395	2.320333	1.585767
21	1	-2.132014	3.787545	0.721979
22	6	0.130113	2.537927	-1.652859
23	1	0.207381	3.610390	-1.877328
24	1	0.838853	2.004745	-2.295926
25	1	-0.873733	2.209333	-1.933417
26	6	1.363724	-2.170611	1.393722
27	7	1.534431	-1.371642	0.407292
28	6	0.461041	-1.430931	2.334416
29	6	0.968383	-1.287176	3.757874
30	1	0.325204	-0.618809	4.335259
31	1	0.959039	-2.267644	4.253480
32	1	1.993867	-0.906296	3.789488
33	6	1.971995	-3.513534	1.624293
34	1	1.211044	-4.221515	1.967349
35	1	2.450005	-3.896080	0.721539
36	1	2.727424	-3.437668	2.416907
37	6	-0.884728	-1.170686	2.000946
38	1	-1.459217	-0.750459	2.822211
39	8	2.215329	-1.852639	-0.732515
40	6	3.438489	-1.252553	-0.964890
41	8	3.943781	-0.503475	-0.173638

42	6	3.991712	-1.678559	-2.327346
43	6	3.092144	-1.050772	-3.429673
44	1	3.065058	0.041946	-3.347461
45	1	3.503153	-1.307274	-4.411721
46	1	2.068410	-1.432788	-3.374784
47	6	5.436112	-1.151176	-2.459234
48	1	5.834920	-1.440721	-3.436679
49	1	5.472413	-0.060316	-2.381745
50	1	6.085716	-1.571449	-1.684434
51	6	3.977039	-3.225317	-2.451903
52	1	4.413564	-3.506846	-3.415761
53	1	4.572497	-3.693006	-1.659736
54	1	2.959935	-3.623871	-2.406843
55	6	-1.117971	-0.685931	-0.288969
56	1	-1.845884	0.014229	-0.697971
57	1	-0.628685	-1.211987	-1.110922
58	6	-1.715984	-1.626210	0.781776
59	6	-1.574721	-3.127534	0.460070
60	1	-0.540501	-3.402757	0.235312
61	1	-1.923015	-3.742991	1.299301
62	1	-2.168632	-3.382869	-0.424627
63	6	-3.195999	-1.278619	1.102076
64	1	-3.498890	-1.832530	2.002286
65	1	-3.253648	-0.212615	1.353887
66	6	-4.184734	-1.574121	-0.033632
67	1	-4.317043	-2.649676	-0.190851
68	1	-3.813556	-1.169941	-0.986755
69	6	-5.554024	-0.968032	0.204668
70	8	-5.824553	-0.118404	1.044977
71	8	-6.471659	-1.474667	-0.655319
72	6	-7.846961	-0.939975	-0.563536
73	1	-7.804467	0.138295	-0.741153
74	1	-8.211293	-1.112799	0.452795
75	6	-8.680131	-1.663406	-1.605737
76	1	-9.709902	-1.292105	-1.572233
77	1	-8.287514	-1.491648	-2.612905
78	1	-8.699018	-2.741226	-1.416170

24 (E = -1414.3925027 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.832423	0.057612	0.441001
2	6	-1.315710	-1.972967	-0.698544
3	6	-1.425643	-0.759805	-1.521297
4	6	-2.472113	0.048982	-0.967474
5	6	-2.891376	-0.537078	0.301129
6	6	-2.105553	-1.709585	0.525015
7	6	-0.843213	-0.528100	-2.897136
8	1	-1.293746	0.356891	-3.350452
9	1	0.236971	-0.373346	-2.877301
10	1	-1.061371	-1.378962	-3.552006
11	6	-3.169540	1.194278	-1.641221
12	1	-4.004781	0.802176	-2.237708
13	1	-3.578742	1.895536	-0.911165
14	1	-2.508279	1.749492	-2.307382
15	6	-4.018879	-0.034767	1.154357
16	1	-3.911864	-0.344365	2.195818
17	1	-4.086761	1.055500	1.125862
18	1	-4.966880	-0.441963	0.777106
19	6	-2.208515	-2.556522	1.768836

20	1	-2.480053	-1.927296	2.619026
21	1	-2.981092	-3.327751	1.665147
22	1	-1.261660	-3.040477	2.013674
23	8	-0.233006	0.058531	2.436540
24	6	-0.045159	1.085636	3.216953
25	8	-0.317994	2.252857	2.936835
26	6	0.523162	0.706407	4.578919
27	1	0.866512	1.596383	5.110320
28	1	-0.259437	0.220300	5.174260
29	1	1.346566	-0.006110	4.472725
30	6	0.917668	2.590538	-0.443465
31	7	0.782572	1.396361	0.026057
32	6	-0.293351	3.342629	-0.852019
33	6	-0.307223	3.883271	-2.267425
34	1	-1.233110	4.436645	-2.446826
35	1	0.535394	4.558663	-2.456006
36	1	-0.239826	3.070952	-3.001539
37	6	2.260624	3.261900	-0.574869
38	1	2.137436	4.322137	-0.796912
39	1	2.830147	3.155827	0.351907
40	1	2.844529	2.802694	-1.381634
41	6	-1.248475	3.582033	0.051896
42	1	-2.105876	4.192913	-0.210046
43	1	-1.176095	3.201037	1.064275
44	8	2.012015	0.852443	0.534838
45	6	2.706077	0.035910	-0.329536
46	8	2.370298	-0.131182	-1.471977
47	6	3.907124	-0.598104	0.382677
48	6	3.366679	-1.637648	1.405001
49	1	2.773158	-2.412497	0.906679
50	1	4.215261	-2.124281	1.897180
51	1	2.749894	-1.160758	2.172044
52	6	4.786952	-1.304631	-0.671134
53	1	5.642096	-1.769201	-0.169615
54	1	4.231181	-2.085778	-1.198440
55	1	5.168382	-0.595629	-1.413388
56	6	4.733973	0.485837	1.122907
57	1	5.596611	0.008405	1.599306
58	1	5.109375	1.245042	0.427677
59	1	4.145821	0.982196	1.899350
60	7	-0.596765	-3.065375	-0.950981
61	6	-0.832959	-4.363776	-0.282878
62	1	-0.730568	-5.143390	-1.042247
63	1	-0.095785	-4.545305	0.505607
64	1	-1.838784	-4.417763	0.123024
65	6	0.518167	-3.110547	-1.923816
66	1	0.184785	-3.519233	-2.882576
67	1	0.957069	-2.127700	-2.061163
68	1	1.287129	-3.769302	-1.512342

TS24-25 (E = -1414.3759916 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.935418	0.426628	0.148045
2	6	-1.138841	-1.628575	-1.208606
3	6	-1.882842	-0.434997	-1.630148
4	6	-2.882841	-0.161126	-0.594707
5	6	-2.569259	-0.957533	0.545923
6	6	-1.397970	-1.761825	0.227278
7	6	-2.023305	0.104912	-3.037802

8	1	-2.830298	0.839518	-3.078378
9	1	-1.120371	0.599560	-3.400399
10	1	-2.277142	-0.700675	-3.736539
11	6	-4.095562	0.710355	-0.759163
12	1	-4.870454	0.160824	-1.309759
13	1	-4.510055	1.000026	0.209028
14	1	-3.877016	1.623386	-1.318961
15	6	-3.352699	-1.033132	1.825413
16	1	-2.699777	-1.182094	2.688554
17	1	-3.932447	-0.122760	1.993256
18	1	-4.050439	-1.879690	1.780518
19	6	-0.783122	-2.724585	1.215021
20	1	-0.824768	-2.296860	2.220204
21	1	-1.326333	-3.678555	1.241103
22	1	0.263727	-2.928649	0.989127
23	8	-0.492386	0.736737	2.238304
24	6	-0.598095	1.908953	2.718181
25	8	-0.879882	2.923836	2.018308
26	6	-0.377671	2.086769	4.202420
27	1	0.416147	2.821680	4.370641
28	1	-1.292562	2.478419	4.660050
29	1	-0.109897	1.139992	4.672771
30	6	1.330090	2.251948	-0.688777
31	7	1.102397	1.085595	-0.140523
32	6	0.118823	2.904012	-1.165750
33	6	0.189824	4.022284	-2.177347
34	1	-0.817454	4.358054	-2.437763
35	1	0.742742	4.885083	-1.784244
36	1	0.694564	3.704408	-3.098748
37	6	2.688945	2.881112	-0.782406
38	1	2.840407	3.566525	0.061858
39	1	3.486453	2.138307	-0.759833
40	1	2.769091	3.468235	-1.700125
41	6	-1.038905	2.432907	-0.602539
42	1	-1.975990	2.867999	-0.941960
43	1	-0.996258	2.496979	0.732069
44	8	2.198789	0.603673	0.617007
45	6	2.649841	-0.652327	0.275322
46	8	2.240143	-1.249956	-0.682325
47	6	3.727814	-1.116063	1.263300
48	6	3.128084	-1.172851	2.694253
49	1	2.275571	-1.859546	2.742368
50	1	3.894823	-1.535792	3.387011
51	1	2.799447	-0.185522	3.030131
52	6	4.213842	-2.517577	0.837909
53	1	4.984951	-2.858067	1.536507
54	1	3.394704	-3.243626	0.848804
55	1	4.643596	-2.502222	-0.168689
56	6	4.913828	-0.113260	1.228783
57	1	5.699725	-0.468692	1.903574
58	1	5.340454	-0.037191	0.222024
59	1	4.606112	0.883839	1.556266
60	7	-0.319443	-2.372141	-1.950249
61	6	0.131842	-3.718981	-1.547331
62	1	1.134728	-3.684302	-1.111296
63	1	-0.569292	-4.170493	-0.850136
64	1	0.159628	-4.338249	-2.448220
65	6	0.301880	-1.898705	-3.205439
66	1	-0.261732	-2.236900	-4.080456
67	1	0.391035	-0.816619	-3.210412
68	1	1.310634	-2.314108	-3.251981

25 (E = -1414.3958097 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-1.007226	0.438010	0.025124
2	6	-1.182862	-1.803967	-1.056167
3	6	-1.808689	-0.600391	-1.680840
4	6	-2.899447	-0.177001	-0.806725
5	6	-2.727525	-0.878065	0.425921
6	6	-1.643363	-1.840022	0.302638
7	6	-1.672895	-0.129279	-3.110211
8	1	-1.967041	0.920607	-3.182529
9	1	-0.644262	-0.203919	-3.467603
10	1	-2.320960	-0.700759	-3.786957
11	6	-4.050267	0.712904	-1.187077
12	1	-4.846368	0.112392	-1.646927
13	1	-4.471193	1.221785	-0.316011
14	1	-3.753450	1.475352	-1.912206
15	6	-3.625559	-0.767155	1.627601
16	1	-3.055975	-0.803306	2.560019
17	1	-4.197331	0.163465	1.613229
18	1	-4.339902	-1.601217	1.635816
19	6	-1.368536	-2.897600	1.352011
20	1	-2.164696	-2.895386	2.101042
21	1	-1.349163	-3.896258	0.902206
22	1	-0.424715	-2.751430	1.886408
23	8	-0.733500	0.939286	2.199158
24	6	-0.787605	2.016953	2.795170
25	8	-0.946847	3.177196	2.187168
26	6	-0.675611	2.112977	4.287550
27	1	0.196739	2.719947	4.552646
28	1	-1.560550	2.613776	4.693819
29	1	-0.578760	1.119024	4.722451
30	6	1.308287	2.281869	-0.449524
31	7	1.053046	1.060849	-0.055731
32	6	0.130190	2.979195	-0.953451
33	6	0.262224	4.321796	-1.642634
34	1	-0.724181	4.673586	-1.959600
35	1	0.696560	5.084756	-0.984233
36	1	0.900477	4.257989	-2.533349
37	6	2.656027	2.935777	-0.392804
38	1	2.567350	3.937535	0.039583
39	1	3.376759	2.363894	0.188076
40	1	3.043261	3.059169	-1.412291
41	6	-1.039695	2.308183	-0.747888
42	1	-1.962879	2.777979	-1.088035
43	1	-0.980699	3.041851	1.211688
44	8	2.106579	0.417956	0.652759
45	6	2.892743	-0.432112	-0.088737
46	8	2.746895	-0.588757	-1.271812
47	6	3.967507	-1.076409	0.800715
48	6	3.314668	-1.760198	2.030274
49	1	2.618576	-2.549914	1.727224
50	1	4.099468	-2.220749	2.639555
51	1	2.775194	-1.039798	2.651229
52	6	4.745816	-2.114933	-0.035184
53	1	5.522702	-2.567706	0.589473
54	1	4.089827	-2.912776	-0.397540
55	1	5.227230	-1.650028	-0.900969
56	6	4.938938	0.039024	1.280993
57	1	5.739976	-0.418570	1.871307
58	1	5.399088	0.559224	0.433202
59	1	4.427570	0.772385	1.911669

60	7	-0.299046	-2.628584	-1.644290
61	6	0.714605	-3.393783	-0.897955
62	1	1.675938	-3.274199	-1.407068
63	1	0.816836	-3.013518	0.113767
64	1	0.463956	-4.459715	-0.867595
65	6	-0.219345	-2.832768	-3.102324
66	1	0.609133	-2.269384	-3.546048
67	1	-0.045089	-3.898789	-3.278648
68	1	-1.154008	-2.562451	-3.586556

1-N(CH_3)$_2$ (E = -817.8647376 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.122013	0.051871	-0.727291
2	6	0.478382	0.851143	1.419295
3	6	1.331185	1.278843	0.286731
4	6	2.002793	0.125385	-0.249424
5	6	1.383082	-1.037155	0.319803
6	6	0.323748	-0.601295	1.230926
7	7	-0.111141	1.631820	2.315130
8	6	1.611344	2.686223	-0.171754
9	1	1.842386	2.685453	-1.239984
10	1	0.752960	3.342434	-0.019205
11	1	2.476689	3.111343	0.351753
12	6	3.142031	0.130019	-1.227917
13	1	4.095153	0.100851	-0.683468
14	1	3.106763	-0.739911	-1.888724
15	1	3.139981	1.028636	-1.848841
16	6	1.789038	-2.457963	0.067513
17	1	0.931555	-3.134846	0.075264
18	1	2.295173	-2.560035	-0.895062
19	1	2.484581	-2.784219	0.852504
20	6	-0.462932	-1.565843	2.081270
21	1	-0.333891	-2.584903	1.712117
22	1	-0.101665	-1.537878	3.116423
23	1	-1.529971	-1.344026	2.073523
24	8	-2.015319	-0.192462	-1.390947
25	6	-3.144512	-0.290233	-0.705744
26	8	-3.224802	-0.156751	0.505560
27	6	-4.343943	-0.578832	-1.587250
28	1	-4.198752	-1.528989	-2.113141
29	1	-5.255701	-0.627530	-0.990009
30	1	-4.443777	0.202423	-2.348526
31	6	-1.306338	1.211526	3.089126
32	1	-1.022008	0.626959	3.968110
33	1	-1.816121	2.116722	3.422055
34	1	-1.988709	0.650735	2.453114
35	6	0.352686	3.004313	2.617952
36	1	0.309592	3.130870	3.702371
37	1	1.382299	3.145847	2.302123
38	1	-0.294322	3.753033	2.150846

26 (E = -1185.239128 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.727221	0.459343	0.020407
2	6	-1.978808	-1.580357	-0.237461

3	6	-2.749441	-0.348152	0.029333
4	6	-2.362327	0.124157	1.330385
5	6	-1.270656	-0.731412	1.805563
6	6	-1.012926	-1.741295	0.840263
7	7	-2.072457	-2.346640	-1.333443
8	6	-3.885586	0.235980	-0.775535
9	1	-4.013323	1.291538	-0.523496
10	1	-3.699033	0.178592	-1.849812
11	1	-4.835469	-0.268924	-0.559064
12	6	-3.066863	1.163287	2.155235
13	1	-3.845701	0.685030	2.764722
14	1	-2.374783	1.673354	2.830029
15	1	-3.547494	1.919092	1.529719
16	6	-0.640328	-0.628280	3.163602
17	1	0.384368	-1.006729	3.165605
18	1	-0.621175	0.407456	3.511364
19	1	-1.222149	-1.214003	3.888700
20	6	-0.112541	-2.932754	1.077149
21	1	-0.654362	-3.863297	0.874830
22	1	0.787748	-2.932225	0.458358
23	1	0.204331	-2.960786	2.122360
24	6	1.408874	2.453122	-0.421221
25	7	1.247223	1.211049	-0.052111
26	6	0.146184	3.155353	-0.703103
27	6	0.164074	4.615257	-1.105731
28	1	-0.861967	4.972753	-1.234525
29	1	0.648532	5.245170	-0.348492
30	1	0.696294	4.775661	-2.052406
31	6	2.737236	3.133549	-0.528009
32	1	2.833793	3.867776	0.282971
33	1	3.570981	2.437406	-0.464631
34	1	2.795231	3.689524	-1.468967
35	6	-0.963945	2.389955	-0.551888
36	1	-1.935738	2.847975	-0.735374
37	8	2.433970	0.535392	0.324516
38	6	2.734690	-0.567654	-0.436593
39	8	2.072511	-0.900316	-1.385504
40	6	4.006921	-1.248350	0.086044
41	6	3.832722	-1.625617	1.581294
42	1	2.992526	-2.313398	1.725395
43	1	4.742158	-2.126006	1.930337
44	1	3.668763	-0.739839	2.201387
45	6	4.272274	-2.514352	-0.755843
46	1	5.185562	-2.999322	-0.396357
47	1	3.448819	-3.231032	-0.674183
48	1	4.406324	-2.268270	-1.813763
49	6	5.195220	-0.257413	-0.067147
50	1	6.117901	-0.758260	0.244316
51	1	5.316777	0.060948	-1.108777
52	1	5.060679	0.629229	0.559318
53	6	-0.936557	-3.125391	-1.871269
54	1	0.009523	-2.705789	-1.538410
55	1	-1.005437	-4.180983	-1.590118
56	1	-0.972529	-3.053352	-2.961994
57	6	-3.304965	-2.468075	-2.136637
58	1	-4.176201	-2.170516	-1.559427
59	1	-3.243404	-1.877497	-3.056849
60	1	-3.420294	-3.521522	-2.407903

27 (E = -1648.9820178 au)

Center Number	Atomic	Coordinates (Angstroms)		

	Number	X	Y	Z
1	77	0.174594	0.171621	0.722656
2	6	1.677511	2.190115	0.541327
3	6	0.951490	1.991527	1.793186
4	6	-0.474094	2.110998	1.509633
5	6	-0.618975	2.199252	0.087066
6	6	0.684998	2.107587	-0.523387
7	7	3.002228	2.367333	0.413550
8	6	1.505115	2.146495	3.193316
9	1	0.696707	2.098155	3.925684
10	1	2.232954	1.380675	3.463417
11	1	1.985777	3.127264	3.298139
12	6	-1.547314	2.378485	2.531521
13	1	-1.525029	3.433256	2.836159
14	1	-2.540952	2.164468	2.131576
15	1	-1.416349	1.770474	3.430381
16	6	-1.870634	2.574976	-0.658015
17	1	-2.026214	1.979541	-1.561707
18	1	-2.762911	2.497499	-0.035132
19	1	-1.778662	3.622221	-0.975578
20	6	0.893953	2.182885	-2.018046
21	1	0.927881	3.221950	-2.372071
22	1	1.814463	1.686043	-2.326600
23	1	0.067262	1.692384	-2.538861
24	6	1.857413	-2.156804	1.527169
25	7	1.618460	-1.372520	0.503844
26	6	1.116336	-1.785161	2.716433
27	6	1.324056	-2.503067	4.036292
28	1	0.665656	-2.072168	4.796950
29	1	1.095282	-3.574051	3.964585
30	1	2.356755	-2.409650	4.395584
31	6	2.769677	-3.346716	1.437669
32	1	2.958123	-3.765327	2.426380
33	1	2.321307	-4.127422	0.811728
34	1	3.728145	-3.075654	0.984882
35	6	0.205702	-0.796469	2.510696
36	1	-0.436514	-0.489672	3.334474
37	8	2.083069	-1.882839	-0.739467
38	6	3.202080	-1.282677	-1.266644
39	8	3.827201	-0.443164	-0.677663
40	6	3.517933	-1.861885	-2.653323
41	6	2.301501	-1.664990	-3.596642
42	1	2.040576	-0.605433	-3.696208
43	1	2.557523	-2.044890	-4.591500
44	1	1.423245	-2.209238	-3.238511
45	6	4.749655	-1.126181	-3.222378
46	1	4.990200	-1.537385	-4.208185
47	1	4.556430	-0.054473	-3.334623
48	1	5.622897	-1.249925	-2.574484
49	6	3.828871	-3.377307	-2.508225
50	1	4.094781	-3.781026	-3.490924
51	1	4.674111	-3.547198	-1.831748
52	1	2.962723	-3.930375	-2.133681
53	6	-0.917202	-0.831259	-0.898080
54	1	-1.371715	-0.074688	-1.527287
55	1	-0.271300	-1.525501	-1.421799
56	6	-1.601967	-1.267415	0.257114
57	6	-1.428943	-2.707333	0.713414
58	1	-0.423345	-3.084780	0.522627
59	1	-1.655512	-2.830633	1.776466
60	1	-2.124932	-3.340690	0.146188
61	6	-2.929948	-0.636208	0.662986

62	1	-3.014585	-0.625339	1.755822
63	1	-2.966935	0.399806	0.326995
64	6	-4.141189	-1.384858	0.066527
65	1	-4.225645	-2.402095	0.466257
66	1	-4.033100	-1.490695	-1.021387
67	6	-5.453371	-0.676187	0.337534
68	8	-5.583638	0.373326	0.955513
69	8	-6.495838	-1.355592	-0.199322
70	6	-7.844335	-0.777349	-0.014263
71	1	-7.843086	0.229975	-0.439638
72	1	-8.036971	-0.703874	1.059673
73	6	-8.826271	-1.698484	-0.714903
74	1	-9.841965	-1.305506	-0.599540
75	1	-8.606094	-1.768266	-1.784796
76	1	-8.798155	-2.704698	-0.285094
77	6	3.625075	2.931027	-0.797876
78	1	4.021196	2.144977	-1.449195
79	1	2.917716	3.551059	-1.343383
80	1	4.452932	3.570584	-0.477784
81	6	3.970254	1.886179	1.420971
82	1	4.181717	2.645524	2.180127
83	1	3.608052	0.973192	1.889741
84	1	4.897242	1.641147	0.900112

TS27-28 (E = -1648.9394332 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.272079	0.376348	0.370702
2	6	1.768148	2.303634	0.614920
3	6	0.836800	2.259655	1.697100
4	6	-0.500692	2.311238	1.141054
5	6	-0.412836	2.354316	-0.293616
6	6	0.977116	2.209345	-0.644795
7	7	3.115058	2.370504	0.713438
8	6	1.139690	2.415574	3.169215
9	1	0.288076	2.873788	3.680588
10	1	1.349247	1.465478	3.672804
11	1	2.004417	3.070563	3.317077
12	6	-1.741939	2.559681	1.953695
13	1	-1.755253	3.602277	2.299302
14	1	-2.648270	2.396704	1.366280
15	1	-1.787708	1.918930	2.839443
16	6	-1.540464	2.643167	-1.247060
17	1	-1.379836	2.170289	-2.219419
18	1	-2.501818	2.297503	-0.858355
19	1	-1.616490	3.726448	-1.410119
20	6	1.498315	2.271892	-2.059697
21	1	1.672159	3.310676	-2.372854
22	1	2.432745	1.720252	-2.172382
23	1	0.768713	1.840390	-2.749947
24	6	1.604156	-2.137153	1.319768
25	7	1.567388	-1.294154	0.304722
26	6	0.703822	-1.764675	2.375873
27	6	0.893814	-2.246770	3.794463
28	1	0.206850	-1.724317	4.466276
29	1	0.688251	-3.322570	3.882357
30	1	1.917479	-2.079984	4.150461
31	6	2.471815	-3.363506	1.331392
32	1	2.561293	-3.757030	2.345061
33	1	2.039458	-4.149263	0.700126

34	1	3.471711	-3.146751	0.945618
35	6	-0.331246	-0.929595	1.979248
36	1	-0.971156	-0.547683	2.767028
37	8	2.106320	-1.858749	-0.886461
38	6	3.207538	-1.224185	-1.411496
39	8	3.786427	-0.344278	-0.834019
40	6	3.564039	-1.825036	-2.777793
41	6	2.359300	-1.662849	-3.743538
42	1	2.087066	-0.608682	-3.867189
43	1	2.634911	-2.059572	-4.726514
44	1	1.482730	-2.209920	-3.385156
45	6	4.794518	-1.081046	-3.337942
46	1	5.062833	-1.510699	-4.308577
47	1	4.586014	-0.015823	-3.479675
48	1	5.655962	-1.174937	-2.669317
49	6	3.894737	-3.332470	-2.598919
50	1	4.187371	-3.749374	-3.568384
51	1	4.727786	-3.477033	-1.901566
52	1	3.029502	-3.891972	-2.232165
53	6	-1.112390	-0.793643	-0.675445
54	1	-1.898220	-0.171961	-1.097658
55	1	-0.692934	-1.465093	-1.422826
56	6	-1.462690	-1.458743	0.622372
57	6	-1.310322	-2.986010	0.564771
58	1	-0.334393	-3.285337	0.180301
59	1	-1.467168	-3.445059	1.545930
60	1	-2.059490	-3.377226	-0.134572
61	6	-2.820938	-1.024068	1.215472
62	1	-2.927822	-1.432500	2.227309
63	1	-2.843044	0.064559	1.304859
64	6	-4.022315	-1.483986	0.369350
65	1	-4.135561	-2.573154	0.384022
66	1	-3.894231	-1.203119	-0.684622
67	6	-5.328446	-0.876684	0.844563
68	8	-5.440498	0.021927	1.669115
69	8	-6.385999	-1.450925	0.223299
70	6	-7.729810	-0.936322	0.565351
71	1	-7.752634	0.132480	0.335256
72	1	-7.878396	-1.066690	1.640787
73	6	-8.732994	-1.725165	-0.256160
74	1	-9.745778	-1.374896	-0.030512
75	1	-8.556035	-1.591895	-1.328035
76	1	-8.680617	-2.793146	-0.022429
77	6	3.969460	2.961389	-0.327509
78	1	4.432513	2.192590	-0.955404
79	1	3.402042	3.655523	-0.944822
80	1	4.762703	3.528269	0.171980
81	6	3.862712	1.711632	1.796961
82	1	4.323678	2.444557	2.468921
83	1	3.209536	1.052750	2.365081
84	1	4.652164	1.100199	1.347281

28 (E = -1648.9702251 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.423384	0.372100	0.941350
2	6	1.894446	2.388436	0.605506
3	6	1.578757	2.176823	1.998742
4	6	0.142404	2.205196	2.128203
5	6	-0.456526	2.339357	0.823782

6	6	0.620984	2.293596	-0.144448
7	7	3.119298	2.578383	0.087786
8	6	2.520589	2.307311	3.177056
9	1	1.957388	2.534413	4.085837
10	1	3.107800	1.405686	3.377589
11	1	3.224265	3.131658	3.015919
12	6	-0.607530	2.323858	3.427603
13	1	-0.651886	3.378541	3.730820
14	1	-1.633736	1.962206	3.329524
15	1	-0.125822	1.766236	4.233405
16	6	-1.890680	2.696138	0.538793
17	1	-2.231168	2.293895	-0.418736
18	1	-2.563210	2.327982	1.317778
19	1	-1.995165	3.788938	0.494496
20	6	0.398702	2.455164	-1.630828
21	1	0.352064	3.512147	-1.924554
22	1	1.181434	1.967539	-2.214080
23	1	-0.553527	1.997725	-1.912800
24	6	1.428610	-2.163319	1.509468
25	7	1.640476	-1.429309	0.478339
26	6	0.526617	-1.372674	2.399895
27	6	0.990449	-1.201555	3.835955
28	1	0.325857	-0.530192	4.384738
29	1	0.978103	-2.172662	4.349432
30	1	2.010784	-0.808600	3.889499
31	6	1.982239	-3.517489	1.819998
32	1	2.730035	-3.426588	2.618574
33	1	1.190325	-4.175632	2.191127
34	1	2.456754	-3.969298	0.948844
35	6	-0.813356	-1.121109	2.025790
36	1	-1.413869	-0.691136	2.823412
37	8	2.282951	-2.081237	-0.596246
38	6	2.979278	-1.278886	-1.475291
39	8	3.157595	-0.108192	-1.288249
40	6	3.456584	-2.109685	-2.672877
41	6	2.211532	-2.601235	-3.462631
42	1	1.599227	-1.758995	-3.804587
43	1	2.545741	-3.157566	-4.344797
44	1	1.588453	-3.263320	-2.854358
45	6	4.332844	-1.213669	-3.573069
46	1	4.671792	-1.794552	-4.436855
47	1	3.773994	-0.346727	-3.938613
48	1	5.214456	-0.850775	-3.034833
49	6	4.280940	-3.327068	-2.175100
50	1	4.657044	-3.879685	-3.042526
51	1	5.141443	-3.006555	-1.576814
52	1	3.671287	-4.007809	-1.574495
53	6	-0.982284	-0.670311	-0.277409
54	1	-1.700132	0.024545	-0.712438
55	1	-0.475500	-1.206585	-1.082097
56	6	-1.608963	-1.597845	0.789158
57	6	-1.456292	-3.103196	0.491578
58	1	-0.415558	-3.379048	0.302048
59	1	-1.828584	-3.707994	1.328412
60	1	-2.022930	-3.372137	-0.406952
61	6	-3.099020	-1.251348	1.060480
62	1	-3.426996	-1.794099	1.958698
63	1	-3.167666	-0.182125	1.295758
64	6	-4.051490	-1.566290	-0.100572
65	1	-4.165917	-2.644743	-0.253032
66	1	-3.658112	-1.165460	-1.045993
67	6	-5.435866	-0.979578	0.093076
68	8	-5.752094	-0.151333	0.938710

69	8	-6.310826	-1.480450	-0.813978
70	6	-7.697369	-0.970671	-0.765799
71	1	-7.666591	0.112808	-0.911064
72	1	-8.101309	-1.178899	0.228781
73	6	-8.472867	-1.677384	-1.862661
74	1	-9.509936	-1.325415	-1.862162
75	1	-8.041620	-1.469178	-2.846907
76	1	-8.479303	-2.760510	-1.705114
77	6	3.354770	3.204842	-1.224063
78	1	3.528328	2.452627	-2.000543
79	1	2.522288	3.846333	-1.502859
80	1	4.248329	3.831175	-1.137046
81	6	4.349326	2.050758	0.707131
82	1	4.945175	2.853766	1.154391
83	1	4.115948	1.302257	1.459217
84	1	4.940560	1.567130	-0.075860

29 (E = -1580.0040143 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.571522	0.672627	1.023885
2	6	1.306200	2.375374	-0.322466
3	6	1.764458	2.455965	1.062228
4	6	0.572239	2.653539	1.891043
5	6	-0.575643	2.564827	1.042864
6	6	-0.111620	2.426036	-0.331461
7	6	2.176301	2.388752	-1.534519
8	9	3.448591	1.941813	-1.294181
9	9	2.309257	3.672401	-2.034948
10	9	1.688570	1.630783	-2.572983
11	6	3.176052	2.579541	1.555559
12	1	3.219427	2.444195	2.637788
13	1	3.836462	1.849144	1.088357
14	1	3.553486	3.584691	1.324444
15	6	0.577573	2.975646	3.355112
16	1	0.727911	4.055507	3.482956
17	1	-0.369919	2.710604	3.828885
18	1	1.382246	2.459011	3.883179
19	6	-2.009502	2.778430	1.441742
20	1	-2.687633	2.159190	0.849174
21	1	-2.170560	2.542960	2.495861
22	1	-2.286935	3.828635	1.283452
23	6	-1.044860	2.358624	-1.500884
24	1	-1.468228	3.358034	-1.668987
25	1	-0.554696	2.031946	-2.415807
26	1	-1.882460	1.686803	-1.290072
27	6	1.394842	-2.075400	1.675936
28	7	1.726289	-1.103695	0.868090
29	6	0.571196	-1.628537	2.816016
30	6	1.789255	-3.498467	1.433539
31	1	1.224813	-4.169913	2.079533
32	1	1.623077	-3.767387	0.387266
33	1	2.857403	-3.639717	1.641777
34	6	0.101742	-0.359261	2.695537
35	1	-0.505288	0.060635	3.493321
36	8	2.357902	-1.514218	-0.328549
37	6	3.707619	-1.206295	-0.398284
38	8	4.286396	-0.662295	0.500940
39	6	4.319112	-1.720901	-1.706788
40	6	3.345839	-1.583719	-2.902339

41	1	3.059617	-0.540647	-3.067111
42	1	3.845539	-1.946189	-3.806761
43	1	2.437605	-2.174591	-2.755361
44	6	5.617607	-0.928984	-1.982303
45	1	6.086050	-1.316573	-2.892681
46	1	5.409583	0.135620	-2.130681
47	1	6.328298	-1.029637	-1.157174
48	6	4.661834	-3.223607	-1.479744
49	1	5.164730	-3.609407	-2.372707
50	1	5.334560	-3.353365	-0.625019
51	1	3.759003	-3.819699	-1.313626
52	6	0.310858	-2.508956	3.986752
53	6	1.361854	-3.169060	4.657180
54	6	-1.003526	-2.656794	4.475786
55	6	1.102965	-3.951818	5.787592
56	1	2.383911	-3.052048	4.309796
57	6	-1.259452	-3.442449	5.605103
58	1	-1.822551	-2.167247	3.957990
59	6	-0.207581	-4.092293	6.263489
60	1	1.922913	-4.446962	6.297235
61	1	-2.277137	-3.551249	5.965283
62	1	-0.406551	-4.703258	7.137598

30 (E = -2043.7587236 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.131831	0.305159	0.740215
2	6	1.042749	2.172220	-0.207025
3	6	1.502605	2.070929	1.169605
4	6	0.343864	2.202716	2.003355
5	6	-0.821297	2.345724	1.167138
6	6	-0.375924	2.381171	-0.202258
7	6	1.914198	2.320333	-1.408910
8	9	3.162752	1.780133	-1.246511
9	9	2.113055	3.654714	-1.721436
10	9	1.386918	1.746828	-2.542657
11	6	2.921401	2.045420	1.666743
12	1	2.953216	1.800791	2.730158
13	1	3.537019	1.324775	1.130804
14	1	3.363737	3.041713	1.537308
15	6	0.349258	2.302489	3.501738
16	1	0.528374	3.347480	3.786500
17	1	-0.608712	2.002225	3.931350
18	1	1.133809	1.691493	3.952801
19	6	-2.195880	2.709593	1.659837
20	1	-2.963310	2.550333	0.901064
21	1	-2.475790	2.136545	2.547250
22	1	-2.212076	3.773311	1.930700
23	6	-1.245795	2.740818	-1.372855
24	1	-1.292025	3.835982	-1.438879
25	1	-0.857929	2.366211	-2.319778
26	1	-2.269801	2.383290	-1.246159
27	6	1.573061	-2.090046	1.718062
28	7	1.514095	-1.258825	0.705510
29	6	0.658436	-1.729204	2.789114
30	6	2.427751	-3.321407	1.711885
31	1	2.075878	-4.030114	2.461919
32	1	2.416281	-3.800131	0.729674
33	1	3.467735	-3.065539	1.947118
34	6	-0.184171	-0.712024	2.463948

35	1	-0.949674	-0.398994	3.169038
36	8	2.189353	-1.640269	-0.473806
37	6	3.542667	-1.343167	-0.534887
38	8	4.130636	-0.841199	0.382105
39	6	4.136276	-1.810693	-1.868784
40	6	3.212887	-1.454105	-3.060193
41	1	3.039437	-0.375468	-3.122178
42	1	3.695854	-1.775296	-3.989001
43	1	2.245810	-1.959098	-2.986801
44	6	5.517181	-1.140956	-2.045657
45	1	5.965104	-1.487725	-2.982365
46	1	5.427260	-0.050633	-2.091506
47	1	6.192690	-1.395655	-1.223996
48	6	4.308402	-3.356029	-1.783943
49	1	4.790698	-3.707605	-2.701981
50	1	4.940644	-3.641830	-0.936196
51	1	3.342048	-3.861697	-1.692445
52	6	-0.792976	-0.671283	-1.023492
53	1	-1.141461	0.125101	-1.669041
54	1	-0.067318	-1.339146	-1.471094
55	6	-1.640919	-1.153301	-0.014846
56	6	-1.534860	-2.601037	0.418381
57	1	-0.517051	-2.985492	0.347079
58	1	-1.909207	-2.759634	1.432720
59	1	-2.152910	-3.202265	-0.262156
60	6	-2.982610	-0.488799	0.256859
61	1	-3.179879	-0.467718	1.334568
62	1	-2.964298	0.545595	-0.088149
63	6	-4.140384	-1.219140	-0.457422
64	1	-4.298444	-2.224119	-0.051761
65	1	-3.916118	-1.347185	-1.525250
66	6	-5.449287	-0.460499	-0.348649
67	8	-5.587470	0.652449	0.143045
68	8	-6.468845	-1.172595	-0.881723
69	6	-7.809211	-0.545621	-0.869268
70	1	-7.744001	0.403123	-1.408925
71	1	-8.076633	-0.340371	0.170879
72	6	-8.765304	-1.521695	-1.529769
73	1	-9.773429	-1.094072	-1.540707
74	1	-8.468906	-1.725020	-2.563568
75	1	-8.801750	-2.468956	-0.982696
76	6	0.631222	-2.440372	4.099041
77	6	1.806803	-2.602182	4.860978
78	6	-0.584998	-2.922791	4.623138
79	6	1.765081	-3.230675	6.110706
80	1	2.750631	-2.219172	4.484514
81	6	-0.624877	-3.548889	5.874679
82	1	-1.496586	-2.816748	4.043259
83	6	0.549715	-3.706299	6.621070
84	1	2.678039	-3.342627	6.686426
85	1	-1.569290	-3.917597	6.261500
86	1	0.519149	-4.194464	7.589458

TS30-31 (E = -2043.7207324 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.237444	0.403796	0.568231
2	6	1.122006	2.229854	-0.238675
3	6	1.615392	2.173886	1.149038
4	6	0.490148	2.255197	1.994573

5	6	-0.702499	2.369892	1.167576
6	6	-0.306778	2.434185	-0.208774
7	6	1.986593	2.418319	-1.437218
8	9	3.201754	1.784936	-1.337180
9	9	2.278197	3.759019	-1.641499
10	9	1.416622	1.978082	-2.606649
11	6	3.052060	2.153233	1.588076
12	1	3.128038	1.952081	2.658526
13	1	3.638184	1.403596	1.056899
14	1	3.503459	3.135734	1.396662
15	6	0.490893	2.286477	3.497476
16	1	0.448511	3.326284	3.847379
17	1	-0.376869	1.765387	3.910753
18	1	1.390199	1.827836	3.913978
19	6	-2.079610	2.638139	1.706615
20	1	-2.859121	2.446097	0.967057
21	1	-2.292413	2.036813	2.594821
22	1	-2.152341	3.693804	2.000255
23	6	-1.214946	2.755356	-1.363914
24	1	-1.194541	3.837790	-1.544500
25	1	-0.909714	2.254868	-2.283052
26	1	-2.248038	2.476718	-1.144850
27	6	1.352046	-2.186764	1.504619
28	7	1.469490	-1.271487	0.573438
29	6	0.302772	-1.851412	2.459096
30	6	2.134007	-3.468022	1.502853
31	1	1.747964	-4.154881	2.255549
32	1	2.076793	-3.947957	0.521331
33	1	3.192534	-3.278589	1.713843
34	6	-0.650951	-0.972322	1.961805
35	1	-1.393198	-0.611048	2.662518
36	8	2.230068	-1.655935	-0.555314
37	6	3.579948	-1.341708	-0.517527
38	8	4.094015	-0.857882	0.452275
39	6	4.266204	-1.763355	-1.821192
40	6	3.420144	-1.372719	-3.058846
41	1	3.246179	-0.292998	-3.097844
42	1	3.964222	-1.663649	-3.963429
43	1	2.452662	-1.882127	-3.063354
44	6	5.650489	-1.080492	-1.883477
45	1	6.163621	-1.396797	-2.797259
46	1	5.555263	0.010099	-1.903699
47	1	6.270709	-1.355682	-1.025528
48	6	4.444205	-3.309562	-1.773885
49	1	4.987908	-3.628532	-2.669172
50	1	5.022222	-3.618209	-0.895938
51	1	3.478123	-3.823540	-1.760847
52	6	-0.991382	-0.689901	-0.747071
53	1	-1.669132	-0.010945	-1.257054
54	1	-0.444072	-1.312838	-1.450650
55	6	-1.578223	-1.422555	0.411539
56	6	-1.449110	-2.946789	0.298027
57	1	-0.436363	-3.257872	0.038453
58	1	-1.759745	-3.452167	1.217088
59	1	-2.097689	-3.276085	-0.523203
60	6	-2.995920	-0.963481	0.807791
61	1	-3.276510	-1.407650	1.769233
62	1	-3.003743	0.121336	0.937094
63	6	-4.056636	-1.348968	-0.241874
64	1	-4.229945	-2.429189	-0.266906
65	1	-3.733752	-1.063478	-1.252349
66	6	-5.387499	-0.666343	0.015380
67	8	-5.566511	0.283343	0.767354

68	8	-6.373178	-1.233231	-0.717266
69	6	-7.724781	-0.641382	-0.602347
70	1	-7.660839	0.408554	-0.901059
71	1	-8.026627	-0.690022	0.447362
72	6	-8.642409	-1.444539	-1.505607
73	1	-9.657423	-1.037283	-1.449354
74	1	-8.311526	-1.395434	-2.547729
75	1	-8.677798	-2.494313	-1.197990
76	6	0.299791	-2.370876	3.835355
77	6	1.509578	-2.550864	4.545743
78	6	-0.919734	-2.654565	4.493072
79	6	1.496444	-2.995361	5.870097
80	1	2.456651	-2.312770	4.072620
81	6	-0.926088	-3.109841	5.813203
82	1	-1.858320	-2.541524	3.960840
83	6	0.280487	-3.279858	6.506460
84	1	2.432021	-3.115844	6.405304
85	1	-1.868980	-3.336295	6.298959
86	1	0.273096	-3.631593	7.532386

31 (E = -2043.7485758 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.178730	0.201452	0.942947
2	6	0.703143	2.126554	0.107690
3	6	1.679973	2.036381	1.203929
4	6	0.955749	1.978557	2.407034
5	6	-0.465518	2.035573	2.089455
6	6	-0.625848	2.250095	0.682885
7	6	1.056448	2.453147	-1.304152
8	9	2.208311	1.837153	-1.730850
9	9	1.270398	3.812194	-1.472178
10	9	0.080154	2.111340	-2.207043
11	6	3.175652	2.080093	1.065350
12	1	3.665476	1.795381	1.998018
13	1	3.537775	1.421658	0.275637
14	1	3.488558	3.102652	0.816514
15	6	1.507210	1.946615	3.802460
16	1	1.419829	2.943101	4.255593
17	1	0.957603	1.246755	4.437261
18	1	2.560478	1.660455	3.820044
19	6	-1.554623	2.118419	3.122866
20	1	-2.535685	1.884855	2.704580
21	1	-1.367088	1.439217	3.958663
22	1	-1.594570	3.138701	3.526388
23	6	-1.896087	2.670367	-0.003306
24	1	-1.917513	3.766023	-0.069142
25	1	-1.977378	2.275688	-1.016188
26	1	-2.774597	2.354883	0.563146
27	6	1.068455	-2.380158	1.338448
28	7	1.352448	-1.490484	0.460411
29	6	0.083155	-1.712460	2.259481
30	6	1.601678	-3.767520	1.459824
31	1	0.848509	-4.423292	1.903414
32	1	1.904719	-4.158562	0.486111
33	1	2.477767	-3.774526	2.119571
34	6	-1.194669	-1.354095	1.778462
35	1	-1.851043	-0.941072	2.537275
36	8	2.146960	-1.826384	-0.642300
37	6	3.519511	-1.657947	-0.447652

38	8	3.965479	-1.314632	0.609662
39	6	4.282973	-2.005966	-1.726389
40	6	3.744189	-1.163909	-2.913190
41	1	3.845043	-0.091099	-2.718263
42	1	4.326757	-1.403897	-3.808567
43	1	2.692944	-1.383908	-3.118449
44	6	5.779572	-1.705405	-1.495533
45	1	6.338464	-1.962073	-2.400974
46	1	5.944843	-0.645265	-1.278446
47	1	6.181216	-2.292666	-0.664099
48	6	4.085938	-3.520638	-2.019537
49	1	4.667069	-3.785035	-2.908934
50	1	4.441486	-4.137108	-1.186312
51	1	3.036121	-3.759314	-2.213264
52	6	-1.128745	-0.710405	-0.474920
53	1	-1.774687	0.046372	-0.914468
54	1	-0.544722	-1.186788	-1.262517
55	6	-1.880516	-1.700714	0.439665
56	6	-1.742478	-3.179781	0.027414
57	1	-0.698959	-3.483521	-0.087041
58	1	-2.215653	-3.836501	0.767638
59	1	-2.225985	-3.346299	-0.940996
60	6	-3.379180	-1.322729	0.595519
61	1	-3.809059	-1.925204	1.408031
62	1	-3.443132	-0.274928	0.912308
63	6	-4.218384	-1.509406	-0.675811
64	1	-4.365651	-2.567300	-0.915453
65	1	-3.712204	-1.066741	-1.546099
66	6	-5.585612	-0.860486	-0.579698
67	8	-5.929257	-0.037448	0.260168
68	8	-6.402237	-1.293756	-1.570082
69	6	-7.759623	-0.710388	-1.629588
70	1	-7.658915	0.372336	-1.745685
71	1	-8.259161	-0.915872	-0.678888
72	6	-8.471300	-1.353173	-2.806079
73	1	-9.484956	-0.946547	-2.886609
74	1	-7.945467	-1.149015	-3.744060
75	1	-8.547212	-2.437270	-2.675801
76	6	0.443558	-1.690466	3.706269
77	6	1.793287	-1.562679	4.099831
78	6	-0.541604	-1.847259	4.703242
79	6	2.145310	-1.584643	5.451897
80	1	2.565758	-1.425029	3.349010
81	6	-0.185105	-1.862351	6.056295
82	1	-1.580795	-1.985309	4.425608
83	6	1.156855	-1.731630	6.434832
84	1	3.186713	-1.483135	5.737522
85	1	-0.953808	-1.990157	6.810709
86	1	1.430963	-1.750481	7.484004

32 (E = -1917.031809 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.567464	0.694269	0.984186
2	6	1.302412	2.384845	-0.377414
3	6	1.769625	2.472276	1.004138
4	6	0.583315	2.682811	1.837954
5	6	-0.570445	2.596356	0.997114
6	6	-0.115277	2.445911	-0.378192
7	6	2.166345	2.383167	-1.594445

8	9	3.434602	1.922906	-1.358289
9	9	2.310736	3.662855	-2.100738
10	9	1.664523	1.625741	-2.626254
11	6	3.184638	2.592783	1.487810
12	1	3.234830	2.461367	2.570185
13	1	3.839939	1.859022	1.018827
14	1	3.563061	3.596071	1.250315
15	6	0.599031	3.017223	3.298960
16	1	0.755889	4.097460	3.415451
17	1	-0.347221	2.762412	3.780663
18	1	1.404424	2.501808	3.827054
19	6	-1.999795	2.826654	1.402754
20	1	-2.688033	2.214248	0.814949
21	1	-2.158486	2.595945	2.458268
22	1	-2.265608	3.879685	1.243234
23	6	-1.056222	2.374106	-1.540955
24	1	-1.481867	3.372605	-1.708554
25	1	-0.572316	2.045368	-2.458366
26	1	-1.891846	1.702192	-1.322204
27	6	1.458356	-2.019765	1.715110
28	7	1.740292	-1.071030	0.862748
29	6	0.636852	-1.553241	2.845403
30	6	1.895674	-3.437710	1.518530
31	1	1.383484	-4.102454	2.213120
32	1	1.694279	-3.757351	0.492626
33	1	2.976274	-3.532403	1.683936
34	6	0.118541	-0.308085	2.680041
35	1	-0.497720	0.119455	3.466609
36	8	2.353551	-1.507098	-0.333373
37	6	3.704267	-1.207072	-0.430780
38	8	4.299925	-0.652966	0.450772
39	6	4.288932	-1.744162	-1.742342
40	6	3.297987	-1.607456	-2.923545
41	1	3.022721	-0.562577	-3.095465
42	1	3.778303	-1.986395	-3.831683
43	1	2.384810	-2.184894	-2.755348
44	6	5.592217	-0.971272	-2.047065
45	1	6.040184	-1.373370	-2.961415
46	1	5.395040	0.094436	-2.202115
47	1	6.315547	-1.073327	-1.233176
48	6	4.616947	-3.248519	-1.504847
49	1	5.100477	-3.649493	-2.401782
50	1	5.302083	-3.377693	-0.659948
51	1	3.710007	-3.831990	-1.317919
52	6	0.432237	-2.382523	4.063362
53	6	1.519140	-2.985636	4.729811
54	6	-0.861260	-2.538146	4.600220
55	6	1.319492	-3.721484	5.898214
56	1	2.526771	-2.862907	4.347870
57	6	-1.067194	-3.272785	5.769746
58	1	-1.709526	-2.095739	4.089747
59	6	0.023898	-3.869765	6.415068
60	1	2.165788	-4.175090	6.400889
61	1	-2.069006	-3.388285	6.165355
62	6	-0.175831	-4.629712	7.690657
63	9	-1.458627	-5.096024	7.847750
64	9	0.084228	-3.854952	8.812000
65	9	0.656719	-5.722208	7.798401

33 (E = -2380.7868907 au)

Center Number	Atomic	Coordinates (Angstroms)		

	Number	X	Y	Z
1	77	0.136473	0.319569	0.730180
2	6	1.051727	2.175378	-0.234411
3	6	1.509926	2.082644	1.143777
4	6	0.350221	2.226069	1.975171
5	6	-0.813151	2.365975	1.136197
6	6	-0.365436	2.389675	-0.233093
7	6	1.924827	2.311183	-1.437105
8	9	3.172333	1.771105	-1.268134
9	9	2.124819	3.642187	-1.761089
10	9	1.397559	1.727459	-2.565369
11	6	2.928016	2.057288	1.642666
12	1	2.958231	1.819375	2.707634
13	1	3.542851	1.332268	1.111777
14	1	3.372231	3.051955	1.507415
15	6	0.354136	2.338634	3.472627
16	1	0.535647	3.385688	3.748089
17	1	-0.605073	2.044997	3.904035
18	1	1.137033	1.730133	3.929940
19	6	-2.186881	2.740387	1.623147
20	1	-2.952046	2.586688	0.860955
21	1	-2.475427	2.170799	2.510019
22	1	-2.195720	3.804533	1.892548
23	6	-1.233350	2.740940	-1.407420
24	1	-1.281722	3.835673	-1.478951
25	1	-0.842539	2.362337	-2.351498
26	1	-2.257007	2.382161	-1.281030
27	6	1.573143	-2.077007	1.713916
28	7	1.514319	-1.249924	0.698440
29	6	0.660512	-1.706183	2.783055
30	6	2.421636	-3.312943	1.708964
31	1	2.073157	-4.018981	2.463097
32	1	2.398524	-3.796096	0.729106
33	1	3.465370	-3.061893	1.932274
34	6	-0.181420	-0.687930	2.455441
35	1	-0.941662	-0.367961	3.163103
36	8	2.186189	-1.638642	-0.479301
37	6	3.541803	-1.345810	-0.542279
38	8	4.130080	-0.840999	0.372564
39	6	4.133863	-1.823098	-1.873036
40	6	3.210122	-1.475235	-3.066704
41	1	3.037048	-0.397076	-3.136954
42	1	3.692852	-1.803669	-3.993064
43	1	2.242947	-1.979452	-2.989396
44	6	5.515115	-1.155415	-2.055345
45	1	5.962405	-1.509467	-2.989593
46	1	5.425772	-0.065436	-2.109404
47	1	6.190816	-1.404392	-1.232106
48	6	4.305109	-3.367954	-1.776294
49	1	4.786696	-3.726607	-2.691925
50	1	4.937663	-3.647759	-0.926813
51	1	3.338501	-3.872373	-1.680651
52	6	-0.799982	-0.669768	-1.025046
53	1	-1.146795	0.124550	-1.673970
54	1	-0.075267	-1.340921	-1.469219
55	6	-1.649844	-1.146079	-0.016440
56	6	-1.544253	-2.590145	0.427617
57	1	-0.526729	-2.975949	0.360249
58	1	-1.921385	-2.741612	1.442044
59	1	-2.161385	-3.195767	-0.249845
60	6	-2.988583	-0.476330	0.255031
61	1	-3.184572	-0.450221	1.332769

62	1	-2.968328	0.556524	-0.094549
63	6	-4.148265	-1.208416	-0.454606
64	1	-4.303540	-2.213129	-0.047004
65	1	-3.928059	-1.337492	-1.523002
66	6	-5.457956	-0.451842	-0.340466
67	8	-5.598420	0.654333	0.165515
68	8	-6.474908	-1.158251	-0.885503
69	6	-7.816760	-0.534401	-0.867039
70	1	-7.752482	0.421917	-1.393229
71	1	-8.086712	-0.344418	0.175351
72	6	-8.769205	-1.503286	-1.543184
73	1	-9.778260	-1.077798	-1.550312
74	1	-8.470152	-1.691441	-2.579088
75	1	-8.804682	-2.458188	-1.009500
76	6	0.638035	-2.398679	4.101232
77	6	1.822207	-2.583662	4.845031
78	6	-0.580461	-2.840461	4.653329
79	6	1.789922	-3.193343	6.099416
80	1	2.769911	-2.232580	4.451416
81	6	-0.620474	-3.447351	5.910744
82	1	-1.499716	-2.721081	4.090738
83	6	0.567065	-3.629655	6.631145
84	1	2.709114	-3.325396	6.658546
85	1	-1.566048	-3.785151	6.317219
86	6	0.540468	-4.245812	7.995911
87	9	-0.592988	-4.983382	8.236695
88	9	0.595002	-3.295356	9.005684
89	9	1.611467	-5.083473	8.225124

TS33-34 (E = -2380.7466804 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.229261	0.383526	0.563386
2	6	1.146109	2.211463	-0.165658
3	6	1.618860	2.132517	1.230300
4	6	0.481621	2.201280	2.055357
5	6	-0.698668	2.339082	1.209964
6	6	-0.281653	2.433964	-0.157427
7	6	2.033030	2.420228	-1.346839
8	9	3.240063	1.774353	-1.241687
9	9	2.336281	3.762531	-1.511083
10	9	1.477371	2.012130	-2.533941
11	6	3.049247	2.083089	1.686446
12	1	3.108349	1.883038	2.758105
13	1	3.624236	1.318998	1.162783
14	1	3.525446	3.054189	1.497994
15	6	0.451830	2.193559	3.557957
16	1	0.360232	3.221610	3.931920
17	1	-0.402109	1.628277	3.941424
18	1	1.360672	1.760950	3.981057
19	6	-2.081767	2.606424	1.732687
20	1	-2.850761	2.431059	0.978111
21	1	-2.311367	1.994167	2.609002
22	1	-2.151877	3.658144	2.040876
23	6	-1.166110	2.793137	-1.319553
24	1	-1.131065	3.879232	-1.473599
25	1	-0.850414	2.310725	-2.244723
26	1	-2.205540	2.520486	-1.124438
27	6	1.336489	-2.224973	1.468473
28	7	1.454805	-1.307251	0.541491

29	6	0.293854	-1.885662	2.429117
30	6	2.109963	-3.511186	1.460531
31	1	1.745568	-4.186060	2.234630
32	1	2.013744	-4.005143	0.488686
33	1	3.176495	-3.326556	1.629954
34	6	-0.675624	-1.023064	1.939630
35	1	-1.410128	-0.661150	2.648038
36	8	2.205635	-1.691332	-0.591975
37	6	3.557521	-1.375926	-0.561036
38	8	4.075537	-0.897743	0.408960
39	6	4.233213	-1.786835	-1.873028
40	6	3.401038	-1.331175	-3.098440
41	1	3.264885	-0.245300	-3.106102
42	1	3.934754	-1.614614	-4.011518
43	1	2.416530	-1.806584	-3.116385
44	6	5.639191	-1.148738	-1.914777
45	1	6.143131	-1.455774	-2.836760
46	1	5.580478	-0.055518	-1.903532
47	1	6.248613	-1.468954	-1.064612
48	6	4.359208	-3.338589	-1.871266
49	1	4.891478	-3.649009	-2.776327
50	1	4.927568	-3.691699	-1.003781
51	1	3.376664	-3.820307	-1.871328
52	6	-1.007564	-0.664868	-0.765041
53	1	-1.693878	0.022318	-1.252047
54	1	-0.475139	-1.277800	-1.488537
55	6	-1.580918	-1.422621	0.392401
56	6	-1.444540	-2.943915	0.231361
57	1	-0.428421	-3.244128	-0.026663
58	1	-1.764016	-3.478416	1.130479
59	1	-2.081736	-3.248091	-0.607646
60	6	-3.006241	-0.987214	0.797033
61	1	-3.284546	-1.466289	1.742280
62	1	-3.023079	0.092619	0.964052
63	6	-4.063046	-1.346050	-0.264544
64	1	-4.199127	-2.428927	-0.351679
65	1	-3.764403	-0.991195	-1.259792
66	6	-5.415182	-0.732703	0.050243
67	8	-5.633811	0.099162	0.921719
68	8	-6.370869	-1.217224	-0.775193
69	6	-7.741338	-0.684331	-0.606766
70	1	-7.704169	0.397934	-0.758489
71	1	-8.057784	-0.884254	0.420494
72	6	-8.620455	-1.381492	-1.628548
73	1	-9.647742	-1.013125	-1.537634
74	1	-8.274692	-1.182067	-2.647661
75	1	-8.629915	-2.463940	-1.466941
76	6	0.328011	-2.367597	3.821626
77	6	1.557372	-2.521396	4.502508
78	6	-0.868871	-2.640906	4.519071
79	6	1.587847	-2.932447	5.833598
80	1	2.490624	-2.293478	4.000320
81	6	-0.841541	-3.057997	5.849907
82	1	-1.823639	-2.548941	4.014905
83	6	0.387455	-3.206386	6.506075
84	1	2.538585	-3.037641	6.343158
85	1	-1.768651	-3.274096	6.365968
86	6	0.439884	-3.619058	7.946994
87	9	-0.737449	-4.157252	8.399991
88	9	0.723132	-2.552860	8.785259
89	9	1.423182	-4.553058	8.194652

34 (E = -2380.7745303 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.148957	0.110207	0.997316
2	6	0.667962	2.064678	0.232336
3	6	1.665837	1.922474	1.302154
4	6	0.966426	1.822106	2.518305
5	6	-0.459319	1.903299	2.234363
6	6	-0.648321	2.171898	0.840116
7	6	0.993024	2.448236	-1.173068
8	9	2.126953	1.839991	-1.653594
9	9	1.217002	3.810591	-1.285055
10	9	-0.007920	2.155155	-2.065688
11	6	3.158643	1.959916	1.137786
12	1	3.663132	1.588424	2.031205
13	1	3.496861	1.372587	0.284281
14	1	3.478766	2.997613	0.975171
15	6	1.553824	1.742506	3.897242
16	1	1.535768	2.737692	4.361363
17	1	0.983292	1.070211	4.542699
18	1	2.590058	1.399129	3.882882
19	6	-1.527012	1.956655	3.291127
20	1	-2.515155	1.727439	2.887852
21	1	-1.319377	1.261982	4.108832
22	1	-1.563319	2.968296	3.716297
23	6	-1.930087	2.632848	0.202950
24	1	-1.949444	3.730528	0.202357
25	1	-2.031303	2.299182	-0.829720
26	1	-2.798710	2.285955	0.766252
27	6	0.997770	-2.495660	1.275577
28	7	1.310175	-1.571440	0.444237
29	6	0.007835	-1.847675	2.207453
30	6	1.501880	-3.896788	1.345489
31	1	0.707337	-4.565392	1.687433
32	1	1.872908	-4.231861	0.374831
33	1	2.322996	-3.963331	2.069451
34	6	-1.263765	-1.460302	1.729122
35	1	-1.927818	-1.075192	2.496314
36	8	2.121713	-1.862374	-0.656103
37	6	3.494853	-1.744010	-0.417082
38	8	3.919625	-1.481260	0.671116
39	6	4.280580	-2.019067	-1.699744
40	6	3.867594	-0.994478	-2.790974
41	1	4.069504	0.032492	-2.469001
42	1	4.453323	-1.188784	-3.695364
43	1	2.807071	-1.080463	-3.043136
44	6	5.785789	-1.881719	-1.385248
45	1	6.359801	-2.079852	-2.295909
46	1	6.029842	-0.873034	-1.037287
47	1	6.100629	-2.595384	-0.617509
48	6	3.966708	-3.462186	-2.184272
49	1	4.566927	-3.672055	-3.075435
50	1	4.223770	-4.204276	-1.420142
51	1	2.911504	-3.577632	-2.447568
52	6	-1.152077	-0.710860	-0.483939
53	1	-1.780951	0.078476	-0.888266
54	1	-0.560867	-1.150003	-1.287301
55	6	-1.929186	-1.738630	0.365156
56	6	-1.791114	-3.196397	-0.116815
57	1	-0.747658	-3.498182	-0.236414
58	1	-2.274911	-3.886892	0.584649
59	1	-2.264500	-3.313003	-1.097350

60	6	-3.428001	-1.358299	0.512511
61	1	-3.876680	-1.999223	1.284317
62	1	-3.491426	-0.328194	0.882742
63	6	-4.244660	-1.471693	-0.781866
64	1	-4.390154	-2.514341	-1.082203
65	1	-3.723067	-0.983354	-1.617793
66	6	-5.612547	-0.825929	-0.672721
67	8	-5.975096	-0.064741	0.216043
68	8	-6.405120	-1.183943	-1.711265
69	6	-7.760593	-0.594996	-1.760422
70	1	-7.657269	0.493422	-1.782516
71	1	-8.286698	-0.878559	-0.844727
72	6	-8.438102	-1.135918	-3.006267
73	1	-9.449659	-0.722957	-3.080731
74	1	-7.886407	-0.854017	-3.908582
75	1	-8.516179	-2.227047	-2.969881
76	6	0.344434	-1.898308	3.661430
77	6	1.685562	-1.780257	4.083588
78	6	-0.653866	-2.122485	4.629543
79	6	2.019287	-1.878888	5.433307
80	1	2.470320	-1.594104	3.357664
81	6	-0.324652	-2.214314	5.984246
82	1	-1.686623	-2.254709	4.329928
83	6	1.011915	-2.098068	6.384853
84	1	3.054407	-1.787434	5.740474
85	1	-1.103504	-2.394624	6.714901
86	6	1.375962	-2.164997	7.838309
87	9	0.437046	-2.814678	8.600358
88	9	1.517370	-0.905838	8.400121
89	9	2.575391	-2.804615	8.056888

35 (E = -1633.5270491 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.910487	0.388264	0.306804
2	6	-1.177574	-1.681469	-0.381640
3	6	-1.301406	-0.797263	-1.539064
4	6	-2.422348	0.054641	-1.295437
5	6	-2.993449	-0.286249	0.000157
6	6	-2.251498	-1.389223	0.538094
7	6	-0.259688	-2.853812	-0.282704
8	9	0.898475	-2.695293	-1.002106
9	9	-0.860058	-4.000287	-0.776681
10	9	0.119366	-3.150438	1.002306
11	6	-0.520638	-0.856465	-2.822271
12	1	-0.683585	0.045253	-3.415627
13	1	0.549552	-0.967605	-2.654469
14	1	-0.867221	-1.714603	-3.412666
15	6	-3.008232	1.041318	-2.263909
16	1	-3.738328	0.527993	-2.903238
17	1	-3.534760	1.847892	-1.748229
18	1	-2.249805	1.483571	-2.913839
19	6	-4.256396	0.284593	0.581121
20	1	-4.218626	0.299052	1.671742
21	1	-4.430378	1.306741	0.235904
22	1	-5.113809	-0.325187	0.267944
23	6	-2.583255	-2.113362	1.809829
24	1	-3.142977	-1.467939	2.487207
25	1	-3.205914	-2.984360	1.566078
26	1	-1.691531	-2.469125	2.325558

27	8	-0.193967	0.420844	2.302354
28	6	-0.954883	0.624627	3.341274
29	8	-2.159173	0.873229	3.307973
30	6	-0.210724	0.503909	4.666735
31	1	-0.606173	1.229783	5.382755
32	1	-0.382482	-0.499869	5.075285
33	1	0.865141	0.645319	4.543306
34	6	1.116004	2.436482	-0.304275
35	7	1.046270	1.198096	0.029970
36	6	-0.276791	2.968955	-0.429426
37	6	2.340773	3.267038	-0.499047
38	1	2.136209	4.312744	-0.257616
39	1	3.155556	2.903125	0.129544
40	1	2.672292	3.215481	-1.544334
41	6	-1.185365	2.559864	0.594234
42	1	-2.200209	2.931630	0.492497
43	1	-0.788751	2.667797	1.599413
44	8	2.244717	0.560531	0.369956
45	6	2.957798	-0.000074	-0.693647
46	8	2.607175	0.144908	-1.829165
47	6	4.196634	-0.729081	-0.171110
48	6	3.804681	-1.734929	0.942785
49	1	3.086043	-2.474548	0.576519
50	1	4.704935	-2.265803	1.269205
51	1	3.372717	-1.227054	1.809287
52	6	4.854371	-1.471494	-1.354550
53	1	5.748261	-1.991185	-0.995615
54	1	4.175024	-2.213690	-1.785747
55	1	5.152547	-0.777169	-2.145852
56	6	5.178975	0.333874	0.400140
57	1	6.093964	-0.172935	0.723551
58	1	5.451630	1.074378	-0.359945
59	1	4.752425	0.851651	1.264471
60	7	-0.583439	3.692684	-1.483090
61	1	-1.500173	4.119607	-1.573106
62	1	0.057992	3.833723	-2.256987

TS35-36 (E = -1633.5108702 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.968753	0.291412	0.236151
2	6	-1.108039	-1.827570	-0.464366
3	6	-1.278266	-0.918367	-1.594370
4	6	-2.452974	-0.135977	-1.334552
5	6	-2.994277	-0.530188	-0.045191
6	6	-2.175305	-1.597866	0.469832
7	6	-0.145757	-2.961235	-0.397641
8	9	1.014937	-2.734404	-1.095694
9	9	-0.689090	-4.116466	-0.940308
10	9	0.227200	-3.290733	0.882253
11	6	-0.509152	-0.912125	-2.885515
12	1	-0.699835	0.005345	-3.445603
13	1	0.564998	-1.000310	-2.731606
14	1	-0.840883	-1.758273	-3.501692
15	6	-3.092784	0.833711	-2.286620
16	1	-3.778957	0.290794	-2.949412
17	1	-3.673094	1.593164	-1.757962
18	1	-2.353697	1.343063	-2.908838
19	6	-4.287482	-0.041674	0.548750
20	1	-4.280322	-0.097383	1.639676

21	1	-4.488413	0.995214	0.269079
22	1	-5.121084	-0.655141	0.183183
23	6	-2.420506	-2.329592	1.758592
24	1	-3.200439	-1.840885	2.344243
25	1	-2.753789	-3.351264	1.537826
26	1	-1.517968	-2.394346	2.368274
27	8	-0.454388	0.295506	2.341086
28	6	-0.633772	1.246082	3.156180
29	8	-1.054701	2.399822	2.826083
30	6	-0.326653	0.996303	4.613670
31	1	0.441308	1.700525	4.950447
32	1	-1.226409	1.178229	5.210835
33	1	0.017888	-0.026465	4.768441
34	6	1.071941	2.453016	-0.136901
35	7	0.949823	1.173313	0.023998
36	6	-0.251834	3.105045	-0.284502
37	6	2.359643	3.213029	-0.146890
38	1	2.241417	4.168619	0.372387
39	1	3.160074	2.652226	0.333864
40	1	2.664274	3.422627	-1.180841
41	6	-1.319208	2.375782	0.227127
42	1	-2.312575	2.776430	0.030410
43	1	-1.175122	2.436518	1.568947
44	8	2.129406	0.478980	0.359474
45	6	2.850003	-0.027860	-0.717942
46	8	2.529374	0.191139	-1.851732
47	6	4.083878	-0.791925	-0.228924
48	6	3.751417	-1.703743	0.977863
49	1	2.982793	-2.438893	0.721922
50	1	4.657596	-2.244775	1.269390
51	1	3.407220	-1.124822	1.839142
52	6	4.626211	-1.635372	-1.404486
53	1	5.527378	-2.163829	-1.077787
54	1	3.892138	-2.378725	-1.732126
55	1	4.885002	-1.006656	-2.261314
56	6	5.145635	0.267350	0.191016
57	1	6.065983	-0.252329	0.476858
58	1	5.381270	0.946905	-0.635360
59	1	4.807425	0.854515	1.050667
60	7	-0.302402	4.321246	-0.852146
61	1	-1.190431	4.793047	-0.966186
62	1	0.523167	4.833323	-1.132556

36 (E = -1633.5225425 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	-0.950105	0.344001	0.125345
2	6	-1.075463	-1.849900	-0.466775
3	6	-1.246923	-0.968386	-1.618321
4	6	-2.443270	-0.196091	-1.385339
5	6	-2.966296	-0.543899	-0.082872
6	6	-2.130454	-1.589532	0.462034
7	6	-0.101127	-2.971380	-0.367599
8	9	1.031560	-2.776008	-1.117273
9	9	-0.652706	-4.159762	-0.822958
10	9	0.323159	-3.228098	0.914845
11	6	-0.494199	-1.003180	-2.918480
12	1	-0.713354	-0.115334	-3.514610
13	1	0.583200	-1.059494	-2.773718
14	1	-0.814624	-1.883057	-3.492044

15	6	-3.103174	0.716751	-2.378752
16	1	-3.746370	0.122375	-3.040400
17	1	-3.730811	1.462222	-1.885700
18	1	-2.373374	1.242538	-2.998091
19	6	-4.264772	-0.061959	0.506196
20	1	-4.241443	-0.068278	1.598643
21	1	-4.496632	0.955482	0.182405
22	1	-5.086995	-0.713262	0.182800
23	6	-2.382132	-2.265108	1.778141
24	1	-2.907031	-1.599135	2.465821
25	1	-3.024077	-3.139821	1.608335
26	1	-1.463107	-2.605216	2.253290
27	8	-0.435690	0.449818	2.276693
28	6	-0.708634	1.285867	3.147571
29	8	-1.266381	2.446097	2.887418
30	6	-0.415652	1.037124	4.595683
31	1	0.300640	1.782957	4.956799
32	1	-1.333013	1.150803	5.182367
33	1	-0.006845	0.036941	4.732156
34	6	1.091034	2.494709	-0.141516
35	7	0.982185	1.197591	-0.079344
36	6	-0.208539	3.164527	-0.260825
37	6	2.375413	3.258604	-0.087711
38	1	2.365999	3.946134	0.767348
39	1	3.245073	2.612229	0.002423
40	1	2.473268	3.864796	-0.995928
41	6	-1.285064	2.353068	-0.069719
42	1	-2.285618	2.771541	-0.168951
43	1	-1.355189	2.549081	1.905910
44	8	2.159497	0.498967	0.277397
45	6	2.852145	-0.068887	-0.778536
46	8	2.525855	0.098137	-1.921124
47	6	4.083007	-0.831032	-0.273309
48	6	3.777208	-1.624587	1.020567
49	1	2.973899	-2.350485	0.862461
50	1	4.677138	-2.171884	1.319870
51	1	3.491151	-0.962413	1.842346
52	6	4.553177	-1.790235	-1.389910
53	1	5.456681	-2.310829	-1.056634
54	1	3.788884	-2.540759	-1.616465
55	1	4.785829	-1.247124	-2.310302
56	6	5.191293	0.225980	0.009325
57	1	6.106982	-0.294658	0.308647
58	1	5.413814	0.819888	-0.884138
59	1	4.903905	0.900077	0.822732
60	7	-0.225386	4.510761	-0.646479
61	1	-1.147699	4.931372	-0.587074
62	1	0.456791	5.106442	-0.186070

37 (E = -1404.3590729 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	1.018419	0.462079	-0.047513
2	6	0.969411	-1.821717	-0.066025
3	6	1.109103	-1.334788	1.273086
4	6	2.350582	-0.555679	1.313547
5	6	2.939104	-0.564116	0.002778
6	6	2.062333	-1.327149	-0.862553
7	6	-0.060964	-2.763970	-0.590228
8	9	-1.059922	-3.038478	0.304076

9	9	0.505634	-3.983337	-0.921278
10	9	-0.677709	-2.321582	-1.741149
11	6	0.277472	-1.657582	2.480103
12	1	0.472345	-0.946441	3.284870
13	1	-0.789605	-1.645368	2.263718
14	1	0.543871	-2.659358	2.843127
15	6	2.959493	0.024061	2.555618
16	1	3.510100	-0.761894	3.089776
17	1	3.660349	0.827556	2.320191
18	1	2.198961	0.421729	3.231611
19	6	4.279184	-0.003109	-0.384859
20	1	4.289349	0.328549	-1.426151
21	1	4.553266	0.848337	0.242562
22	1	5.052673	-0.772552	-0.267029
23	6	2.331093	-1.623648	-2.307378
24	1	2.963398	-2.519394	-2.376642
25	1	1.414554	-1.810586	-2.868487
26	1	2.869639	-0.800888	-2.783162
27	6	-0.895571	2.683910	-0.460702
28	7	-0.918538	1.419927	-0.203171
29	6	0.469171	3.278578	-0.271982
30	6	-2.067690	3.499736	-0.896281
31	1	-1.854110	3.973127	-1.862409
32	1	-2.967707	2.898046	-0.998345
33	1	-2.254287	4.297897	-0.167824
34	6	1.488533	2.398032	-0.034041
35	1	2.489224	2.791203	0.128871
36	8	-2.123697	0.766316	-0.523909
37	6	-2.790660	0.228418	0.565806
38	8	-2.384658	0.356026	1.687203
39	6	-4.102465	-0.439096	0.139629
40	6	-4.096362	-0.894091	-1.337592
41	1	-3.293412	-1.611434	-1.532655
42	1	-5.051051	-1.382216	-1.559060
43	1	-3.980588	-0.049611	-2.022921
44	6	-4.354608	-1.649386	1.070978
45	1	-5.327281	-2.089193	0.828243
46	1	-3.588120	-2.419373	0.936749
47	1	-4.363814	-1.346473	2.121691
48	6	-5.217779	0.626679	0.360036
49	1	-6.186506	0.179245	0.114558
50	1	-5.245356	0.959400	1.402749
51	1	-5.073700	1.499576	-0.285638
52	7	0.555732	4.641858	-0.278864
53	1	1.480816	5.053956	-0.260565
54	1	-0.143083	5.204884	-0.745932

38 (E = -1868.1072956 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.109207	0.249952	0.725366
2	6	1.035397	2.136295	-0.150514
3	6	1.481890	2.005984	1.227597
4	6	0.316742	2.112132	2.051650
5	6	-0.842339	2.274396	1.208407
6	6	-0.385583	2.345278	-0.154643
7	6	1.918487	2.304855	-1.340812
8	9	3.158722	1.742424	-1.182427
9	9	2.139821	3.643525	-1.617797
10	9	1.393191	1.767508	-2.493170

11	6	2.894693	1.970971	1.739674
12	1	2.917588	1.667527	2.788079
13	1	3.526664	1.290265	1.172473
14	1	3.323904	2.979233	1.671797
15	6	0.306695	2.171288	3.551720
16	1	0.481425	3.208471	3.866575
17	1	-0.655397	1.857851	3.962483
18	1	1.087498	1.549007	3.993900
19	6	-2.222436	2.614818	1.702257
20	1	-2.979457	2.499733	0.925221
21	1	-2.515463	1.992032	2.551309
22	1	-2.241240	3.661396	2.032820
23	6	-1.240998	2.743934	-1.323473
24	1	-1.264502	3.840861	-1.369009
25	1	-0.854815	2.380039	-2.275283
26	1	-2.272382	2.404550	-1.209278
27	6	1.527781	-2.167711	1.673327
28	7	1.497668	-1.311013	0.684160
29	6	0.585592	-1.834705	2.729949
30	6	2.388526	-3.389723	1.714798
31	1	1.873313	-4.180104	2.266321
32	1	2.640267	-3.747668	0.716235
33	1	3.324353	-3.167024	2.243883
34	6	-0.251469	-0.811366	2.431303
35	1	-1.052549	-0.535561	3.112244
36	8	2.208587	-1.653902	-0.485534
37	6	3.562799	-1.356342	-0.500300
38	8	4.127875	-0.893815	0.451128
39	6	4.189416	-1.773687	-1.836040
40	6	3.271069	-1.430627	-3.034942
41	1	3.058280	-0.358289	-3.080992
42	1	3.779634	-1.717056	-3.961473
43	1	2.322401	-1.972231	-2.985879
44	6	5.547761	-1.051623	-1.981816
45	1	6.022186	-1.369953	-2.915585
46	1	5.418342	0.035162	-2.016211
47	1	6.219212	-1.292352	-1.152711
48	6	4.417108	-3.313244	-1.775323
49	1	4.922177	-3.630799	-2.693547
50	1	5.050062	-3.590393	-0.925247
51	1	3.468756	-3.855551	-1.705363
52	6	-0.768951	-0.662428	-1.086662
53	1	-1.109778	0.149939	-1.715842
54	1	-0.031081	-1.311835	-1.541796
55	6	-1.628022	-1.179269	-0.102490
56	6	-1.518392	-2.639468	0.287788
57	1	-0.498838	-3.016844	0.204509
58	1	-1.889107	-2.826602	1.298973
59	1	-2.134540	-3.224204	-0.408480
60	6	-2.979099	-0.534779	0.174971
61	1	-3.176063	-0.537037	1.253279
62	1	-2.971723	0.506441	-0.149617
63	6	-4.134292	-1.261071	-0.547623
64	1	-4.268540	-2.282502	-0.177723
65	1	-3.924858	-1.344294	-1.623359
66	6	-5.453421	-0.528788	-0.391446
67	8	-5.589382	0.603232	0.055683
68	8	-6.486635	-1.286863	-0.826396
69	6	-7.837565	-0.686570	-0.761741
70	1	-7.832234	0.224771	-1.366028
71	1	-8.038129	-0.416547	0.278629
72	6	-8.813155	-1.723294	-1.287574
73	1	-9.829559	-1.316792	-1.256131

74	1	-8.583793	-1.990848	-2.323768
75	1	-8.789302	-2.631625	-0.677391
76	7	0.514662	-2.683860	3.861551
77	1	-0.168731	-2.347514	4.534725
78	1	1.407296	-2.789017	4.339847

TS38-39 (E = -1868.082908 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.228922	0.386133	0.526181
2	6	1.138504	2.229155	-0.438315
3	6	1.606562	2.152051	0.946786
4	6	0.459802	2.266448	1.787831
5	6	-0.714208	2.388586	0.947779
6	6	-0.281697	2.415930	-0.424057
7	6	2.004608	2.378348	-1.635552
8	9	3.245160	1.802683	-1.487915
9	9	2.250862	3.714030	-1.932002
10	9	1.468159	1.843459	-2.784920
11	6	3.032538	2.158357	1.425229
12	1	3.087671	1.889468	2.482016
13	1	3.665970	1.470047	0.868431
14	1	3.446249	3.169536	1.312532
15	6	0.458125	2.348332	3.289482
16	1	0.491091	3.399449	3.605360
17	1	-0.446481	1.902861	3.711618
18	1	1.320216	1.838893	3.726335
19	6	-2.100570	2.704855	1.442937
20	1	-2.870790	2.416132	0.724065
21	1	-2.315912	2.201894	2.389399
22	1	-2.194709	3.785489	1.613868
23	6	-1.173400	2.690171	-1.603634
24	1	-1.123983	3.760083	-1.844577
25	1	-0.873199	2.132705	-2.491471
26	1	-2.215699	2.454404	-1.378875
27	6	1.251628	-2.275011	1.318849
28	7	1.425671	-1.275042	0.481292
29	6	0.163960	-2.009790	2.240439
30	6	2.033680	-3.552671	1.316710
31	1	1.389291	-4.394868	1.585671
32	1	2.473779	-3.756323	0.340683
33	1	2.847219	-3.499792	2.051862
34	6	-0.606253	-0.903094	1.906612
35	1	-1.396331	-0.605769	2.588013
36	8	2.339693	-1.507471	-0.573505
37	6	3.680789	-1.319204	-0.281278
38	8	4.060118	-1.015849	0.816048
39	6	4.560480	-1.622433	-1.500988
40	6	3.824109	-1.404749	-2.842937
41	1	3.475602	-0.373280	-2.946158
42	1	4.519002	-1.614303	-3.662758
43	1	2.965019	-2.073507	-2.946264
44	6	5.815380	-0.719859	-1.423865
45	1	6.483745	-0.968203	-2.254529
46	1	5.549141	0.339114	-1.504223
47	1	6.356851	-0.871551	-0.485953
48	6	4.987938	-3.115822	-1.376486
49	1	5.685491	-3.349783	-2.187473
50	1	5.492174	-3.308014	-0.423653
51	1	4.128378	-3.788623	-1.467303

52	6	-1.166609	-0.684405	-0.751995
53	1	-1.815662	0.084698	-1.160972
54	1	-0.613102	-1.213399	-1.524543
55	6	-1.798909	-1.540866	0.237214
56	6	-1.612006	-3.034183	0.108745
57	1	-0.616103	-3.297285	-0.253082
58	1	-1.824125	-3.565790	1.040263
59	1	-2.323736	-3.390467	-0.650999
60	6	-3.140156	-1.101167	0.809628
61	1	-3.345611	-1.635430	1.743127
62	1	-3.116225	-0.032304	1.036015
63	6	-4.290326	-1.371612	-0.187035
64	1	-4.424102	-2.443836	-0.366699
65	1	-4.079541	-0.917215	-1.163667
66	6	-5.612926	-0.815307	0.307342
67	8	-5.768106	-0.142012	1.317743
68	8	-6.621387	-1.156379	-0.526616
69	6	-7.976511	-0.670582	-0.181661
70	1	-7.945246	0.421879	-0.147521
71	1	-8.226649	-1.046357	0.814141
72	6	-8.921692	-1.188936	-1.249697
73	1	-9.940015	-0.850847	-1.030652
74	1	-8.642329	-0.813827	-2.239213
75	1	-8.923135	-2.283070	-1.276922
76	7	-0.107968	-2.892218	3.250885
77	1	-0.743610	-2.581391	3.975761
78	1	0.626668	-3.502613	3.586669

39 (E = -1868.1058286 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.217757	0.472990	0.725240
2	6	0.860239	2.333232	-0.220943
3	6	1.735903	2.293732	0.959630
4	6	0.912903	2.317933	2.098051
5	6	-0.476864	2.386929	1.655568
6	6	-0.511142	2.499890	0.229285
7	6	1.336164	2.571855	-1.610119
8	9	2.524969	1.940386	-1.896020
9	9	1.566555	3.921393	-1.850029
10	9	0.446925	2.171428	-2.578349
11	6	3.239203	2.312642	0.948001
12	1	3.641753	2.118385	1.943966
13	1	3.658959	1.576128	0.262761
14	1	3.589441	3.303218	0.629714
15	6	1.342229	2.324081	3.538590
16	1	1.233261	3.330893	3.962695
17	1	0.728532	1.648072	4.142892
18	1	2.386011	2.023190	3.654329
19	6	-1.643989	2.569071	2.586882
20	1	-2.595201	2.337284	2.103755
21	1	-1.549836	1.939864	3.476250
22	1	-1.682939	3.613576	2.923151
23	6	-1.716143	2.849568	-0.600518
24	1	-1.729143	3.932138	-0.781991
25	1	-1.711300	2.347360	-1.568603
26	1	-2.640724	2.587440	-0.081468
27	6	1.239420	-2.074469	1.490998
28	7	1.396707	-1.259265	0.511312
29	6	0.204374	-1.478199	2.392235

30	6	1.921530	-3.379744	1.731491
31	1	1.262875	-4.058618	2.277798
32	1	2.222995	-3.842255	0.789511
33	1	2.824996	-3.224699	2.336091
34	6	-1.013811	-1.006006	1.844356
35	1	-1.662950	-0.570615	2.601052
36	8	2.167619	-1.678602	-0.583208
37	6	3.541237	-1.463636	-0.468267
38	8	4.026946	-1.024424	0.534681
39	6	4.257975	-1.913656	-1.742700
40	6	3.550047	-1.353583	-3.002969
41	1	3.510801	-0.259708	-2.985050
42	1	4.114706	-1.660750	-3.889307
43	1	2.530416	-1.737042	-3.096778
44	6	5.716651	-1.410132	-1.681213
45	1	6.248117	-1.746251	-2.577117
46	1	5.758681	-0.316485	-1.647460
47	1	6.238297	-1.801787	-0.803017
48	6	4.235600	-3.469828	-1.772054
49	1	4.790733	-3.812389	-2.651314
50	1	4.714105	-3.892727	-0.881743
51	1	3.213387	-3.853782	-1.842963
52	6	-1.109072	-0.624121	-0.506605
53	1	-1.819293	0.044871	-0.991776
54	1	-0.565824	-1.179678	-1.272952
55	6	-1.757328	-1.518556	0.573483
56	6	-1.590595	-3.031370	0.322196
57	1	-0.542723	-3.313447	0.186602
58	1	-2.001854	-3.614458	1.155848
59	1	-2.114135	-3.323020	-0.594676
60	6	-3.257527	-1.170543	0.781565
61	1	-3.615760	-1.679463	1.687288
62	1	-3.338465	-0.092963	0.969917
63	6	-4.164435	-1.537031	-0.400895
64	1	-4.273456	-2.621822	-0.507637
65	1	-3.737368	-1.180188	-1.348772
66	6	-5.556606	-0.948016	-0.285350
67	8	-5.923707	-0.132832	0.552141
68	8	-6.372527	-1.434880	-1.252274
69	6	-7.761052	-0.928950	-1.282504
70	1	-7.724568	0.157601	-1.400494
71	1	-8.227957	-1.161452	-0.321383
72	6	-8.460365	-1.611962	-2.443817
73	1	-9.497314	-1.264559	-2.501896
74	1	-7.967740	-1.378035	-3.392846
75	1	-8.470572	-2.698634	-2.313137
76	7	0.486732	-1.445339	3.706320
77	1	-0.194343	-1.072835	4.357498
78	1	1.442103	-1.482062	4.041064

40 (E = -1663.4798623 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.128616	0.252618	0.735154
2	6	1.017390	2.138778	-0.203234
3	6	1.469939	2.035909	1.176603
4	6	0.304130	2.146621	2.002805
5	6	-0.857093	2.276910	1.159523
6	6	-0.403462	2.324875	-0.206813
7	6	1.893964	2.304413	-1.397818

8	9	3.149678	1.781413	-1.228896
9	9	2.077676	3.642997	-1.705033
10	9	1.384078	1.728553	-2.538672
11	6	2.885639	2.035584	1.683959
12	1	2.914261	1.783862	2.745908
13	1	3.519673	1.330717	1.148720
14	1	3.309285	3.041306	1.565053
15	6	0.296286	2.240805	3.501727
16	1	0.451049	3.287927	3.793026
17	1	-0.658498	1.917803	3.922160
18	1	1.089868	1.643900	3.955939
19	6	-2.239683	2.619396	1.645884
20	1	-2.991891	2.495868	0.865228
21	1	-2.535881	2.006447	2.500944
22	1	-2.261922	3.669775	1.964018
23	6	-1.272989	2.670680	-1.382108
24	1	-1.346497	3.764591	-1.443481
25	1	-0.868893	2.309798	-2.327597
26	1	-2.288264	2.285510	-1.265087
27	6	1.591721	-2.131320	1.696208
28	7	1.527716	-1.295503	0.688124
29	6	0.665103	-1.799966	2.762772
30	6	0.641950	-2.583968	4.058470
31	1	-0.095961	-2.151015	4.740254
32	1	0.372988	-3.635709	3.898247
33	1	1.617355	-2.565723	4.559788
34	6	2.493167	-3.326652	1.738514
35	1	2.008577	-4.145599	2.275266
36	1	2.768667	-3.671298	0.741892
37	1	3.412460	-3.073857	2.282280
38	6	-0.178712	-0.785042	2.453394
39	1	-0.960145	-0.495209	3.152170
40	8	2.238662	-1.632653	-0.484936
41	6	3.586284	-1.312811	-0.505202
42	8	4.146334	-0.831740	0.440599
43	6	4.222352	-1.732126	-1.836293
44	6	3.293248	-1.437501	-3.039234
45	1	3.046930	-0.373273	-3.102336
46	1	3.809847	-1.722677	-3.961707
47	1	2.361972	-2.007469	-2.980099
48	6	5.558420	-0.972057	-1.995577
49	1	6.041616	-1.289612	-2.925156
50	1	5.396502	0.109709	-2.045851
51	1	6.237392	-1.180134	-1.163811
52	6	4.497769	-3.262693	-1.750381
53	1	5.008109	-3.580602	-2.665586
54	1	5.143123	-3.505006	-0.898963
55	1	3.567154	-3.832994	-1.665817
56	6	-0.799710	-0.738974	-1.019810
57	1	-1.163511	0.053459	-1.662101
58	1	-0.065416	-1.393885	-1.473398
59	6	-1.642843	-1.242431	-0.018088
60	6	-1.504492	-2.687007	0.413648
61	1	-0.482221	-3.055128	0.321411
62	1	-1.856177	-2.850102	1.435617
63	1	-2.129119	-3.294762	-0.254620
64	6	-2.995402	-0.607986	0.259794
65	1	-3.184005	-0.591535	1.340868
66	1	-2.992444	0.429074	-0.086806
67	6	-4.160600	-1.353678	-0.442994
68	1	-4.259648	-2.367505	-0.034555
69	1	-3.931152	-1.461005	-1.513147
70	6	-5.501737	-0.614705	-0.280342

71	1	-5.717001	-0.488998	0.790194
72	1	-5.409961	0.398738	-0.695598
73	6	-6.671447	-1.344714	-0.959042
74	1	-6.807240	-2.348417	-0.537824
75	1	-7.610634	-0.795891	-0.827704
76	1	-6.494889	-1.455126	-2.036079

TS40-41 (E = -1663.4394018 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.201722	0.401328	0.518853
2	6	1.088787	2.214638	-0.282078
3	6	1.570698	2.204080	1.113146
4	6	0.438218	2.277778	1.941335
5	6	-0.751202	2.355851	1.098557
6	6	-0.343774	2.409887	-0.273485
7	6	1.965517	2.394398	-1.473254
8	9	3.181449	1.764913	-1.354067
9	9	2.256856	3.734075	-1.686234
10	9	1.410129	1.942076	-2.644744
11	6	3.004498	2.212440	1.562380
12	1	3.074218	2.060417	2.641437
13	1	3.598306	1.442356	1.069634
14	1	3.453737	3.186980	1.329855
15	6	0.417918	2.330911	3.443504
16	1	0.330650	3.372899	3.778333
17	1	-0.434708	1.782789	3.853754
18	1	1.328724	1.913478	3.878200
19	6	-2.136331	2.615692	1.622131
20	1	-2.904226	2.420254	0.871126
21	1	-2.357084	2.009883	2.505454
22	1	-2.219684	3.670152	1.917334
23	6	-1.239709	2.710248	-1.443855
24	1	-1.213814	3.788233	-1.648772
25	1	-0.928446	2.187480	-2.348520
26	1	-2.275487	2.439201	-1.228115
27	6	1.337899	-2.162607	1.501731
28	7	1.448415	-1.274797	0.547089
29	6	0.282391	-1.813841	2.443157
30	6	0.321784	-2.327993	3.855973
31	1	-0.475315	-1.876367	4.451164
32	1	0.186276	-3.418233	3.880003
33	1	1.284632	-2.113940	4.335480
34	6	2.176278	-3.398147	1.624098
35	1	1.615351	-4.198520	2.111312
36	1	2.522510	-3.749192	0.651561
37	1	3.057223	-3.183019	2.242903
38	6	-0.699514	-0.987705	1.940153
39	1	-1.447010	-0.640521	2.643707
40	8	2.247738	-1.649116	-0.558234
41	6	3.590063	-1.313729	-0.478479
42	8	4.066271	-0.823968	0.507752
43	6	4.326483	-1.726373	-1.757735
44	6	3.495519	-1.405700	-3.024726
45	1	3.269093	-0.337208	-3.092782
46	1	4.077242	-1.688209	-3.908327
47	1	2.554930	-1.962925	-3.042611
48	6	5.678420	-0.979616	-1.801868
49	1	6.229292	-1.291711	-2.694900
50	1	5.532364	0.104409	-1.850662

51	1	6.288228	-1.205630	-0.922450
52	6	4.578079	-3.260838	-1.669449
53	1	5.155601	-3.573552	-2.545581
54	1	5.151948	-3.520352	-0.772976
55	1	3.637835	-3.821424	-1.665163
56	6	-1.026311	-0.724891	-0.756143
57	1	-1.723004	-0.070660	-1.273222
58	1	-0.480917	-1.353902	-1.456915
59	6	-1.603485	-1.455993	0.413606
60	6	-1.456205	-2.980518	0.310322
61	1	-0.435739	-3.284118	0.070797
62	1	-1.777890	-3.478724	1.230193
63	1	-2.090116	-3.320763	-0.517171
64	6	-3.034288	-1.022720	0.796633
65	1	-3.304835	-1.471381	1.760928
66	1	-3.051422	0.064812	0.926021
67	6	-4.105442	-1.418351	-0.246992
68	1	-4.189768	-2.511168	-0.305019
69	1	-3.807479	-1.068720	-1.244863
70	6	-5.486923	-0.831517	0.102955
71	1	-5.775969	-1.162087	1.110510
72	1	-5.413686	0.264076	0.149565
73	6	-6.577147	-1.232937	-0.902968
74	1	-6.694734	-2.322837	-0.942618
75	1	-7.546216	-0.800786	-0.629712
76	1	-6.327999	-0.886451	-1.913591

41 (E = -1663.4688728 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.229055	0.400968	0.821611
2	6	0.768071	2.249049	-0.171100
3	6	1.686892	2.284216	0.978353
4	6	0.899895	2.319568	2.141509
5	6	-0.504341	2.324915	1.746894
6	6	-0.590041	2.400824	0.319556
7	6	1.194892	2.443948	-1.586688
8	9	2.382449	1.818279	-1.883865
9	9	1.392423	3.784569	-1.877620
10	9	0.280681	1.990109	-2.504889
11	6	3.185981	2.366276	0.919732
12	1	3.624566	2.212962	1.907366
13	1	3.617615	1.632583	0.239585
14	1	3.480785	3.364412	0.569930
15	6	1.389361	2.414387	3.559267
16	1	1.398482	3.464484	3.879814
17	1	0.739086	1.869751	4.248746
18	1	2.402844	2.021907	3.669038
19	6	-1.655250	2.503025	2.698957
20	1	-2.596069	2.146680	2.274330
21	1	-1.486255	1.978766	3.642677
22	1	-1.772674	3.570021	2.929772
23	6	-1.831683	2.716367	-0.467595
24	1	-1.902967	3.804092	-0.598285
25	1	-1.826317	2.260894	-1.457930
26	1	-2.728384	2.385377	0.060652
27	6	1.192112	-2.084786	1.500165
28	7	1.459233	-1.296493	0.525485
29	6	0.163548	-1.348023	2.306621
30	6	0.478450	-1.155446	3.775922

31	1	-0.249967	-0.491641	4.247137
32	1	0.427543	-2.125028	4.289082
33	1	1.482507	-0.748523	3.927912
34	6	1.790478	-3.410017	1.824035
35	1	1.024155	-4.090008	2.206601
36	1	2.274422	-3.855071	0.953171
37	1	2.542961	-3.283977	2.613575
38	6	-1.121673	-1.118702	1.779017
39	1	-1.812087	-0.675332	2.491556
40	8	2.260794	-1.743724	-0.534462
41	6	3.612819	-1.423224	-0.434983
42	8	4.061094	-0.873923	0.530656
43	6	4.364784	-1.911702	-1.674826
44	6	3.672755	-1.398164	-2.964559
45	1	3.630679	-0.304221	-2.985319
46	1	4.250307	-1.733621	-3.832142
47	1	2.655503	-1.788055	-3.058449
48	6	5.814440	-1.385537	-1.602626
49	1	6.367744	-1.742416	-2.477047
50	1	5.840656	-0.290983	-1.602957
51	1	6.324586	-1.741104	-0.702430
52	6	4.363045	-3.467494	-1.657248
53	1	4.945498	-3.830123	-2.510425
54	1	4.822997	-3.855948	-0.741601
55	1	3.348367	-3.867981	-1.740850
56	6	-1.028732	-0.677239	-0.523298
57	1	-1.699019	0.015645	-1.026670
58	1	-0.417395	-1.192846	-1.264244
59	6	-1.756835	-1.614570	0.462015
60	6	-1.531625	-3.115628	0.191670
61	1	-0.470795	-3.372810	0.130007
62	1	-1.991425	-3.726544	0.978430
63	1	-1.981666	-3.393643	-0.766851
64	6	-3.278037	-1.304857	0.542955
65	1	-3.693875	-1.845637	1.407092
66	1	-3.393675	-0.231893	0.757864
67	6	-4.098598	-1.649704	-0.713357
68	1	-4.122204	-2.737666	-0.861570
69	1	-3.616962	-1.222388	-1.605184
70	6	-5.547833	-1.132565	-0.631360
71	1	-6.026070	-1.540606	0.270718
72	1	-5.535321	-0.040944	-0.501626
73	6	-6.386813	-1.494687	-1.866701
74	1	-6.445467	-2.582388	-1.997854
75	1	-7.410001	-1.112136	-1.779679
76	1	-5.947084	-1.072076	-2.778815

42 (E = -3042.231943 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.116988	0.239618	0.728766
2	6	1.007602	2.129681	-0.194769
3	6	1.454237	2.025980	1.186497
4	6	0.284478	2.131683	2.007401
5	6	-0.873167	2.262600	1.159391
6	6	-0.413863	2.314866	-0.204780
7	6	1.889024	2.301087	-1.385752
8	9	3.145509	1.782330	-1.212465
9	9	2.067970	3.640748	-1.688423
10	9	1.385439	1.725392	-2.529270

11	6	2.867369	2.026172	1.700436
12	1	2.891802	1.769574	2.761291
13	1	3.505544	1.325584	1.164560
14	1	3.288875	3.033548	1.588147
15	6	0.269473	2.222209	3.506311
16	1	0.421042	3.269152	3.799950
17	1	-0.686629	1.896926	3.921895
18	1	1.062317	1.626244	3.962946
19	6	-2.257750	2.603138	1.641790
20	1	-3.004552	2.500180	0.852893
21	1	-2.564356	1.976422	2.483104
22	1	-2.276256	3.647446	1.979304
23	6	-1.276531	2.665944	-1.383524
24	1	-1.345027	3.760255	-1.443224
25	1	-0.869351	2.305325	-2.327762
26	1	-2.294228	2.285466	-1.272700
27	6	1.597489	-2.132925	1.692475
28	7	1.525752	-1.300396	0.682588
29	6	0.668586	-1.806715	2.759508
30	6	0.652055	-2.589512	4.055919
31	1	-0.088926	-2.161811	4.737591
32	1	0.391530	-3.643435	3.896567
33	1	1.627602	-2.562847	4.556487
34	6	2.507492	-3.321427	1.736723
35	1	2.028305	-4.143158	2.274065
36	1	2.786230	-3.665195	0.740759
37	1	3.424358	-3.061284	2.281096
38	6	-0.182878	-0.798976	2.450491
39	1	-0.966761	-0.514829	3.148655
40	8	2.238906	-1.632488	-0.489787
41	6	3.586096	-1.306798	-0.508992
42	8	4.142638	-0.823764	0.437589
43	6	4.224511	-1.723156	-1.839711
44	6	3.294437	-1.433299	-3.043070
45	1	3.042482	-0.370398	-3.106266
46	1	3.813120	-1.715590	-3.965231
47	1	2.366255	-2.008371	-2.984689
48	6	5.556921	-0.956558	-1.998468
49	1	6.042193	-1.272231	-2.927587
50	1	5.389740	0.124364	-2.049422
51	1	6.236399	-1.160956	-1.166210
52	6	4.507385	-3.252382	-1.753360
53	1	5.019218	-3.567865	-2.668552
54	1	5.154060	-3.491314	-0.901999
55	1	3.579620	-3.827295	-1.668737
56	6	-0.790261	-0.741353	-1.037875
57	1	-1.156782	0.049991	-1.679825
58	1	-0.053331	-1.393082	-1.491353
59	6	-1.625531	-1.245661	-0.028561
60	6	-1.489685	-2.693799	0.395823
61	1	-0.466419	-3.059626	0.307171
62	1	-1.844745	-2.862359	1.415708
63	1	-2.107835	-3.301573	-0.278423
64	6	-2.984137	-0.616296	0.245428
65	1	-3.179781	-0.608705	1.324864
66	1	-2.981705	0.422456	-0.094248
67	6	-4.133328	-1.370663	-0.476172
68	1	-4.230720	-2.382943	-0.072582
69	1	-3.895958	-1.459912	-1.542513
70	6	-5.459322	-0.613355	-0.295991
71	1	-5.694008	-0.513242	0.768608
72	1	-5.375128	0.397868	-0.706310
73	6	-6.684801	-1.253187	-0.957572

74	17	-8.150276	-0.208986	-0.644108
75	17	-6.468122	-1.396624	-2.761194
76	17	-7.017272	-2.912117	-0.281477

TS42-43 (E = -3042.1914008 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.196936	0.394041	0.514737
2	6	1.081592	2.209296	-0.288896
3	6	1.558655	2.196508	1.107555
4	6	0.422821	2.270328	1.932794
5	6	-0.763127	2.349059	1.086338
6	6	-0.350735	2.402249	-0.284522
7	6	1.961418	2.389553	-1.477978
8	9	3.178969	1.764649	-1.353471
9	9	2.248049	3.729613	-1.692732
10	9	1.410848	1.932411	-2.649778
11	6	2.990435	2.207675	1.562707
12	1	3.056458	2.048806	2.640963
13	1	3.589886	1.443855	1.067368
14	1	3.435632	3.186019	1.338475
15	6	0.399048	2.324715	3.434797
16	1	0.316657	3.367592	3.768030
17	1	-0.457331	1.781626	3.843702
18	1	1.306638	1.903052	3.872056
19	6	-2.150545	2.608564	1.603924
20	1	-2.915380	2.409767	0.850539
21	1	-2.373571	2.006705	2.489378
22	1	-2.236701	3.664116	1.894237
23	6	-1.243158	2.700318	-1.458028
24	1	-1.217487	3.778194	-1.663443
25	1	-0.928231	2.177540	-2.361390
26	1	-2.279509	2.428953	-1.245704
27	6	1.341197	-2.166888	1.499224
28	7	1.450457	-1.276401	0.546222
29	6	0.281928	-1.825389	2.438069
30	6	0.311936	-2.351235	3.846647
31	1	-0.491697	-1.908004	4.439328
32	1	0.181584	-3.442230	3.860845
33	1	1.269997	-2.136556	4.335467
34	6	2.184007	-3.399365	1.621115
35	1	1.620992	-4.206582	2.094594
36	1	2.544367	-3.740697	0.650395
37	1	3.055718	-3.185179	2.253143
38	6	-0.695808	-0.993686	1.935767
39	1	-1.448645	-0.652274	2.636492
40	8	2.254506	-1.643979	-0.557385
41	6	3.596690	-1.307576	-0.470837
42	8	4.067878	-0.820968	0.519216
43	6	4.339186	-1.715664	-1.747955
44	6	3.510048	-1.402772	-3.017965
45	1	3.276311	-0.336053	-3.088516
46	1	4.096690	-1.682501	-3.899186
47	1	2.573524	-1.966726	-3.038204
48	6	5.686000	-0.959336	-1.788748
49	1	6.241644	-1.268382	-2.679864
50	1	5.532454	0.123579	-1.839092
51	1	6.294766	-1.180269	-0.907341
52	6	4.601566	-3.248239	-1.656854

53	1	5.184282	-3.557706	-2.530680
54	1	5.174262	-3.502500	-0.758144
55	1	3.665386	-3.815643	-1.655292
56	6	-1.020618	-0.735379	-0.770612
57	1	-1.714380	-0.080048	-1.290068
58	1	-0.469951	-1.362726	-1.468267
59	6	-1.596724	-1.465494	0.397840
60	6	-1.447109	-2.989711	0.299257
61	1	-0.425074	-3.290509	0.063835
62	1	-1.770367	-3.487000	1.218849
63	1	-2.075172	-3.334790	-0.530946
64	6	-3.027641	-1.032651	0.783147
65	1	-3.299862	-1.484938	1.744561
66	1	-3.045382	0.054133	0.914406
67	6	-4.087247	-1.434492	-0.271790
68	1	-4.172047	-2.524172	-0.323469
69	1	-3.786410	-1.079723	-1.263031
70	6	-5.451853	-0.831205	0.104216
71	1	-5.751064	-1.167094	1.102263
72	1	-5.385377	0.260857	0.136131
73	6	-6.610479	-1.173080	-0.838888
74	17	-8.133061	-0.364847	-0.236188
75	17	-6.287465	-0.580261	-2.531558
76	17	-6.910586	-2.969066	-0.901963

43 (E = -3042.2219713 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.225753	0.400481	0.816456
2	6	0.766451	2.248441	-0.174372
3	6	1.684058	2.280729	0.975997
4	6	0.895643	2.315732	2.138526
5	6	-0.508081	2.324324	1.742476
6	6	-0.591992	2.401449	0.315090
7	6	1.194438	2.443441	-1.589872
8	9	2.382724	1.818892	-1.885580
9	9	1.390334	3.784006	-1.880630
10	9	0.281298	1.987992	-2.508303
11	6	3.183250	2.361215	0.919917
12	1	3.620383	2.200548	1.906996
13	1	3.615096	1.632123	0.235074
14	1	3.479304	3.361571	0.577561
15	6	1.384135	2.408868	3.556663
16	1	1.398388	3.459234	3.876095
17	1	0.730293	1.868325	4.245933
18	1	2.395494	2.011339	3.667745
19	6	-1.659605	2.503344	2.693537
20	1	-2.600895	2.150043	2.267438
21	1	-1.492826	1.977376	3.636664
22	1	-1.774710	3.570260	2.925794
23	6	-1.832323	2.718842	-0.473304
24	1	-1.902933	3.806851	-0.601842
25	1	-1.825597	2.265689	-1.464695
26	1	-2.730052	2.387508	0.053032
27	6	1.193816	-2.083493	1.494480
28	7	1.458550	-1.294879	0.519366
29	6	0.162451	-1.349782	2.300246
30	6	0.474577	-1.157972	3.770129
31	1	-0.255767	-0.496264	4.241233
32	1	0.424983	-2.128348	4.281871

33	1	1.477613	-0.749332	3.923888
34	6	1.796386	-3.406454	1.819555
35	1	1.033354	-4.087274	2.207125
36	1	2.277846	-3.852678	0.947887
37	1	2.551958	-3.276524	2.605500
38	6	-1.122532	-1.121607	1.771296
39	1	-1.814744	-0.681041	2.483679
40	8	2.262445	-1.738319	-0.539716
41	6	3.615795	-1.423079	-0.433295
42	8	4.061531	-0.879489	0.536592
43	6	4.371091	-1.909782	-1.671677
44	6	3.681996	-1.397081	-2.963239
45	1	3.638219	-0.303210	-2.983949
46	1	4.262677	-1.731417	-3.829150
47	1	2.665690	-1.788613	-3.060343
48	6	5.820037	-1.382141	-1.595489
49	1	6.376005	-1.738419	-2.468453
50	1	5.845129	-0.287550	-1.595779
51	1	6.328122	-1.737242	-0.693966
52	6	4.370893	-3.465662	-1.653937
53	1	4.956225	-3.827673	-2.505387
54	1	4.828548	-3.853570	-0.736920
55	1	3.356867	-3.867175	-1.740606
56	6	-1.029222	-0.676788	-0.531216
57	1	-1.701150	0.016307	-1.032318
58	1	-0.418380	-1.189609	-1.274295
59	6	-1.753307	-1.619255	0.452542
60	6	-1.523071	-3.119259	0.180167
61	1	-0.461170	-3.372321	0.126627
62	1	-1.986796	-3.733723	0.961614
63	1	-1.961774	-3.397751	-0.783585
64	6	-3.275582	-1.315356	0.537019
65	1	-3.690508	-1.861299	1.397243
66	1	-3.396482	-0.243836	0.752266
67	6	-4.080882	-1.669114	-0.729049
68	1	-4.095989	-2.753807	-0.874608
69	1	-3.603998	-1.227914	-1.611963
70	6	-5.524467	-1.151176	-0.608949
71	1	-6.001978	-1.571125	0.282380
72	1	-5.525965	-0.062599	-0.493443
73	6	-6.447701	-1.467661	-1.789839
74	17	-8.104519	-0.768849	-1.464820
75	17	-5.821704	-0.738715	-3.338696
76	17	-6.631520	-3.264916	-2.030572

44 (E = -1718.824193 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.142983	0.253387	0.738635
2	6	1.035148	2.139556	-0.196334
3	6	1.484607	2.035733	1.184411
4	6	0.317134	2.146440	2.008155
5	6	-0.842273	2.277679	1.162418
6	6	-0.385679	2.326270	-0.202913
7	6	1.914603	2.306188	-1.388668
8	9	3.169304	1.781378	-1.217922
9	9	2.100676	3.645173	-1.692927
10	9	1.406599	1.733115	-2.531713
11	6	2.899269	2.033885	1.694659
12	1	2.925574	1.781579	2.756535

13	1	3.533664	1.328671	1.160278
14	1	3.324136	3.039255	1.577120
15	6	0.306126	2.239734	3.507129
16	1	0.460673	3.286618	3.799397
17	1	-0.649659	1.916820	3.925361
18	1	1.098523	1.642257	3.962669
19	6	-2.225864	2.620112	1.646052
20	1	-2.976399	2.496874	0.863749
21	1	-2.523849	2.006770	2.500210
22	1	-2.248745	3.670349	1.964624
23	6	-1.252293	2.673336	-1.380005
24	1	-1.323300	3.767375	-1.442118
25	1	-0.847267	2.311073	-2.324556
26	1	-2.268556	2.290314	-1.264734
27	6	1.601394	-2.132450	1.702280
28	7	1.540934	-1.295964	0.694487
29	6	0.672522	-1.800663	2.766621
30	6	0.645240	-2.585326	4.061848
31	1	-0.093492	-2.151596	4.742252
32	1	0.374901	-3.636536	3.900394
33	1	1.619549	-2.568998	4.565356
34	6	2.501591	-3.328715	1.745988
35	1	2.015748	-4.147006	2.282583
36	1	2.777676	-3.673925	0.749719
37	1	3.420634	-3.076585	2.290501
38	6	-0.169672	-0.784854	2.455554
39	1	-0.952527	-0.494702	3.152602
40	8	2.253456	-1.634210	-0.477283
41	6	3.601148	-1.314878	-0.496145
42	8	4.160368	-0.833600	0.450057
43	6	4.238151	-1.734857	-1.826599
44	6	3.311695	-1.435549	-3.030500
45	1	3.068907	-0.370439	-3.092442
46	1	3.828674	-1.721093	-3.952646
47	1	2.378501	-2.002575	-2.973470
48	6	5.576859	-0.978908	-1.982967
49	1	6.060267	-1.296713	-2.912352
50	1	5.418513	0.103447	-2.031898
51	1	6.254050	-1.190368	-1.150591
52	6	4.508417	-3.266396	-1.742328
53	1	5.019059	-3.584818	-2.657188
54	1	5.151745	-3.511979	-0.890296
55	1	3.575837	-3.833768	-1.659865
56	6	-0.779446	-0.737211	-1.019859
57	1	-1.139545	0.055350	-1.664071
58	1	-0.044157	-1.393269	-1.470085
59	6	-1.627509	-1.238996	-0.021463
60	6	-1.493137	-2.683508	0.411692
61	1	-0.471149	-3.053444	0.323639
62	1	-1.849028	-2.845384	1.432423
63	1	-2.116285	-3.290376	-0.258710
64	6	-2.981364	-0.603464	0.248295
65	1	-3.176159	-0.585295	1.328382
66	1	-2.975067	0.433342	-0.099258
67	6	-4.139628	-1.351127	-0.464285
68	1	-4.246748	-2.361297	-0.048498
69	1	-3.902356	-1.465603	-1.528879
70	6	-5.477902	-0.607014	-0.313121
71	1	-5.708801	-0.485565	0.754196
72	1	-5.386466	0.409413	-0.724163
73	6	-6.666645	-1.312681	-0.984167
74	1	-6.726884	-2.348868	-0.628398
75	1	-7.596863	-0.810550	-0.676676

76	7	-6.508166	-1.359191	-2.461696
77	1	-7.290334	-1.872130	-2.868440
78	1	-6.578057	-0.411453	-2.835428

TS44-45 (E = -1718.7846091 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.197230	0.401657	0.526991
2	6	1.096589	2.211182	-0.263622
3	6	1.560045	2.200646	1.138527
4	6	0.415881	2.277651	1.949993
5	6	-0.761976	2.358939	1.090545
6	6	-0.335161	2.409778	-0.275608
7	6	1.987177	2.378305	-1.447261
8	9	3.210822	1.771755	-1.296490
9	9	2.258513	3.717030	-1.687986
10	9	1.455449	1.889039	-2.615624
11	6	2.987244	2.206089	1.608403
12	1	3.040153	2.061286	2.689434
13	1	3.584637	1.430273	1.129277
14	1	3.444283	3.176885	1.375756
15	6	0.375356	2.331270	3.451913
16	1	0.299011	3.374470	3.785694
17	1	-0.491049	1.796190	3.850192
18	1	1.273629	1.900167	3.899336
19	6	-2.153377	2.628194	1.592794
20	1	-2.911866	2.431916	0.832190
21	1	-2.390275	2.030060	2.477053
22	1	-2.235083	3.685040	1.879918
23	6	-1.213647	2.706638	-1.459486
24	1	-1.199859	3.786378	-1.656016
25	1	-0.876938	2.194537	-2.361099
26	1	-2.248941	2.418368	-1.264745
27	6	1.337882	-2.165724	1.496202
28	7	1.449650	-1.271311	0.548301
29	6	0.282696	-1.821668	2.440079
30	6	0.327498	-2.337352	3.852075
31	1	-0.461822	-1.879962	4.453119
32	1	0.182739	-3.426463	3.876247
33	1	1.295381	-2.132065	4.325041
34	6	2.174600	-3.403690	1.606620
35	1	1.625122	-4.197353	2.116774
36	1	2.489594	-3.764383	0.626644
37	1	3.075268	-3.186767	2.195624
38	6	-0.702842	-0.997032	1.941059
39	1	-1.450579	-0.656423	2.647795
40	8	2.246520	-1.640234	-0.559790
41	6	3.589713	-1.306253	-0.483876
42	8	4.069820	-0.816821	0.500494
43	6	4.320411	-1.720172	-1.766116
44	6	3.490558	-1.384705	-3.030190
45	1	3.276514	-0.313448	-3.093912
46	1	4.066864	-1.671007	-3.916139
47	1	2.543581	-1.930970	-3.047965
48	6	5.679384	-0.986344	-1.808317
49	1	6.226577	-1.299254	-2.703349
50	1	5.543864	0.099340	-1.851452
51	1	6.287864	-1.222334	-0.930519
52	6	4.556270	-3.257554	-1.687054
53	1	5.131247	-3.570797	-2.564662

54	1	5.126188	-3.529129	-0.791686
55	1	3.610036	-3.807926	-1.687348
56	6	-1.015427	-0.730157	-0.754727
57	1	-1.708386	-0.081722	-1.284520
58	1	-0.460498	-1.360407	-1.446820
59	6	-1.603620	-1.458572	0.412602
60	6	-1.464803	-2.984398	0.311591
61	1	-0.444217	-3.293947	0.080468
62	1	-1.796226	-3.479355	1.229869
63	1	-2.094329	-3.322482	-0.520153
64	6	-3.034668	-1.016809	0.785020
65	1	-3.312334	-1.454355	1.752238
66	1	-3.048591	0.071867	0.902101
67	6	-4.099378	-1.421130	-0.261957
68	1	-4.200881	-2.513372	-0.291198
69	1	-3.780124	-1.103746	-1.263803
70	6	-5.470169	-0.795137	0.055279
71	1	-5.785280	-1.095293	1.065499
72	1	-5.387475	0.299344	0.065250
73	6	-6.554344	-1.200105	-0.951818
74	1	-6.264103	-0.867857	-1.956217
75	1	-6.630516	-2.298925	-0.983325
76	7	-7.846742	-0.545485	-0.624179
77	1	-8.540845	-0.793231	-1.329419
78	1	-8.202993	-0.921951	0.255410

45 (E = -1718.8148219 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.214905	0.383754	0.821017
2	6	0.701654	2.238141	-0.188889
3	6	1.648904	2.284796	0.935945
4	6	0.892695	2.311696	2.120399
5	6	-0.520555	2.299307	1.762908
6	6	-0.645235	2.370002	0.337932
7	6	1.082786	2.441943	-1.616406
8	9	2.276611	1.848183	-1.949470
9	9	1.234638	3.787175	-1.913608
10	9	0.153808	1.962813	-2.506891
11	6	3.145224	2.380450	0.841689
12	1	3.612862	2.171918	1.805541
13	1	3.561723	1.693489	0.105989
14	1	3.423706	3.400247	0.544292
15	6	1.420687	2.416434	3.523559
16	1	1.444014	3.469256	3.834365
17	1	0.786404	1.881321	4.234821
18	1	2.435028	2.019991	3.609461
19	6	-1.648984	2.462342	2.744001
20	1	-2.596490	2.097939	2.341600
21	1	-1.451538	1.937099	3.681689
22	1	-1.771122	3.527405	2.981121
23	6	-1.910619	2.671145	-0.416472
24	1	-1.993873	3.757460	-0.551814
25	1	-1.929399	2.209794	-1.403935
26	1	-2.789804	2.336909	0.138367
27	6	1.213685	-2.089122	1.501361
28	7	1.466664	-1.299859	0.523899
29	6	0.180806	-1.363140	2.311975
30	6	0.503054	-1.165608	3.779162
31	1	-0.230390	-0.510960	4.255305

32	1	0.467261	-2.135733	4.292683
33	1	1.503128	-0.746742	3.924855
34	6	1.830452	-3.405742	1.825664
35	1	1.074239	-4.094745	2.212207
36	1	2.316792	-3.846441	0.953901
37	1	2.584100	-3.268647	2.612169
38	6	-1.110457	-1.148353	1.792849
39	1	-1.799966	-0.710728	2.509820
40	8	2.276040	-1.734945	-0.534721
41	6	3.628239	-1.417166	-0.419684
42	8	4.067934	-0.876428	0.554546
43	6	4.390058	-1.895092	-1.657563
44	6	3.715088	-1.358465	-2.947047
45	1	3.682123	-0.263956	-2.953334
46	1	4.298709	-1.686625	-3.813362
47	1	2.695729	-1.738625	-3.056474
48	6	5.842627	-1.380671	-1.563496
49	1	6.402277	-1.730312	-2.436812
50	1	5.877017	-0.286444	-1.549290
51	1	6.340915	-1.751772	-0.662910
52	6	4.376766	-3.450830	-1.661596
53	1	4.965776	-3.805979	-2.513407
54	1	4.824087	-3.855354	-0.746612
55	1	3.360192	-3.842580	-1.761544
56	6	-1.037836	-0.713547	-0.511671
57	1	-1.718028	-0.030322	-1.014890
58	1	-0.425148	-1.226283	-1.253487
59	6	-1.750278	-1.654257	0.481946
60	6	-1.513941	-3.154123	0.214941
61	1	-0.451232	-3.401977	0.147618
62	1	-1.963447	-3.766494	1.006484
63	1	-1.967095	-3.439393	-0.740047
64	6	-3.273694	-1.357298	0.572576
65	1	-3.680841	-1.903307	1.437334
66	1	-3.397310	-0.285936	0.789780
67	6	-4.095407	-1.707590	-0.681874
68	1	-4.113604	-2.795833	-0.827068
69	1	-3.615270	-1.279789	-1.573938
70	6	-5.545886	-1.194512	-0.597930
71	1	-6.032605	-1.607720	0.297768
72	1	-5.544299	-0.101514	-0.475448
73	6	-6.382578	-1.559260	-1.837424
74	1	-5.907127	-1.146443	-2.736297
75	1	-6.401891	-2.649471	-1.960927
76	7	-7.788696	-1.088418	-1.822206
77	1	-8.263987	-1.462280	-0.999974
78	1	-7.806683	-0.073584	-1.714775

46 (E = -1662.2278953 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.317495	0.413776	0.652621
2	6	1.120303	2.219467	-0.268412
3	6	1.646494	2.273510	1.108509
4	6	0.537896	2.356305	1.970483
5	6	-0.679039	2.368852	1.165548
6	6	-0.314175	2.372208	-0.220735
7	6	1.956475	2.366948	-1.492478
8	9	3.190689	1.772358	-1.381732
9	9	2.208062	3.702391	-1.772261

10	9	1.380135	1.850030	-2.626590
11	6	3.093918	2.334064	1.509512
12	1	3.199270	2.255842	2.593489
13	1	3.683839	1.540532	1.049860
14	1	3.520315	3.296696	1.198509
15	6	0.565232	2.473172	3.469111
16	1	0.451395	3.525009	3.762781
17	1	-0.252336	1.913702	3.932096
18	1	1.504575	2.107178	3.889123
19	6	-2.053849	2.628071	1.716926
20	1	-2.840210	2.349680	1.012062
21	1	-2.225868	2.090542	2.653511
22	1	-2.162033	3.700030	1.929800
23	6	-1.255073	2.593578	-1.373306
24	1	-1.251619	3.658402	-1.639701
25	1	-0.969299	2.024406	-2.258182
26	1	-2.278576	2.323329	-1.104923
27	6	1.599989	-2.075094	1.646269
28	7	1.624757	-1.213982	0.660338
29	6	0.597982	-1.723376	2.642073
30	6	0.746833	-2.180865	4.067758
31	1	-0.091779	-1.829547	4.673514
32	1	0.786688	-3.275675	4.138384
33	1	1.677748	-1.799891	4.507597
34	6	2.476713	-3.284780	1.756141
35	1	1.918862	-4.127483	2.173351
36	1	2.890985	-3.578930	0.792796
37	1	3.309356	-3.070772	2.438768
38	6	-0.427178	-0.927015	2.176576
39	1	-1.140717	-0.579404	2.912700
40	8	2.359020	-1.598939	-0.485580
41	6	3.693097	-1.225938	-0.510949
42	8	4.224404	-0.692646	0.423189
43	6	4.347682	-1.662728	-1.826542
44	6	3.417476	-1.413566	-3.039500
45	1	3.153931	-0.355336	-3.129354
46	1	3.941566	-1.713434	-3.952972
47	1	2.495408	-1.996944	-2.967697
48	6	5.668701	-0.879314	-1.995886
49	1	6.163371	-1.208748	-2.915165
50	1	5.484778	0.197246	-2.072460
51	1	6.347123	-1.054282	-1.155996
52	6	4.652798	-3.185247	-1.704851
53	1	5.174286	-3.513058	-2.610175
54	1	5.298756	-3.395382	-0.845287
55	1	3.733437	-3.772276	-1.612405
56	6	-3.486516	-1.848750	2.287804
57	6	-2.869846	-1.061501	1.113444
58	6	-1.315199	-3.026211	0.632453
59	6	-1.926701	-3.795965	1.815506
60	6	-3.385246	-3.369338	2.068329
61	1	-3.484139	-1.238620	0.216932
62	1	-2.902659	0.014823	1.302032
63	1	-2.994226	-1.583265	3.233088
64	1	-4.536608	-1.549710	2.393445
65	1	-1.867066	-3.293598	-0.283799
66	1	-0.278254	-3.320207	0.446797
67	1	-1.877015	-4.870065	1.597981
68	1	-1.335118	-3.635995	2.726112
69	1	-4.002420	-3.654820	1.203304
70	1	-3.790052	-3.903247	2.936206
71	6	-1.447089	-1.490047	0.702466
72	6	-0.929770	-0.804849	-0.513439

73	1	-0.389117	-1.455433	-1.198657
74	1	-1.665523	-0.200789	-1.039456

TS46-47 (E = -1662.2278953 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.317495	0.413776	0.652621
2	6	1.120303	2.219467	-0.268412
3	6	1.646494	2.273510	1.108509
4	6	0.537896	2.356305	1.970483
5	6	-0.679039	2.368852	1.165548
6	6	-0.314175	2.372208	-0.220735
7	6	1.956475	2.366948	-1.492478
8	9	3.190689	1.772358	-1.381732
9	9	2.208062	3.702391	-1.772261
10	9	1.380135	1.850030	-2.626590
11	6	3.093918	2.334064	1.509512
12	1	3.199270	2.255842	2.593489
13	1	3.683839	1.540532	1.049860
14	1	3.520315	3.296696	1.198509
15	6	0.565232	2.473172	3.469111
16	1	0.451395	3.525009	3.762781
17	1	-0.252336	1.913702	3.932096
18	1	1.504575	2.107178	3.889123
19	6	-2.053849	2.628071	1.716926
20	1	-2.840210	2.349680	1.012062
21	1	-2.225868	2.090542	2.653511
22	1	-2.162033	3.700030	1.929800
23	6	-1.255073	2.593578	-1.373306
24	1	-1.251619	3.658402	-1.639701
25	1	-0.969299	2.024406	-2.258182
26	1	-2.278576	2.323329	-1.104923
27	6	1.599989	-2.075094	1.646269
28	7	1.624757	-1.213982	0.660338
29	6	0.597982	-1.723376	2.642073
30	6	0.746833	-2.180865	4.067758
31	1	-0.091779	-1.829547	4.673514
32	1	0.786688	-3.275675	4.138384
33	1	1.677748	-1.799891	4.507597
34	6	2.476713	-3.284780	1.756141
35	1	1.918862	-4.127483	2.173351
36	1	2.890985	-3.578930	0.792796
37	1	3.309356	-3.070772	2.438768
38	6	-0.427178	-0.927015	2.176576
39	1	-1.140717	-0.579404	2.912700
40	8	2.359020	-1.598939	-0.485580
41	6	3.693097	-1.225938	-0.510949
42	8	4.224404	-0.692646	0.423189
43	6	4.347682	-1.662728	-1.826542
44	6	3.417476	-1.413566	-3.039500
45	1	3.153931	-0.355336	-3.129354
46	1	3.941566	-1.713434	-3.952972
47	1	2.495408	-1.996944	-2.967697
48	6	5.668701	-0.879314	-1.995886
49	1	6.163371	-1.208748	-2.915165
50	1	5.484778	0.197246	-2.072460
51	1	6.347123	-1.054282	-1.155996
52	6	4.652798	-3.185247	-1.704851
53	1	5.174286	-3.513058	-2.610175
54	1	5.298756	-3.395382	-0.845287

55	1	3.733437	-3.772276	-1.612405
56	6	-3.486516	-1.848750	2.287804
57	6	-2.869846	-1.061501	1.113444
58	6	-1.315199	-3.026211	0.632453
59	6	-1.926701	-3.795965	1.815506
60	6	-3.385246	-3.369338	2.068329
61	1	-3.484139	-1.238620	0.216932
62	1	-2.902659	0.014823	1.302032
63	1	-2.994226	-1.583265	3.233088
64	1	-4.536608	-1.549710	2.393445
65	1	-1.867066	-3.293598	-0.283799
66	1	-0.278254	-3.320207	0.446797
67	1	-1.877015	-4.870065	1.597981
68	1	-1.335118	-3.635995	2.726112
69	1	-4.002420	-3.654820	1.203304
70	1	-3.790052	-3.903247	2.936206
71	6	-1.447089	-1.490047	0.702466
72	6	-0.929770	-0.804849	-0.513439
73	1	-0.389117	-1.455433	-1.198657
74	1	-1.665523	-0.200789	-1.039456

47 (E = -1662.260602 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.390733	0.429405	0.849770
2	6	0.835249	2.247222	-0.243998
3	6	1.759512	2.396445	0.891348
4	6	0.981500	2.455801	2.058711
5	6	-0.424013	2.366326	1.679000
6	6	-0.524848	2.358758	0.250766
7	6	1.241269	2.395367	-1.671035
8	9	2.460769	1.824703	-1.947443
9	9	1.360668	3.729267	-2.028961
10	9	0.348214	1.846280	-2.557226
11	6	3.252317	2.541744	0.806012
12	1	3.701373	2.548616	1.800857
13	1	3.713055	1.737986	0.231550
14	1	3.500639	3.492154	0.316562
15	6	1.473984	2.650830	3.465004
16	1	1.414439	3.712978	3.736848
17	1	0.865809	2.096863	4.184687
18	1	2.511915	2.331754	3.583242
19	6	-1.575019	2.547834	2.630032
20	1	-2.498080	2.110146	2.244453
21	1	-1.368609	2.106077	3.607666
22	1	-1.750274	3.620934	2.783239
23	6	-1.783805	2.581387	-0.540627
24	1	-1.883976	3.653969	-0.752655
25	1	-1.780159	2.052457	-1.493955
26	1	-2.665082	2.270824	0.024367
27	6	1.442107	-1.993990	1.635289
28	7	1.685846	-1.237191	0.630001
29	6	0.397353	-1.254436	2.418699
30	6	0.720580	-0.987908	3.875138
31	1	-0.031719	-0.340926	4.331938
32	1	0.719139	-1.938384	4.425542
33	1	1.707451	-0.532406	3.999492
34	6	2.081309	-3.288001	2.005526
35	1	1.338160	-3.981325	2.409134
36	1	2.584010	-3.744374	1.151423

37	1	2.825605	-3.110239	2.792899
38	6	-0.898981	-1.089829	1.894308
39	1	-1.591228	-0.629356	2.592892
40	8	2.484283	-1.718091	-0.418675
41	6	3.812694	-1.304141	-0.395740
42	8	4.256997	-0.656897	0.509599
43	6	4.550453	-1.826792	-1.630517
44	6	3.801051	-1.399497	-2.920270
45	1	3.713973	-0.310233	-2.988433
46	1	4.366320	-1.751563	-3.789365
47	1	2.798144	-1.833036	-2.964695
48	6	5.979268	-1.242113	-1.626329
49	1	6.522333	-1.619798	-2.498450
50	1	5.961634	-0.148781	-1.679181
51	1	6.527831	-1.533448	-0.725455
52	6	4.612248	-3.378575	-1.545701
53	1	5.177297	-3.755569	-2.404421
54	1	5.121459	-3.707727	-0.632911
55	1	3.612867	-3.822706	-1.572985
56	6	-3.809140	-2.255257	1.665351
57	6	-3.054234	-1.401232	0.626573
58	6	-1.298885	-3.184489	0.397335
59	6	-2.022049	-4.047334	1.451157
60	6	-3.535401	-3.757841	1.464826
61	1	-3.435439	-1.630336	-0.379097
62	1	-3.239827	-0.332689	0.799769
63	1	-3.507296	-1.963321	2.683023
64	1	-4.884778	-2.050757	1.593939
65	1	-1.686498	-3.429084	-0.603195
66	1	-0.228754	-3.421500	0.371957
67	1	-1.838998	-5.109602	1.247147
68	1	-1.604857	-3.841942	2.449042
69	1	-3.972701	-4.081774	0.508332
70	1	-4.027302	-4.341923	2.252459
71	6	-1.524837	-1.665964	0.606708
72	6	-0.816385	-0.774377	-0.428700
73	1	-0.179617	-1.323069	-1.123996
74	1	-1.505943	-0.146821	-0.990790

48 (E = -1662.2712109 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.163594	0.219103	0.910729
2	6	0.940346	2.062912	-0.193337
3	6	1.475150	2.063528	1.160970
4	6	0.358252	2.200089	2.046932
5	6	-0.853845	2.239214	1.269054
6	6	-0.483672	2.210638	-0.123541
7	6	1.754081	2.179143	-1.437168
8	9	3.001346	1.619280	-1.325384
9	9	1.963830	3.505624	-1.777677
10	9	1.168135	1.599743	-2.537053
11	6	2.916890	2.133344	1.582491
12	1	3.018878	1.906653	2.645555
13	1	3.549031	1.444266	1.025419
14	1	3.287751	3.153625	1.418739
15	6	0.438070	2.397166	3.533486
16	1	0.567081	3.467313	3.742065
17	1	-0.474912	2.069690	4.035173
18	1	1.282774	1.864557	3.975353

19	6	-2.215992	2.574960	1.814199
20	1	-3.013853	2.318576	1.115341
21	1	-2.415709	2.061564	2.758299
22	1	-2.274634	3.654938	2.002782
23	6	-1.437215	2.456911	-1.258364
24	1	-1.553204	3.542284	-1.378528
25	1	-1.084366	2.052211	-2.206329
26	1	-2.428189	2.048007	-1.049817
27	6	1.769621	-2.046128	1.933297
28	7	1.612527	-1.285709	0.877554
29	6	0.903772	-1.666814	3.034471
30	6	0.991630	-2.356244	4.380380
31	1	0.293629	-1.889833	5.081960
32	1	0.737781	-3.421894	4.314469
33	1	1.999471	-2.282850	4.806693
34	6	2.713600	-3.207422	1.995156
35	1	2.311195	-3.987096	2.645471
36	1	2.907467	-3.632674	1.009998
37	1	3.670374	-2.880744	2.422356
38	6	0.006000	-0.703555	2.712731
39	1	-0.739841	-0.388929	3.438800
40	8	2.256100	-1.684825	-0.314558
41	6	3.587493	-1.325855	-0.447222
42	8	4.191925	-0.768091	0.426313
43	6	4.148384	-1.809494	-1.790254
44	6	3.126416	-1.637589	-2.940465
45	1	2.827569	-0.591308	-3.056212
46	1	3.590813	-1.964376	-3.876758
47	1	2.228911	-2.240309	-2.777177
48	6	5.434422	-1.008463	-2.095096
49	1	5.863461	-1.367499	-3.036061
50	1	5.221170	0.060165	-2.201431
51	1	6.179393	-1.133780	-1.304287
52	6	4.499500	-3.317659	-1.622600
53	1	4.967609	-3.675085	-2.545825
54	1	5.205926	-3.474006	-0.800066
55	1	3.603623	-3.920225	-1.441211
56	6	-2.520582	-3.664096	0.256050
57	6	-1.442032	-2.754375	0.908321
58	6	-2.970648	-0.749600	0.634210
59	6	-4.063584	-1.666877	0.015763
60	6	-3.936899	-3.117916	0.509412
61	1	-1.585240	-2.768041	1.994482
62	1	-0.446075	-3.151792	0.694801
63	1	-2.335532	-3.730863	-0.825747
64	1	-2.418970	-4.677973	0.661739
65	1	-3.141453	-0.667202	1.715435
66	1	-3.055349	0.251716	0.205870
67	1	-5.050651	-1.257959	0.263092
68	1	-3.970868	-1.641669	-1.079575
69	1	-4.154853	-3.159437	1.587129
70	1	-4.681388	-3.751120	0.011492
71	6	-1.596506	-1.341169	0.370002
72	6	-0.816111	-0.914483	-0.716201
73	1	-1.223394	-0.186332	-1.407387
74	1	-0.088526	-1.591536	-1.147062

TS48-49 (E = -1662.2313266 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	77	0.235896	0.371745	0.718215
2	6	1.032027	2.139976	-0.253234
3	6	1.577462	2.246439	1.114501
4	6	0.481226	2.354435	1.985768
5	6	-0.747626	2.338962	1.196436
6	6	-0.402900	2.300211	-0.193979
7	6	1.854071	2.256488	-1.491223
8	9	3.086670	1.658857	-1.382931
9	9	2.107344	3.584835	-1.799676
10	9	1.261147	1.719294	-2.606474
11	6	3.031023	2.311176	1.491308
12	1	3.151523	2.281595	2.576063
13	1	3.605427	1.490367	1.060079
14	1	3.463523	3.253148	1.129888
15	6	0.525060	2.512264	3.480083
16	1	0.392482	3.568947	3.747112
17	1	-0.274639	1.948337	3.968430
18	1	1.477120	2.177335	3.897357
19	6	-2.113584	2.616890	1.760240
20	1	-2.910553	2.331087	1.070494
21	1	-2.277545	2.097462	2.708283
22	1	-2.211257	3.693463	1.954101
23	6	-1.357229	2.491183	-1.341036
24	1	-1.345805	3.545427	-1.646433
25	1	-1.090926	1.886637	-2.208386
26	1	-2.379535	2.242503	-1.048490
27	6	1.540944	-2.088720	1.766320
28	7	1.548649	-1.262721	0.752524
29	6	0.564815	-1.697944	2.774688
30	6	0.744677	-2.111414	4.210097
31	1	-0.032932	-1.668344	4.836717
32	1	0.685334	-3.203275	4.316503
33	1	1.724147	-1.804177	4.597148
34	6	2.408194	-3.302829	1.897568
35	1	1.850099	-4.123106	2.356970
36	1	2.795744	-3.634762	0.935303
37	1	3.259159	-3.074677	2.552333
38	6	-0.481942	-0.932043	2.310658
39	1	-1.177333	-0.560810	3.054293
40	8	2.259322	-1.687126	-0.393765
41	6	3.593737	-1.317848	-0.452150
42	8	4.141034	-0.758587	0.457303
43	6	4.226959	-1.793637	-1.764494
44	6	3.276174	-1.582830	-2.968616
45	1	3.007718	-0.528339	-3.084822
46	1	3.786064	-1.907646	-3.881591
47	1	2.357347	-2.166375	-2.864416
48	6	5.543461	-1.013730	-1.979933
49	1	6.022104	-1.369649	-2.897803
50	1	5.356313	0.059857	-2.084991
51	1	6.237033	-1.162843	-1.147480
52	6	4.537634	-3.311091	-1.600843
53	1	5.048095	-3.665261	-2.502518
54	1	5.195314	-3.493581	-0.743808
55	1	3.621249	-3.897235	-1.478118
56	6	-2.453559	-3.694290	0.026561
57	6	-1.378345	-3.056095	0.940245
58	6	-2.913070	-1.070062	1.336998
59	6	-3.991230	-1.721087	0.434895
60	6	-3.871715	-3.254867	0.430889
61	1	-1.517420	-3.408615	1.970045
62	1	-0.384982	-3.368938	0.605486
63	1	-2.262545	-3.416134	-1.019272

64	1	-2.356714	-4.785428	0.087003
65	1	-3.095168	-1.375760	2.375080
66	1	-2.993563	0.019513	1.291423
67	1	-4.980145	-1.412763	0.795570
68	1	-3.894110	-1.340105	-0.591095
69	1	-4.099932	-3.641271	1.435490
70	1	-4.611896	-3.690081	-0.251420
71	6	-1.502791	-1.515367	0.905718
72	6	-1.028047	-0.897884	-0.370392
73	1	-1.777088	-0.321590	-0.907583
74	1	-0.505203	-1.581370	-1.036469

49 (E = -1662.2603997 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	77	0.288359	0.379473	0.963436
2	6	0.739683	2.158736	-0.187775
3	6	1.670850	2.335039	0.939161
4	6	0.897958	2.436576	2.106505
5	6	-0.510618	2.345765	1.735219
6	6	-0.616842	2.298201	0.308579
7	6	1.139990	2.258563	-1.620585
8	9	2.355815	1.673269	-1.882698
9	9	1.263886	3.579215	-2.022802
10	9	0.240738	1.684648	-2.484492
11	6	3.164438	2.467078	0.842427
12	1	3.616581	2.514225	1.834865
13	1	3.617867	1.635646	0.302310
14	1	3.417765	3.393591	0.311589
15	6	1.395833	2.672548	3.504523
16	1	1.331961	3.741656	3.746406
17	1	0.793696	2.136157	4.242508
18	1	2.435899	2.362215	3.626793
19	6	-1.657676	2.560308	2.684184
20	1	-2.588288	2.137858	2.299612
21	1	-1.462699	2.121354	3.665512
22	1	-1.811280	3.637876	2.828686
23	6	-1.877440	2.502872	-0.484963
24	1	-1.978009	3.570395	-0.720935
25	1	-1.875687	1.952398	-1.426028
26	1	-2.757860	2.205404	0.088492
27	6	1.345508	-2.024336	1.795895
28	7	1.568058	-1.298164	0.763064
29	6	0.327439	-1.255408	2.585882
30	6	0.692937	-0.942072	4.022175
31	1	-0.040063	-0.270742	4.474805
32	1	0.697829	-1.872211	4.606073
33	1	1.686947	-0.492191	4.102167
34	6	1.980692	-3.314591	2.185448
35	1	1.238260	-3.989222	2.620934
36	1	2.460439	-3.797179	1.332688
37	1	2.743196	-3.124291	2.952151
38	6	-0.980332	-1.094671	2.091482
39	1	-1.655283	-0.610366	2.792284
40	8	2.324259	-1.822058	-0.296795
41	6	3.652816	-1.413099	-0.344693
42	8	4.137736	-0.737803	0.518424
43	6	4.334533	-1.979080	-1.592926
44	6	3.530215	-1.589611	-2.861645
45	1	3.447239	-0.502557	-2.962128

46	1	4.053278	-1.975161	-3.742848
47	1	2.523557	-2.016388	-2.846298
48	6	5.763764	-1.401227	-1.671020
49	1	6.264153	-1.804938	-2.556899
50	1	5.747462	-0.309667	-1.752749
51	1	6.352944	-1.670619	-0.789190
52	6	4.394845	-3.527657	-1.461395
53	1	4.923453	-3.934104	-2.329817
54	1	4.939380	-3.830275	-0.559872
55	1	3.393782	-3.968122	-1.433965
56	6	-2.206160	-3.844722	-0.471966
57	6	-1.423717	-3.238948	0.712504
58	6	-3.170044	-1.431146	0.934077
59	6	-3.956008	-2.027590	-0.248851
60	6	-3.711761	-3.542803	-0.372058
61	1	-1.747768	-3.718420	1.648739
62	1	-0.358171	-3.463224	0.586742
63	1	-1.814517	-3.438086	-1.416246
64	1	-2.034148	-4.927973	-0.502691
65	1	-3.545294	-1.866940	1.873042
66	1	-3.336517	-0.347267	0.995020
67	1	-5.025578	-1.820768	-0.118180
68	1	-3.652431	-1.533081	-1.183401
69	1	-4.127362	-4.051865	0.511073
70	1	-4.238747	-3.944238	-1.246497
71	6	-1.645006	-1.709411	0.846225
72	6	-0.961314	-0.857778	-0.243634
73	1	-1.655874	-0.239099	-0.807708
74	1	-0.345153	-1.428574	-0.938803

a_1 (E = -596.5115126 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	7.779023	-2.802874	2.169087
2	7	6.665248	-3.431328	2.321158
3	6	7.981101	-1.685677	3.128235
4	6	6.894790	-1.412642	4.148465
5	1	7.177375	-0.568486	4.783820
6	1	5.942372	-1.180813	3.658998
7	1	6.720538	-2.288011	4.783892
8	6	8.830023	-3.119565	1.130690
9	1	8.534091	-3.962874	0.509937
10	1	8.997611	-2.250303	0.485541
11	1	9.781851	-3.358448	1.617307
12	6	9.098021	-0.944653	3.084154
13	1	9.245811	-0.129716	3.783433
14	1	9.890854	-1.115048	2.367819
15	8	6.524572	-4.485924	1.378220
16	6	5.362333	-5.196792	1.499360
17	8	4.518285	-4.971162	2.327950
18	6	5.309178	-6.302317	0.433030
19	6	6.521165	-7.254327	0.621939
20	1	7.469235	-6.728578	0.477378
21	1	6.519730	-7.703380	1.622001
22	1	6.460781	-8.063856	-0.113705
23	6	3.993240	-7.090897	0.598102
24	1	3.121156	-6.441783	0.470263
25	1	3.948278	-7.881106	-0.158757
26	1	3.929422	-7.556959	1.586549
27	6	5.361313	-5.653519	-0.976814

28	1	5.283438	-6.438419	-1.737090
29	1	4.528486	-4.955700	-1.122547
30	1	6.299657	-5.114175	-1.134346

a_2 (E = -612.5634646 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.952295	0.404943	-0.000300
2	7	0.983213	-0.439856	0.011178
3	6	3.302959	-0.226227	0.027262
4	6	1.810447	1.907349	-0.018067
5	1	0.777839	2.198677	-0.202525
6	1	2.121775	2.329093	0.944618
7	1	2.446683	2.342114	-0.794004
8	6	4.412697	0.524825	0.169983
9	1	5.392899	0.064259	0.210127
10	1	4.368320	1.599853	0.246275
11	8	-0.279218	0.199062	0.008830
12	6	-1.345852	-0.662118	0.028957
13	8	-1.238581	-1.860207	0.052731
14	6	-2.660284	0.132320	0.015941
15	6	-2.729816	0.978168	-1.284814
16	1	-1.921943	1.714237	-1.327186
17	1	-2.669594	0.341419	-2.175063
18	1	-3.685113	1.513463	-1.314236
19	6	-3.841197	-0.859865	0.059487
20	1	-3.813276	-1.472737	0.966118
21	1	-4.782766	-0.300837	0.050598
22	1	-3.830489	-1.530070	-0.805867
23	6	-2.708698	1.065019	1.256390
24	1	-3.663731	1.601523	1.265130
25	1	-2.633304	0.490555	2.186954
26	1	-1.900811	1.801880	1.235151
27	7	3.334443	-1.610718	-0.146446
28	1	2.481905	-2.086165	0.127509
29	1	4.164163	-2.063449	0.219827

AcOH (E = -229.1515754 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	0.626114	1.208100	0.000017
2	6	0.090277	0.122259	-0.000034
3	8	0.795751	-1.029765	0.000058
4	6	-1.395295	-0.126133	-0.000065
5	1	-1.677718	-0.706631	0.884536
6	1	-1.930359	0.823288	-0.002609
7	1	-1.677300	-0.711439	-0.881559
8	1	1.740568	-0.808661	-0.000371

AcO^- (E = -228.681307 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	8	0.758792	1.126072	0.001846
2	6	0.189029	0.000003	-0.009927
3	8	0.765587	-1.122615	0.001879
4	6	-1.353680	-0.003231	-0.004000
5	1	-1.703438	0.016953	1.037258
6	1	-1.752697	0.882327	-0.508413
7	1	-1.750992	-0.907559	-0.475084

$^{t}BuCO_2^-$ (E = -346.5891108 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1.626616	-1.115749	0.000000
2	6	-1.046595	0.005607	0.000000
3	8	-1.624012	1.126344	0.000000
4	6	0.524390	-0.022003	0.000000
5	6	1.003952	-0.780856	-1.262906
6	1	2.100360	-0.841546	-1.280417
7	1	0.599986	-1.797647	-1.278781
8	1	0.680728	-0.267034	-2.177740
9	6	1.128903	1.397387	0.000000
10	1	0.817361	1.962797	0.884694
11	1	2.225907	1.338700	0.000000
12	1	0.817361	1.962797	-0.884694
13	6	1.003952	-0.780856	1.262906
14	1	2.100360	-0.841546	1.280417
15	1	0.680728	-0.267034	2.177740
16	1	0.599986	-1.797647	1.278781

b_1 (E = -463.7318419 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.486031	-1.565137	-0.439953
2	1	-1.866562	-2.297949	0.067095
3	1	-3.535775	-1.535881	-0.165949
4	6	-1.980046	-0.738983	-1.360803
5	6	-2.838419	0.277656	-2.083152
6	1	-3.887048	0.200487	-1.780153
7	1	-2.502641	1.303240	-1.882084
8	1	-2.778806	0.129713	-3.169972
9	6	-0.512076	-0.795891	-1.748883
10	1	-0.042468	-1.665234	-1.275281
11	1	-0.431280	-0.940361	-2.835470
12	6	0.265148	0.475279	-1.357014
13	1	0.198264	0.648583	-0.275296
14	1	-0.161215	1.366750	-1.834242
15	6	1.731038	0.415275	-1.734741
16	8	2.274621	-0.493760	-2.350058
17	8	2.393056	1.518140	-1.304076
18	6	3.836615	1.600776	-1.609910
19	1	3.957800	1.550772	-2.695593
20	1	4.329163	0.732942	-1.162524
21	6	4.341771	2.910880	-1.033162
22	1	5.412981	3.011631	-1.237567
23	1	3.825783	3.764506	-1.483855
24	1	4.195621	2.946059	0.051024

b_2 (E = -275.1496827 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.782158	0.399353	1.080023
2	1	3.499733	1.241749	1.703733
3	1	4.742141	-0.063506	1.286444
4	6	2.984269	-0.045297	0.103087
5	6	3.377660	-1.213007	-0.776967
6	1	4.377358	-1.582791	-0.528361
7	1	2.670293	-2.045669	-0.673781
8	1	3.369163	-0.917681	-1.835152
9	6	1.641843	0.603609	-0.184000
10	1	1.550296	1.520242	0.413782
11	1	1.611928	0.905518	-1.243127
12	6	0.423468	-0.306087	0.102504
13	1	0.461265	-0.636451	1.150861
14	1	0.477405	-1.212670	-0.516009
15	6	-0.919318	0.399136	-0.161105
16	1	-0.977550	1.307389	0.455793
17	1	-0.948560	0.739441	-1.206308
18	6	-2.136571	-0.494820	0.123223
19	1	-3.075141	0.035863	-0.073109
20	1	-2.120990	-1.393307	-0.506299
21	1	-2.148687	-0.821970	1.170389

b_3 (E = -1653.9033865 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.669139	-1.115643	-0.363326
2	1	3.346799	-2.151771	-0.385540
3	1	4.674981	-0.907105	-0.713651
4	6	2.865478	-0.142221	0.076488
5	6	3.309772	1.304347	0.120419
6	1	4.351838	1.410664	-0.196186
7	1	2.690970	1.933434	-0.532176
8	1	3.212441	1.707367	1.137672
9	6	1.462326	-0.442529	0.575339
10	1	1.321822	-1.529926	0.622643
11	1	1.358765	-0.057281	1.601563
12	6	0.348550	0.177204	-0.304444
13	1	0.459316	-0.186446	-1.332478
14	1	0.452383	1.267110	-0.328338
15	6	-1.040291	-0.197110	0.238934
16	1	-1.157204	-1.285644	0.254338
17	1	-1.145766	0.153822	1.270774
18	6	-2.236158	0.361578	-0.538211
19	17	-3.787145	-0.193641	0.255171
20	17	-2.231747	2.184675	-0.549427
21	17	-2.245247	-0.225915	-2.263456

b_4 (E = -330.495065 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.599549	-1.021787	-0.379417
2	1	2.339249	-2.075502	-0.363233
3	1	3.578580	-0.764459	-0.771394
4	6	1.753326	-0.086061	0.064224

5	6	2.114576	1.384355	0.054221
6	1	3.134255	1.543425	-0.310227
7	1	1.430891	1.958612	-0.583896
8	1	2.036644	1.806972	1.065329
9	6	0.384956	-0.449284	0.613497
10	1	0.312017	-1.540985	0.704988
11	1	0.287127	-0.033458	1.628911
12	6	-0.796798	0.063213	-0.243824
13	1	-0.689657	-0.323855	-1.267348
14	1	-0.760367	1.158762	-0.314374
15	6	-2.162637	-0.361448	0.323675
16	1	-2.216143	-1.456360	0.389133
17	1	-2.263416	0.017851	1.351796
18	6	-3.342594	0.143196	-0.515928
19	1	-3.278187	1.239310	-0.611663
20	1	-3.276935	-0.273080	-1.528790
21	7	-4.635324	-0.303935	0.065014
22	1	-4.772072	0.148784	0.969863
23	1	-5.402482	0.022336	-0.522908

b_5 (E = -273.9397298 au)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-4.667881	-0.872092	-0.051407
2	6	-3.126782	-0.869646	-0.057390
3	6	-2.565451	0.574362	-0.036601
4	6	-4.665203	1.371362	1.167830
5	6	-5.225137	-0.073191	1.143105
6	1	-1.470578	0.563410	0.022898
7	1	-2.757340	-1.410298	0.826403
8	1	-2.746678	-1.400702	-0.939052
9	1	-5.034603	-0.426661	-0.989071
10	1	-5.043358	-1.902942	-0.023381
11	1	-5.016128	1.907080	2.057890
12	1	-5.052731	1.909990	0.287607
13	1	-4.951306	-0.579977	2.080139
14	1	-6.321313	-0.043398	1.104622
15	1	-2.836883	1.067010	-0.984653
16	6	-3.149566	1.373856	1.112477
17	6	-2.392303	1.998816	2.019012
18	1	-2.832437	2.555972	2.840608
19	1	-1.308015	1.977197	1.965276