

Electronic Supplementary Information for

Theoretical Investigations to the Iridium-Catalyzed Direct Borylation of B(3,6)-H of *o*-Carborane: the Actual Catalyst, Mechanism, and Origin of Regioselectivity

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Part 1: The NAO analysis^[1] to the lowest-lying delocalized π orbital of *o*-C₂B₁₀H₁₂

All results were shown in Table S1 and Fig. S1. As we can see, the equatorial plane of the π orbital locates at the xz plane, in which the cage B(3,6,8,10) atoms locate as well. So these four atoms contribute their 2p_y orbitals to the molecule orbital. While the cage C(1,2), B(4,5,7,11), and the H(17,24) atoms locate out of the plane, and they contribute their valence s (2s or 1s) and the p_y orbitals to construct the molecule orbital. In another word, this π orbital is formed by the linear combination (hybridization) of the valence atomic orbitals of the cage carbon and borane atoms, which is in accordance with the LOL analysis which concludes the 26-electron-delocalization structure of carborane. The second and third lowest-lying π orbitals are with the xy (HOMO-22) and yz (HOMO-21) plane as the equatorial planes, respectively. They have similar components with HOMO-23.

Table S1 Percentage of the major components that contribute to the lowest-lying π orbital (HOMO-23) of *o*-C₂B₁₀H₁₂ (M06-L/6-31G(d, p))

	C(1,2)	B(3,6)	B(4,5,7,11)	B(8,10)	B(9,12)	H(17,24)
1s						2.8%
2s	15.4%		4.1%			
2p _x			2.0%			
2p _y	5.1%	5.2%		1.2%		
2p _z	1.1%		0.9%		0.8%	

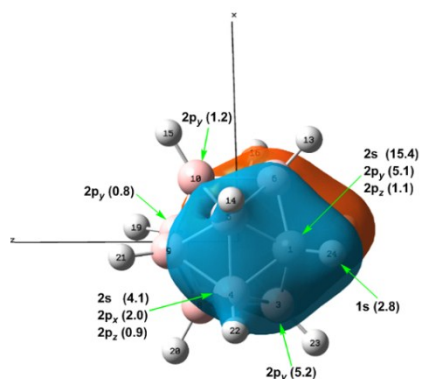


Fig. S1 A brief map to illustrate the major components that contribute to the HOMO-23 orbital of $o\text{-C}_2\text{B}_{10}\text{H}_{12}$.

Obviously, these π orbitals are quite comparable with the lowest-lying π orbital of benzene, and the o -carborane also has π orbitals with one or more nodal planes (Fig. S2). The differences lie mainly in: (1) the benzene has only one this type of π orbital, but the o -carborane has three quasi degenerate ones (be exactly degenerate for $\text{B}_{12}\text{H}_{12}^{2-}$). (2) the lowest-lying π orbital of benzene consists of six delocalized 2p orbitals with the same phase, but these of the carborane consist of 26 atomic orbitals (see the LOL analysis in main text), including not only 2p orbitals, but also s orbitals.

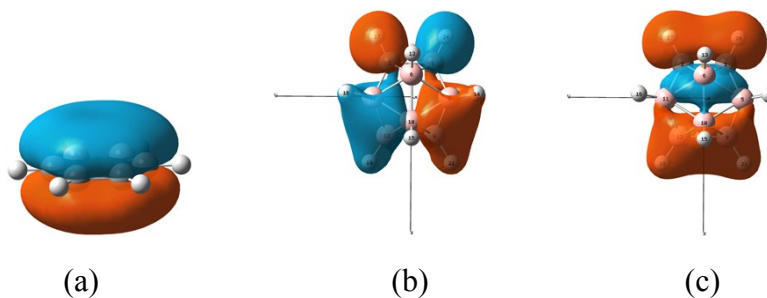


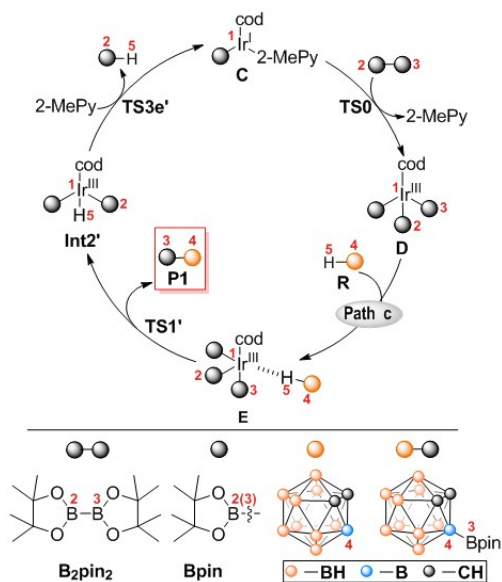
Fig. S2 The lowest-lying π orbitals of benzene (a), the π orbitals of o -carborane with one nodal plane (b) or two nodal planes (c).

Reference

- [1]. Reed, A. E.; Weinstock, R. B.; Weinhold, F., Natural population analysis. *J. Chem. Phys.* 1985, 83, 735-746.

Part 2: Details of Mechanism III

This mechanism indicates that, with approach of the **R** to **D**, a precursory intermediate **E** generates with the H5 atom oriented to the Ir atom, followed by the nucleophilic attack of the H5 atom to the Ir^{III} atom and simultaneous release of the product **P1**. Finally, the byproduct HBpin eliminates to regenerate the Ir^I catalyst **C**.



Scheme S1 The proposed catalytic cycle of Mechanism III. The number labels aside the shaded balls indicate labels for the boron atom of the Bpin group (black balls) or the cage B(3) atom (orange balls).

Part 3: Flexible scanning results from Int4

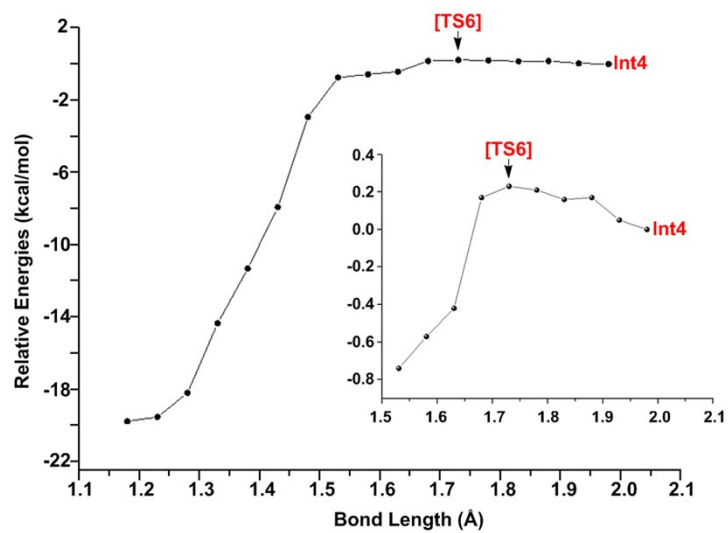


Fig. S3 The flexible scanning curve to the bond length of H6-B7 from the optimized structure of **Int4**.

Part 4: Hydrogen bond distributions in Int3s and Int5s

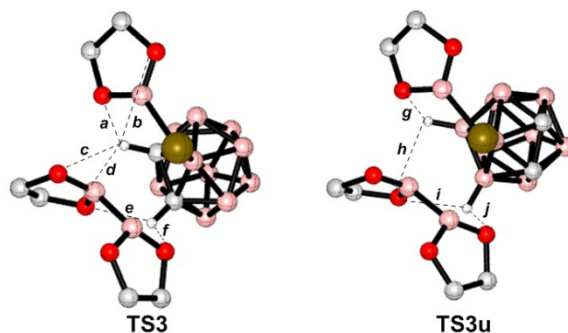


Fig. S4 Hydrogen bonds distributions in **TS3** and **TS3u**^a. The Bpin group bonded to the cage B(3) atom is omitted for brevity.

^a The B–H···O is not an actual hydrogen bond, and we plot them after the way we do for the C–H···O just for the sake of visual comparison.

Table S2 The bond lengths of hydrogen bonds in **TS3** and **TS3u**^a.

Stationary Point	Hydrogen Bond	Bond Length (Å)				
		O-H	C-H	B-H	C-O	B-O
TS3	<i>a</i>	2.34	1.08	–	3.12	–
	<i>b</i>	3.95	1.08	–	4.22	–
	<i>c</i>	3.73	1.08	–	4.55	–
	<i>d</i>	2.48	1.08	–	3.11	–
	<i>e</i>	2.22	1.08	–	2.98	–
	<i>f</i>	2.36	1.08	–	3.06	–
TS3u	<i>g</i>	2.70	–	1.18	–	3.39
	<i>h</i>	2.97	–	1.18	–	3.42
	<i>i</i>	2.47	–	1.17	–	3.13
	<i>j</i>	2.60	–	1.17	–	3.22

^a The geometry parameters of the B–H···O “interactions” are also listed after the way we do for the C–H···O interactions, although they are not actual hydrogen bonds.

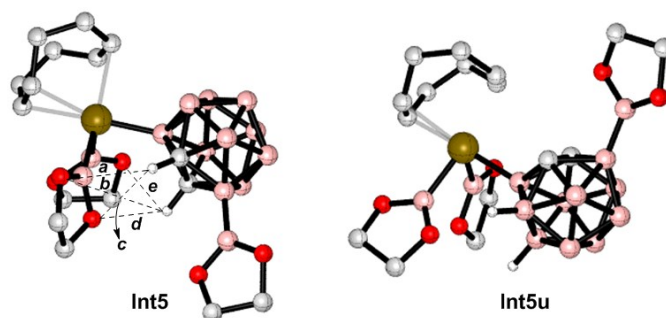


Fig. S5 Hydrogen bonds distributions in **Int5** and **Int5u**^a. The Bpin group bonded to the cage B(3) atom is omitted for brevity.

^a The B–H···O is not an actual hydrogen bond, and we plot them after the way we do for the C–H···O just for the sake of visual comparison.

Table S3 The bond lengths of hydrogen bonds in **Int5** and **Int5u**^a.

	Hydrogen Bond	Bond Length (Å)				
		O-H	C-H	B-H	C-O	B-O
Int5	<i>a</i>	2.81	1.09	–	3.72	–
	<i>b</i>	4.00	1.09	–	4.34	–
	<i>c</i>	2.96	1.09	–	3.47	–
	<i>d</i>	2.37	1.09	–	3.17	–
	<i>e</i>	3.43	1.09	–	3.63	–
Int5u	<i>f</i>	2.53	–	1.18	–	3.07
	<i>g</i>	2.90	–	1.18	–	3.30
	<i>h</i>	2.98	–	1.18	–	3.55

^a The geometry parameters of the B–H···O “interactions” are also listed after the way we do for the C–H···O interactions, although they are not actual hydrogen bonds.

Part 5: List of Cartesian coordinates of all structures involved in this work

2-MePy

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.522523	-0.164385	0.000197
2	6	0	1.929401	-0.164385	0.000197
3	6	0	2.596092	1.062222	0.000197
4	6	0	1.842019	2.237009	-0.000044
5	6	0	0.438817	2.134204	-0.000185
6	7	0	-0.220713	0.959253	0.000000
7	1	0	3.694636	1.101998	-0.000753
8	1	0	-0.043024	-1.113206	0.000319
9	1	0	2.484133	-1.111286	0.000461
10	1	0	2.326055	3.221933	-0.000145
11	6	0	-0.444133	3.395949	-0.000298
12	1	0	-0.236699	3.976509	0.874243
13	1	0	-0.234023	3.978225	-0.873057
14	1	0	-1.475153	3.109780	-0.002157

B₂pin₂

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.305603	-1.247878	0.000000
2	5	0	1.454397	-1.247878	0.000000
3	8	0	-1.075603	0.085801	0.000000
4	8	0	-1.075603	-2.581557	0.000000
5	8	0	2.224397	-1.245292	1.333677
6	6	0	-2.505603	-2.581557	0.000000
7	6	0	-2.481655	-0.174794	-0.002614
8	8	0	2.224397	-1.250464	-1.333677
9	6	0	3.630038	-1.209918	1.073250
10	6	0	3.630321	-1.249957	-1.072374
11	6	0	4.302090	0.009196	-1.651044
12	1	0	5.353254	-0.024873	-1.454084
13	1	0	4.138261	0.047190	-2.707745

14	1	0	3.881504	0.880137	-1.193367
15	6	0	4.294186	-2.533972	-1.603588
16	1	0	4.156043	-2.594925	-2.662880
17	1	0	5.340563	-2.512835	-1.380991
18	1	0	3.847210	-3.386297	-1.135982
19	6	0	4.260734	0.090684	1.604529
20	1	0	4.175494	0.118795	2.670758
21	1	0	5.293899	0.124830	1.328297
22	1	0	3.751020	0.932092	1.183668
23	6	0	4.333503	-2.451613	1.651980
24	1	0	5.363474	-2.445552	1.362111
25	1	0	4.263339	-2.436135	2.719565
26	1	0	3.862469	-3.335889	1.276369
27	6	0	-3.144926	0.383247	-1.275509
28	1	0	-4.202892	0.232487	-1.221834
29	1	0	-2.937438	1.429822	-1.356313
30	1	0	-2.755294	-0.124839	-2.132792
31	6	0	-3.150173	0.386060	1.266294
32	1	0	-2.988682	1.442574	1.317263
33	1	0	-4.200990	0.187041	1.233507
34	1	0	-2.725336	-0.081753	2.129755
35	6	0	-3.103138	-3.171775	1.290812
36	1	0	-4.154977	-2.977407	1.318294
37	1	0	-2.935015	-4.228290	1.311071
38	1	0	-2.634592	-2.719714	2.139932
39	6	0	-3.103138	-3.174577	-1.289527
40	1	0	-2.936213	-4.231334	-1.306844
41	1	0	-4.154740	-2.979083	-1.318087
42	1	0	-2.633632	-2.725347	-2.139618

BH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.000000	0.000000	0.000000
2	5	0	0.000000	0.000000	2.902961
3	5	0	2.514167	0.000000	1.451931
4	5	0	-0.238527	-1.003000	1.469813
5	5	0	1.391965	-1.003000	2.374109

6	5	0	-0.824544	0.641000	1.476474
7	5	0	1.689921	0.641000	2.878929
8	5	0	0.327662	1.672000	0.606381
9	5	0	0.361033	1.672000	2.316246
10	5	0	1.825472	1.672000	1.432266
11	1	0	3.672828	-0.223391	1.452895
12	1	0	1.771633	-1.925031	3.005069
13	1	0	2.280092	0.870055	3.874737
14	1	0	2.524234	2.622646	1.412170
15	1	0	2.214595	0.869897	-1.010102
16	1	0	-0.039026	2.622848	0.011546
17	1	0	0.029167	2.622835	2.931207
18	1	0	-1.982018	0.870046	1.490355
19	1	0	-0.579764	-0.223539	3.906108
20	1	0	-0.975043	-1.924833	1.482799
21	1	0	-0.578626	-0.223373	-1.003841
22	1	0	1.716453	-1.925136	-0.133354
23	6	0	1.647821	0.641000	-0.000759
24	6	0	1.359760	-1.003000	0.510723

C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.249817	-0.465803	-0.186623
2	8	0	2.069242	0.062671	0.809685
3	8	0	2.010677	-1.172958	-1.104703
4	6	0	3.393099	-0.934883	-0.785035
5	6	0	3.374786	-0.508735	0.672292
6	6	0	4.173582	-2.220261	-1.008257
7	1	0	4.121872	-2.499553	-2.064246
8	1	0	5.231901	-2.089756	-0.745118
9	1	0	3.767079	-3.049603	-0.417622
10	6	0	3.891486	0.126974	-1.762437
11	1	0	4.948381	0.369537	-1.597296
12	1	0	3.781955	-0.242689	-2.787236
13	1	0	3.301701	1.050393	-1.674060
14	6	0	3.465463	-1.628293	1.711730
15	1	0	4.441326	-2.127806	1.694181

16	1	0	3.314607	-1.208787	2.712834
17	1	0	2.682930	-2.381331	1.540722
18	6	0	4.403596	0.567208	0.984728
19	1	0	4.287823	0.890462	2.023527
20	1	0	5.424169	0.181796	0.862635
21	1	0	4.283870	1.449104	0.341543
22	7	0	-0.503105	1.915957	-0.122676
23	6	0	-0.180616	2.723276	0.920339
24	6	0	-0.670637	2.468298	-1.343951
25	6	0	-0.052987	4.102847	0.737476
26	6	0	-0.559266	3.828005	-1.580119
27	1	0	-0.899740	1.763797	-2.139476
28	6	0	-0.249477	4.666126	-0.514607
29	1	0	0.208520	4.722005	1.591123
30	1	0	-0.709412	4.214296	-2.583813
31	1	0	-0.150741	5.737751	-0.660224
32	6	0	0.052108	2.073185	2.244920
33	1	0	-0.894357	1.762173	2.695847
34	1	0	0.670000	1.176716	2.107578
35	1	0	0.547214	2.746525	2.952287
36	77	0	-0.792148	-0.242126	-0.032346
37	6	0	-1.369036	-1.749041	-1.320647
38	6	0	-3.123322	0.051621	0.150319
39	6	0	-2.591602	-0.363220	1.349285
40	6	0	-1.093874	-2.340989	-0.041737
41	6	0	-2.759759	-1.498328	-1.863704
42	1	0	-0.611329	-1.879334	-2.097231
43	6	0	-3.760114	-0.878988	-0.852050
44	1	0	-3.269698	1.121722	0.011460
45	6	0	-2.647136	-1.772406	1.881675
46	1	0	-2.446228	0.402655	2.112452
47	6	0	-2.198775	-2.841092	0.875439
48	1	0	-0.163417	-2.903084	0.030682
49	1	0	-2.657452	-0.821960	-2.723340
50	1	0	-3.181283	-2.431787	-2.272198
51	1	0	-4.530640	-0.335268	-1.408540
52	1	0	-4.296528	-1.676444	-0.320873
53	1	0	-1.996827	-1.821135	2.762894
54	1	0	-3.662860	-1.989706	2.247861
55	1	0	-3.051719	-3.196796	0.283732
56	1	0	-1.847523	-3.718435	1.428555

D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.125913	1.043002	0.294871
2	8	0	0.262429	1.529608	1.588869
3	8	0	0.042841	2.076579	-0.615528
4	6	0	-0.108321	2.931932	1.556557
5	6	0	0.228442	3.328920	0.086816
6	6	0	1.674971	3.768044	-0.082333
7	1	0	1.921081	3.827806	-1.146355
8	1	0	1.840481	4.754158	0.364199
9	1	0	2.357013	3.047922	0.372462
10	6	0	-0.712007	4.345903	-0.532254
11	1	0	-0.714979	5.281938	0.037308
12	1	0	-0.389165	4.576985	-1.552455
13	1	0	-1.732606	3.958797	-0.584182
14	6	0	0.681492	3.661057	2.623248
15	1	0	0.482341	4.737757	2.590009
16	1	0	0.391329	3.297780	3.613480
17	1	0	1.756154	3.504580	2.507741
18	6	0	-1.601609	2.997289	1.845228
19	1	0	-1.808390	2.548018	2.821560
20	1	0	-1.969312	4.028205	1.863883
21	1	0	-2.153092	2.439113	1.082448
22	5	0	1.912452	-0.366617	-0.920361
23	8	0	2.828848	-1.348733	-1.285422
24	8	0	2.563888	0.837449	-0.695318
25	6	0	3.992792	0.598527	-0.698162
26	6	0	4.121589	-0.738667	-1.495966
27	6	0	4.425201	0.466580	0.756399
28	1	0	5.513518	0.399570	0.852047
29	1	0	4.083855	1.343929	1.315099
30	1	0	3.989610	-0.420677	1.224795
31	6	0	4.683881	1.789839	-1.333543
32	1	0	4.551231	2.678959	-0.710736
33	1	0	5.759682	1.607509	-1.431261
34	1	0	4.279963	2.011485	-2.323596

35	6	0	4.311378	-0.528479	-2.990250
36	1	0	5.301162	-0.119692	-3.216029
37	1	0	4.221706	-1.489896	-3.506499
38	1	0	3.550409	0.143005	-3.388735
39	6	0	5.177616	-1.698867	-0.978786
40	1	0	5.158742	-2.616912	-1.573464
41	1	0	6.179631	-1.263981	-1.061053
42	1	0	5.005518	-1.975351	0.063433
43	77	0	0.020048	-0.979670	-0.157448
44	6	0	-1.650776	-1.222417	1.619231
45	6	0	1.228852	-1.193686	1.837157
46	6	0	1.389864	-2.389478	1.142295
47	6	0	-1.489366	-2.488126	1.106855
48	6	0	-1.077017	-0.750812	2.920662
49	1	0	-2.433100	-0.598650	1.200867
50	6	0	0.415935	-1.057746	3.106583
51	1	0	1.980874	-0.422386	1.692426
52	6	0	0.718807	-3.692032	1.471556
53	1	0	2.265062	-2.475336	0.503616
54	6	0	-0.758755	-3.572981	1.851225
55	1	0	-2.110246	-2.771911	0.262632
56	1	0	-1.228323	0.327232	2.990827
57	1	0	-1.652734	-1.202065	3.743510
58	1	0	0.857929	-0.260036	3.710462
59	1	0	0.541191	-1.983198	3.683085
60	1	0	0.808905	-4.349363	0.601884
61	1	0	1.276924	-4.195722	2.276557
62	1	0	-0.865754	-3.398072	2.928752
63	1	0	-1.252790	-4.529482	1.650627
64	5	0	-1.848517	-0.281658	-0.992483
65	8	0	-2.759901	-1.293314	-1.244318
66	8	0	-2.492988	0.943160	-0.860875
67	6	0	-3.928490	0.738436	-0.939804
68	6	0	-4.062168	-0.722923	-1.502735
69	6	0	-5.085732	-1.586273	-0.786277
70	1	0	-6.098023	-1.186313	-0.909694
71	1	0	-5.068195	-2.594942	-1.208038
72	1	0	-4.873175	-1.667582	0.282569
73	6	0	-4.308293	-0.776727	-3.003361
74	1	0	-4.266976	-1.816086	-3.337653
75	1	0	-5.292635	-0.372152	-3.260534

76	1	0	-3.537890	-0.226556	-3.545991
77	6	0	-4.530507	1.816799	-1.824942
78	1	0	-5.622343	1.730451	-1.843737
79	1	0	-4.277907	2.803030	-1.424072
80	1	0	-4.172596	1.768581	-2.852322
81	6	0	-4.507924	0.921612	0.460511
82	1	0	-4.291587	1.933347	0.814510
83	1	0	-5.594796	0.795898	0.453513
84	1	0	-4.100707	0.218890	1.190742

HBpin

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.000000	2.021146	0.000001
2	8	0	-1.333679	1.251146	0.000003
3	8	0	1.333679	1.251146	-0.000001
4	6	0	1.073082	-0.154909	0.000000
5	6	0	-1.073082	-0.154909	0.000000
6	6	0	-1.628332	-0.822522	-1.271845
7	1	0	-1.575398	-1.886201	-1.168477
8	1	0	-2.647275	-0.528196	-1.413367
9	1	0	-1.048115	-0.517029	-2.117375
10	6	0	-1.628332	-0.822526	1.271843
11	1	0	-2.668234	-0.590969	1.371268
12	1	0	-1.504218	-1.882956	1.201252
13	1	0	-1.098333	-0.457516	2.126694
14	6	0	1.628332	-0.822523	1.271844
15	1	0	1.404211	-1.868608	1.252446
16	1	0	2.688759	-0.685652	1.312605
17	1	0	1.177817	-0.377172	2.134166
18	6	0	1.628332	-0.822524	-1.271844
19	1	0	2.690676	-0.699061	-1.304730
20	1	0	1.390705	-1.865736	-1.259849
21	1	0	1.189404	-0.366639	-2.134637
22	1	0	0.000000	3.201146	0.000000

Int1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.183577	1.514918	-0.484276
2	5	0	-2.162909	-0.149840	0.409941
3	5	0	2.137231	0.034523	0.564561
4	8	0	3.216297	-0.397939	1.305128
5	8	0	-2.744898	0.930817	-0.254929
6	8	0	-3.153510	-1.040340	0.802355
7	8	0	-0.429726	1.525228	-1.850197
8	8	0	0.062463	2.776482	0.012550
9	8	0	2.565483	0.748634	-0.564278
10	6	0	-4.446218	-0.456047	0.510002
11	6	0	-4.098597	0.567725	-0.617301
12	6	0	4.411858	0.251103	0.811586
13	6	0	4.025176	0.676806	-0.638373
14	6	0	-0.296346	3.719910	-1.045326
15	6	0	-0.176217	2.860678	-2.345922
16	6	0	-1.714495	4.170128	-0.750342
17	1	0	-1.749853	4.627649	0.242455
18	1	0	-2.064631	4.909893	-1.481990
19	1	0	-2.395128	3.307283	-0.759651
20	6	0	-1.201221	3.162049	-3.412517
21	1	0	-1.095258	4.184700	-3.777550
22	1	0	-1.073224	2.487653	-4.254282
23	1	0	-2.219194	3.035411	-3.026982
24	6	0	1.237299	2.841003	-2.927883
25	1	0	1.281344	2.074587	-3.706521
26	1	0	1.505547	3.803889	-3.375955
27	1	0	1.970932	2.581217	-2.158616
28	6	0	0.669242	4.883449	-0.976085
29	1	0	0.492605	5.585988	-1.799979
30	1	0	0.539006	5.431303	-0.036959
31	1	0	1.713468	4.557726	-1.027488
32	6	0	4.551979	2.031852	-1.069213
33	1	0	5.644902	2.047601	-1.021948
34	1	0	4.263141	2.237480	-2.097023
35	1	0	4.166905	2.834653	-0.432840

36	6	0	4.367587	-0.363014	-1.697036
37	1	0	3.908413	-0.073829	-2.657522
38	1	0	5.450280	-0.437514	-1.854739
39	1	0	3.988698	-1.353939	-1.434681
40	6	0	4.660719	1.440450	1.720529
41	1	0	4.761445	1.097339	2.751485
42	1	0	5.582456	1.980838	1.452934
43	1	0	3.831087	2.153828	1.688368
44	6	0	5.558987	-0.734333	0.900331
45	1	0	6.477666	-0.312421	0.481367
46	1	0	5.750388	-0.989697	1.938908
47	1	0	5.328714	-1.658313	0.362232
48	6	0	-4.014130	-0.078670	-1.992314
49	1	0	-5.006982	-0.308235	-2.405098
50	1	0	-3.506097	0.597128	-2.679629
51	1	0	-3.448527	-1.019107	-1.953738
52	6	0	-4.956816	1.807394	-0.654120
53	1	0	-4.646252	2.456041	-1.475201
54	1	0	-6.014457	1.551881	-0.811002
55	1	0	-4.887735	2.383601	0.271773
56	6	0	-4.936319	0.226566	1.780987
57	1	0	-5.942590	0.644607	1.655034
58	1	0	-4.961381	-0.498064	2.599138
59	1	0	-4.261358	1.044531	2.067188
60	6	0	-5.398387	-1.560438	0.093317
61	1	0	-5.583932	-2.230331	0.934586
62	1	0	-6.358826	-1.146827	-0.224418
63	1	0	-4.978985	-2.155696	-0.724672
64	5	0	0.134369	-1.836115	-0.605376
65	5	0	1.628443	-2.801064	-0.908526
66	5	0	0.482809	-2.370235	-3.472015
67	5	0	-0.981475	-3.182350	-2.940124
68	1	0	-0.947183	-0.790867	-2.427547
69	5	0	1.843740	-3.110019	-2.626265
70	1	0	1.601870	-0.749181	-2.174371
71	5	0	1.224529	-4.367886	-1.583186
72	1	0	2.570165	-2.522530	-0.242166
73	5	0	-0.525167	-4.421800	-1.778022
74	1	0	0.092124	-4.049815	0.733303
75	1	0	-2.266921	-2.700601	-0.793305
76	5	0	0.507256	-4.106247	-3.182518

77	1	0	0.575419	-1.729546	-4.450059
78	1	0	-1.919627	-3.140239	-3.648537
79	1	0	2.918483	-2.991360	-3.116752
80	1	0	1.884817	-5.331848	-1.331005
81	1	0	-1.158380	-5.421637	-1.669517
82	1	0	0.625465	-4.854451	-4.090901
83	77	0	-0.014666	-0.215032	0.821627
84	6	0	-0.703691	-1.735753	2.351380
85	6	0	-0.831111	1.084680	2.527325
86	6	0	0.570516	1.236929	2.502142
87	6	0	0.696084	-1.594222	2.463016
88	6	0	-1.664023	-1.192558	3.382020
89	1	0	-1.087723	-2.559619	1.768065
90	6	0	-1.505081	0.316148	3.641388
91	1	0	-1.411303	1.867687	2.049662
92	6	0	1.471397	0.608542	3.540607
93	1	0	0.954655	2.124094	2.013531
94	6	0	1.319047	-0.910700	3.663108
95	1	0	1.310169	-2.337014	1.957024
96	1	0	-2.668951	-1.408708	3.043490
97	1	0	-1.525245	-1.757193	4.327208
98	1	0	-2.496654	0.746188	3.827986
99	1	0	-0.937277	0.484081	4.573341
100	1	0	2.504070	0.839969	3.286854
101	1	0	1.274865	1.095491	4.505982
102	1	0	0.716727	-1.155369	4.551857
103	1	0	2.303791	-1.351769	3.840603
104	1	0	0.708453	0.147232	-0.771154
105	6	0	1.113673	-1.714713	-2.048524
106	6	0	-0.479728	-1.745880	-2.209369
107	5	0	-1.182798	-2.887648	-1.210002
108	5	0	0.183332	-3.609437	-0.368463

Intlu

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.131311	1.603752	-0.460020
2	5	0	-2.145333	-0.027024	0.429847
3	5	0	2.167520	0.047144	0.426598
4	8	0	3.218915	-0.531815	1.105473
5	8	0	-2.838061	1.184342	0.394738
6	8	0	-3.021313	-1.081777	0.234004
7	8	0	-0.544654	1.665628	-1.775348
8	8	0	0.256849	2.822434	0.019037
9	8	0	2.613117	0.837331	-0.619543
10	6	0	-4.383702	-0.570952	0.123345
11	6	0	-4.138615	0.935840	-0.215278
12	6	0	4.446122	0.073015	0.640493
13	6	0	4.046509	0.648635	-0.759998
14	6	0	-0.113113	3.811630	-0.979698
15	6	0	-0.169699	2.968299	-2.288072
16	6	0	-1.478470	4.351431	-0.575483
17	1	0	-1.406043	4.774795	0.435891
18	1	0	-1.829999	5.136374	-1.248837
19	1	0	-2.210254	3.548432	-0.544306
20	6	0	-1.207147	3.413480	-3.300505
21	1	0	-0.971034	4.401966	-3.686251
22	1	0	-1.215547	2.714118	-4.140889
23	1	0	-2.207255	3.437817	-2.874026
24	6	0	1.193502	2.801567	-2.953786
25	1	0	1.116032	2.054115	-3.749257
26	1	0	1.533147	3.746246	-3.402738
27	1	0	1.935177	2.456595	-2.241889
28	6	0	0.938790	4.910518	-0.987355
29	1	0	0.742562	5.622452	-1.784086
30	1	0	0.916879	5.449438	-0.032053
31	1	0	1.936813	4.492907	-1.115970
32	6	0	4.669600	2.002940	-1.080344
33	1	0	5.762591	1.933767	-1.087563
34	1	0	4.361065	2.324440	-2.079097
35	1	0	4.372453	2.769585	-0.365516

36	6	0	4.283029	-0.317331	-1.907990
37	1	0	3.808776	0.083017	-2.818372
38	1	0	5.343040	-0.447555	-2.109769
39	1	0	3.833242	-1.294848	-1.716975
40	6	0	4.821478	1.159603	1.643759
41	1	0	4.925461	0.708448	2.635677
42	1	0	5.763806	1.640647	1.390613
43	1	0	4.040026	1.925194	1.693369
44	6	0	5.519794	-0.996177	0.596190
45	1	0	6.454793	-0.604143	0.185160
46	1	0	5.712943	-1.362459	1.609895
47	1	0	5.207624	-1.855543	-0.009463
48	6	0	-3.982527	1.199634	-1.703042
49	1	0	-4.929493	1.046640	-2.237312
50	1	0	-3.680842	2.243210	-1.847354
51	1	0	-3.210436	0.567620	-2.140464
52	6	0	-5.152000	1.887244	0.388942
53	1	0	-4.894918	2.919333	0.125381
54	1	0	-6.157995	1.679487	0.009195
55	1	0	-5.174741	1.820770	1.487560
56	6	0	-5.059460	-0.782881	1.462407
57	1	0	-6.119335	-0.504056	1.432760
58	1	0	-4.995879	-1.838337	1.739005
59	1	0	-4.567461	-0.189891	2.251628
60	6	0	-5.086269	-1.360060	-0.968312
61	1	0	-5.199166	-2.402438	-0.656279
62	1	0	-6.075800	-0.955162	-1.168753
63	1	0	-4.506693	-1.357621	-1.894349
64	5	0	0.142850	-1.780823	-0.714730
65	5	0	-0.813491	-1.896636	-2.233159
66	5	0	0.940787	-1.832968	-2.333103
67	5	0	1.586504	-2.796336	-1.020048
68	6	0	0.243102	-3.431481	-0.273971
69	6	0	-1.116114	-2.913141	-0.958970
70	5	0	0.049421	-2.902169	-3.412455
71	5	0	-1.311732	-3.563576	-2.500821
72	1	0	-1.566923	-1.011415	-2.436573
73	5	0	1.533522	-3.466077	-2.654330
74	1	0	1.497708	-0.847014	-2.698813
75	5	0	1.096973	-4.472761	-1.277753
76	1	0	2.534130	-2.582046	-0.348591

77	5	0	-0.661404	-4.527348	-1.186304
78	1	0	0.197152	-3.623527	0.794977
79	1	0	-1.970415	-2.744657	-0.314442
80	5	0	0.134736	-4.545135	-2.747861
81	1	0	-0.046951	-2.696684	-4.566932
82	1	0	-2.411488	-3.798646	-2.854652
83	1	0	2.540299	-3.663150	-3.244348
84	1	0	1.706093	-5.346889	-0.760965
85	1	0	-1.267364	-5.356410	-0.602391
86	1	0	0.106819	-5.524976	-3.415711
87	77	0	0.012652	-0.166821	0.768624
88	6	0	-0.735089	-1.656623	2.284012
89	6	0	-0.683094	1.167425	2.486810
90	6	0	0.730008	1.240317	2.442069
91	6	0	0.674637	-1.574145	2.410715
92	6	0	-1.681193	-1.053954	3.286588
93	1	0	-1.166962	-2.480630	1.721131
94	6	0	-1.410155	0.428155	3.587221
95	1	0	-1.214738	1.980138	2.003549
96	6	0	1.616222	0.555327	3.455458
97	1	0	1.146436	2.101167	1.940299
98	6	0	1.328469	-0.934163	3.624406
99	1	0	1.285681	-2.317450	1.907704
100	1	0	-2.693436	-1.167252	2.875861
101	1	0	-1.661891	-1.645715	4.221644
102	1	0	-2.362328	0.936491	3.775707
103	1	0	-0.831105	0.525722	4.514099
104	1	0	2.653050	0.685012	3.150505
105	1	0	1.512678	1.078666	4.414906
106	1	0	0.683006	-1.104122	4.488109
107	1	0	2.260754	-1.463776	3.831260
108	1	0	0.570337	0.072752	-0.948764

Int2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.292524	-0.518679	-0.909294
2	5	0	0.171311	0.617719	1.175453
3	8	0	-0.282362	1.450976	2.184482
4	8	0	1.246671	-1.903434	-1.037425
5	8	0	2.616778	-0.080400	-0.939867
6	8	0	1.028922	-0.350748	1.684914
7	6	0	0.431090	1.154874	3.408850
8	6	0	1.106645	-0.239225	3.125779
9	6	0	3.449323	-1.185485	-1.353776
10	6	0	2.590799	-2.429827	-0.967448
11	6	0	3.624803	-1.045801	-2.860076
12	1	0	4.053585	-0.064696	-3.084908
13	1	0	4.282113	-1.815092	-3.278975
14	1	0	2.648508	-1.116917	-3.351178
15	6	0	2.688620	-3.600157	-1.927223
16	1	0	3.712919	-3.985578	-1.978430
17	1	0	2.040954	-4.413192	-1.586200
18	1	0	2.370067	-3.318935	-2.933787
19	6	0	2.816510	-2.893257	0.464213
20	1	0	2.060118	-3.641806	0.722202
21	1	0	3.802993	-3.349685	0.593788
22	1	0	2.712660	-2.055198	1.157030
23	6	0	4.784001	-1.088072	-0.643317
24	1	0	5.416385	-1.952069	-0.875769
25	1	0	5.315299	-0.187846	-0.964173
26	1	0	4.655377	-1.035416	0.440058
27	6	0	2.572512	-0.316008	3.522475
28	1	0	2.699305	-0.140542	4.596055
29	1	0	2.964444	-1.313718	3.304234
30	1	0	3.180338	0.409600	2.977478
31	6	0	0.366604	-1.430703	3.716682
32	1	0	0.819687	-2.353706	3.340674
33	1	0	0.435498	-1.444255	4.808811
34	1	0	-0.688891	-1.439486	3.439310
35	6	0	1.437237	2.280856	3.609789

36	1	0	0.904111	3.235376	3.647860
37	1	0	1.997260	2.168092	4.543080
38	1	0	2.155250	2.326787	2.784985
39	6	0	-0.569061	1.146747	4.549427
40	1	0	-0.083436	0.881927	5.494797
41	1	0	-1.007912	2.141447	4.664018
42	1	0	-1.381681	0.440705	4.367296
43	5	0	-1.694513	-0.727235	-0.334463
44	5	0	-2.408981	-1.171282	1.243733
45	5	0	-1.977350	-3.623296	-0.129207
46	5	0	-3.054803	-3.081646	-1.409895
47	1	0	-0.741059	-2.399041	-1.716783
48	5	0	-2.540096	-2.921939	1.382447
49	1	0	-0.280517	-2.241389	0.768748
50	5	0	-3.973679	-1.955551	1.036577
51	1	0	-2.057384	-0.541471	2.179740
52	5	0	-4.288927	-2.053538	-0.691424
53	1	0	-3.991126	0.442866	0.016609
54	1	0	-2.923455	-0.829429	-2.598690
55	5	0	-3.702133	-3.485189	0.180861
56	1	0	-1.266417	-4.563546	-0.205021
57	1	0	-3.112891	-3.731434	-2.397296
58	1	0	-2.231152	-3.457802	2.391528
59	1	0	-4.827935	-1.827523	1.848128
60	1	0	-5.377888	-1.997609	-1.156420
61	1	0	-4.357213	-4.456215	0.355839
62	77	0	-0.299308	0.786147	-0.818214
63	6	0	-2.094228	2.337228	-1.403452
64	6	0	0.805157	2.449532	-1.999290
65	6	0	1.172470	2.591953	-0.666234
66	6	0	-1.728097	2.663745	-0.124057
67	6	0	-1.640019	3.060910	-2.643693
68	1	0	-2.903287	1.620247	-1.533512
69	6	0	-0.138225	3.406567	-2.703984
70	1	0	1.480115	1.869673	-2.630428
71	6	0	0.633761	3.657743	0.247258
72	1	0	2.098035	2.113066	-0.351929
73	6	0	-0.890659	3.873482	0.209934
74	1	0	-2.233205	2.161878	0.698259
75	1	0	-1.893951	2.445297	-3.511511
76	1	0	-2.224968	3.985971	-2.759740

77	1	0	0.151695	3.462147	-3.758388
78	1	0	0.028057	4.411394	-2.295476
79	1	0	0.924470	3.408321	1.268388
80	1	0	1.138188	4.608573	0.014068
81	1	0	-1.136843	4.667087	-0.506227
82	1	0	-1.203875	4.247705	1.189952
83	6	0	-1.327030	-2.190651	0.483865
84	6	0	-1.617401	-2.281103	-1.088578
85	5	0	-2.910804	-1.329839	-1.522935
86	5	0	-3.473460	-0.625354	-0.024917

Int2u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.347629	-0.653430	-0.913673
2	5	0	0.218475	0.589410	1.171215
3	8	0	-0.308138	1.435843	2.137780
4	8	0	1.306673	-2.009506	-1.192255
5	8	0	2.666195	-0.216671	-0.787589
6	8	0	1.105452	-0.310261	1.728610
7	6	0	0.365985	1.183397	3.397583
8	6	0	1.070579	-0.203022	3.169696
9	6	0	3.534640	-1.307536	-1.168026
10	6	0	2.626507	-2.548427	-0.927235
11	6	0	3.882157	-1.100233	-2.637318
12	1	0	4.350531	-0.119357	-2.759779
13	1	0	4.579741	-1.859565	-3.006258
14	1	0	2.978571	-1.118321	-3.256929
15	6	0	2.882470	-3.721311	-1.850930
16	1	0	3.877328	-4.143114	-1.669963
17	1	0	2.145173	-4.507141	-1.663468
18	1	0	2.817134	-3.441920	-2.902963
19	6	0	2.635118	-3.018808	0.521261
20	1	0	1.840875	-3.757247	0.661215
21	1	0	3.590447	-3.483247	0.787382
22	1	0	2.437283	-2.183190	1.196437
23	6	0	4.780235	-1.256889	-0.306341
24	1	0	5.423378	-2.124071	-0.493576

25	1	0	5.358493	-0.356307	-0.531637
26	1	0	4.524539	-1.237556	0.755507
27	6	0	2.501964	-0.274826	3.675763
28	1	0	2.545059	-0.118258	4.759080
29	1	0	2.915356	-1.266008	3.467471
30	1	0	3.144661	0.463205	3.191274
31	6	0	0.289282	-1.395623	3.701579
32	1	0	0.765876	-2.316935	3.355372
33	1	0	0.276364	-1.406699	4.796126
34	1	0	-0.741055	-1.405831	3.342095
35	6	0	1.349649	2.326320	3.608807
36	1	0	0.808651	3.277325	3.588580
37	1	0	1.862520	2.247950	4.572347
38	1	0	2.109849	2.349591	2.821863
39	6	0	-0.675141	1.186173	4.500381
40	1	0	-0.220448	0.945956	5.467496
41	1	0	-1.130314	2.177237	4.580302
42	1	0	-1.470231	0.464095	4.303907
43	5	0	-1.587101	-0.814131	-0.305262
44	5	0	-1.793295	-2.365126	-1.181763
45	5	0	-1.487204	-2.385038	0.545101
46	5	0	-2.445233	-1.093251	1.250694
47	6	0	-3.287174	-0.445766	-0.018044
48	6	0	-2.921006	-1.155965	-1.390492
49	5	0	-2.619247	-3.551531	-0.165654
50	5	0	-3.497769	-2.731187	-1.451817
51	1	0	-1.040363	-2.586324	-2.063981
52	5	0	-3.020192	-2.759231	1.354388
53	1	0	-0.440605	-2.702921	0.997604
54	5	0	-4.153428	-1.458599	1.003435
55	1	0	-2.175999	-0.376155	2.150648
56	5	0	-4.453293	-1.447726	-0.725529
57	1	0	-3.526074	0.611139	-0.061983
58	1	0	-2.939481	-0.545258	-2.286753
59	5	0	-4.273065	-2.976598	0.115406
60	1	0	-2.363319	-4.705978	-0.249591
61	1	0	-3.844506	-3.149807	-2.502980
62	1	0	-3.053697	-3.323944	2.396957
63	1	0	-4.963913	-0.966639	1.709747
64	1	0	-5.381184	-0.930568	-1.240296
65	1	0	-5.206912	-3.694207	0.240700

66	77	0	-0.212747	0.701248	-0.838362
67	6	0	-1.913280	2.329194	-1.525461
68	6	0	1.002545	2.279491	-2.025986
69	6	0	1.329894	2.454166	-0.687954
70	6	0	-1.574934	2.679659	-0.244436
71	6	0	-1.390435	3.007278	-2.766047
72	1	0	-2.756962	1.658058	-1.682617
73	6	0	0.133156	3.256682	-2.795849
74	1	0	1.657822	1.635495	-2.611606
75	6	0	0.813212	3.570462	0.175191
76	1	0	2.213196	1.935242	-0.321861
77	6	0	-0.694481	3.861638	0.071434
78	1	0	-2.108640	2.230379	0.589948
79	1	0	-1.674407	2.395288	-3.629735
80	1	0	-1.913191	3.965207	-2.907701
81	1	0	0.457065	3.258250	-3.842120
82	1	0	0.342632	4.268128	-2.425710
83	1	0	1.048391	3.333902	1.213278
84	1	0	1.373667	4.488797	-0.058948
85	1	0	-0.875691	4.635203	-0.684768
86	1	0	-1.024595	4.290635	1.023188

Int3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.828371	0.749786	-0.890119
2	8	0	2.953701	-0.048257	-1.038217
3	8	0	2.125681	1.931441	-0.232105
4	6	0	4.058609	0.567783	-0.336236
5	6	0	3.562831	2.043021	-0.129478
6	6	0	4.006985	2.996572	-1.234586
7	1	0	3.506938	3.959270	-1.098239
8	1	0	5.083827	3.172568	-1.215654
9	1	0	3.731512	2.612420	-2.218139
10	6	0	3.880567	2.630072	1.238343
11	1	0	4.961364	2.673274	1.403163
12	1	0	3.485634	3.645358	1.302644
13	1	0	3.422452	2.036003	2.032701

14	6	0	5.285943	0.438370	-1.225909
15	1	0	6.154715	0.924747	-0.772448
16	1	0	5.530458	-0.627926	-1.357244
17	1	0	5.124992	0.875486	-2.216670
18	6	0	4.282417	-0.185759	0.954732
19	1	0	4.506301	-1.236315	0.734618
20	1	0	5.121201	0.233436	1.527807
21	1	0	3.379119	-0.166363	1.571100
22	5	0	-0.686608	1.861159	-0.260229
23	8	0	-0.889660	2.209306	1.064182
24	8	0	-0.786634	2.975835	-1.079453
25	6	0	-0.871164	4.167279	-0.272674
26	6	0	-1.246802	3.617751	1.154647
27	6	0	-1.922007	5.086729	-0.883995
28	1	0	-2.058534	5.977831	-0.267459
29	1	0	-1.602527	5.397642	-1.876452
30	1	0	-2.882500	4.581174	-0.984424
31	6	0	0.501748	4.824617	-0.337976
32	1	0	0.743955	5.033164	-1.383582
33	1	0	0.525171	5.775742	0.211883
34	1	0	1.274141	4.160564	0.059460
35	6	0	-0.437521	4.234851	2.281988
36	1	0	-0.558472	5.322710	2.300509
37	1	0	-0.775959	3.855315	3.246646
38	1	0	0.627224	4.013430	2.171310
39	6	0	-2.727216	3.693079	1.480139
40	1	0	-2.919401	3.161032	2.422058
41	1	0	-3.051188	4.727515	1.618780
42	1	0	-3.343911	3.232222	0.706039
43	5	0	-2.300444	-0.501535	-0.649831
44	5	0	-3.603204	0.741275	-0.646141
45	5	0	-3.703596	-0.558437	-1.801447
46	5	0	-3.196797	-2.022998	-0.993226
47	6	0	-2.895659	-1.556209	0.565114
48	6	0	-3.127844	0.013621	0.764154
49	5	0	-5.175826	0.019847	-0.998943
50	5	0	-4.755549	0.422252	0.654934
51	1	0	-3.281406	1.855726	-0.867632
52	5	0	-4.920474	-1.705117	-1.219145
53	1	0	-3.524423	-0.359990	-2.957727
54	5	0	-4.338782	-2.365864	0.301624

55	1	0	-2.595639	-2.946807	-1.441709
56	5	0	-4.241044	-1.043284	1.458416
57	1	0	-2.478763	0.519740	1.472924
58	5	0	-5.570807	-1.097655	0.313569
59	1	0	-6.002372	0.632853	-1.589032
60	1	0	-5.140594	1.322206	1.332919
61	1	0	-5.568377	-2.371812	-1.965250
62	1	0	-4.438041	-3.464372	0.727983
63	1	0	-4.205341	-1.195140	2.631201
64	1	0	-6.679571	-1.315629	0.687553
65	77	0	-0.207311	0.015013	-1.059263
66	6	0	1.103520	-1.715018	-2.598219
67	6	0	0.928933	1.115534	-2.642406
68	6	0	-0.507304	0.860871	-2.939220
69	6	0	-0.213012	-2.001914	-2.726756
70	6	0	1.920250	-1.019453	-3.652244
71	1	0	1.654284	-2.153037	-1.766160
72	6	0	1.962508	0.513566	-3.587156
73	1	0	1.099927	2.170453	-2.426741
74	6	0	-0.927254	0.000155	-4.122294
75	1	0	-1.131165	1.751059	-2.842918
76	6	0	-1.047006	-1.515334	-3.872185
77	1	0	-0.676153	-2.676173	-2.024257
78	1	0	2.950249	-1.401592	-3.604294
79	1	0	1.531982	-1.324292	-4.632727
80	1	0	2.956920	0.839766	-3.284350
81	1	0	1.790955	0.939691	-4.585268
82	1	0	-1.897032	0.366831	-4.475435
83	1	0	-0.227842	0.187667	-4.942181
84	1	0	-0.777724	-2.057359	-4.790786
85	1	0	-2.090342	-1.768774	-3.674717
86	5	0	0.623612	-1.780237	0.438730
87	5	0	0.211623	-0.409334	1.502183
88	8	0	-0.204749	-2.842106	0.133765
89	8	0	1.879509	-2.206413	0.837808
90	8	0	1.175463	0.365474	2.105414
91	6	0	1.940309	-3.664425	0.779901
92	6	0	0.453847	-4.094762	0.469932
93	8	0	-0.729012	-0.850091	2.408555
94	6	0	1.030921	0.225218	3.549429
95	6	0	-0.455168	-0.258730	3.721561

96	6	0	0.298276	-5.033365	-0.709065
97	1	0	0.779340	-5.995591	-0.505511
98	1	0	-0.759376	-5.209779	-0.907562
99	1	0	0.733619	-4.613402	-1.622958
100	6	0	-0.314957	-4.633768	1.670621
101	1	0	-1.360664	-4.801778	1.375999
102	1	0	0.095764	-5.571964	2.030930
103	1	0	-0.321273	-3.904231	2.496204
104	6	0	2.466168	-4.156966	2.131859
105	1	0	2.569588	-5.242302	2.138450
106	1	0	3.449269	-3.719120	2.325144
107	1	0	1.808643	-3.863382	2.963001
108	6	0	2.956032	-4.047367	-0.295434
109	1	0	3.918882	-3.601509	-0.043287
110	1	0	3.075805	-5.133113	-0.349796
111	1	0	2.668702	-3.690227	-1.286476
112	1	0	-2.119136	-1.996816	1.171999
113	6	0	-1.455254	0.862983	3.942167
114	1	0	-2.474186	0.467697	3.889894
115	1	0	-1.330852	1.317871	4.927561
116	1	0	-1.345093	1.635615	3.177574
117	6	0	-0.657579	-1.345663	4.772637
118	1	0	-1.698929	-1.664354	4.770872
119	1	0	-0.030140	-2.221774	4.581657
120	1	0	-0.418417	-0.956897	5.769062
121	6	0	1.321452	1.554230	4.213430
122	1	0	0.702918	2.358611	3.801471
123	1	0	1.144443	1.496921	5.301069
124	1	0	2.369933	1.830443	4.067544
125	6	0	2.050906	-0.813482	3.987071
126	1	0	1.902466	-1.762832	3.458832
127	1	0	3.053139	-0.457666	3.745799
128	1	0	2.006827	-1.003024	5.063191

Int3u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.719131	0.651814	-1.149104

2	8	0	2.779310	-0.232681	-1.326157
3	8	0	2.156811	1.847317	-0.615193
4	6	0	3.991156	0.366725	-0.834170
5	6	0	3.591469	1.884831	-0.640806
6	6	0	3.994958	2.769665	-1.812648
7	1	0	3.568891	3.772674	-1.662283
8	1	0	5.074186	2.870154	-1.907052
9	1	0	3.600309	2.384168	-2.762224
10	6	0	4.065672	2.497436	0.666460
11	1	0	5.160409	2.521314	0.723613
12	1	0	3.698773	3.521869	0.745076
13	1	0	3.680027	1.931464	1.516055
14	6	0	5.077209	0.121473	-1.868229
15	1	0	6.029660	0.578473	-1.559680
16	1	0	5.242921	-0.948378	-1.970792
17	1	0	4.806615	0.519168	-2.852944
18	6	0	4.367479	-0.331466	0.465368
19	1	0	4.530708	-1.388384	0.276101
20	1	0	5.284213	0.089799	0.892976
21	1	0	3.553221	-0.259790	1.197288
22	5	0	-0.675975	1.886705	-0.218752
23	8	0	-0.640881	2.356159	1.085958
24	8	0	-0.925085	2.926664	-1.104981
25	6	0	-0.856664	4.182055	-0.384567
26	6	0	-1.083041	3.734630	1.093133
27	6	0	-1.920749	5.114617	-0.934156
28	1	0	-1.953409	6.044396	-0.363518
29	1	0	-1.693094	5.365013	-1.972676
30	1	0	-2.914709	4.651593	-0.911386
31	6	0	0.533815	4.760836	-0.640608
32	1	0	0.684169	4.869421	-1.718892
33	1	0	0.655311	5.741271	-0.179401
34	1	0	1.303511	4.077030	-0.267091
35	6	0	-0.243884	4.510077	2.100313
36	1	0	-0.471842	5.574520	2.049596
37	1	0	-0.479771	4.169918	3.115341
38	1	0	0.823602	4.365852	1.926455
39	6	0	-2.541357	3.753757	1.515482
40	1	0	-2.648822	3.274633	2.487898
41	1	0	-2.924437	4.779741	1.598780
42	1	0	-3.168816	3.212996	0.811148

43	5	0	-2.325234	-0.435638	-0.141917
44	5	0	-3.674972	0.736969	-0.351740
45	5	0	-5.158727	-0.081491	-0.853510
46	5	0	-4.971587	0.435623	0.814623
47	1	0	-3.401184	1.768020	-0.868264
48	5	0	-4.807712	-1.798236	-0.950605
49	1	0	-3.310830	-0.604316	-2.313013
50	5	0	-4.392354	-2.354461	0.671115
51	1	0	-2.611583	-2.684664	-0.920839
52	5	0	-4.491890	-0.975049	1.759613
53	1	0	-2.711185	0.883178	2.026912
54	5	0	-5.674371	-1.155543	0.441797
55	1	0	-5.828021	0.390036	-1.712228
56	1	0	-5.602289	1.327545	1.261086
57	1	0	-5.154449	-2.507068	-1.829715
58	1	0	-4.519848	-3.504056	0.910666
59	1	0	-4.785058	-1.130259	2.902015
60	1	0	-6.810592	-1.425486	0.605756
61	77	0	-0.351824	-0.009656	-0.947728
62	6	0	0.803382	-1.918974	-2.657148
63	6	0	0.646689	0.940672	-2.721692
64	6	0	-0.825600	0.710869	-2.835799
65	6	0	-0.525790	-2.173537	-2.642154
66	6	0	1.503309	-1.248600	-3.811845
67	1	0	1.419943	-2.296764	-1.856320
68	6	0	1.544819	0.295921	-3.777418
69	1	0	0.847094	2.001351	-2.621983
70	6	0	-1.400621	-0.169099	-3.938976
71	1	0	-1.391737	1.637521	-2.757587
72	6	0	-1.456785	-1.694630	-3.714409
73	1	0	-0.909994	-2.796062	-1.847657
74	1	0	2.524891	-1.633790	-3.863562
75	1	0	1.007600	-1.576479	-4.735417
76	1	0	2.580322	0.623492	-3.626154
77	1	0	1.241980	0.690911	-4.755398
78	1	0	-2.411174	0.179265	-4.163790
79	1	0	-0.831265	0.039079	-4.857257
80	1	0	-1.228834	-2.214451	-4.660816
81	1	0	-2.473214	-2.018297	-3.467844
82	5	0	0.666000	-1.745078	0.575583
83	5	0	0.411053	-0.308406	1.574983

84	8	0	-0.164487	-2.792437	0.238661
85	8	0	1.912990	-2.205006	0.970090
86	8	0	1.459942	0.507812	1.949546
87	6	0	1.956659	-3.653898	0.892679
88	6	0	0.447450	-4.054351	0.641352
89	8	0	-0.393128	-0.650343	2.633146
90	6	0	1.505895	0.528149	3.404149
91	6	0	0.079284	0.017366	3.829048
92	6	0	0.235902	-5.065115	-0.468218
93	1	0	0.693849	-6.023567	-0.218529
94	1	0	-0.841217	-5.235076	-0.602550
95	1	0	0.641310	-4.715280	-1.414182
96	6	0	-0.288483	-4.471733	1.908891
97	1	0	-1.358033	-4.602500	1.666079
98	1	0	0.093093	-5.418056	2.308629
99	1	0	-0.230167	-3.696762	2.677052
100	6	0	2.523384	-4.176684	2.205941
101	1	0	2.567488	-5.271895	2.212452
102	1	0	3.546466	-3.791653	2.333690
103	1	0	1.932118	-3.848476	3.068941
104	6	0	2.904056	-4.027772	-0.248792
105	1	0	3.900695	-3.637347	-0.022138
106	1	0	2.984012	-5.123834	-0.353041
107	1	0	2.595091	-3.613788	-1.210605
108	1	0	-2.132959	-2.134633	1.771799
109	6	0	-0.907758	1.137941	4.150270
110	1	0	-1.901459	0.708699	4.292491
111	1	0	-0.622590	1.677125	5.059735
112	1	0	-0.972026	1.841426	3.315532
113	6	0	0.090410	-1.008638	4.948242
114	1	0	-0.931446	-1.327730	5.157210
115	1	0	0.676570	-1.903529	4.679855
116	1	0	0.507600	-0.592837	5.875192
117	6	0	1.820696	1.942513	3.858668
118	1	0	1.119532	2.656770	3.434219
119	1	0	1.786846	2.012438	4.957841
120	1	0	2.828839	2.229321	3.540776
121	6	0	2.636531	-0.409800	3.810753
122	1	0	2.486426	-1.413145	3.395467
123	1	0	3.586123	-0.026216	3.419978
124	1	0	2.728878	-0.484936	4.899592

125	6	0	-3.627572	-0.636586	-1.285825
126	5	0	-2.922149	-1.518071	1.164621
127	5	0	-3.268660	0.190619	1.255761
128	6	0	-3.195811	-1.911526	-0.430337

Int4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.632303	-0.110116	1.569153
2	5	0	-0.592242	2.396925	-0.199485
3	5	0	-1.999199	-1.679332	-0.045180
4	8	0	-2.999469	-2.393395	-0.688565
5	8	0	0.555782	2.422567	0.609066
6	8	0	-0.807274	3.617836	-0.778181
7	8	0	0.644324	-0.614305	1.732276
8	8	0	-1.216166	0.241903	2.763568
9	8	0	-1.290323	-2.514857	0.816915
10	6	0	0.102492	4.579208	-0.145918
11	6	0	1.253000	3.672286	0.372481
12	6	0	-3.086966	-3.732971	-0.126307
13	6	0	-1.719202	-3.887394	0.637066
14	6	0	-0.166090	0.211860	3.789308
15	6	0	0.897650	-0.741693	3.151353
16	6	0	0.317898	1.642721	3.935617
17	1	0	-0.523395	2.282347	4.231527
18	1	0	1.088545	1.729438	4.709226
19	1	0	0.714922	2.017912	2.989483
20	6	0	2.338879	-0.331013	3.388379
21	1	0	2.581400	-0.300418	4.459327
22	1	0	3.013669	-1.053541	2.910376
23	1	0	2.548461	0.650766	2.942604
24	6	0	0.682511	-2.208772	3.493644
25	1	0	1.322550	-2.821681	2.852058
26	1	0	0.927405	-2.428254	4.536651
27	1	0	-0.355996	-2.503572	3.289061
28	6	0	-0.773891	-0.297661	5.081739
29	1	0	0.000794	-0.392490	5.847527
30	1	0	-1.519054	0.418474	5.446817

31	1	0	-1.257458	-1.265856	4.947619
32	6	0	-1.843616	-4.545255	1.997335
33	1	0	-2.268293	-5.555975	1.907347
34	1	0	-0.851088	-4.651092	2.448263
35	1	0	-2.465202	-3.968133	2.676675
36	6	0	-0.639405	-4.598462	-0.171584
37	1	0	0.314031	-4.500879	0.365226
38	1	0	-0.855870	-5.657955	-0.288224
39	1	0	-0.510371	-4.162515	-1.159125
40	6	0	-4.290139	-3.741570	0.797884
41	1	0	-5.187520	-3.465199	0.231866
42	1	0	-4.469283	-4.738592	1.232956
43	1	0	-4.174475	-3.035282	1.618578
44	6	0	-3.296025	-4.718495	-1.262538
45	1	0	-3.299563	-5.746410	-0.883413
46	1	0	-4.251178	-4.524652	-1.745702
47	1	0	-2.508501	-4.625363	-2.013469
48	6	0	2.338499	3.398331	-0.654075
49	1	0	2.953436	4.282898	-0.834202
50	1	0	2.981944	2.593879	-0.293292
51	1	0	1.905291	3.075528	-1.609149
52	6	0	1.885675	4.139504	1.675678
53	1	0	2.649375	3.423638	1.984245
54	1	0	2.374739	5.104316	1.531476
55	1	0	1.159300	4.233591	2.475181
56	6	0	-0.683716	5.242911	0.977692
57	1	0	-0.106517	6.031842	1.463231
58	1	0	-1.599660	5.679350	0.559931
59	1	0	-0.978279	4.507782	1.738115
60	6	0	0.511213	5.585977	-1.198781
61	1	0	-0.356426	6.166948	-1.513784
62	1	0	1.251763	6.284700	-0.792633
63	1	0	0.927881	5.105791	-2.080713
64	5	0	-0.305738	-0.211499	-1.791151
65	5	0	-0.187214	-1.797268	-2.614749
66	5	0	2.495902	-1.057681	-1.991277
67	5	0	2.298604	0.392358	-2.990056
68	1	0	1.647427	0.690838	-0.703246
69	5	0	1.490373	-2.309412	-2.702693
70	1	0	0.836654	-1.716424	-0.406676
71	5	0	0.684669	-1.648105	-4.130668

72	1	0	-1.031063	-2.576270	-2.356745
73	5	0	1.178836	0.032365	-4.301509
74	1	0	-1.419485	-0.103244	-4.124443
75	1	0	0.347328	2.048299	-2.795178
76	5	0	2.353882	-1.188891	-3.756754
77	1	0	3.155201	1.209578	-2.943500
78	1	0	1.763998	-3.439643	-2.463124
79	1	0	0.404969	-2.342343	-5.050191
80	1	0	1.275945	0.571885	-5.358591
81	1	0	3.291478	-1.539177	-4.393698
82	77	0	-1.657940	0.462088	-0.297697
83	6	0	-2.778001	1.547811	-1.910039
84	6	0	-3.139139	1.812223	0.908060
85	6	0	-3.566694	0.487138	1.061928
86	6	0	-3.319561	0.246558	-1.768170
87	6	0	-3.513671	2.782388	-1.462875
88	1	0	-2.052859	1.696241	-2.709069
89	6	0	-3.893369	2.797837	0.025284
90	1	0	-2.566464	2.227236	1.733642
91	6	0	-4.750216	-0.088952	0.336943
92	1	0	-3.291901	-0.012410	1.977817
93	6	0	-4.716077	0.059586	-1.183304
94	1	0	-2.995902	-0.511131	-2.474370
95	1	0	-2.882905	3.648533	-1.679783
96	1	0	-4.416581	2.891718	-2.080039
97	1	0	-3.749259	3.800461	0.427299
98	1	0	-4.967290	2.583281	0.141430
99	1	0	-4.808477	-1.153557	0.576589
100	1	0	-5.677168	0.361746	0.740114
101	1	0	-5.329027	0.914002	-1.495365
102	1	0	-5.168045	-0.822627	-1.645190
103	1	0	-0.071254	0.885670	0.432055
104	6	0	0.914350	-1.360414	-1.427907
105	6	0	1.375788	0.160183	-1.613492
106	5	0	0.607387	0.897333	-2.883831
107	5	0	-0.395611	-0.346592	-3.571552
108	5	0	3.854949	-1.104808	-1.019099
109	8	0	4.896283	-1.991716	-1.098064
110	8	0	4.071616	-0.107975	-0.083385
111	6	0	5.813144	-1.677592	-0.016322
112	6	0	5.491209	-0.180141	0.252011

113	6	0	7.232514	-1.943942	-0.491265
114	1	0	7.959957	-1.628696	0.274085
115	1	0	7.375838	-3.013121	-0.666264
116	1	0	7.452923	-1.418269	-1.419432
117	6	0	5.459118	-2.583586	1.147376
118	1	0	5.493196	-3.625677	0.822068
119	1	0	6.141484	-2.458001	1.983654
120	1	0	4.439896	-2.380296	1.502243
121	6	0	5.673744	0.274198	1.685429
122	1	0	6.726477	0.219965	1.982593
123	1	0	5.349974	1.314598	1.796119
124	1	0	5.097967	-0.327977	2.391797
125	6	0	6.206971	0.763145	-0.698073
126	1	0	5.774650	1.763884	-0.615519
127	1	0	7.274042	0.830224	-0.475605
128	1	0	6.089346	0.436045	-1.736597

Int4u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-2.282814	1.122045	0.282047
2	5	0	0.232817	1.887394	-0.305900
3	5	0	-2.087452	-1.747276	-0.457372
4	8	0	-2.057366	-2.996601	-1.055677
5	8	0	-0.447939	3.104696	-0.396451
6	8	0	1.570262	2.133824	-0.004426
7	8	0	-2.313606	1.592873	1.581939
8	8	0	-3.442643	1.418873	-0.397646
9	8	0	-3.154275	-1.640502	0.421251
10	6	0	1.803159	3.560228	0.059845
11	6	0	0.358675	4.131798	0.226927
12	6	0	-3.266770	-3.706473	-0.694304
13	6	0	-3.753563	-2.954082	0.584882
14	6	0	-4.220748	2.308501	0.442307
15	6	0	-3.682197	1.979436	1.873619
16	6	0	-3.899816	3.726549	-0.000979
17	1	0	-4.134822	3.829874	-1.066878
18	1	0	-4.484962	4.473173	0.555496

19	1	0	-2.836851	3.933506	0.135742
20	6	0	-3.670465	3.139792	2.835043
21	1	0	-4.695125	3.477608	3.051344
22	1	0	-3.204818	2.832729	3.778077
23	1	0	-3.114968	3.992304	2.450315
24	6	0	-4.354784	0.767630	2.496964
25	1	0	-3.808552	0.486068	3.404623
26	1	0	-5.393516	0.977858	2.773439
27	1	0	-4.337743	-0.090405	1.809802
28	6	0	-5.687364	1.984485	0.237465
29	1	0	-6.318725	2.573306	0.928782
30	1	0	-5.986654	2.242414	-0.786278
31	1	0	-5.892402	0.926907	0.392242
32	6	0	-5.260145	-2.774508	0.683437
33	1	0	-5.774443	-3.746284	0.701819
34	1	0	-5.520988	-2.253316	1.606667
35	1	0	-5.654737	-2.194927	-0.153983
36	6	0	-3.225470	-3.551189	1.883971
37	1	0	-3.455527	-2.868909	2.709701
38	1	0	-3.684973	-4.515863	2.094128
39	1	0	-2.140233	-3.677495	1.854490
40	6	0	-4.227074	-3.548546	-1.873793
41	1	0	-3.747527	-3.940812	-2.779414
42	1	0	-5.157986	-4.093841	-1.713999
43	1	0	-4.470100	-2.496294	-2.040365
44	6	0	-2.927569	-5.166087	-0.482687
45	1	0	-3.802492	-5.725404	-0.149270
46	1	0	-2.576207	-5.608112	-1.423931
47	1	0	-2.133312	-5.282661	0.255935
48	6	0	-0.081326	4.228526	1.681597
49	1	0	0.480992	4.998588	2.217154
50	1	0	-1.136405	4.483717	1.710375
51	1	0	0.042910	3.275880	2.194226
52	6	0	0.115089	5.445612	-0.488889
53	1	0	-0.919232	5.762838	-0.340803
54	1	0	0.768006	6.233229	-0.101645
55	1	0	0.277217	5.356596	-1.571240
56	6	0	2.464611	3.970206	-1.246644
57	1	0	2.736204	5.024493	-1.252808
58	1	0	3.368227	3.380345	-1.400475
59	1	0	1.797777	3.789773	-2.096687

60	6	0	2.737443	3.829446	1.224001
61	1	0	3.719561	3.394836	1.036426
62	1	0	2.875159	4.910463	1.376915
63	1	0	2.345067	3.392992	2.155673
64	5	0	0.335943	-0.877470	1.005191
65	5	0	0.761393	-0.013541	2.508377
66	5	0	-0.218362	-1.465354	2.613857
67	5	0	0.427771	-2.620463	1.458375
68	6	0	1.737905	-1.857991	0.799499
69	6	0	1.924841	-0.384058	1.384498
70	5	0	1.041868	-1.160519	3.822333
71	5	0	2.411525	-0.418628	2.996560
72	1	0	0.381798	1.104811	2.582644
73	5	0	0.830216	-2.784022	3.168885
74	1	0	-1.381971	-1.418795	2.855935
75	5	0	2.061108	-3.035043	1.939649
76	1	0	-0.171228	-3.369259	0.768310
77	5	0	3.061833	-1.585518	1.838755
78	1	0	2.052256	-1.998805	-0.233076
79	1	0	2.312756	0.372145	0.703557
80	5	0	2.460112	-2.139392	3.407369
81	1	0	0.771944	-0.874849	4.940889
82	1	0	3.137753	0.433514	3.369583
83	1	0	0.409475	-3.697922	3.806721
84	1	0	2.534594	-4.052141	1.560658
85	1	0	3.222700	-2.557558	4.203329
86	77	0	-0.747092	-0.042648	-0.674420
87	6	0	1.095020	-0.280623	-1.959788
88	6	0	-1.268594	1.156000	-2.559403
89	6	0	-2.087642	0.003102	-2.564199
90	6	0	0.298533	-1.427571	-2.128395
91	6	0	1.221244	0.799071	-3.017132
92	1	0	1.964810	-0.332478	-1.298512
93	6	0	-0.116373	1.316956	-3.527119
94	1	0	-1.727569	2.062791	-2.184154
95	6	0	-1.845441	-1.163127	-3.498000
96	1	0	-3.101429	0.123483	-2.196899
97	6	0	-0.425247	-1.713026	-3.434101
98	1	0	0.544202	-2.313761	-1.547877
99	1	0	1.792540	1.625234	-2.570700
100	1	0	1.848169	0.426339	-3.848337

101	1	0	-0.026100	2.380310	-3.772353
102	1	0	-0.387716	0.823493	-4.470003
103	1	0	-2.556492	-1.952070	-3.237717
104	1	0	-2.094180	-0.839058	-4.522845
105	1	0	0.174629	-1.311991	-4.263867
106	1	0	-0.455021	-2.795709	-3.579165
107	1	0	-1.429489	-0.252631	0.914849
108	5	0	4.476945	-1.354357	0.976460
109	8	0	5.737683	-1.083235	1.428530
110	8	0	4.352187	-1.229494	-0.397202
111	6	0	6.587739	-0.922532	0.245018
112	6	0	5.548199	-0.539596	-0.850367
113	6	0	7.241927	-2.267257	-0.006121
114	1	0	7.960710	-2.213334	-0.829401
115	1	0	7.774934	-2.579852	0.894683
116	1	0	6.501337	-3.035928	-0.244648
117	6	0	7.621975	0.141977	0.544813
118	1	0	8.293003	-0.199986	1.336532
119	1	0	8.228332	0.352624	-0.342677
120	1	0	7.158349	1.072821	0.876596
121	6	0	5.198353	0.942977	-0.854136
122	1	0	6.014773	1.558413	-1.244498
123	1	0	4.315929	1.099436	-1.472784
124	1	0	4.965098	1.290409	0.156200
125	6	0	5.888909	-1.005945	-2.245960
126	1	0	5.084822	-0.717484	-2.940812
127	1	0	6.812637	-0.552670	-2.604809
128	1	0	5.994800	-2.091621	-2.297305

Int5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.517412	0.851473	-1.170883
2	5	0	-2.112701	0.603133	0.983858
3	8	0	-2.039012	0.210697	2.308864
4	8	0	-0.216991	1.096246	-2.520339
5	8	0	0.217698	1.715375	-0.361684
6	8	0	-2.412586	1.961809	0.891799

7	6	0	-1.847754	1.414961	3.092723
8	6	0	-2.603286	2.470971	2.235342
9	6	0	0.748879	2.766308	-1.202521
10	6	0	0.891016	2.037130	-2.567223
11	6	0	-0.289528	3.879121	-1.246081
12	1	0	-0.512364	4.209057	-0.229054
13	1	0	0.065863	4.741012	-1.819975
14	1	0	-1.224922	3.524613	-1.690066
15	6	0	0.727979	2.929459	-3.781635
16	1	0	1.447171	3.755620	-3.753459
17	1	0	0.914888	2.364768	-4.700530
18	1	0	-0.278409	3.349137	-3.840767
19	6	0	2.179946	1.236004	-2.665602
20	1	0	2.085823	0.488223	-3.457139
21	1	0	3.032290	1.883547	-2.894118
22	1	0	2.406345	0.716656	-1.727844
23	6	0	2.048031	3.256312	-0.594666
24	1	0	2.555353	3.960654	-1.264807
25	1	0	1.844228	3.780128	0.344744
26	1	0	2.723797	2.425896	-0.373038
27	6	0	-4.097050	2.495646	2.526647
28	1	0	-4.310611	2.972463	3.488495
29	1	0	-4.614043	3.060002	1.744949
30	1	0	-4.510981	1.482530	2.553720
31	6	0	-2.032592	3.873514	2.301143
32	1	0	-2.601774	4.542227	1.648398
33	1	0	-2.087871	4.270625	3.320616
34	1	0	-0.989042	3.893237	1.979419
35	6	0	-2.404863	1.182767	4.481321
36	1	0	-1.822129	0.409371	4.988727
37	1	0	-2.346286	2.096926	5.082397
38	1	0	-3.445582	0.853806	4.452834
39	6	0	-0.349590	1.690140	3.153073
40	1	0	-0.130220	2.566647	3.771341
41	1	0	0.165549	0.829653	3.587383
42	1	0	0.052746	1.862176	2.148367
43	5	0	-0.261105	-1.657068	0.341802
44	5	0	0.312467	-1.823211	2.034153
45	5	0	2.685552	-1.780567	0.434122
46	5	0	2.123102	-3.221826	-0.401988
47	1	0	1.310678	-1.167506	-1.393006

48	5	0	2.072532	-1.860822	2.085293
49	1	0	1.284633	0.078613	0.857366
50	5	0	1.157876	-3.355202	2.271546
51	1	0	-0.246372	-1.222517	2.874411
52	5	0	1.182722	-4.196591	0.729594
53	1	0	-1.286805	-3.763209	1.454670
54	1	0	-0.186431	-3.545086	-1.422121
55	5	0	2.624777	-3.329032	1.280273
56	1	0	2.713797	-3.568652	-1.367761
57	1	0	2.645119	-1.236435	2.914088
58	1	0	1.111297	-3.909478	3.318427
59	1	0	1.145345	-5.377090	0.624652
60	1	0	3.639386	-3.855160	1.594301
61	77	0	-1.831967	-0.619745	-0.640160
62	6	0	-3.145995	-2.629593	-0.701857
63	6	0	-3.413644	-0.200745	-2.366312
64	6	0	-3.771722	0.612740	-1.313681
65	6	0	-3.696213	-1.879305	0.309668
66	6	0	-3.690877	-2.757870	-2.099594
67	1	0	-2.377775	-3.350151	-0.429305
68	6	0	-4.177121	-1.449260	-2.749113
69	1	0	-2.736726	0.211633	-3.113768
70	6	0	-4.886361	0.329221	-0.347033
71	1	0	-3.378315	1.625720	-1.280325
72	6	0	-4.994842	-1.120670	0.166335
73	1	0	-3.301641	-2.017535	1.314480
74	1	0	-2.908205	-3.195386	-2.728563
75	1	0	-4.513171	-3.489411	-2.106789
76	1	0	-4.118587	-1.566981	-3.835085
77	1	0	-5.236743	-1.290119	-2.516808
78	1	0	-4.750952	1.002778	0.501956
79	1	0	-5.846559	0.619847	-0.800430
80	1	0	-5.658285	-1.697832	-0.488511
81	1	0	-5.494313	-1.098683	1.141092
82	6	0	1.237454	-1.007097	0.906865
83	6	0	1.270049	-1.773371	-0.492177
84	5	0	0.361923	-3.168986	-0.441208
85	5	0	-0.246917	-3.249122	1.197021
86	5	0	4.061543	-0.869088	0.155678
87	8	0	5.296073	-1.421745	-0.078519
88	8	0	4.116481	0.501670	0.313614

89	6	0	6.281917	-0.403805	0.236529
90	6	0	5.481654	0.917853	0.023726
91	6	0	7.475527	-0.581852	-0.678647
92	1	0	8.211735	0.212955	-0.516745
93	1	0	7.962786	-1.537939	-0.472142
94	1	0	7.183221	-0.573985	-1.730354
95	6	0	6.680264	-0.628182	1.688707
96	1	0	7.042032	-1.652152	1.806926
97	1	0	7.473187	0.057360	2.003075
98	1	0	5.823990	-0.497523	2.357504
99	6	0	5.847403	2.046061	0.966482
100	1	0	6.896063	2.335009	0.837258
101	1	0	5.229663	2.924258	0.757058
102	1	0	5.691900	1.766278	2.009731
103	6	0	5.510121	1.400588	-1.417943
104	1	0	4.803809	2.226900	-1.537652
105	1	0	6.504363	1.760210	-1.699890
106	1	0	5.221578	0.602537	-2.109073

Int5u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	2.137980	-0.306143	-1.380704
2	5	0	1.781642	0.385721	1.179468
3	8	0	1.585597	0.968275	2.424944
4	8	0	2.095992	-1.594508	-1.887899
5	8	0	3.362957	0.296650	-1.669210
6	8	0	2.887698	-0.443265	1.187135
7	6	0	2.707278	0.628011	3.279406
8	6	0	3.384111	-0.580477	2.537499
9	6	0	4.087561	-0.579646	-2.561494
10	6	0	3.448873	-1.964369	-2.251266
11	6	0	3.799877	-0.100273	-3.979290
12	1	0	4.097014	0.948387	-4.071386
13	1	0	4.351420	-0.678486	-4.728312
14	1	0	2.728650	-0.166069	-4.200200
15	6	0	3.403596	-2.928229	-3.419124
16	1	0	4.416552	-3.216579	-3.721319

17	1	0	2.867978	-3.836228	-3.127679
18	1	0	2.896778	-2.502503	-4.286228
19	6	0	4.068522	-2.644916	-1.037833
20	1	0	3.450428	-3.501592	-0.755351
21	1	0	5.081479	-3.002882	-1.250238
22	1	0	4.096932	-1.959355	-0.187731
23	6	0	5.566185	-0.478095	-2.246149
24	1	0	6.143561	-1.200535	-2.833929
25	1	0	5.935959	0.522439	-2.487957
26	1	0	5.757029	-0.662152	-1.186442
27	6	0	4.901839	-0.518436	2.485830
28	1	0	5.330570	-0.528096	3.493880
29	1	0	5.287446	-1.392858	1.953581
30	1	0	5.257091	0.372915	1.964391
31	6	0	2.954165	-1.947262	3.050196
32	1	0	3.337307	-2.717311	2.374885
33	1	0	3.352342	-2.140265	4.051570
34	1	0	1.868186	-2.051562	3.081946
35	6	0	3.599546	1.860071	3.348450
36	1	0	3.015543	2.709331	3.716100
37	1	0	4.446243	1.711320	4.025727
38	1	0	3.996592	2.120107	2.362223
39	6	0	2.170248	0.298541	4.658731
40	1	0	2.978280	-0.018070	5.327145
41	1	0	1.699503	1.183107	5.096647
42	1	0	1.423417	-0.496941	4.618550
43	5	0	-0.306707	-1.017862	0.199377
44	5	0	-0.726180	-2.404105	-0.858390
45	5	0	0.182400	-2.690784	0.614521
46	5	0	-0.529088	-1.673415	1.859016
47	6	0	-1.802456	-0.924966	1.119605
48	6	0	-1.908587	-1.329172	-0.403940
49	5	0	-1.068864	-3.845138	0.104387
50	5	0	-2.395360	-2.922901	-0.597755
51	1	0	-0.335990	-2.371317	-1.972937
52	5	0	-0.939661	-3.390954	1.799550
53	1	0	1.336991	-2.955201	0.608515
54	5	0	-2.194526	-2.200618	2.139055
55	1	0	0.003655	-1.103383	2.747085
56	5	0	-3.109413	-1.919652	0.665478
57	1	0	-2.106013	0.085173	1.371985

58	1	0	-2.292644	-0.569752	-1.076346
59	5	0	-2.541953	-3.540616	1.047478
60	1	0	-0.797198	-4.925974	-0.300364
61	1	0	-3.069319	-3.176984	-1.539389
62	1	0	-0.565410	-4.132212	2.646770
63	1	0	-2.707984	-1.946271	3.174105
64	1	0	-3.322706	-4.385722	1.329699
65	77	0	0.623583	0.758114	-0.475302
66	6	0	-1.372857	2.205097	-0.169418
67	6	0	1.143561	2.670804	-1.674699
68	6	0	1.938314	2.684080	-0.534975
69	6	0	-0.602028	2.404700	0.943989
70	6	0	-1.406394	3.128919	-1.360103
71	1	0	-2.166199	1.457374	-0.140204
72	6	0	-0.032621	3.609520	-1.875183
73	1	0	1.584077	2.238867	-2.572743
74	6	0	1.694272	3.554760	0.665054
75	1	0	2.937329	2.262311	-0.623667
76	6	0	0.237294	3.638900	1.152557
77	1	0	-0.736493	1.754993	1.806272
78	1	0	-1.936383	2.614222	-2.171074
79	1	0	-2.027413	4.007017	-1.124288
80	1	0	-0.125977	3.821384	-2.945967
81	1	0	0.212853	4.572652	-1.410530
82	1	0	2.311368	3.183796	1.484213
83	1	0	2.060330	4.570484	0.448411
84	1	0	-0.270272	4.484604	0.672845
85	1	0	0.250491	3.867227	2.223512
86	5	0	-4.522107	-1.066616	0.390389
87	8	0	-5.789064	-1.516287	0.140081
88	8	0	-4.395946	0.300473	0.183257
89	6	0	-6.620634	-0.347078	-0.111389
90	6	0	-5.571457	0.712159	-0.562571
91	6	0	-7.292777	0.012079	1.204621
92	1	0	-8.000283	0.838056	1.082924
93	1	0	-7.840043	-0.856183	1.578649
94	1	0	-6.555102	0.297915	1.959816
95	6	0	-7.649839	-0.707845	-1.161872
96	1	0	-8.337766	-1.460785	-0.769478
97	1	0	-8.238772	0.171350	-1.444858
98	1	0	-7.182377	-1.116260	-2.059723

99	6	0	-5.199846	0.589012	-2.035297
100	1	0	-6.002574	0.939534	-2.691826
101	1	0	-4.305104	1.187917	-2.234777
102	1	0	-4.964668	-0.449390	-2.295998
103	6	0	-5.900107	2.145540	-0.205419
104	1	0	-5.089880	2.804788	-0.531659
105	1	0	-6.819848	2.470920	-0.703104
106	1	0	-6.025415	2.274045	0.871191

Int6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-3.066054	0.125521	0.312180
2	8	0	-3.643409	1.375556	0.472056
3	8	0	-3.296443	-0.685969	1.410451
4	6	0	-4.243540	1.460841	1.781249
5	6	0	-4.275340	-0.051326	2.254736
6	6	0	-5.603089	-0.742200	1.964024
7	1	0	-5.504836	-1.808316	2.190838
8	1	0	-6.425398	-0.335947	2.580362
9	1	0	-5.887898	-0.641551	0.913726
10	6	0	-3.865302	-0.267389	3.692908
11	1	0	-4.541855	0.252679	4.389165
12	1	0	-3.885692	-1.334843	3.933161
13	1	0	-2.853817	0.095707	3.854428
14	6	0	-5.620444	2.093552	1.615898
15	1	0	-6.148665	2.150602	2.572960
16	1	0	-5.497008	3.119374	1.240496
17	1	0	-6.242235	1.544073	0.904494
18	6	0	-3.373012	2.349077	2.645136
19	1	0	-3.288011	3.334738	2.178424
20	1	0	-3.794359	2.473518	3.644430
21	1	0	-2.362585	1.940418	2.724728
22	5	0	-1.221409	-1.992237	0.007873
23	8	0	-0.413012	-2.274516	1.095457
24	8	0	-2.010562	-3.080979	-0.313705
25	6	0	-1.898219	-4.087834	0.708404
26	6	0	-0.599776	-3.667206	1.485272

27	6	0	-1.814467	-5.446259	0.029781
28	1	0	-1.662997	-6.237687	0.772049
29	1	0	-2.745168	-5.657064	-0.499464
30	1	0	-0.996942	-5.487075	-0.691776
31	6	0	-3.165987	-4.003852	1.548057
32	1	0	-4.030986	-4.154932	0.887878
33	1	0	-3.200043	-4.769267	2.329341
34	1	0	-3.264299	-3.021031	2.000232
35	6	0	-0.743446	-3.735286	2.995915
36	1	0	-1.018250	-4.749210	3.314989
37	1	0	0.209481	-3.482433	3.472029
38	1	0	-1.501960	-3.039355	3.353503
39	6	0	0.655113	-4.428947	1.061886
40	1	0	1.528400	-3.975887	1.542638
41	1	0	0.602313	-5.480795	1.372972
42	1	0	0.816722	-4.396991	-0.016662
43	5	0	0.553777	-0.749318	-1.877341
44	5	0	1.067628	-2.475671	-2.058222
45	5	0	0.868691	-1.515969	-3.493555
46	5	0	1.505722	0.086029	-3.151341
47	6	0	2.078899	-0.020662	-1.599353
48	6	0	1.829486	-1.480482	-0.971670
49	5	0	2.217357	-2.663782	-3.381263
50	5	0	2.786571	-2.645282	-1.710858
51	1	0	0.313611	-3.293159	-1.668422
52	5	0	2.488728	-1.058689	-4.068915
53	1	0	-0.028992	-1.707427	-4.242593
54	5	0	3.224353	-0.065822	-2.824427
55	1	0	1.106972	1.127953	-3.544991
56	5	0	3.411300	-1.042615	-1.350865
57	1	0	1.612791	-1.518485	0.086521
58	5	0	3.677091	-1.758819	-2.944716
59	1	0	2.248324	-3.656729	-4.028135
60	1	0	3.176856	-3.541975	-1.042611
61	1	0	2.724819	-0.879060	-5.213889
62	1	0	3.935962	0.883765	-2.934695
63	1	0	4.780069	-2.083023	-3.268136
64	77	0	-1.404976	-0.231636	-1.057131
65	6	0	-2.676395	1.822292	-2.194133
66	6	0	-3.567123	-0.741867	-1.365055
67	6	0	-2.603085	-1.238351	-2.395226

68	6	0	-1.680460	1.433339	-3.033443
69	6	0	-4.132179	1.517859	-2.429625
70	1	0	-2.455275	2.508508	-1.383296
71	6	0	-4.667778	0.204584	-1.834223
72	1	0	-3.945520	-1.569353	-0.761386
73	6	0	-2.689505	-0.757029	-3.839687
74	1	0	-2.433917	-2.315433	-2.325909
75	6	0	-1.900520	0.520129	-4.193011
76	1	0	-0.691116	1.866583	-2.912696
77	1	0	-4.721371	2.355653	-2.032313
78	1	0	-4.298278	1.516010	-3.513116
79	1	0	-5.336568	0.431664	-1.004551
80	1	0	-5.277497	-0.324975	-2.577600
81	1	0	-2.324955	-1.571464	-4.478809
82	1	0	-3.747356	-0.637931	-4.094078
83	1	0	-2.417133	1.058632	-5.001092
84	1	0	-0.923222	0.236992	-4.600451
85	5	0	-0.376549	1.955716	-0.027990
86	5	0	-0.025468	0.647536	1.092744
87	8	0	0.449285	2.352883	-1.062507
88	8	0	-0.862668	3.033959	0.686851
89	8	0	-0.657475	0.451823	2.293509
90	6	0	-0.346824	4.264827	0.091878
91	6	0	0.804569	3.746105	-0.843917
92	8	0	1.355879	0.600140	1.219886
93	6	0	0.344437	0.569924	3.359880
94	6	0	1.699290	0.312535	2.612332
95	6	0	0.895849	4.432385	-2.199794
96	1	0	1.134016	5.495511	-2.085331
97	1	0	1.693990	3.961374	-2.792142
98	1	0	-0.036876	4.342718	-2.762617
99	6	0	2.176688	3.722322	-0.184794
100	1	0	2.895221	3.214055	-0.834665
101	1	0	2.558303	4.739306	0.015600
102	1	0	2.143679	3.176053	0.764450
103	6	0	0.115493	5.167827	1.221379
104	1	0	0.537334	6.095972	0.835150
105	1	0	-0.736382	5.413406	1.861764
106	1	0	0.871331	4.677123	1.853278
107	6	0	-1.485654	4.929446	-0.658134
108	1	0	-2.339341	5.044874	0.022657

109	1	0	-1.193488	5.926524	-1.012368
110	1	0	-1.815713	4.352838	-1.529619
111	1	0	2.047925	0.808263	-0.904811
112	6	0	2.182046	-1.127536	2.666988
113	1	0	3.029125	-1.251177	1.991062
114	1	0	2.513576	-1.403521	3.679828
115	1	0	1.382956	-1.812280	2.351728
116	6	0	2.830346	1.249903	3.007060
117	1	0	3.658345	1.093579	2.314429
118	1	0	2.542221	2.303432	2.943841
119	1	0	3.169711	1.041744	4.023326
120	6	0	0.037988	-0.431466	4.448438
121	1	0	-0.047690	-1.440105	4.045252
122	1	0	0.815195	-0.413413	5.210229
123	1	0	-0.908975	-0.182284	4.938073
124	6	0	0.204982	1.989929	3.898838
125	1	0	0.339347	2.734599	3.102267
126	1	0	-0.791151	2.133924	4.308931
127	1	0	0.932841	2.192242	4.689582
128	5	0	4.623965	-0.580300	-0.287118
129	8	0	5.675981	-1.396504	0.067827
130	8	0	4.783195	0.715193	0.161479
131	6	0	6.565568	-0.618213	0.920321
132	6	0	6.191671	0.847240	0.527288
133	6	0	6.330056	1.868859	1.642477
134	1	0	7.386722	1.978925	1.923121
135	1	0	5.961599	2.832344	1.306593
136	1	0	5.768975	1.581738	2.535538
137	6	0	6.914150	1.323142	-0.723803
138	1	0	6.447710	2.253729	-1.068264
139	1	0	7.967637	1.521425	-0.540424
140	1	0	6.829485	0.592704	-1.533173
141	6	0	6.215297	-0.960295	2.363305
142	1	0	6.261668	-2.034172	2.490987
143	1	0	6.905353	-0.484106	3.063630
144	1	0	5.201994	-0.631268	2.608540
145	6	0	7.989674	-1.014126	0.608631
146	1	0	8.693295	-0.380797	1.167742
147	1	0	8.164896	-2.045259	0.902230
148	1	0	8.214741	-0.918450	-0.458626

Int6u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	2.022017	-0.637650	-1.710737
2	8	0	2.236386	-2.000069	-1.883237
3	8	0	3.223423	0.062397	-1.737096
4	6	0	3.657426	-2.267643	-1.971028
5	6	0	4.272503	-0.824618	-2.173186
6	6	0	4.550684	-0.483815	-3.624131
7	1	0	4.846419	0.563257	-3.702221
8	1	0	5.350435	-1.096811	-4.048423
9	1	0	3.659359	-0.614589	-4.246647
10	6	0	5.494460	-0.541503	-1.320343
11	1	0	6.321892	-1.213928	-1.583417
12	1	0	5.830908	0.487133	-1.478114
13	1	0	5.264858	-0.659347	-0.260719
14	6	0	3.863727	-3.215570	-3.134428
15	1	0	4.926068	-3.433735	-3.273776
16	1	0	3.354093	-4.155385	-2.924330
17	1	0	3.473072	-2.819188	-4.074993
18	6	0	4.092986	-2.941634	-0.680829
19	1	0	3.542517	-3.877725	-0.556523
20	1	0	5.163208	-3.162630	-0.691968
21	1	0	3.863408	-2.315772	0.183209
22	5	0	1.388209	1.904766	-0.535326
23	8	0	2.220814	2.359244	0.472189
24	8	0	1.390436	2.786385	-1.610735
25	6	0	2.420572	3.772756	-1.403547
26	6	0	2.654984	3.706260	0.138809
27	6	0	1.927700	5.112416	-1.914806
28	1	0	2.653651	5.903287	-1.706344
29	1	0	1.784214	5.063864	-2.997271
30	1	0	0.967787	5.382682	-1.454752
31	6	0	3.635158	3.312633	-2.213584
32	1	0	3.342724	3.210018	-3.263624
33	1	0	4.452573	4.036298	-2.162203
34	1	0	3.986016	2.342424	-1.865825
35	6	0	4.095173	3.864878	0.556724

36	1	0	4.491944	4.842318	0.220379
37	1	0	4.190262	3.836345	1.647006
38	1	0	4.730659	3.085200	0.132389
39	6	0	1.777490	4.671346	0.921668
40	1	0	1.857944	4.452144	1.987489
41	1	0	2.085139	5.707251	0.759163
42	1	0	0.723448	4.575806	0.647180
43	5	0	-1.005846	1.145449	0.805131
44	5	0	-1.491350	2.864820	0.589727
45	5	0	-3.229470	3.070933	0.812747
46	5	0	-2.110853	3.540940	2.094326
47	1	0	-0.975476	3.457623	-0.312442
48	5	0	-3.910881	1.498113	1.223175
49	1	0	-2.757929	1.373611	-0.813597
50	5	0	-3.190739	0.991373	2.754273
51	1	0	-2.695303	-0.517617	0.943531
52	5	0	-2.089337	2.254031	3.293903
53	1	0	0.317962	2.677917	2.415980
54	5	0	-3.613456	2.678993	2.488642
55	1	0	-3.842554	3.752870	0.064145
56	1	0	-1.944591	4.682365	2.360520
57	1	0	-3.780111	0.191796	3.394207
58	1	0	-1.909022	2.450666	4.449065
59	1	0	-4.527023	3.185367	3.056724
60	77	0	0.270168	0.172165	-0.649574
61	6	0	-0.670322	-2.199862	-1.935559
62	6	0	0.740154	0.103756	-2.862156
63	6	0	-0.481613	0.862880	-2.443520
64	6	0	-1.766635	-1.558938	-1.459284
65	6	0	-0.288547	-2.211579	-3.377713
66	1	0	-0.091421	-2.816692	-1.255128
67	6	0	0.560739	-1.023692	-3.869721
68	1	0	1.492496	0.828478	-3.198421
69	6	0	-1.861634	0.472347	-2.985647
70	1	0	-0.342000	1.938168	-2.537879
71	6	0	-2.623233	-0.691184	-2.316210
72	1	0	-2.043756	-1.726323	-0.432119
73	1	0	0.254546	-3.138395	-3.580555
74	1	0	-1.214861	-2.256126	-3.976325
75	1	0	1.545535	-1.390781	-4.184407
76	1	0	0.113856	-0.588379	-4.775632

77	1	0	-2.499690	1.364655	-2.958788
78	1	0	-1.738517	0.266694	-4.066336
79	1	0	-3.107105	-1.305725	-3.103453
80	1	0	-3.461284	-0.296964	-1.723225
81	5	0	0.703144	-1.678456	0.957802
82	5	0	1.765571	-0.346370	1.471000
83	8	0	-0.610044	-1.969646	1.273511
84	8	0	1.500549	-2.805459	1.054403
85	8	0	3.107676	-0.328380	1.206444
86	6	0	0.704131	-3.938898	1.504813
87	6	0	-0.691353	-3.299920	1.843742
88	8	0	1.466292	-0.059791	2.780918
89	6	0	3.808549	-0.223728	2.485837
90	6	0	2.700653	0.281237	3.475169
91	6	0	-1.881877	-4.005769	1.205057
92	1	0	-1.983840	-5.020052	1.600812
93	1	0	-2.802848	-3.466647	1.443853
94	1	0	-1.787568	-4.070280	0.119602
95	6	0	-0.941430	-3.093015	3.325681
96	1	0	-1.884643	-2.550514	3.459660
97	1	0	-1.010896	-4.045521	3.866916
98	1	0	-0.150344	-2.476320	3.778889
99	6	0	1.421627	-4.559531	2.700766
100	1	0	0.867732	-5.430223	3.091890
101	1	0	2.417058	-4.909240	2.395056
102	1	0	1.558513	-3.845996	3.514137
103	6	0	0.681992	-4.956753	0.355376
104	1	0	1.712875	-5.277611	0.146942
105	1	0	0.099127	-5.847177	0.629352
106	1	0	0.270886	-4.535653	-0.574020
107	1	0	-0.942474	-0.103523	3.057477
108	6	0	2.695176	1.790357	3.682278
109	1	0	1.813108	2.063934	4.263194
110	1	0	3.583442	2.121702	4.224227
111	1	0	2.638606	2.309969	2.721805
112	6	0	2.679230	-0.432864	4.818594
113	1	0	1.844688	-0.055147	5.411966
114	1	0	2.562756	-1.514548	4.701685
115	1	0	3.605758	-0.238898	5.375122
116	6	0	4.972297	0.726450	2.329339
117	1	0	4.647932	1.695089	1.928965

118	1	0	5.467960	0.894124	3.294847
119	1	0	5.717509	0.316759	1.638072
120	6	0	4.317429	-1.624451	2.800357
121	1	0	3.500249	-2.352284	2.801156
122	1	0	5.035280	-1.935987	2.031586
123	1	0	4.830091	-1.658906	3.766689
124	6	0	-2.553167	1.660292	0.211987
125	5	0	-1.450304	0.803767	2.519975
126	5	0	-0.779260	2.366193	2.110423
127	6	0	-2.531200	0.494951	1.299661
128	5	0	-5.245453	0.795755	0.487576
129	8	0	-6.128070	-0.061062	1.092409
130	8	0	-5.459544	0.915225	-0.870145
131	6	0	-6.830623	-0.757572	0.022460
132	6	0	-6.719600	0.250624	-1.168207
133	6	0	-6.611734	-0.388844	-2.531392
134	1	0	-7.523279	-0.948344	-2.767321
135	1	0	-6.499261	0.387707	-3.300598
136	1	0	-5.761376	-1.069835	-2.606473
137	6	0	-7.797430	1.313818	-1.143699
138	1	0	-7.535080	2.105039	-1.849885
139	1	0	-8.774261	0.910070	-1.426743
140	1	0	-7.884720	1.773421	-0.151237
141	6	0	-6.068630	-2.053351	-0.226181
142	1	0	-5.999771	-2.603778	0.718618
143	1	0	-6.565996	-2.682419	-0.960297
144	1	0	-5.049176	-1.852042	-0.565999
145	6	0	-8.247019	-1.047438	0.472260
146	1	0	-8.827847	-1.507329	-0.339537
147	1	0	-8.238175	-1.750650	1.308829
148	1	0	-8.757348	-0.140743	0.801478

P1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	3.219005	0.002546	1.559389
2	5	0	3.548045	-0.884889	-1.132335
3	5	0	0.988978	-0.000487	-0.231856

4	5	0	3.342123	-1.427031	0.533537
5	5	0	1.966403	-1.428862	-0.571351
6	5	0	4.325295	0.000349	0.194446
7	5	0	2.083095	-0.002797	-1.606398
8	5	0	3.342016	1.428668	0.528640
9	5	0	3.547874	0.881071	-1.135448
10	5	0	1.966666	1.426853	-0.575995
11	1	0	1.395327	-2.436163	-0.802060
12	1	0	1.645828	-0.004647	-2.705368
13	1	0	1.395735	2.433499	-0.809936
14	1	0	1.239972	1.283925	1.737550
15	1	0	3.692046	2.436501	1.034369
16	1	0	4.168645	1.525866	-1.909589
17	1	0	5.492725	0.000668	0.384314
18	1	0	4.169070	-1.532090	-1.904258
19	1	0	3.692261	-2.433095	1.042697
20	1	0	3.403377	0.004486	2.723310
21	1	0	1.239773	-1.277921	1.741875
22	6	0	1.850079	0.808508	0.978667
23	6	0	1.849914	-0.805211	0.981456
24	5	0	-0.767833	-0.000249	-0.125955
25	8	0	-1.536620	-1.333824	-0.079643
26	8	0	-1.536256	1.333534	-0.079604
27	6	0	-2.940091	-1.073038	0.004968
28	6	0	-2.939799	1.073127	0.004997
29	6	0	-3.530041	-1.628225	1.314672
30	6	0	-3.683103	-1.628169	-1.224407
31	6	0	-3.682657	1.628495	-1.224365
32	6	0	-3.529600	1.628439	1.314715
33	1	0	-4.598005	-1.575144	1.275495
34	1	0	-3.227872	-2.647210	1.438214
35	1	0	-3.174146	-1.048066	2.140296
36	1	0	-3.458090	-2.668101	-1.337598
37	1	0	-4.737347	-1.503914	-1.090134
38	1	0	-3.370120	-1.098202	-2.099665
39	1	0	-4.725709	1.404514	-1.142060
40	1	0	-3.548342	2.688904	-1.273273
41	1	0	-3.290060	1.177938	-2.111927
42	1	0	-3.404237	2.690766	1.340127
43	1	0	-4.571676	1.390954	1.365510
44	1	0	-3.022685	1.189431	2.148507

P2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-2.835661	0.225949	0.014477
2	8	0	-2.620562	-1.096955	0.335367
3	8	0	-4.128079	0.504269	-0.318862
4	6	0	-4.918000	-0.682426	0.002972
5	6	0	-3.846121	-1.818212	0.004416
6	6	0	-5.996773	-0.835004	-1.049711
7	1	0	-6.569655	-1.753263	-0.882817
8	1	0	-6.690616	0.007161	-0.994392
9	1	0	-5.581849	-0.863855	-2.058996
10	6	0	-5.533823	-0.436901	1.368680
11	1	0	-6.140266	0.471358	1.322166
12	1	0	-6.175577	-1.263760	1.687826
13	1	0	-4.780437	-0.291278	2.154323
14	6	0	-4.079629	-2.896160	1.042489
15	1	0	-4.982515	-3.466823	0.798124
16	1	0	-3.236273	-3.593610	1.058201
17	1	0	-4.212687	-2.484754	2.046888
18	6	0	-3.614212	-2.432537	-1.368143
19	1	0	-2.735459	-3.081805	-1.332041
20	1	0	-4.468629	-3.033665	-1.692044
21	1	0	-3.435145	-1.659260	-2.121690
22	5	0	-1.554875	1.310736	0.005594
23	5	0	-0.933647	2.135208	-1.430449
24	5	0	-1.411380	3.070642	-0.015794
25	5	0	-0.914797	2.169478	1.413076
26	6	0	-0.135031	0.816520	0.806158
27	6	0	-0.142872	0.797686	-0.797993
28	5	0	0.059763	3.499985	-0.910447
29	5	0	0.827675	2.003524	-1.440999
30	1	0	-1.532513	1.994627	-2.438960
31	5	0	0.069380	3.520349	0.853434
32	1	0	-2.394944	3.728935	-0.012461
33	5	0	0.843255	2.034561	1.411747
34	1	0	-1.497472	2.059525	2.435517

35	5	0	1.318887	1.104584	-0.006715
36	1	0	-0.217355	-0.153360	1.286145
37	1	0	-0.219594	-0.183170	-1.254348
38	5	0	1.457762	2.855279	-0.027209
39	1	0	0.134357	4.480910	-1.568075
40	1	0	1.394941	1.773238	-2.450618
41	1	0	0.147896	4.515288	1.489386
42	1	0	1.416965	1.824786	2.423401
43	1	0	2.527170	3.360854	-0.038730
44	5	0	2.531173	-0.171305	0.001714
45	8	0	3.060244	-0.721935	1.339058
46	8	0	3.062852	-0.737077	-1.328256
47	6	0	4.432066	-1.118560	-1.171331
48	6	0	4.431414	-1.099803	1.190703
49	6	0	5.391188	-0.063123	-1.752484
50	1	0	6.367013	-0.488686	-1.860004
51	1	0	5.033580	0.255399	-2.709333
52	1	0	5.439373	0.777240	-1.091903
53	6	0	4.702583	-2.526688	-1.733110
54	1	0	4.530208	-2.528567	-2.789133
55	1	0	5.718384	-2.799830	-1.537047
56	1	0	4.047114	-3.230042	-1.263479
57	6	0	4.707345	-2.497597	1.775196
58	1	0	5.705178	-2.796104	1.529994
59	1	0	4.595147	-2.467913	2.838883
60	1	0	4.013430	-3.199969	1.362819
61	6	0	5.385056	-0.030766	1.755794
62	1	0	5.182716	0.113385	2.796552
63	1	0	6.397395	-0.353899	1.630676
64	1	0	5.237652	0.890987	1.232780

TS0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.583625	1.637796	-0.508211
2	5	0	2.010284	-0.291248	-0.002431
3	5	0	-1.979961	0.678511	-0.338973
4	8	0	-0.426506	2.629032	0.449328

5	8	0	0.023657	1.969764	-1.701348
6	8	0	-2.628894	0.464911	0.872900
7	8	0	-2.875334	0.664066	-1.397701
8	8	0	2.816156	-0.860944	0.996566
9	8	0	2.790910	0.557888	-0.796150
10	6	0	0.387389	3.366994	-1.640066
11	6	0	0.426025	3.662943	-0.100834
12	6	0	4.184089	0.294465	-0.498914
13	6	0	4.120577	-0.245341	0.959759
14	6	0	-4.185952	0.330687	-0.872268
15	6	0	-4.036908	0.699221	0.634209
16	6	0	-0.720664	4.121244	-2.365007
17	1	0	-0.526484	5.197714	-2.406577
18	1	0	-0.797599	3.744676	-3.387786
19	1	0	-1.689145	3.960356	-1.880225
20	6	0	1.715013	3.550510	-2.349428
21	1	0	1.596253	3.344794	-3.416700
22	1	0	2.077772	4.579194	-2.243617
23	1	0	2.463856	2.860709	-1.955200
24	6	0	-0.149907	5.009002	0.298824
25	1	0	-0.097652	5.127071	1.384636
26	1	0	0.419564	5.826912	-0.156131
27	1	0	-1.195495	5.108955	0.000474
28	6	0	1.803228	3.481339	0.514231
29	1	0	2.497463	4.268017	0.199410
30	1	0	1.716541	3.521935	1.605170
31	1	0	2.222439	2.515219	0.223696
32	6	0	-5.219438	1.144600	-1.625310
33	1	0	-5.250888	0.831979	-2.672351
34	1	0	-6.218111	0.996570	-1.199676
35	1	0	-4.986895	2.211124	-1.600608
36	6	0	-4.409655	-1.156228	-1.093356
37	1	0	-5.403174	-1.469575	-0.756677
38	1	0	-4.324489	-1.385416	-2.159208
39	1	0	-3.652512	-1.740930	-0.562127
40	6	0	-4.851216	-0.146645	1.591991
41	1	0	-4.603140	0.122825	2.623376
42	1	0	-5.923229	0.024442	1.446162
43	1	0	-4.656865	-1.213771	1.467361
44	6	0	-4.273295	2.180354	0.908052
45	1	0	-5.329723	2.450883	0.814718

46	1	0	-3.942684	2.413101	1.923343
47	1	0	-3.692324	2.803079	0.220512
48	6	0	5.163197	-1.295625	1.294157
49	1	0	6.176986	-0.895207	1.179381
50	1	0	5.047072	-1.619633	2.331986
51	1	0	5.064582	-2.176644	0.656849
52	6	0	4.141359	0.857017	2.011207
53	1	0	3.873542	0.429962	2.981932
54	1	0	5.130379	1.318629	2.099779
55	1	0	3.418669	1.645441	1.779286
56	6	0	4.975468	1.575165	-0.674609
57	1	0	6.021117	1.431817	-0.379998
58	1	0	4.964042	1.884539	-1.723893
59	1	0	4.560610	2.391874	-0.078238
60	6	0	4.656224	-0.763247	-1.488713
61	1	0	4.466793	-0.414594	-2.507854
62	1	0	5.726589	-0.969918	-1.388778
63	1	0	4.110365	-1.701560	-1.343902
64	7	0	-0.192295	-0.576953	2.056838
65	6	0	0.533047	0.484661	2.466739
66	6	0	-1.064707	-1.101473	2.956049
67	6	0	0.471212	1.038355	3.734803
68	6	0	-1.165336	-0.598777	4.255294
69	6	0	-0.390265	0.475081	4.663538
70	1	0	1.094038	1.895655	3.968547
71	1	0	-1.874371	-1.063363	4.933809
72	1	0	-0.468667	0.866735	5.673886
73	77	0	0.121851	-1.141903	-0.177989
74	6	0	-0.038424	-3.282236	0.019692
75	6	0	1.131322	-1.744547	-1.994376
76	6	0	-0.120695	-1.144646	-2.296410
77	6	0	-1.314415	-3.000244	-0.525733
78	6	0	1.107750	-3.918954	-0.734240
79	1	0	0.001751	-3.506797	1.088677
80	6	0	1.392480	-3.235756	-2.071232
81	1	0	2.000941	-1.118858	-2.178762
82	6	0	-1.319739	-1.903135	-2.801777
83	1	0	-0.080080	-0.103327	-2.619418
84	6	0	-1.648775	-3.161463	-1.988952
85	1	0	-2.158613	-3.050431	0.152995
86	1	0	2.000435	-3.838813	-0.101049

87	1	0	0.920746	-4.995650	-0.872456
88	1	0	2.437995	-3.404925	-2.353006
89	1	0	0.796821	-3.677658	-2.878125
90	1	0	-2.173140	-1.219218	-2.764347
91	1	0	-1.169632	-2.146934	-3.866613
92	1	0	-1.141981	-4.040636	-2.407537
93	1	0	-2.719241	-3.376699	-2.090574
94	1	0	1.180692	0.924125	1.721419
95	6	0	-1.982244	-2.193800	2.540214
96	1	0	-2.551897	-1.858595	1.670944
97	1	0	-1.453423	-3.106272	2.257539
98	1	0	-2.676958	-2.437899	3.346981

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.000866	-0.818727	1.167509
2	5	0	-2.249356	-0.389229	-0.360015
3	5	0	1.999753	-0.439493	-0.486823
4	8	0	2.967052	-0.772264	-1.424591
5	8	0	-2.733793	-0.813718	0.866880
6	8	0	-3.245896	0.222619	-1.100754
7	8	0	-0.219756	0.127195	2.167876
8	8	0	0.279886	-2.060051	1.711062
9	8	0	2.599770	-0.270700	0.763592
10	6	0	-4.505285	0.014226	-0.401350
11	6	0	-4.022372	-0.173794	1.064066
12	6	0	4.182716	-1.142678	-0.729061
13	6	0	4.038772	-0.401569	0.638091
14	6	0	0.057480	-2.006936	3.137926
15	6	0	0.082090	-0.468864	3.454085
16	6	0	-1.297026	-2.658663	3.390723
17	1	0	-1.264739	-3.692681	3.032402
18	1	0	-1.553748	-2.673512	4.451867
19	1	0	-2.081874	-2.137773	2.835687
20	6	0	-0.971473	-0.015172	4.445991
21	1	0	-0.795756	-0.457330	5.433272
22	1	0	-0.930337	1.072784	4.557677

23	1	0	-1.979096	-0.289317	4.122055
24	6	0	1.450301	0.050214	3.871519
25	1	0	1.412725	1.144530	3.939595
26	1	0	1.757161	-0.335164	4.847690
27	1	0	2.203178	-0.213184	3.127860
28	6	0	1.157294	-2.799464	3.819299
29	1	0	1.051274	-2.759767	4.908882
30	1	0	1.098942	-3.848889	3.516237
31	1	0	2.146637	-2.422956	3.554734
32	6	0	4.555673	-1.181945	1.831266
33	1	0	5.620343	-1.411296	1.716552
34	1	0	4.442315	-0.593484	2.748746
35	1	0	4.015501	-2.123499	1.962984
36	6	0	4.627880	0.999905	0.642485
37	1	0	4.317687	1.516664	1.556840
38	1	0	5.721705	0.979543	0.624321
39	1	0	4.279966	1.590871	-0.208566
40	6	0	4.157562	-2.658541	-0.575925
41	1	0	4.110986	-3.120188	-1.566848
42	1	0	5.054266	-3.032298	-0.074543
43	1	0	3.280159	-2.984758	-0.006791
44	6	0	5.369982	-0.709353	-1.563629
45	1	0	6.311670	-0.916025	-1.039280
46	1	0	5.384081	-1.261443	-2.505449
47	1	0	5.330391	0.357020	-1.795153
48	6	0	-3.761619	1.151523	1.763348
49	1	0	-4.691251	1.666670	2.019636
50	1	0	-3.198147	0.973428	2.682003
51	1	0	-3.169609	1.818540	1.126368
52	6	0	-4.888916	-1.074616	1.918323
53	1	0	-4.476070	-1.144010	2.930870
54	1	0	-5.904457	-0.677177	1.999283
55	1	0	-4.942849	-2.087319	1.508713
56	6	0	-5.138579	-1.244163	-0.973570
57	1	0	-6.124318	-1.433331	-0.537452
58	1	0	-5.260306	-1.128412	-2.054753
59	1	0	-4.510797	-2.119999	-0.791594
60	6	0	-5.388483	1.222444	-0.638780
61	1	0	-5.667320	1.281191	-1.691923
62	1	0	-6.310402	1.150275	-0.050241
63	1	0	-4.882140	2.151885	-0.372380

64	5	0	0.106539	2.030094	-0.489260
65	5	0	1.695353	2.685728	-0.902373
66	5	0	0.899562	3.867815	1.575358
67	5	0	-0.535676	4.538467	0.795392
68	1	0	-0.823700	2.256672	1.655544
69	5	0	2.185051	3.797851	0.373184
70	1	0	1.582475	1.607949	1.283537
71	5	0	1.551424	4.423881	-1.147175
72	1	0	2.485721	1.954296	-1.385411
73	5	0	-0.130772	4.880145	-0.888047
74	1	0	0.025728	3.123836	-2.821922
75	1	0	-2.166573	3.168892	-0.646124
76	5	0	1.063852	5.160539	0.391948
77	1	0	1.075168	3.841738	2.740638
78	1	0	-1.354910	5.038689	1.481734
79	1	0	3.302516	3.781921	0.757824
80	1	0	2.259840	4.978021	-1.914547
81	1	0	-0.655731	5.766909	-1.470371
82	1	0	1.414635	6.238384	0.734077
83	77	0	-0.133543	-0.396975	-0.855911
84	6	0	-0.775452	0.122998	-3.090886
85	6	0	-1.301932	-2.162533	-1.436495
86	6	0	0.118213	-2.445570	-1.341757
87	6	0	0.552522	-0.263928	-3.133935
88	6	0	-1.905893	-0.774940	-3.534137
89	1	0	-1.004622	1.187290	-3.037131
90	6	0	-1.992998	-2.118496	-2.797293
91	1	0	-1.891445	-2.617805	-0.636805
92	6	0	0.969244	-2.732817	-2.556111
93	1	0	0.406352	-3.027238	-0.464128
94	6	0	0.948369	-1.635581	-3.628164
95	1	0	1.326960	0.501418	-3.100169
96	1	0	-2.839859	-0.230195	-3.395736
97	1	0	-1.807216	-0.952303	-4.615301
98	1	0	-3.047085	-2.380870	-2.664879
99	1	0	-1.566641	-2.925080	-3.411726
100	1	0	1.994954	-2.865134	-2.213246
101	1	0	0.667978	-3.700125	-2.990680
102	1	0	0.257159	-1.914485	-4.436109
103	1	0	1.939278	-1.570927	-4.091244
104	1	0	-0.835966	1.143925	-0.498823

105	6	0	1.227550	2.456598	0.700530
106	5	0	-1.021097	3.420944	-0.474243
107	5	0	0.258173	3.335998	-1.680809
108	6	0	-0.303251	2.882881	0.938628

TS1u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.026343	1.546343	-0.456788
2	5	0	-2.200625	0.043169	0.483930
3	5	0	2.085415	0.096580	0.422121
4	8	0	3.107323	-0.460643	1.178342
5	8	0	-2.930596	1.214940	0.440214
6	8	0	-3.000369	-1.048412	0.171940
7	8	0	-0.430148	1.525073	-1.778964
8	8	0	0.315477	2.818701	-0.041924
9	8	0	2.603080	0.879907	-0.592920
10	6	0	-4.374971	-0.592006	0.028484
11	6	0	-4.187055	0.932862	-0.235072
12	6	0	4.364666	0.143471	0.777942
13	6	0	4.043721	0.724829	-0.637746
14	6	0	-0.060566	3.737877	-1.099129
15	6	0	-0.099699	2.813967	-2.357143
16	6	0	-1.426960	4.293664	-0.722674
17	1	0	-1.358563	4.782258	0.253303
18	1	0	-1.784281	5.029042	-1.450690
19	1	0	-2.160711	3.485901	-0.639302
20	6	0	-1.157384	3.176673	-3.380251
21	1	0	-0.950318	4.159134	-3.818348
22	1	0	-1.156519	2.440685	-4.189232
23	1	0	-2.158528	3.199981	-2.947019
24	6	0	1.254122	2.665031	-3.036514
25	1	0	1.190656	1.871078	-3.785898
26	1	0	1.557475	3.589800	-3.537972
27	1	0	2.017498	2.377373	-2.310949
28	6	0	0.973362	4.843714	-1.162192
29	1	0	0.771817	5.519375	-2.000796
30	1	0	0.948382	5.434686	-0.242380

31	1	0	1.981346	4.439339	-1.278711
32	6	0	4.657012	2.085775	-0.915666
33	1	0	5.750361	2.041147	-0.862137
34	1	0	4.388703	2.416968	-1.923197
35	1	0	4.305329	2.839936	-0.208390
36	6	0	4.366651	-0.228035	-1.777802
37	1	0	3.948654	0.168180	-2.707561
38	1	0	5.447453	-0.343109	-1.907851
39	1	0	3.931023	-1.216769	-1.615337
40	6	0	4.685708	1.222674	1.803607
41	1	0	4.754571	0.770932	2.797295
42	1	0	5.639493	1.715168	1.590608
43	1	0	3.904230	1.989172	1.830699
44	6	0	5.437421	-0.927549	0.794863
45	1	0	6.394398	-0.528149	0.441246
46	1	0	5.582729	-1.293162	1.814944
47	1	0	5.166896	-1.778806	0.167404
48	6	0	-3.981623	1.259411	-1.706339
49	1	0	-4.884475	1.066595	-2.293666
50	1	0	-3.737325	2.320264	-1.805101
51	1	0	-3.149954	0.689271	-2.131714
52	6	0	-5.262051	1.820036	0.358853
53	1	0	-5.035263	2.868715	0.148067
54	1	0	-6.239909	1.594326	-0.079803
55	1	0	-5.334186	1.703446	1.441930
56	6	0	-5.085454	-0.886401	1.340456
57	1	0	-6.151935	-0.648176	1.283068
58	1	0	-4.984751	-1.948850	1.578945
59	1	0	-4.652511	-0.309538	2.163472
60	6	0	-5.008100	-1.366850	-1.109726
61	1	0	-5.090621	-2.424461	-0.843209
62	1	0	-6.016629	-0.997385	-1.323603
63	1	0	-4.412197	-1.295148	-2.022322
64	5	0	0.216072	-1.722397	-0.808792
65	5	0	-0.647996	-1.898674	-2.379400
66	5	0	1.104905	-1.758905	-2.349751
67	5	0	1.689286	-2.703985	-0.980598
68	6	0	0.305900	-3.367956	-0.319851
69	6	0	-1.011217	-2.916010	-1.108520
70	5	0	0.314488	-2.884777	-3.472600
71	5	0	-1.080536	-3.582290	-2.649659

72	1	0	-1.426901	-1.049584	-2.645858
73	5	0	1.762654	-3.386311	-2.604936
74	1	0	1.642527	-0.768040	-2.704075
75	5	0	1.261377	-4.392365	-1.249030
76	1	0	2.588080	-2.472421	-0.251950
77	5	0	-0.495930	-4.510697	-1.277528
78	1	0	0.199634	-3.542034	0.744601
79	1	0	-1.903243	-2.745099	-0.510831
80	5	0	0.406758	-4.517323	-2.786491
81	1	0	0.294604	-2.690414	-4.640295
82	1	0	-2.147264	-3.848848	-3.082602
83	1	0	2.809632	-3.560009	-3.132479
84	1	0	1.863357	-5.237292	-0.684430
85	1	0	-1.110109	-5.350675	-0.722923
86	1	0	0.460606	-5.504413	-3.436749
87	77	0	-0.051504	-0.129473	0.814177
88	6	0	-0.788282	-1.716687	2.305552
89	6	0	-0.784444	1.127487	2.493296
90	6	0	0.633364	1.207853	2.463965
91	6	0	0.602576	-1.616578	2.455060
92	6	0	-1.766745	-1.113758	3.284138
93	1	0	-1.210043	-2.524426	1.707925
94	6	0	-1.519923	0.370344	3.587529
95	1	0	-1.316226	1.964337	2.048246
96	6	0	1.496200	0.542066	3.506259
97	1	0	1.047198	2.106720	2.012355
98	6	0	1.222602	-0.955354	3.670624
99	1	0	1.248813	-2.319886	1.934827
100	1	0	-2.766565	-1.234432	2.855341
101	1	0	-1.770782	-1.697009	4.218453
102	1	0	-2.482204	0.864477	3.763710
103	1	0	-0.958044	0.480100	4.524597
104	1	0	2.540573	0.683993	3.230029
105	1	0	1.357242	1.068693	4.463732
106	1	0	0.566751	-1.131899	4.533308
107	1	0	2.161474	-1.467775	3.901133
108	1	0	-0.584405	-0.545527	-0.681391

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.023702	1.509877	-0.435148
2	5	0	-2.233223	-0.052280	0.446692
3	5	0	2.055965	0.059927	0.532948
4	8	0	3.076234	-0.316582	1.390171
5	8	0	-2.765798	1.040824	-0.230517
6	8	0	-3.217625	-0.992041	0.692302
7	8	0	-0.254660	1.444117	-1.803037
8	8	0	0.214184	2.799424	-0.016289
9	8	0	2.584803	0.700951	-0.588730
10	6	0	-4.497319	-0.411623	0.323782
11	6	0	-4.072292	0.652721	-0.723811
12	6	0	4.299430	0.340003	0.974506
13	6	0	4.036559	0.654089	-0.531623
14	6	0	-0.120257	3.689815	-1.113528
15	6	0	-0.013983	2.757520	-2.366899
16	6	0	-1.534855	4.185161	-0.848759
17	1	0	-1.557305	4.695401	0.118139
18	1	0	-1.870207	4.891885	-1.614550
19	1	0	-2.232884	3.345224	-0.801942
20	6	0	-1.060621	3.017389	-3.432356
21	1	0	-0.952900	4.024020	-3.850719
22	1	0	-0.945018	2.301490	-4.251581
23	1	0	-2.072636	2.916623	-3.033291
24	6	0	1.378025	2.722490	-2.979183
25	1	0	1.422106	1.917848	-3.720631
26	1	0	1.629548	3.662500	-3.480405
27	1	0	2.126167	2.511012	-2.212857
28	6	0	0.860146	4.845437	-1.107251
29	1	0	0.684108	5.509425	-1.960593
30	1	0	0.736312	5.434042	-0.194463
31	1	0	1.894698	4.498256	-1.148575
32	6	0	4.580782	1.991963	-0.997948
33	1	0	5.664965	2.043902	-0.849744
34	1	0	4.388234	2.127088	-2.066180
35	1	0	4.119189	2.824250	-0.461430

36	6	0	4.494542	-0.445101	-1.477480
37	1	0	4.114833	-0.236486	-2.483558
38	1	0	5.586084	-0.496603	-1.537521
39	1	0	4.123364	-1.426205	-1.171144
40	6	0	4.431056	1.598704	1.823049
41	1	0	4.463112	1.321413	2.880256
42	1	0	5.345294	2.154325	1.592849
43	1	0	3.575182	2.266010	1.672857
44	6	0	5.461996	-0.596936	1.232556
45	1	0	6.401678	-0.163819	0.872506
46	1	0	5.565072	-0.775490	2.306138
47	1	0	5.316184	-1.562618	0.744466
48	6	0	-3.861742	0.057986	-2.110655
49	1	0	-4.810308	-0.173939	-2.605026
50	1	0	-3.313450	0.773245	-2.730854
51	1	0	-3.273276	-0.864483	-2.053320
52	6	0	-4.957168	1.879814	-0.794289
53	1	0	-4.591570	2.565308	-1.565159
54	1	0	-5.985165	1.605417	-1.054800
55	1	0	-4.972765	2.419655	0.155021
56	6	0	-5.084074	0.212947	1.581726
57	1	0	-6.086414	0.615986	1.405894
58	1	0	-5.155532	-0.544727	2.367039
59	1	0	-4.446667	1.025080	1.946612
60	6	0	-5.393274	-1.511936	-0.204290
61	1	0	-5.631176	-2.218957	0.594772
62	1	0	-6.336457	-1.099792	-0.579640
63	1	0	-4.912194	-2.068657	-1.010923
64	5	0	0.186065	-1.834793	-0.663396
65	5	0	1.692773	-2.780480	-0.795989
66	5	0	0.742349	-2.466226	-3.463273
67	5	0	-0.757793	-3.279841	-3.020664
68	1	0	-0.782778	-0.878206	-2.633798
69	5	0	2.037031	-3.143218	-2.485917
70	1	0	1.698849	-0.750634	-2.119713
71	5	0	1.343275	-4.380556	-1.443626
72	1	0	2.575129	-2.478185	-0.071520
73	5	0	-0.388174	-4.460530	-1.771181
74	1	0	0.020239	-3.988349	0.755284
75	1	0	-2.199758	-2.677800	-0.987900
76	5	0	0.753156	-4.184955	-3.103966

77	1	0	0.906950	-1.866804	-4.465353
78	1	0	-1.641973	-3.273787	-3.804884
79	1	0	3.143294	-3.045188	-2.891163
80	1	0	1.981782	-5.317701	-1.103078
81	1	0	-1.016670	-5.459354	-1.675608
82	1	0	0.956858	-4.972374	-3.963168
83	77	0	-0.092432	-0.182445	0.845823
84	6	0	-0.838035	-1.787050	2.354858
85	6	0	-0.984555	1.045873	2.491881
86	6	0	0.432321	1.181898	2.519125
87	6	0	0.543305	-1.647704	2.523166
88	6	0	-1.834996	-1.232216	3.339818
89	1	0	-1.207515	-2.593469	1.727402
90	6	0	-1.709805	0.277299	3.584267
91	1	0	-1.528205	1.871753	2.036137
92	6	0	1.280873	0.564698	3.602543
93	1	0	0.826274	2.097713	2.084937
94	6	0	1.119141	-0.953921	3.741586
95	1	0	1.193556	-2.353994	2.011705
96	1	0	-2.833891	-1.459757	2.966098
97	1	0	-1.730592	-1.774232	4.292461
98	1	0	-2.709377	0.706267	3.714121
99	1	0	-1.185779	0.467751	4.531467
100	1	0	2.324675	0.792406	3.384643
101	1	0	1.051336	1.066065	4.556423
102	1	0	0.474660	-1.185771	4.601185
103	1	0	2.093052	-1.396816	3.968276
104	1	0	-0.244937	-0.384781	-0.747609
105	6	0	1.248215	-1.736705	-2.022518
106	6	0	-0.325414	-1.817866	-2.331563
107	5	0	-1.091530	-2.905553	-1.326195
108	5	0	0.199159	-3.588601	-0.343842

TS2u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.552401	1.492321	-0.665391
2	5	0	-2.042830	-0.234558	0.528052
3	5	0	2.286148	0.253868	0.393789
4	8	0	3.386936	-0.307308	1.005824
5	8	0	-2.914836	0.846320	0.477180
6	8	0	-2.762488	-1.419627	0.505526
7	8	0	-1.166499	1.465662	-1.895543
8	8	0	-0.336360	2.763775	-0.191153
9	8	0	2.662344	1.184583	-0.563051
10	6	0	-4.185619	-1.130336	0.501582
11	6	0	-4.222642	0.366810	0.064152
12	6	0	4.585201	0.352969	0.509653
13	6	0	4.088939	1.062874	-0.794122
14	6	0	-0.979177	3.675898	-1.127052
15	6	0	-1.029928	2.813631	-2.426174
16	6	0	-2.352987	4.005645	-0.567266
17	1	0	-2.240836	4.427721	0.435320
18	1	0	-2.875626	4.738195	-1.190240
19	1	0	-2.961510	3.101850	-0.482271
20	6	0	-2.195268	3.107549	-3.344911
21	1	0	-2.118806	4.123894	-3.745724
22	1	0	-2.189966	2.411311	-4.187419
23	1	0	-3.154674	3.012912	-2.833758
24	6	0	0.282990	2.831959	-3.199730
25	1	0	0.253113	2.059119	-3.971758
26	1	0	0.454430	3.798585	-3.683356
27	1	0	1.129697	2.611982	-2.540461
28	6	0	-0.120521	4.919150	-1.231851
29	1	0	-0.503338	5.589516	-2.008915
30	1	0	-0.131186	5.464428	-0.284409
31	1	0	0.916163	4.669698	-1.467579
32	6	0	4.654039	2.453377	-1.018107
33	1	0	5.742790	2.419568	-1.133779
34	1	0	4.234966	2.876207	-1.935557
35	1	0	4.414264	3.131874	-0.197185

36	6	0	4.268014	0.226778	-2.052793
37	1	0	3.739525	0.707744	-2.880551
38	1	0	5.323609	0.134308	-2.326631
39	1	0	3.850513	-0.776011	-1.936019
40	6	0	5.034129	1.328540	1.587365
41	1	0	5.165007	0.791127	2.531228
42	1	0	5.986039	1.803381	1.330043
43	1	0	4.294360	2.118965	1.744574
44	6	0	5.647353	-0.705734	0.287938
45	1	0	6.549187	-0.266535	-0.152211
46	1	0	5.926707	-1.159783	1.242515
47	1	0	5.291847	-1.499376	-0.372171
48	6	0	-4.312367	0.543088	-1.444102
49	1	0	-5.274249	0.194088	-1.831693
50	1	0	-4.215979	1.604381	-1.687543
51	1	0	-3.506177	0.014022	-1.960406
52	6	0	-5.279770	1.207215	0.753578
53	1	0	-5.222105	2.240429	0.399614
54	1	0	-6.284186	0.833210	0.527441
55	1	0	-5.150930	1.217303	1.837776
56	6	0	-4.700356	-1.354637	1.915112
57	1	0	-5.788250	-1.248085	1.967294
58	1	0	-4.441862	-2.366213	2.240342
59	1	0	-4.257315	-0.646197	2.620878
60	6	0	-4.851813	-2.093768	-0.461511
61	1	0	-4.761713	-3.117854	-0.087731
62	1	0	-5.918711	-1.869759	-0.567606
63	1	0	-4.388597	-2.055288	-1.449816
64	5	0	0.337594	-1.751284	-0.757934
65	5	0	-0.740199	-1.944529	-2.113701
66	5	0	0.962187	-1.606830	-2.376834
67	5	0	1.866153	-2.502089	-1.167600
68	6	0	0.712016	-3.330797	-0.310036
69	6	0	-0.760344	-3.024970	-0.846706
70	5	0	0.127105	-2.790359	-3.397490
71	5	0	-1.014302	-3.663686	-2.380631
72	1	0	-1.651205	-1.201177	-2.231242
73	5	0	1.750534	-3.136659	-2.807152
74	1	0	1.335449	-0.553290	-2.777850
75	5	0	1.606961	-4.221932	-1.427378
76	1	0	2.845432	-2.177326	-0.592344

77	5	0	-0.101887	-4.547067	-1.164826
78	1	0	0.807686	-3.528703	0.752847
79	1	0	-1.559454	-2.999600	-0.114233
80	5	0	0.521661	-4.416961	-2.802742
81	1	0	-0.115505	-2.578797	-4.538073
82	1	0	-2.101583	-4.050484	-2.640161
83	1	0	2.707259	-3.171337	-3.507388
84	1	0	2.389881	-5.002345	-1.008953
85	1	0	-0.516620	-5.465509	-0.551144
86	1	0	0.571032	-5.377465	-3.493412
87	77	0	0.148171	-0.122549	0.744781
88	6	0	-0.328802	-1.548602	2.337006
89	6	0	-0.641552	1.284715	2.437985
90	6	0	0.730380	1.539337	2.298638
91	6	0	1.073969	-1.282630	2.373484
92	6	0	-1.285502	-1.018352	3.379981
93	1	0	-0.666338	-2.481250	1.884459
94	6	0	-1.199081	0.496233	3.605667
95	1	0	-1.319244	1.954393	1.917532
96	6	0	1.763841	1.027040	3.269573
97	1	0	1.008217	2.395861	1.688777
98	6	0	1.708424	-0.485157	3.499961
99	1	0	1.735039	-2.005679	1.900329
100	1	0	-2.294289	-1.281731	3.052259
101	1	0	-1.131472	-1.554074	4.329902
102	1	0	-2.196818	0.883588	3.841222
103	1	0	-0.585042	0.707714	4.491001
104	1	0	2.753889	1.293432	2.897380
105	1	0	1.650155	1.560023	4.226450
106	1	0	1.160756	-0.706109	4.426041
107	1	0	2.724506	-0.859389	3.654890
108	1	0	0.545141	0.019415	-0.913591

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-1.919274	-0.565429	-0.831834
2	8	0	-2.942327	0.325712	-1.109771
3	8	0	-2.370171	-1.625941	-0.066315
4	6	0	-4.123323	-0.068961	-0.371189
5	6	0	-3.811757	-1.559015	0.014470
6	6	0	-4.349517	-2.569019	-0.990898
7	1	0	-3.969228	-3.564061	-0.743618
8	1	0	-5.443215	-2.609687	-0.987105
9	1	0	-4.019356	-2.331339	-2.007381
10	6	0	-4.217972	-1.944312	1.423765
11	1	0	-5.297727	-1.833198	1.571108
12	1	0	-3.960106	-2.991155	1.612923
13	1	0	-3.693670	-1.328407	2.157658
14	6	0	-5.322148	0.109167	-1.286097
15	1	0	-6.244025	-0.221870	-0.795505
16	1	0	-5.437609	1.167580	-1.536405
17	1	0	-5.212434	-0.446278	-2.220678
18	6	0	-4.244577	0.860110	0.827308
19	1	0	-4.310711	1.892643	0.474029
20	1	0	-5.142105	0.636701	1.414020
21	1	0	-3.364213	0.787433	1.468145
22	5	0	0.384899	-1.949573	-0.108616
23	8	0	0.503685	-2.153185	1.257265
24	8	0	0.362452	-3.157631	-0.785422
25	6	0	0.257195	-4.242223	0.158661
26	6	0	0.658986	-3.574364	1.522853
27	6	0	1.186638	-5.354996	-0.290669
28	1	0	1.184459	-6.182201	0.427503
29	1	0	0.850913	-5.747599	-1.254027
30	1	0	2.212898	-5.002350	-0.411184
31	6	0	-1.188244	-4.722046	0.114144
32	1	0	-1.428047	-5.019302	-0.911248
33	1	0	-1.353095	-5.586265	0.765298
34	1	0	-1.871532	-3.918939	0.396881
35	6	0	-0.257131	-3.942132	2.677477

36	1	0	-0.286891	-5.027301	2.822514
37	1	0	0.110026	-3.500048	3.609268
38	1	0	-1.275608	-3.583997	2.504396
39	6	0	2.109581	-3.805318	1.921268
40	1	0	2.348312	-3.201092	2.802604
41	1	0	2.292668	-4.853546	2.177183
42	1	0	2.801200	-3.519754	1.125719
43	5	0	2.331283	0.069465	-0.714492
44	5	0	3.428763	-1.359140	-0.577352
45	5	0	3.723355	-0.197279	-1.841029
46	5	0	3.455282	1.398321	-1.169338
47	6	0	3.087385	1.115979	0.423845
48	6	0	3.070313	-0.445884	0.760920
49	5	0	5.091026	-0.924321	-0.974541
50	5	0	4.613156	-1.112416	0.705538
51	1	0	2.930975	-2.424749	-0.705382
52	5	0	5.107719	0.797098	-1.347011
53	1	0	3.519475	-0.466465	-2.977413
54	5	0	4.640919	1.667895	0.106128
55	1	0	2.996727	2.351236	-1.702152
56	5	0	4.334166	0.487689	1.374148
57	1	0	2.346468	-0.770243	1.501643
58	5	0	5.656055	0.232487	0.245130
59	1	0	5.814436	-1.706723	-1.494133
60	1	0	4.857733	-1.992127	1.459652
61	1	0	5.848741	1.280939	-2.136079
62	1	0	4.908404	2.773192	0.435425
63	1	0	4.320521	0.740424	2.529102
64	1	0	6.779522	0.301860	0.614710
65	77	0	0.167269	-0.168946	-1.140066
66	6	0	-0.906180	1.506859	-2.732169
67	6	0	-1.022200	-1.304150	-2.626339
68	6	0	0.419471	-1.218353	-2.914746
69	6	0	0.447464	1.665393	-2.844030
70	6	0	-1.752920	0.837455	-3.787284
71	1	0	-1.450907	2.053122	-1.972895
72	6	0	-1.993714	-0.667378	-3.597483
73	1	0	-1.322122	-2.292200	-2.272973
74	6	0	0.939906	-0.469089	-4.136539
75	1	0	0.973434	-2.131570	-2.704659
76	6	0	1.246636	1.025844	-3.938491

77	1	0	0.955282	2.377385	-2.200002
78	1	0	-2.718181	1.353650	-3.814142
79	1	0	-1.282524	1.016304	-4.762204
80	1	0	-3.018867	-0.836036	-3.257073
81	1	0	-1.904337	-1.193163	-4.560060
82	1	0	1.854181	-0.964395	-4.476748
83	1	0	0.215162	-0.601058	-4.952279
84	1	0	1.079947	1.564165	-4.883737
85	1	0	2.306978	1.150982	-3.707607
86	5	0	-0.319537	1.951040	0.310805
87	5	0	-0.188214	0.715834	1.575392
88	8	0	0.717920	2.823282	0.045624
89	8	0	-1.518738	2.622058	0.448334
90	8	0	-1.260076	0.151209	2.207945
91	6	0	-1.288611	4.047787	0.247506
92	6	0	0.268337	4.164444	0.373113
93	8	0	0.844576	1.022043	2.433870
94	6	0	-1.078639	0.384483	3.634412
95	6	0	0.468913	0.581024	3.775030
96	6	0	0.927325	5.137638	-0.582613
97	1	0	0.578137	6.159199	-0.399489
98	1	0	2.010800	5.118538	-0.437263
99	1	0	0.727333	4.885663	-1.625958
100	6	0	0.736455	4.424138	1.798727
101	1	0	1.822224	4.301931	1.849974
102	1	0	0.486628	5.436161	2.130649
103	1	0	0.292013	3.706838	2.495480
104	6	0	-2.070494	4.787986	1.317314
105	1	0	-1.881092	5.865041	1.260087
106	1	0	-3.141965	4.626981	1.170551
107	1	0	-1.815384	4.448061	2.322918
108	6	0	-1.822338	4.436466	-1.122868
109	1	0	-2.844862	4.062153	-1.231603
110	1	0	-1.842004	5.525129	-1.233326
111	1	0	-1.223427	4.028063	-1.938064
112	1	0	2.391545	1.732673	0.975165
113	6	0	1.228866	-0.701916	4.058854
114	1	0	2.304422	-0.512865	3.982248
115	1	0	1.022744	-1.069571	5.069045
116	1	0	0.960643	-1.471469	3.334947
117	6	0	0.890211	1.662507	4.750849

118	1	0	1.977932	1.771341	4.730165
119	1	0	0.449979	2.632906	4.513000
120	1	0	0.598389	1.394339	5.771722
121	6	0	-1.634898	-0.798275	4.397112
122	1	0	-1.208076	-1.736807	4.040483
123	1	0	-1.426256	-0.700509	5.467836
124	1	0	-2.720208	-0.849213	4.273002
125	6	0	-1.869110	1.646778	3.950755
126	1	0	-1.496453	2.498625	3.372160
127	1	0	-2.916708	1.497276	3.675367
128	1	0	-1.824052	1.899374	5.014244

TS3u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.632223	1.063836	-0.947043
2	8	0	2.852510	0.411683	-1.075252
3	8	0	1.770404	2.251660	-0.244229
4	6	0	3.875468	1.172718	-0.387732
5	6	0	3.175690	2.559484	-0.134350
6	6	0	3.475538	3.593879	-1.212827
7	1	0	2.847872	4.475097	-1.052992
8	1	0	4.522772	3.911681	-1.198655
9	1	0	3.250598	3.204268	-2.211189
10	6	0	3.419625	3.147136	1.242578
11	1	0	4.484658	3.341422	1.409135
12	1	0	2.886450	4.098129	1.339872
13	1	0	3.054485	2.472567	2.019808
14	6	0	5.088011	1.232677	-1.302114
15	1	0	5.891906	1.825315	-0.851985
16	1	0	5.469174	0.220127	-1.464950
17	1	0	4.850902	1.662257	-2.278389
18	6	0	4.239582	0.433085	0.889094
19	1	0	4.606030	-0.565339	0.638104
20	1	0	5.026568	0.961804	1.437465
21	1	0	3.367942	0.309993	1.531564
22	5	0	-0.988426	1.762662	-0.243954
23	8	0	-1.193751	2.024931	1.102294

24	8	0	-1.284098	2.877880	-1.012088
25	6	0	-1.511481	4.013347	-0.153667
26	6	0	-1.748790	3.359772	1.255339
27	6	0	-2.702216	4.785490	-0.692169
28	1	0	-2.949262	5.630792	-0.040648
29	1	0	-2.464827	5.184405	-1.681878
30	1	0	-3.586159	4.151838	-0.788289
31	6	0	-0.256439	4.874042	-0.226603
32	1	0	-0.081261	5.151231	-1.270574
33	1	0	-0.356322	5.794611	0.357073
34	1	0	0.615823	4.316681	0.119721
35	6	0	-1.008967	4.057105	2.383462
36	1	0	-1.293556	5.113119	2.442267
37	1	0	-1.264939	3.598419	3.344029
38	1	0	0.074130	3.993547	2.248110
39	6	0	-3.215593	3.200818	1.629202
40	1	0	-3.294525	2.613905	2.550279
41	1	0	-3.690044	4.170291	1.810332
42	1	0	-3.781254	2.679220	0.854725
43	5	0	-2.200789	-0.819552	-0.605938
44	5	0	-3.687326	0.199631	-0.536409
45	5	0	-5.129112	-0.755538	-0.869518
46	5	0	-4.728954	-0.321776	0.786078
47	1	0	-3.544092	1.354808	-0.744756
48	5	0	-4.608876	-2.416057	-1.138986
49	1	0	-3.491914	-0.823655	-2.876734
50	5	0	-3.890195	-3.004987	0.353184
51	1	0	-2.127047	-3.262694	-1.445534
52	5	0	-3.959955	-1.710032	1.541642
53	1	0	-2.466480	0.113210	1.544977
54	5	0	-5.300536	-1.950387	0.430154
55	1	0	-6.062070	-0.272298	-1.418307
56	1	0	-5.232061	0.483088	1.494028
57	1	0	-5.163518	-3.156606	-1.880322
58	1	0	-3.801728	-4.115495	0.752520
59	1	0	-3.865818	-1.871661	2.708963
60	1	0	-6.344598	-2.343858	0.828035
61	77	0	-0.271002	0.050370	-1.128767
62	6	0	1.294708	-1.463773	-2.655554
63	6	0	0.739914	1.325187	-2.664617
64	6	0	-0.656392	0.890970	-2.962229

65	6	0	0.024949	-1.925380	-2.787835
66	6	0	2.002309	-0.648614	-3.706092
67	1	0	1.894390	-1.820252	-1.824660
68	6	0	1.831883	0.880149	-3.622671
69	1	0	0.762579	2.398005	-2.455167
70	6	0	-0.966314	-0.016467	-4.149187
71	1	0	-1.386333	1.692015	-2.862380
72	6	0	-0.877992	-1.536648	-3.915647
73	1	0	-0.334243	-2.667627	-2.084527
74	1	0	3.069302	-0.889244	-3.656117
75	1	0	1.653516	-0.997043	-4.687071
76	1	0	2.781047	1.337164	-3.329519
77	1	0	1.595314	1.287012	-4.616460
78	1	0	-1.978164	0.215167	-4.495566
79	1	0	-0.302174	0.273770	-4.976535
80	1	0	-0.549684	-2.029948	-4.842404
81	1	0	-1.875430	-1.930667	-3.706133
82	5	0	0.988101	-1.731383	0.565733
83	5	0	0.393528	-0.504459	1.641988
84	8	0	0.313780	-2.831561	0.097743
85	8	0	2.290549	-2.019687	0.901842
86	8	0	1.182185	0.455954	2.218101
87	6	0	2.549431	-3.430489	0.675367
88	6	0	1.120657	-4.015476	0.350805
89	8	0	-0.508009	-1.052786	2.533992
90	6	0	1.053255	0.303529	3.660674
91	6	0	-0.337810	-0.395818	3.826788
92	6	0	1.064898	-4.899459	-0.879158
93	1	0	1.670022	-5.801019	-0.738582
94	1	0	0.032991	-5.210533	-1.063164
95	1	0	1.422252	-4.377259	-1.770002
96	6	0	0.448464	-4.702488	1.531291
97	1	0	-0.574123	-4.971258	1.250850
98	1	0	0.973242	-5.614322	1.830865
99	1	0	0.388518	-4.032446	2.395009
100	6	0	3.178935	-3.978536	1.945616
101	1	0	3.404699	-5.044916	1.843212
102	1	0	4.116554	-3.450903	2.142475
103	1	0	2.531760	-3.848534	2.815633
104	6	0	3.560123	-3.538620	-0.458064
105	1	0	4.468488	-2.996988	-0.181729

106	1	0	3.830955	-4.582644	-0.642516
107	1	0	3.193772	-3.116354	-1.395116
108	1	0	-1.724403	-2.311626	1.172489
109	6	0	-1.493245	0.573565	4.004030
110	1	0	-2.441179	0.028426	3.949868
111	1	0	-1.447131	1.070160	4.978454
112	1	0	-1.480653	1.329570	3.217518
113	6	0	-0.387176	-1.472985	4.893053
114	1	0	-1.377331	-1.936620	4.901830
115	1	0	0.352496	-2.257484	4.718671
116	1	0	-0.207754	-1.044610	5.884773
117	6	0	1.152120	1.665365	4.313256
118	1	0	0.428401	2.363941	3.893144
119	1	0	0.980246	1.587653	5.392284
120	1	0	2.152493	2.081608	4.165791
121	6	0	2.219590	-0.576095	4.093113
122	1	0	2.196256	-1.543917	3.583684
123	1	0	3.159474	-0.086438	3.823206
124	1	0	2.219927	-0.744256	5.174184
125	6	0	-3.603652	-1.073763	-1.723134
126	5	0	-2.581747	-1.980695	0.601436
127	5	0	-3.055926	-0.469426	0.845326
128	6	0	-2.852307	-2.462045	-0.962474

TS3e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.933966	0.025275	0.114027
2	8	0	2.523426	-0.371699	1.329052
3	8	0	2.797899	0.916718	-0.527507
4	6	0	3.673486	0.456895	1.588361
5	6	0	4.071891	0.912452	0.156473
6	6	0	4.956542	-0.104586	-0.553833
7	1	0	5.057514	0.174225	-1.606414
8	1	0	5.958550	-0.151356	-0.116015
9	1	0	4.511876	-1.104922	-0.507564
10	6	0	4.679409	2.297702	0.062834
11	1	0	5.635810	2.343274	0.595323

12	1	0	4.865672	2.553914	-0.984119
13	1	0	4.019680	3.060933	0.482563
14	6	0	4.716204	-0.374283	2.310668
15	1	0	5.631933	0.203178	2.480168
16	1	0	4.330249	-0.683715	3.285945
17	1	0	4.974114	-1.275893	1.751926
18	6	0	3.206841	1.603886	2.476509
19	1	0	2.807591	1.193820	3.409157
20	1	0	4.021041	2.291071	2.728485
21	1	0	2.406799	2.171384	1.991362
22	5	0	-0.848272	1.322287	-0.335608
23	8	0	-0.395009	2.218289	0.646299
24	8	0	-0.818614	1.918111	-1.592316
25	6	0	-0.220669	3.225994	-1.514618
26	6	0	-0.223694	3.525437	0.030629
27	6	0	-1.074155	4.178297	-2.340591
28	1	0	-0.695524	5.204046	-2.270791
29	1	0	-1.032727	3.878340	-3.390544
30	1	0	-2.122217	4.172083	-2.037103
31	6	0	1.163328	3.153418	-2.142303
32	1	0	1.056865	2.787059	-3.167612
33	1	0	1.628625	4.144143	-2.189053
34	1	0	1.829260	2.476269	-1.606863
35	6	0	1.067443	4.132304	0.541212
36	1	0	1.250651	5.105157	0.073066
37	1	0	1.016415	4.282909	1.623807
38	1	0	1.914891	3.479960	0.319449
39	6	0	-1.408777	4.373770	0.476745
40	1	0	-1.453787	4.388751	1.570053
41	1	0	-1.321481	5.407701	0.129405
42	1	0	-2.355859	3.980984	0.093410
43	5	0	-2.309767	0.394515	-0.032651
44	5	0	-3.698313	1.268970	-0.770514
45	5	0	-3.493279	-0.453568	-1.051175
46	5	0	-2.964704	-1.195572	0.460527
47	6	0	-2.927516	0.096960	1.531842
48	6	0	-3.355054	1.469124	0.849012
49	5	0	-5.116563	0.218669	-0.774396
50	5	0	-4.978586	1.498106	0.426972
51	1	0	-3.451013	2.153082	-1.511997
52	5	0	-4.660194	-1.299472	-0.010078

53	1	0	-3.160249	-0.851400	-2.116033
54	5	0	-4.229194	-0.950535	1.665063
55	1	0	-2.230881	-2.090607	0.657992
56	5	0	-4.437795	0.772638	1.931663
57	1	0	-2.205095	0.171640	2.336986
58	1	0	-2.835396	2.344581	1.223189
59	5	0	-5.573983	-0.091291	0.909712
60	1	0	-5.916736	0.284347	-1.644730
61	1	0	-5.538870	2.537225	0.482837
62	1	0	-5.124482	-2.348682	-0.305280
63	1	0	-4.270367	-1.663377	2.607351
64	1	0	-4.544725	1.258088	3.001076
65	1	0	-6.688677	-0.256143	1.271295
66	77	0	0.270244	-1.081946	-0.554373
67	6	0	0.989608	-3.020357	-1.025850
68	6	0	1.170707	-0.567995	-2.440594
69	6	0	-0.201401	-0.844318	-2.650256
70	6	0	-0.430823	-3.147987	-1.140541
71	6	0	2.009929	-2.983095	-2.160462
72	1	0	1.403523	-3.450938	-0.108210
73	6	0	2.210364	-1.596046	-2.821556
74	1	0	1.509178	0.463235	-2.444341
75	6	0	-0.638997	-2.102097	-3.379373
76	1	0	-0.882236	0.002209	-2.709925
77	6	0	-1.218220	-3.127952	-2.419942
78	1	0	-0.939356	-3.673167	-0.330353
79	1	0	2.971035	-3.304768	-1.744996
80	1	0	1.750032	-3.739678	-2.913357
81	1	0	3.196833	-1.197890	-2.564954
82	1	0	2.212478	-1.709470	-3.916466
83	1	0	-1.366747	-1.838200	-4.155062
84	1	0	0.219292	-2.531476	-3.910120
85	1	0	-1.272639	-4.123393	-2.891511
86	1	0	-2.252557	-2.857965	-2.171276
87	7	0	0.065828	-1.510275	1.590242
88	6	0	-0.049349	-2.756866	2.082392
89	6	0	0.087028	-0.493811	2.479194
90	6	0	-0.155491	-3.033250	3.437879
91	1	0	-0.065013	-3.560323	1.355181
92	6	0	-0.029110	-0.687704	3.847900
93	6	0	-0.148280	-1.980878	4.345370

94	1	0	-0.246547	-4.063433	3.764280
95	1	0	-0.013346	0.174311	4.507145
96	1	0	-0.230725	-2.163745	5.412484
97	6	0	0.239567	0.913862	1.873562
98	1	0	-0.665127	1.465725	2.021465
99	1	0	1.049942	1.422392	2.352717
100	1	0	0.439872	0.831527	0.825707

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.883746	0.754350	-0.232619
2	8	0	2.917783	1.248000	-1.011263
3	8	0	2.202933	0.816552	1.110938
4	6	0	4.095994	1.347253	-0.172741
5	6	0	3.483324	1.477599	1.257890
6	6	0	3.230836	2.922988	1.660188
7	1	0	2.618157	2.951041	2.565977
8	1	0	4.171055	3.445354	1.865796
9	1	0	2.685663	3.456099	0.880250
10	6	0	4.253331	0.755200	2.348044
11	1	0	5.276916	1.137431	2.429522
12	1	0	3.762501	0.910940	3.314406
13	1	0	4.291414	-0.320592	2.160348
14	6	0	4.912974	2.536932	-0.635462
15	1	0	5.781852	2.691630	0.013509
16	1	0	5.280913	2.360968	-1.650393
17	1	0	4.321816	3.454974	-0.646284
18	6	0	4.877650	0.055287	-0.362275
19	1	0	5.136014	-0.062747	-1.419198
20	1	0	5.806913	0.051044	0.216463
21	1	0	4.265448	-0.798374	-0.059443
22	5	0	-0.472266	1.870414	-0.048473
23	8	0	-1.756754	2.372459	-0.199326
24	8	0	0.391879	2.867121	0.368470
25	6	0	-0.301771	4.139565	0.293659
26	6	0	-1.804964	3.716847	0.326901
27	6	0	0.104875	4.787015	-1.022552

28	1	0	-0.299518	5.799377	-1.119433
29	1	0	1.196704	4.846256	-1.072306
30	1	0	-0.239225	4.199435	-1.879089
31	6	0	0.139245	5.002655	1.459782
32	1	0	1.193972	5.271789	1.355509
33	1	0	-0.440145	5.931680	1.494686
34	1	0	0.018392	4.483514	2.413110
35	6	0	-2.376970	3.648054	1.734890
36	1	0	-2.492266	4.644145	2.173275
37	1	0	-3.366746	3.180277	1.702781
38	1	0	-1.737360	3.047886	2.383647
39	6	0	-2.725230	4.530617	-0.563557
40	1	0	-3.741526	4.130232	-0.502183
41	1	0	-2.755195	5.578697	-0.246546
42	1	0	-2.417645	4.493721	-1.610660
43	5	0	-2.276659	-0.799308	-0.271892
44	5	0	-3.552514	0.061591	-1.207263
45	5	0	-3.179655	-1.613229	-1.602382
46	5	0	-2.918567	-2.472766	-0.102287
47	6	0	-3.215327	-1.329671	1.067094
48	6	0	-3.563449	0.100652	0.448514
49	5	0	-4.860923	-1.049409	-1.622444
50	5	0	-5.064524	0.093092	-0.299738
51	1	0	-3.277606	1.044444	-1.792738
52	5	0	-4.474491	-2.622860	-0.932893
53	1	0	-2.640656	-1.924887	-2.606075
54	5	0	-4.432065	-2.449720	0.811718
55	1	0	-2.134616	-3.322775	0.128932
56	5	0	-4.802275	-0.772045	1.202368
57	1	0	-3.192832	0.958730	0.999071
58	5	0	-5.641610	-1.565365	-0.118242
59	1	0	-5.455300	-0.918449	-2.639775
60	1	0	-5.700718	1.089809	-0.266495
61	1	0	-4.793338	-3.644532	-1.441094
62	1	0	-4.612729	-3.261305	1.652655
63	1	0	-6.796185	-1.811775	-0.027990
64	77	0	0.050391	0.012559	-0.997908
65	6	0	1.301731	-1.279533	-2.583907
66	6	0	0.587896	1.469839	-2.673416
67	6	0	-0.789518	1.199192	-2.786948
68	6	0	-0.034767	-1.524547	-2.862226

69	6	0	2.200861	-0.391012	-3.389649
70	1	0	1.822383	-2.011362	-1.980245
71	6	0	1.611102	0.988629	-3.683400
72	1	0	0.876316	2.373289	-2.142067
73	6	0	-1.404742	0.360369	-3.871900
74	1	0	-1.470196	1.921454	-2.343829
75	6	0	-0.691181	-0.968778	-4.101857
76	1	0	-0.493516	-2.381434	-2.377758
77	1	0	3.135409	-0.269470	-2.837807
78	1	0	2.456756	-0.908169	-4.328095
79	1	0	2.425357	1.717825	-3.724278
80	1	0	1.137935	1.000585	-4.674295
81	1	0	-2.446709	0.165473	-3.604997
82	1	0	-1.444565	0.944423	-4.805490
83	1	0	0.074154	-0.864782	-4.881564
84	1	0	-1.406596	-1.705482	-4.481339
85	5	0	0.938797	-1.730082	-0.010601
86	5	0	-0.684715	-0.377743	0.994265
87	8	0	0.356021	-2.938646	-0.336039
88	8	0	2.205785	-1.915145	0.527542
89	8	0	-1.051067	0.695547	1.845230
90	6	0	2.544811	-3.327456	0.455291
91	6	0	1.158694	-4.016357	0.192494
92	8	0	-0.411762	-1.485587	1.836186
93	6	0	-0.831200	0.397476	3.238210
94	6	0	-0.297696	-1.088895	3.220994
95	6	0	1.183842	-5.119119	-0.850577
96	1	0	1.826896	-5.948180	-0.536258
97	1	0	0.172657	-5.510984	-0.990083
98	1	0	1.536489	-4.753784	-1.818237
99	6	0	0.483774	-4.521314	1.459238
100	1	0	-0.545572	-4.806923	1.227530
101	1	0	1.002868	-5.394112	1.868333
102	1	0	0.445209	-3.740890	2.219910
103	6	0	3.220652	-3.731688	1.753760
104	1	0	3.493999	-4.792113	1.729568
105	1	0	4.139820	-3.153160	1.886808
106	1	0	2.589092	-3.563921	2.625447
107	6	0	3.555116	-3.521568	-0.672340
108	1	0	4.450225	-2.928086	-0.468967
109	1	0	3.859295	-4.570170	-0.743674

110	1	0	3.174852	-3.223861	-1.651785
111	1	0	-2.675704	-1.330766	2.003346
112	6	0	-1.121110	-2.062504	4.055234
113	1	0	-0.729598	-3.075247	3.928961
114	1	0	-1.059042	-1.810876	5.118956
115	1	0	-2.178868	-2.086251	3.780185
116	6	0	1.166802	-1.218043	3.615335
117	1	0	1.449518	-2.273462	3.594036
118	1	0	1.810968	-0.681879	2.916355
119	1	0	1.341135	-0.853033	4.632171
120	6	0	-2.156073	0.586135	3.969748
121	1	0	-2.956777	-0.051272	3.584808
122	1	0	-2.050256	0.376199	5.038805
123	1	0	-2.485299	1.623648	3.866872
124	6	0	0.178209	1.407225	3.766700
125	1	0	1.090009	1.388261	3.167456
126	1	0	-0.244569	2.415120	3.709149
127	1	0	0.423376	1.213419	4.815906
128	1	0	-5.157990	-0.402327	2.266427

TS4u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	2.039170	-0.222149	-0.216508
2	8	0	3.168978	-0.373823	-1.010652
3	8	0	2.369723	-0.256073	1.121818
4	6	0	4.233317	-0.861594	-0.155501
5	6	0	3.813526	-0.304002	1.238087
6	6	0	4.319737	1.109973	1.479013
7	1	0	3.821503	1.534113	2.355257
8	1	0	5.399908	1.115957	1.658909
9	1	0	4.090777	1.756836	0.630074
10	6	0	4.157555	-1.200858	2.412219
11	1	0	5.238567	-1.368005	2.475569
12	1	0	3.837290	-0.730935	3.347577
13	1	0	3.655633	-2.169040	2.335097
14	6	0	5.552244	-0.344471	-0.690643
15	1	0	6.381064	-0.633095	-0.035187

16	1	0	5.744738	-0.770523	-1.679948
17	1	0	5.549952	0.743176	-0.786137
18	6	0	4.182042	-2.382090	-0.213325
19	1	0	4.300834	-2.714510	-1.249517
20	1	0	4.979095	-2.840080	0.381110
21	1	0	3.215685	-2.738499	0.155618
22	5	0	0.510652	1.896518	-0.110709
23	8	0	-0.405354	2.914153	-0.303366
24	8	0	1.745566	2.398804	0.267971
25	6	0	1.703897	3.842063	0.122642
26	6	0	0.172550	4.151631	0.175842
27	6	0	2.328868	4.171980	-1.226148
28	1	0	2.426755	5.251943	-1.374598
29	1	0	3.327002	3.726009	-1.281265
30	1	0	1.732626	3.769758	-2.051047
31	6	0	2.520033	4.463418	1.239380
32	1	0	3.577830	4.211971	1.119464
33	1	0	2.431600	5.555152	1.223301
34	1	0	2.198784	4.105216	2.219602
35	6	0	-0.334383	4.406375	1.585538
36	1	0	0.000770	5.380557	1.956167
37	1	0	-1.427278	4.390442	1.585384
38	1	0	0.007335	3.628966	2.268606
39	6	0	-0.293124	5.262675	-0.746777
40	1	0	-1.378494	5.370280	-0.665574
41	1	0	0.163235	6.219919	-0.471822
42	1	0	-0.055980	5.053923	-1.792405
43	5	0	-2.472242	0.514162	0.246572
44	5	0	-3.079536	1.497149	-1.105233
45	5	0	-4.426363	0.651844	-1.873206
46	5	0	-4.736356	2.012215	-0.795370
47	1	0	-2.308043	2.057192	-1.790475
48	5	0	-4.731508	-0.834756	-0.974728
49	1	0	-2.509194	-0.815427	-1.704387
50	5	0	-5.213283	-0.390934	0.653511
51	1	0	-3.152826	-1.701064	0.570020
52	5	0	-5.216522	1.366241	0.766945
53	1	0	-3.107845	2.888757	1.061547
54	5	0	-5.761136	0.566398	-0.722369
55	1	0	-4.486615	0.606194	-3.054891
56	1	0	-5.132038	3.041529	-1.228309

57	1	0	-4.932084	-1.884757	-1.476754
58	1	0	-5.828317	-1.184109	1.277953
59	1	0	-5.963059	1.926099	1.496834
60	1	0	-6.887575	0.547546	-1.086020
61	77	0	0.150431	0.034219	-1.007132
62	6	0	0.660463	-1.915619	-2.683024
63	6	0	1.293458	0.938475	-2.756472
64	6	0	-0.050939	1.316137	-2.897375
65	6	0	-0.601162	-1.563953	-3.049785
66	6	0	1.903051	-1.507259	-3.409885
67	1	0	0.777148	-2.673639	-1.913866
68	6	0	2.022530	-0.001714	-3.696139
69	1	0	1.948615	1.640313	-2.245060
70	6	0	-1.015119	0.783407	-3.925923
71	1	0	-0.330318	2.290845	-2.498820
72	6	0	-0.901043	-0.711516	-4.248027
73	1	0	-1.419482	-2.068894	-2.542371
74	1	0	2.764916	-1.822968	-2.821253
75	1	0	1.950873	-2.062262	-4.359071
76	1	0	3.084356	0.258952	-3.675491
77	1	0	1.676119	0.215035	-4.715095
78	1	0	-2.032918	0.993566	-3.579567
79	1	0	-0.910041	1.366848	-4.854430
80	1	0	-0.127411	-0.880370	-5.005909
81	1	0	-1.841219	-1.043955	-4.702135
82	5	0	-0.069659	-1.793105	0.155203
83	5	0	-1.010550	0.177487	1.212884
84	8	0	-1.212414	-2.488102	-0.249724
85	8	0	0.832925	-2.650627	0.757400
86	8	0	-0.489329	1.265330	1.929035
87	6	0	0.326694	-4.009033	0.728256
88	6	0	-1.161875	-3.853667	0.232857
89	8	0	-1.155196	-0.921621	2.102886
90	6	0	-0.381576	0.968500	3.333265
91	6	0	-0.626782	-0.586325	3.412075
92	6	0	-1.538668	-4.755925	-0.929847
93	1	0	-1.521839	-5.810871	-0.637121
94	1	0	-2.554336	-4.517088	-1.260109
95	1	0	-0.869128	-4.624512	-1.783863
96	6	0	-2.201406	-3.980807	1.338655
97	1	0	-3.201883	-3.842278	0.914743

98	1	0	-2.182311	-4.970898	1.803743
99	1	0	-2.047164	-3.219040	2.107230
100	6	0	0.459349	-4.613378	2.116190
101	1	0	0.195124	-5.676245	2.098671
102	1	0	1.497208	-4.528095	2.451439
103	1	0	-0.175769	-4.119908	2.851511
104	6	0	1.223434	-4.808146	-0.212753
105	1	0	2.241831	-4.821948	0.185074
106	1	0	0.884298	-5.844633	-0.299970
107	1	0	1.269987	-4.384923	-1.218950
108	1	0	-3.609039	0.212070	2.528134
109	6	0	-1.671018	-1.006334	4.435898
110	1	0	-1.816828	-2.089886	4.383305
111	1	0	-1.336660	-0.767638	5.451224
112	1	0	-2.637736	-0.527878	4.269136
113	6	0	0.646687	-1.381171	3.654093
114	1	0	0.412125	-2.445340	3.699359
115	1	0	1.371910	-1.226493	2.856556
116	1	0	1.096199	-1.104420	4.613320
117	6	0	-1.442900	1.796860	4.049011
118	1	0	-2.445733	1.582095	3.673632
119	1	0	-1.429115	1.617574	5.128806
120	1	0	-1.249544	2.859509	3.881942
121	6	0	1.001661	1.403723	3.793227
122	1	0	1.778339	0.924335	3.194749
123	1	0	1.102429	2.487602	3.676809
124	1	0	1.158661	1.170507	4.851793
125	5	0	-3.856107	0.446858	1.398482
126	5	0	-3.546533	1.930254	0.521230
127	6	0	-3.617513	-0.763889	0.288171
128	6	0	-3.176228	-0.181236	-1.135319

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.659319	0.106350	1.556869
2	5	0	-0.399855	2.296552	-0.158266
3	5	0	-2.333423	-1.542517	-0.000924

4	8	0	-3.227283	-2.269646	-0.765338
5	8	0	0.817635	2.266910	0.534564
6	8	0	-0.618027	3.567498	-0.659837
7	8	0	0.593808	-0.476064	1.669520
8	8	0	-1.193213	0.419518	2.787599
9	8	0	-1.828492	-2.322866	1.034141
10	6	0	0.354335	4.473929	-0.082980
11	6	0	1.519675	3.519493	0.310301
12	6	0	-3.453697	-3.558092	-0.138786
13	6	0	-2.241809	-3.698940	0.842439
14	6	0	-0.131643	0.280981	3.769982
15	6	0	0.860359	-0.707376	3.073680
16	6	0	0.456116	1.670426	3.957957
17	1	0	-0.334038	2.354808	4.280856
18	1	0	1.250454	1.683231	4.711106
19	1	0	0.858887	2.035295	3.010108
20	6	0	2.327481	-0.415057	3.316815
21	1	0	2.572602	-0.457580	4.383812
22	1	0	2.938849	-1.160969	2.799559
23	1	0	2.606401	0.566281	2.924659
24	6	0	0.544376	-2.168172	3.354304
25	1	0	1.149390	-2.797789	2.693844
26	1	0	0.772402	-2.441295	4.389518
27	1	0	-0.507030	-2.379460	3.147006
28	6	0	-0.734738	-0.232579	5.061054
29	1	0	0.045517	-0.415828	5.807875
30	1	0	-1.423778	0.509886	5.472089
31	1	0	-1.289626	-1.160047	4.906200
32	6	0	-2.592211	-4.294202	2.194780
33	1	0	-3.014297	-5.298736	2.081368
34	1	0	-1.691602	-4.382940	2.809304
35	1	0	-3.311112	-3.677434	2.738099
36	6	0	-1.052772	-4.446179	0.253697
37	1	0	-0.198939	-4.344548	0.930339
38	1	0	-1.264380	-5.513272	0.133392
39	1	0	-0.761699	-4.044294	-0.719730
40	6	0	-4.793993	-3.474485	0.578543
41	1	0	-5.566092	-3.172452	-0.135046
42	1	0	-5.085017	-4.437479	1.009752
43	1	0	-4.770042	-2.735511	1.385170
44	6	0	-3.510501	-4.611812	-1.227603

45	1	0	-3.612266	-5.614347	-0.797578
46	1	0	-4.374766	-4.434094	-1.872989
47	1	0	-2.616005	-4.592301	-1.853506
48	6	0	2.522485	3.280198	-0.809158
49	1	0	3.141417	4.164328	-0.992231
50	1	0	3.184910	2.453770	-0.528086
51	1	0	2.026157	3.011763	-1.745350
52	6	0	2.261653	3.907418	1.575136
53	1	0	3.010764	3.145048	1.812849
54	1	0	2.787305	4.858360	1.434493
55	1	0	1.598452	4.010564	2.435696
56	6	0	-0.317988	5.115812	1.123515
57	1	0	0.320093	5.867899	1.598083
58	1	0	-1.241234	5.605467	0.802125
59	1	0	-0.578619	4.361260	1.873912
60	6	0	0.710671	5.520306	-1.118765
61	1	0	-0.164377	6.134672	-1.347780
62	1	0	1.499538	6.184668	-0.749232
63	1	0	1.051930	5.061464	-2.048915
64	5	0	-0.187067	-0.266067	-1.735186
65	5	0	-0.162971	-1.881541	-2.505924
66	5	0	2.570324	-1.206541	-2.013599
67	5	0	2.365807	0.232316	-3.022542
68	1	0	1.770124	0.581212	-0.695197
69	5	0	1.502387	-2.454182	-2.664240
70	1	0	0.977654	-1.817562	-0.366606
71	5	0	0.655034	-1.790624	-4.061315
72	1	0	-1.015278	-2.634989	-2.193115
73	5	0	1.195361	-0.126565	-4.285973
74	1	0	-1.399291	-0.188325	-4.017512
75	1	0	0.468056	1.948424	-2.790211
76	5	0	2.351247	-1.369433	-3.760332
77	1	0	3.249875	1.020860	-3.026033
78	1	0	1.753154	-3.583715	-2.419117
79	1	0	0.324056	-2.490320	-4.957858
80	1	0	1.264216	0.393243	-5.348119
81	1	0	3.247171	-1.746697	-4.435890
82	77	0	-1.660499	0.515319	-0.277429
83	6	0	-2.655674	1.636701	-2.046358
84	6	0	-3.000583	1.991144	0.750078
85	6	0	-3.552119	0.697295	0.930767

86	6	0	-3.323120	0.417995	-1.883232
87	6	0	-3.267911	2.950087	-1.634997
88	1	0	-1.878309	1.693985	-2.804862
89	6	0	-3.657768	3.022477	-0.151530
90	1	0	-2.446124	2.380873	1.601458
91	6	0	-4.793433	0.231196	0.214074
92	1	0	-3.360640	0.226198	1.892461
93	6	0	-4.724980	0.366729	-1.310831
94	1	0	-3.024145	-0.420340	-2.505908
95	1	0	-2.555999	3.743399	-1.858927
96	1	0	-4.152428	3.136146	-2.264228
97	1	0	-3.414315	4.018448	0.231286
98	1	0	-4.746713	2.918568	-0.038662
99	1	0	-4.963337	-0.816279	0.469630
100	1	0	-5.660385	0.782490	0.611595
101	1	0	-5.257856	1.273092	-1.629570
102	1	0	-5.256851	-0.473180	-1.767576
103	1	0	-0.230557	-0.159559	-0.157177
104	6	0	1.014401	-1.471829	-1.398712
105	6	0	1.502374	0.046100	-1.605444
106	5	0	0.700893	0.790175	-2.863994
107	5	0	-0.364740	-0.451102	-3.503537
108	5	0	3.924106	-1.283941	-1.029032
109	8	0	4.939017	-2.200871	-1.090621
110	8	0	4.153989	-0.289323	-0.097806
111	6	0	5.848066	-1.902420	0.006953
112	6	0	5.557193	-0.395906	0.274784
113	6	0	7.262049	-2.209254	-0.439672
114	1	0	7.983538	-1.915549	0.330352
115	1	0	7.375419	-3.282036	-0.614539
116	1	0	7.513409	-1.689933	-1.365994
117	6	0	5.442132	-2.798937	1.167258
118	1	0	5.459287	-3.841485	0.841212
119	1	0	6.122725	-2.692889	2.017537
120	1	0	4.427282	-2.567865	1.507245
121	6	0	5.723138	0.048660	1.711983
122	1	0	6.768283	-0.043766	2.025960
123	1	0	5.434877	1.099623	1.810023
124	1	0	5.104522	-0.534000	2.396533
125	6	0	6.323198	0.527935	-0.662416
126	1	0	5.923017	1.541833	-0.579501

127	1	0	7.389041	0.559498	-0.417227
128	1	0	6.217801	0.209129	-1.703676

TS5u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-2.303190	1.066380	0.269198
2	5	0	0.206971	1.923636	-0.359856
3	5	0	-2.097959	-1.710656	-0.444773
4	8	0	-2.021779	-2.960692	-1.036062
5	8	0	-0.461232	3.139694	-0.425119
6	8	0	1.538774	2.134541	-0.018651
7	8	0	-2.305593	1.498560	1.582609
8	8	0	-3.459485	1.419347	-0.392783
9	8	0	-3.194383	-1.628182	0.396786
10	6	0	1.793898	3.562625	0.059788
11	6	0	0.357808	4.146849	0.220600
12	6	0	-3.233794	-3.695402	-0.717857
13	6	0	-3.779588	-2.947138	0.541051
14	6	0	-4.215444	2.294882	0.485491
15	6	0	-3.659255	1.919138	1.893759
16	6	0	-3.881535	3.720625	0.072485
17	1	0	-4.131951	3.856396	-0.983387
18	1	0	-4.444481	4.456319	0.655754
19	1	0	-2.810532	3.911750	0.187522
20	6	0	-3.602616	3.064781	2.883089
21	1	0	-4.611721	3.419305	3.120155
22	1	0	-3.137183	2.727874	3.813207
23	1	0	-3.024124	3.908766	2.503533
24	6	0	-4.361087	0.719099	2.514519
25	1	0	-3.806752	0.401994	3.402242
26	1	0	-5.385068	0.961817	2.816476
27	1	0	-4.378303	-0.120071	1.814922
28	6	0	-5.689313	2.003743	0.291111
29	1	0	-6.296762	2.576960	1.000066
30	1	0	-5.998023	2.285795	-0.719208
31	1	0	-5.906165	0.942014	0.428188
32	6	0	-5.289488	-2.797237	0.583628

33	1	0	-5.779710	-3.776914	0.599527
34	1	0	-5.585138	-2.264483	1.492215
35	1	0	-5.666920	-2.235489	-0.273526
36	6	0	-3.280220	-3.522677	1.857429
37	1	0	-3.546236	-2.841061	2.670193
38	1	0	-3.730153	-4.498655	2.065590
39	1	0	-2.192984	-3.633821	1.863031
40	6	0	-4.154920	-3.574700	-1.924136
41	1	0	-3.644110	-3.962324	-2.810485
42	1	0	-5.079049	-4.145182	-1.788477
43	1	0	-4.423488	-2.530509	-2.114734
44	6	0	-2.865511	-5.146605	-0.482093
45	1	0	-3.741836	-5.726479	-0.172103
46	1	0	-2.480296	-5.588909	-1.404909
47	1	0	-2.096164	-5.246390	0.286031
48	6	0	-0.093654	4.224293	1.671609
49	1	0	0.474444	4.971857	2.233783
50	1	0	-1.149163	4.507022	1.701471
51	1	0	-0.000627	3.255792	2.172010
52	6	0	0.127818	5.474746	-0.473773
53	1	0	-0.906524	5.796999	-0.324703
54	1	0	0.782127	6.250515	-0.061136
55	1	0	0.305889	5.408218	-1.548994
56	6	0	2.459850	3.974057	-1.244575
57	1	0	2.745320	5.030587	-1.236100
58	1	0	3.365687	3.379573	-1.395896
59	1	0	1.795393	3.807558	-2.098071
60	6	0	2.719983	3.810819	1.233948
61	1	0	3.700548	3.365968	1.039256
62	1	0	2.868232	4.883596	1.398598
63	1	0	2.327432	3.369564	2.152860
64	5	0	0.308648	-0.880057	1.062961
65	5	0	0.763544	-0.023800	2.574799
66	5	0	-0.230999	-1.471953	2.668083
67	5	0	0.389109	-2.613288	1.484578
68	6	0	1.702064	-1.846540	0.816661
69	6	0	1.907206	-0.384904	1.425739
70	5	0	1.048194	-1.189928	3.863777
71	5	0	2.411135	-0.444713	3.028999
72	1	0	0.396828	1.096727	2.665049
73	5	0	0.818712	-2.801945	3.188515

74	1	0	-1.386301	-1.407007	2.926320
75	5	0	2.038185	-3.044204	1.941384
76	1	0	-0.218204	-3.361103	0.800182
77	5	0	3.036752	-1.591074	1.844359
78	1	0	2.004235	-1.979547	-0.215749
79	1	0	2.274363	0.381061	0.748348
80	5	0	2.461158	-2.163192	3.410038
81	1	0	0.800271	-0.920248	4.990225
82	1	0	3.143644	0.406213	3.403544
83	1	0	0.401743	-3.716679	3.816721
84	1	0	2.497157	-4.058940	1.544523
85	1	0	3.231320	-2.605624	4.192556
86	77	0	-0.749653	-0.012277	-0.702134
87	6	0	1.132925	-0.290967	-1.977098
88	6	0	-1.243383	1.156989	-2.557997
89	6	0	-2.058926	0.000406	-2.554663
90	6	0	0.334001	-1.436090	-2.143795
91	6	0	1.254128	0.787946	-3.023986
92	1	0	1.984989	-0.333804	-1.299495
93	6	0	-0.091494	1.316553	-3.536299
94	1	0	-1.712934	2.073351	-2.211362
95	6	0	-1.827300	-1.155807	-3.490908
96	1	0	-3.081007	0.138764	-2.211231
97	6	0	-0.402762	-1.713412	-3.439796
98	1	0	0.545884	-2.316430	-1.542243
99	1	0	1.820315	1.610897	-2.575809
100	1	0	1.867408	0.423885	-3.864357
101	1	0	0.009498	2.379387	-3.783463
102	1	0	-0.362523	0.821204	-4.478291
103	1	0	-2.530574	-1.951075	-3.242433
104	1	0	-2.079366	-0.834127	-4.513931
105	1	0	0.193850	-1.312409	-4.269943
106	1	0	-0.436910	-2.796363	-3.591605
107	1	0	-0.945723	-0.043180	0.897254
108	5	0	4.453121	-1.359501	0.981309
109	8	0	5.716123	-1.096460	1.431860
110	8	0	4.336732	-1.229871	-0.392060
111	6	0	6.564489	-0.934310	0.257187
112	6	0	5.534185	-0.541842	-0.844045
113	6	0	7.221807	-2.280970	-0.001617
114	1	0	7.939199	-2.226546	-0.826085

115	1	0	7.755193	-2.600287	0.896600
116	1	0	6.477105	-3.045009	-0.242190
117	6	0	7.604241	0.124057	0.559489
118	1	0	8.275520	-0.224520	1.348109
119	1	0	8.209474	0.335942	-0.328490
120	1	0	7.145560	1.055468	0.896507
121	6	0	5.189573	0.942030	-0.838364
122	1	0	6.007261	1.556984	-1.226790
123	1	0	4.306303	1.105075	-1.464159
124	1	0	4.949425	1.284122	0.174595
125	6	0	5.870451	-1.011438	-2.242749
126	1	0	5.076307	-0.715796	-2.934577
127	1	0	6.805375	-0.559593	-2.590734
128	1	0	5.972007	-2.097039	-2.290636

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.605041	-0.351554	1.489346
2	5	0	-0.636588	2.406860	-0.003906
3	5	0	-1.985614	-1.681477	-0.119987
4	8	0	-3.012078	-2.359628	-0.742976
5	8	0	0.621151	2.464770	0.587003
6	8	0	-1.070402	3.664703	-0.351547
7	8	0	0.769197	-0.450373	1.435075
8	8	0	-1.101650	-0.663822	2.740323
9	8	0	-1.118427	-2.576937	0.492558
10	6	0	-0.176270	4.640084	0.253868
11	6	0	1.131461	3.820032	0.491052
12	6	0	-2.956228	-3.768142	-0.421758
13	6	0	-1.558689	-3.944294	0.287431
14	6	0	0.033195	-0.686386	3.645551
15	6	0	1.235848	-0.992905	2.694358
16	6	0	0.108974	0.707270	4.256932
17	1	0	-0.840429	0.935005	4.748818
18	1	0	0.909890	0.788704	4.998192
19	1	0	0.279547	1.461632	3.480272
20	6	0	2.529961	-0.284482	3.039755

21	1	0	2.930511	-0.636202	3.997267
22	1	0	3.264016	-0.487961	2.255897
23	1	0	2.402724	0.799302	3.087840
24	6	0	1.486880	-2.477484	2.483449
25	1	0	2.201232	-2.604616	1.662108
26	1	0	1.908962	-2.949003	3.376559
27	1	0	0.563739	-2.989480	2.207098
28	6	0	-0.213025	-1.732819	4.711698
29	1	0	0.652657	-1.819579	5.377194
30	1	0	-1.077190	-1.453580	5.320152
31	1	0	-0.410486	-2.713125	4.272677
32	6	0	-1.637894	-4.611730	1.652747
33	1	0	-2.079962	-5.610505	1.578618
34	1	0	-0.634314	-4.730444	2.071289
35	1	0	-2.227943	-4.020364	2.357149
36	6	0	-0.497615	-4.640375	-0.551444
37	1	0	0.464041	-4.581720	-0.031629
38	1	0	-0.735981	-5.698577	-0.697326
39	1	0	-0.373476	-4.176837	-1.531350
40	6	0	-4.147736	-4.044026	0.486515
41	1	0	-5.066532	-3.767002	-0.038593
42	1	0	-4.220670	-5.100676	0.761096
43	1	0	-4.095850	-3.452692	1.405701
44	6	0	-3.106965	-4.546285	-1.716627
45	1	0	-3.045887	-5.625121	-1.538880
46	1	0	-4.083126	-4.332416	-2.160051
47	1	0	-2.341874	-4.270980	-2.445291
48	6	0	2.116397	3.864333	-0.666740
49	1	0	2.601136	4.843019	-0.738599
50	1	0	2.893230	3.109610	-0.503809
51	1	0	1.636939	3.645633	-1.622915
52	6	0	1.858945	4.136614	1.784897
53	1	0	2.739860	3.493870	1.874514
54	1	0	2.201092	5.177110	1.793961
55	1	0	1.230418	3.973589	2.662896
56	6	0	-0.847531	5.076987	1.548803
57	1	0	-0.276362	5.855661	2.063435
58	1	0	-1.841279	5.473179	1.323545
59	1	0	-0.969220	4.230947	2.233935
60	6	0	-0.028627	5.809586	-0.696351
61	1	0	-0.988892	6.317569	-0.819066

62	1	0	0.689808	6.538453	-0.306003
63	1	0	0.309818	5.484266	-1.681836
64	5	0	-0.300359	-0.008179	-1.597308
65	5	0	-0.177327	-1.514685	-2.584313
66	5	0	2.496060	-0.771815	-1.954443
67	5	0	2.235859	0.761449	-2.798548
68	1	0	1.599144	0.802010	-0.459099
69	5	0	1.512333	-1.984767	-2.771991
70	1	0	0.910306	-1.658148	-0.436946
71	5	0	0.656437	-1.208996	-4.103347
72	1	0	-0.989592	-2.350188	-2.392586
73	5	0	1.110536	0.491539	-4.121739
74	1	0	-1.476311	0.264876	-3.913926
75	1	0	0.242476	2.333502	-2.433044
76	5	0	2.322229	-0.740729	-3.715769
77	1	0	3.080190	1.586729	-2.694903
78	1	0	1.821906	-3.121292	-2.652351
79	1	0	0.374424	-1.816536	-5.081342
80	1	0	1.168694	1.137998	-5.113693
81	1	0	3.253649	-0.991738	-4.403943
82	77	0	-1.790071	0.498753	-0.115589
83	6	0	-2.913858	1.601568	-1.733427
84	6	0	-3.376657	1.665063	1.077512
85	6	0	-3.687840	0.302748	1.184711
86	6	0	-3.379605	0.269567	-1.658916
87	6	0	-3.724279	2.768242	-1.224633
88	1	0	-2.205648	1.840889	-2.524493
89	6	0	-4.193543	2.621131	0.227320
90	1	0	-2.837569	2.107409	1.914446
91	6	0	-4.816388	-0.320865	0.404684
92	1	0	-3.378934	-0.214222	2.091011
93	6	0	-4.759546	-0.054338	-1.104723
94	1	0	-2.999151	-0.426468	-2.402613
95	1	0	-3.121854	3.670781	-1.321174
96	1	0	-4.592189	2.902408	-1.890402
97	1	0	-4.186692	3.604807	0.708604
98	1	0	-5.239556	2.286332	0.258127
99	1	0	-4.803111	-1.397680	0.578287
100	1	0	-5.770912	0.042030	0.818452
101	1	0	-5.433741	0.772685	-1.367584
102	1	0	-5.141985	-0.933944	-1.630727

103	1	0	-0.888385	1.103203	1.109571
104	6	0	0.949110	-1.182069	-1.410066
105	6	0	1.360751	0.366407	-1.424903
106	5	0	0.543728	1.202880	-2.613895
107	5	0	-0.437785	0.000055	-3.405557
108	5	0	3.885776	-0.880107	-1.024395
109	8	0	4.905925	-1.782919	-1.179365
110	8	0	4.181081	0.097680	-0.088787
111	6	0	5.910896	-1.476740	-0.173424
112	6	0	5.615252	0.019290	0.141059
113	6	0	7.279842	-1.745268	-0.763084
114	1	0	8.068584	-1.441455	-0.066288
115	1	0	7.399820	-2.813269	-0.961738
116	1	0	7.423739	-1.211068	-1.703766
117	6	0	5.646319	-2.394342	1.011243
118	1	0	5.632093	-3.431446	0.667836
119	1	0	6.420236	-2.296415	1.778840
120	1	0	4.676905	-2.177057	1.472569
121	6	0	5.919216	0.456256	1.558586
122	1	0	6.997190	0.422782	1.749152
123	1	0	5.582990	1.486824	1.707366
124	1	0	5.421863	-0.169350	2.301857
125	6	0	6.259127	0.971198	-0.858465
126	1	0	5.837738	1.971322	-0.725954
127	1	0	7.342963	1.032596	-0.721630
128	1	0	6.057119	0.657344	-1.887100

TS6u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-2.343423	1.006581	0.269759
2	5	0	0.214964	1.958553	-0.366502
3	5	0	-2.082919	-1.668598	-0.425462
4	8	0	-2.039064	-2.883377	-1.093235
5	8	0	-0.443429	3.177743	-0.406030
6	8	0	1.537589	2.138823	0.020613
7	8	0	-2.341755	1.413133	1.591011
8	8	0	-3.508575	1.362235	-0.377169

9	8	0	-3.146569	-1.634409	0.459085
10	6	0	1.802712	3.561955	0.152562
11	6	0	0.367598	4.151750	0.300427
12	6	0	-3.251227	-3.621469	-0.790052
13	6	0	-3.754867	-2.948820	0.528077
14	6	0	-4.258363	2.225445	0.517751
15	6	0	-3.690097	1.837392	1.918694
16	6	0	-3.929390	3.655899	0.116033
17	1	0	-4.191209	3.802625	-0.935577
18	1	0	-4.485598	4.385762	0.712958
19	1	0	-2.857100	3.846872	0.221792
20	6	0	-3.617091	2.977245	2.914214
21	1	0	-4.621710	3.335389	3.164627
22	1	0	-3.143478	2.631846	3.837159
23	1	0	-3.038400	3.820816	2.534224
24	6	0	-4.394195	0.640632	2.541518
25	1	0	-3.830380	0.311556	3.418796
26	1	0	-5.411336	0.891868	2.859410
27	1	0	-4.428954	-0.192463	1.836838
28	6	0	-5.733707	1.935130	0.333056
29	1	0	-6.335849	2.502955	1.050837
30	1	0	-6.050377	2.224344	-0.672792
31	1	0	-5.949338	0.872422	0.464474
32	6	0	-5.260566	-2.772144	0.611415
33	1	0	-5.772150	-3.739444	0.557252
34	1	0	-5.529899	-2.309211	1.565266
35	1	0	-5.638823	-2.134599	-0.190952
36	6	0	-3.243800	-3.621878	1.792268
37	1	0	-3.480926	-2.992424	2.654504
38	1	0	-3.710744	-4.600710	1.941510
39	1	0	-2.159476	-3.754921	1.769833
40	6	0	-4.201159	-3.412822	-1.962134
41	1	0	-3.724919	-3.764115	-2.882140
42	1	0	-5.135770	-3.967342	-1.832496
43	1	0	-4.446996	-2.353317	-2.088804
44	6	0	-2.898349	-5.089619	-0.657138
45	1	0	-3.776019	-5.677947	-0.367459
46	1	0	-2.537944	-5.474821	-1.614917
47	1	0	-2.115235	-5.249373	0.086611
48	6	0	-0.120484	4.172206	1.741213
49	1	0	0.436447	4.892470	2.348349

50	1	0	-1.175005	4.459470	1.755104
51	1	0	-0.044906	3.183321	2.203619
52	6	0	0.165783	5.508269	-0.344910
53	1	0	-0.869531	5.833214	-0.209736
54	1	0	0.815017	6.260729	0.116013
55	1	0	0.371774	5.483954	-1.416871
56	6	0	2.500448	4.010596	-1.122449
57	1	0	2.793674	5.063806	-1.072630
58	1	0	3.404730	3.413821	-1.273586
59	1	0	1.853801	3.877726	-1.995458
60	6	0	2.703259	3.761760	1.355321
61	1	0	3.686961	3.321882	1.165183
62	1	0	2.850346	4.826838	1.564701
63	1	0	2.289658	3.286062	2.247554
64	5	0	0.290131	-0.927340	1.028227
65	5	0	0.737806	-0.134897	2.584934
66	5	0	-0.258065	-1.584238	2.602899
67	5	0	0.376680	-2.673618	1.376952
68	6	0	1.695052	-1.873078	0.755744
69	6	0	1.890346	-0.441641	1.430638
70	5	0	1.012488	-1.354015	3.822640
71	5	0	2.382460	-0.569910	3.034554
72	1	0	0.373029	0.982124	2.724449
73	5	0	0.792392	-2.933513	3.074186
74	1	0	-1.412994	-1.531200	2.857766
75	5	0	2.024772	-3.117868	1.829331
76	1	0	-0.215426	-3.400719	0.658710
77	5	0	3.020429	-1.659358	1.805264
78	1	0	2.009141	-1.960758	-0.277648
79	1	0	2.256311	0.355193	0.788255
80	5	0	2.432244	-2.302611	3.339044
81	1	0	0.752518	-1.134806	4.957233
82	1	0	3.106291	0.268371	3.451871
83	1	0	0.373322	-3.876473	3.657710
84	1	0	2.488231	-4.113490	1.391453
85	1	0	3.195750	-2.779669	4.107593
86	77	0	-0.738418	0.028118	-0.718232
87	6	0	1.163455	-0.225184	-1.988186
88	6	0	-1.216466	1.232062	-2.551475
89	6	0	-2.025862	0.070126	-2.573325
90	6	0	0.365922	-1.364861	-2.186167

91	6	0	1.287018	0.874980	-3.012848
92	1	0	2.008870	-0.277964	-1.302973
93	6	0	-0.056826	1.420788	-3.515305
94	1	0	-1.697513	2.138403	-2.193800
95	6	0	-1.789974	-1.070369	-3.527589
96	1	0	-3.051912	0.201384	-2.239484
97	6	0	-0.359362	-1.609120	-3.494932
98	1	0	0.564749	-2.258826	-1.600791
99	1	0	1.857439	1.686877	-2.549572
100	1	0	1.897683	0.525974	-3.861484
101	1	0	0.046914	2.491180	-3.726188
102	1	0	-0.322383	0.957940	-4.475169
103	1	0	-2.479797	-1.876983	-3.278633
104	1	0	-2.057897	-0.740318	-4.544058
105	1	0	0.234279	-1.170009	-4.307575
106	1	0	-0.375790	-2.686392	-3.686025
107	1	0	-0.697828	0.200828	0.885460
108	5	0	4.444061	-1.392559	0.964475
109	8	0	5.701350	-1.140491	1.436818
110	8	0	4.341456	-1.218146	-0.404908
111	6	0	6.561901	-0.938423	0.277442
112	6	0	5.542357	-0.514936	-0.822883
113	6	0	7.227159	-2.274038	-0.015923
114	1	0	7.953319	-2.191511	-0.830310
115	1	0	7.751740	-2.619429	0.877796
116	1	0	6.487940	-3.032660	-0.288556
117	6	0	7.594390	0.113364	0.624499
118	1	0	8.258194	-0.257852	1.409078
119	1	0	8.208654	0.355449	-0.249430
120	1	0	7.128570	1.032019	0.985819
121	6	0	5.194839	0.967577	-0.777419
122	1	0	6.015762	1.594947	-1.138302
123	1	0	4.318546	1.147540	-1.408296
124	1	0	4.942754	1.279642	0.242316
125	6	0	5.894855	-0.941966	-2.231322
126	1	0	5.107338	-0.627565	-2.922413
127	1	0	6.832329	-0.477911	-2.555576
128	1	0	5.999710	-2.025418	-2.310452

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-3.053878	0.127361	0.310360
2	8	0	-3.622342	1.388569	0.442498
3	8	0	-3.268283	-0.638843	1.446726
4	6	0	-4.212440	1.514344	1.757343
5	6	0	-4.242189	0.028625	2.276086
6	6	0	-5.571519	-0.673526	2.024934
7	1	0	-5.474154	-1.732800	2.278712
8	1	0	-6.381753	-0.249685	2.626398
9	1	0	-5.860253	-0.611569	0.970454
10	6	0	-3.820757	-0.140367	3.723269
11	1	0	-4.492658	0.400435	4.398546
12	1	0	-3.850436	-1.199571	3.997763
13	1	0	-2.800692	0.220077	3.870950
14	6	0	-5.582666	2.149353	1.584441
15	1	0	-6.099755	2.237602	2.546189
16	1	0	-5.467513	3.156239	1.172962
17	1	0	-6.220283	1.580257	0.903577
18	6	0	-3.326060	2.436226	2.579358
19	1	0	-3.248304	3.403775	2.076330
20	1	0	-3.743995	2.598654	3.578739
21	1	0	-2.318294	2.030739	2.669736
22	5	0	-1.242712	-2.002618	0.060513
23	8	0	-0.418644	-2.225591	1.154051
24	8	0	-2.038469	-3.109194	-0.189353
25	6	0	-1.900379	-4.061115	0.883843
26	6	0	-0.595005	-3.590055	1.622661
27	6	0	-1.807858	-5.449993	0.278282
28	1	0	-1.647705	-6.206913	1.053865
29	1	0	-2.742377	-5.690008	-0.235646
30	1	0	-0.996526	-5.521499	-0.448898
31	6	0	-3.159961	-3.945668	1.733254
32	1	0	-4.030546	-4.135883	1.098221
33	1	0	-3.170699	-4.672501	2.551659
34	1	0	-3.260193	-2.938057	2.140864
35	6	0	-0.728191	-3.561659	3.135421

36	1	0	-1.001718	-4.549537	3.521309
37	1	0	0.228283	-3.288698	3.592930
38	1	0	-1.483546	-2.839403	3.456459
39	6	0	0.655626	-4.369770	1.241420
40	1	0	1.533031	-3.891064	1.688826
41	1	0	0.612548	-5.398683	1.612132
42	1	0	0.810116	-4.398716	0.161488
43	5	0	0.521448	-0.828925	-1.852807
44	5	0	1.036608	-2.557041	-1.972818
45	5	0	0.826510	-1.642659	-3.441925
46	5	0	1.463714	-0.035204	-3.161524
47	6	0	2.050570	-0.088672	-1.606174
48	6	0	1.805827	-1.518740	-0.928363
49	5	0	2.174545	-2.789447	-3.294959
50	5	0	2.759242	-2.711799	-1.635480
51	1	0	0.282266	-3.362042	-1.548246
52	5	0	2.441710	-1.215197	-4.038803
53	1	0	-0.083049	-1.863629	-4.170582
54	5	0	3.186244	-0.172599	-2.835228
55	1	0	1.068611	0.995334	-3.588279
56	5	0	3.386582	-1.093707	-1.337981
57	1	0	1.586724	-1.523704	0.134177
58	5	0	3.640173	-1.873888	-2.906379
59	1	0	2.195539	-3.807449	-3.902385
60	1	0	3.149681	-3.586641	-0.938858
61	1	0	2.672117	-1.073327	-5.193526
62	1	0	3.894722	0.765139	-2.992698
63	1	0	4.734450	-2.202751	-3.223820
64	77	0	-1.447863	-0.300206	-1.077563
65	6	0	-2.694412	1.734794	-2.236565
66	6	0	-3.621720	-0.783274	-1.317861
67	6	0	-2.686493	-1.332338	-2.344541
68	6	0	-1.715566	1.308461	-3.077359
69	6	0	-4.158649	1.447888	-2.448867
70	1	0	-2.453595	2.443263	-1.450847
71	6	0	-4.707637	0.163199	-1.801420
72	1	0	-4.001823	-1.589899	-0.685596
73	6	0	-2.770107	-0.894564	-3.804602
74	1	0	-2.518633	-2.403678	-2.246725
75	6	0	-1.964388	0.356254	-4.206247
76	1	0	-0.719496	1.727554	-2.978867

77	1	0	-4.724742	2.305323	-2.071060
78	1	0	-4.337891	1.413363	-3.531146
79	1	0	-5.362744	0.424981	-0.965675
80	1	0	-5.336796	-0.381775	-2.519994
81	1	0	-2.432624	-1.728639	-4.427284
82	1	0	-3.831368	-0.754381	-4.056506
83	1	0	-2.480979	0.875027	-5.027404
84	1	0	-0.997206	0.047772	-4.611091
85	5	0	-0.344255	2.000394	-0.018977
86	5	0	0.048087	0.786730	1.160119
87	8	0	0.440411	2.334151	-1.100890
88	8	0	-0.844707	3.118083	0.613967
89	8	0	-0.576122	0.591051	2.362838
90	6	0	-0.349050	4.305816	-0.071285
91	6	0	0.804399	3.734598	-0.966543
92	8	0	1.422207	0.708795	1.255035
93	6	0	0.439442	0.735821	3.397488
94	6	0	1.776307	0.427518	2.640789
95	6	0	0.906150	4.337904	-2.352187
96	1	0	1.147472	5.404579	-2.295144
97	1	0	1.703299	3.839602	-2.910767
98	1	0	-0.021061	4.223204	-2.917600
99	6	0	2.166615	3.741083	-0.282422
100	1	0	2.885568	3.189986	-0.897040
101	1	0	2.544721	4.758115	-0.140851
102	1	0	2.124585	3.239863	0.689811
103	6	0	0.103096	5.285257	0.995728
104	1	0	0.525428	6.187600	0.541204
105	1	0	-0.752333	5.583804	1.608316
106	1	0	0.855949	4.850688	1.656959
107	6	0	-1.501927	4.906468	-0.859408
108	1	0	-2.358081	5.048630	-0.193990
109	1	0	-1.225049	5.879604	-1.276534
110	1	0	-1.817909	4.265984	-1.684384
111	1	0	2.020138	0.766922	-0.944888
112	6	0	2.204894	-1.028892	2.704647
113	1	0	3.041188	-1.190661	2.013255
114	1	0	2.543982	-1.304154	3.708784
115	1	0	1.382814	-1.683958	2.410676
116	6	0	2.940558	1.330289	2.996111
117	1	0	3.758177	1.128789	2.299957

118	1	0	2.687994	2.389668	2.910360
119	1	0	3.287505	1.139154	4.017867
120	6	0	0.134092	-0.214704	4.534401
121	1	0	0.037234	-1.241150	4.181549
122	1	0	0.927741	-0.176007	5.288422
123	1	0	-0.802397	0.067457	5.023339
124	6	0	0.338507	2.179278	3.873910
125	1	0	0.488049	2.880768	3.046926
126	1	0	-0.662999	2.355731	4.276138
127	1	0	1.066443	2.398271	4.660799
128	5	0	4.614241	-0.609245	-0.305757
129	8	0	5.666052	-1.415940	0.052374
130	8	0	4.793209	0.702165	0.101262
131	6	0	6.575795	-0.618526	0.857072
132	6	0	6.206005	0.831816	0.427939
133	6	0	6.379436	1.888452	1.498579
134	1	0	7.439559	2.018413	1.741006
135	1	0	5.996813	2.847563	1.137450
136	1	0	5.849319	1.639434	2.419722
137	6	0	6.899165	1.261511	-0.858593
138	1	0	6.434703	2.180203	-1.226519
139	1	0	7.965542	1.450728	-0.702934
140	1	0	6.792741	0.499029	-1.636589
141	6	0	6.254047	-0.908937	2.315670
142	1	0	6.300716	-1.987160	2.486634
143	1	0	6.964642	-0.421885	2.990826
144	1	0	5.246147	-0.568922	2.575569
145	6	0	7.995677	-1.034680	0.531724
146	1	0	8.716616	-0.393532	1.050594
147	1	0	8.167755	-2.064423	0.855017
148	1	0	8.193508	-0.982717	-0.540242

TS7u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-1.984075	0.519273	-1.758102
2	8	0	-2.178173	1.881445	-1.965757
3	8	0	-3.188260	-0.165977	-1.759105
4	6	0	-3.596554	2.150753	-2.089713
5	6	0	-4.226689	0.712020	-2.234827
6	6	0	-4.498783	0.307385	-3.679306
7	1	0	-4.809393	-0.740849	-3.706370
8	1	0	-5.290010	0.911228	-4.134672
9	1	0	-3.599426	0.401045	-4.296832
10	6	0	-5.460893	0.479246	-1.384294
11	1	0	-6.282091	1.139473	-1.683682
12	1	0	-5.799347	-0.555150	-1.501493
13	1	0	-5.234849	0.642581	-0.329501
14	6	0	-3.779704	3.047219	-3.304204
15	1	0	-4.838364	3.274619	-3.469925
16	1	0	-3.256235	3.993460	-3.136353
17	1	0	-3.378886	2.599551	-4.217087
18	6	0	-4.047759	2.893964	-0.843574
19	1	0	-3.494741	3.833166	-0.760711
20	1	0	-5.116449	3.128831	-0.892446
21	1	0	-3.844470	2.313888	0.055847
22	5	0	-1.355702	-1.960144	-0.488056
23	8	0	-2.213101	-2.324476	0.532527
24	8	0	-1.355284	-2.913173	-1.500218
25	6	0	-2.412063	-3.862662	-1.241119
26	6	0	-2.654960	-3.688528	0.291745
27	6	0	-1.929106	-5.240780	-1.650289
28	1	0	-2.670965	-6.005974	-1.396457
29	1	0	-1.772578	-5.273804	-2.732015
30	1	0	-0.985930	-5.498219	-1.164206
31	6	0	-3.604860	-3.443811	-2.090248
32	1	0	-3.299563	-3.410957	-3.140789
33	1	0	-4.436079	-4.150413	-1.998662
34	1	0	-3.945667	-2.444441	-1.810936
35	6	0	-4.110352	-3.813432	0.699860

36	1	0	-4.503297	-4.798385	0.424007
37	1	0	-4.209634	-3.713609	1.785524
38	1	0	-4.729993	-3.049170	0.224017
39	6	0	-1.797684	-4.608119	1.148141
40	1	0	-1.889082	-4.318393	2.198826
41	1	0	-2.115324	-5.651340	1.051816
42	1	0	-0.740667	-4.539538	0.879777
43	5	0	0.989870	-1.110770	0.867926
44	5	0	1.481779	-2.840300	0.769126
45	5	0	3.216859	-3.016448	1.042827
46	5	0	2.083092	-3.408052	2.327623
47	1	0	0.983995	-3.484484	-0.091851
48	5	0	3.888012	-1.413417	1.357597
49	1	0	2.767704	-1.437682	-0.705939
50	5	0	3.142654	-0.816277	2.838191
51	1	0	2.671799	0.574573	0.926721
52	5	0	2.031958	-2.042650	3.439128
53	1	0	-0.357160	-2.532378	2.549604
54	5	0	3.573572	-2.517492	2.696886
55	1	0	3.846052	-3.742608	0.352454
56	1	0	1.910810	-4.531460	2.668694
57	1	0	3.717090	0.028064	3.436920
58	1	0	1.828966	-2.160722	4.601829
59	1	0	4.479831	-2.981584	3.303273
60	77	0	-0.234931	-0.257294	-0.707137
61	6	0	0.700588	2.072795	-2.053580
62	6	0	-0.720330	-0.266450	-2.910274
63	6	0	0.504806	-1.011509	-2.462023
64	6	0	1.780617	1.448171	-1.540852
65	6	0	0.331616	2.021920	-3.507194
66	1	0	0.109365	2.710398	-1.405158
67	6	0	-0.536438	0.826045	-3.954399
68	1	0	-1.477086	-0.993565	-3.216707
69	6	0	1.890581	-0.643466	-2.992325
70	1	0	0.364730	-2.090291	-2.502998
71	6	0	2.651882	0.539119	-2.347348
72	1	0	2.049977	1.665472	-0.513259
73	1	0	-0.188912	2.950749	-3.760705
74	1	0	1.263401	2.021000	-4.088883
75	1	0	-1.519409	1.192282	-4.265506
76	1	0	-0.094600	0.361769	-4.847623

77	1	0	2.525218	-1.535231	-2.926458
78	1	0	1.784964	-0.461546	-4.072410
79	1	0	3.150844	1.116060	-3.140408
80	1	0	3.469508	0.162983	-1.722732
81	5	0	-0.806710	1.848818	1.009746
82	5	0	-1.831183	0.558758	1.568000
83	8	0	0.537258	2.106917	1.138748
84	8	0	-1.563186	2.998835	1.092788
85	8	0	-3.161215	0.456502	1.250788
86	6	0	-0.690284	4.136834	1.309604
87	6	0	0.692565	3.464963	1.639939
88	8	0	-1.564945	0.264531	2.879774
89	6	0	-3.894379	0.359005	2.505834
90	6	0	-2.807719	-0.127064	3.526461
91	6	0	1.883997	4.094663	0.945611
92	1	0	2.025540	5.129034	1.275816
93	1	0	2.794820	3.539412	1.193668
94	1	0	1.770257	4.090398	-0.141686
95	6	0	0.959497	3.313488	3.130520
96	1	0	1.866968	2.720391	3.274230
97	1	0	1.096798	4.282076	3.620572
98	1	0	0.142024	2.779024	3.624356
99	6	0	-1.279205	4.949858	2.449580
100	1	0	-0.647072	5.812752	2.684221
101	1	0	-2.265613	5.322557	2.159837
102	1	0	-1.397882	4.353425	3.356225
103	6	0	-0.706125	4.976032	0.039549
104	1	0	-1.726418	5.319433	-0.150453
105	1	0	-0.065670	5.857761	0.139146
106	1	0	-0.380739	4.414468	-0.838729
107	1	0	0.874219	0.290098	3.020317
108	6	0	-2.764798	-1.633914	3.714259
109	1	0	-1.890104	-1.895574	4.315621
110	1	0	-3.660397	-1.992238	4.232897
111	1	0	-2.673789	-2.139268	2.751234
112	6	0	-2.853605	0.566397	4.875457
113	1	0	-2.036226	0.200945	5.502013
114	1	0	-2.750170	1.650058	4.782030
115	1	0	-3.795944	0.352787	5.391330
116	6	0	-5.049974	-0.602209	2.327953
117	1	0	-4.705087	-1.556407	1.930659

118	1	0	-5.554722	-0.778823	3.284050
119	1	0	-5.787706	-0.189149	1.634556
120	6	0	-4.411159	1.762849	2.795216
121	1	0	-3.591407	2.485878	2.845581
122	1	0	-5.078424	2.074936	1.986159
123	1	0	-4.975065	1.799757	3.732226
124	6	0	2.550733	-1.652349	0.332572
125	5	0	1.405502	-0.649006	2.553858
126	5	0	0.744656	-2.241614	2.239816
127	6	0	2.510320	-0.414994	1.339724
128	5	0	5.232050	-0.769226	0.595486
129	8	0	6.122030	0.119771	1.145734
130	8	0	5.458540	-0.980755	-0.750352
131	6	0	6.836263	0.739213	0.042836
132	6	0	6.723208	-0.338188	-1.076295
133	6	0	6.639196	0.208237	-2.486444
134	1	0	7.554926	0.749150	-2.748101
135	1	0	6.519911	-0.613045	-3.198209
136	1	0	5.792234	0.886350	-2.609933
137	6	0	7.797532	-1.410731	-0.978866
138	1	0	7.538543	-2.242200	-1.638577
139	1	0	8.777877	-1.027209	-1.277575
140	1	0	7.875574	-1.800497	0.039841
141	6	0	6.081017	2.019774	-0.290365
142	1	0	6.006086	2.636530	0.608836
143	1	0	6.586956	2.601883	-1.066639
144	1	0	5.063744	1.801636	-0.636280
145	6	0	8.249442	1.051677	0.487927
146	1	0	8.839670	1.450252	-0.344278
147	1	0	8.234936	1.803928	1.280652
148	1	0	8.753377	0.165022	0.876216

TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	2.665643	1.064153	0.241355
2	8	0	3.806978	1.719019	-0.202809
3	8	0	2.483107	1.264954	1.595560
4	6	0	4.590413	2.061145	0.968419
5	6	0	3.498820	2.177395	2.075255
6	6	0	2.897958	3.572695	2.158348
7	1	0	2.003538	3.553459	2.787435
8	1	0	3.609717	4.281055	2.595232
9	1	0	2.596972	3.927524	1.171277
10	6	0	3.928590	1.702349	3.450749
11	1	0	4.786806	2.275512	3.818847
12	1	0	3.107434	1.836393	4.162338
13	1	0	4.189319	0.641297	3.437245
14	6	0	5.357921	3.333835	0.676640
15	1	0	5.914197	3.667110	1.559549
16	1	0	6.079798	3.156481	-0.126008
17	1	0	4.694730	4.142017	0.360953
18	6	0	5.541601	0.898292	1.214352
19	1	0	6.175270	0.748319	0.334749
20	1	0	6.194844	1.078602	2.074098
21	1	0	4.970084	-0.018147	1.390864
22	5	0	0.252627	1.669763	-0.534969
23	8	0	-0.861354	1.922987	-1.328856
24	8	0	0.681202	2.834097	0.083139
25	6	0	-0.064014	3.948354	-0.470104
26	6	0	-1.338452	3.259880	-1.055854
27	6	0	0.813090	4.582864	-1.541465
28	1	0	0.374558	5.507674	-1.929417
29	1	0	1.792398	4.819358	-1.113138
30	1	0	0.969735	3.903759	-2.384333
31	6	0	-0.332608	4.950593	0.635875
32	1	0	0.607163	5.385300	0.987954
33	1	0	-0.964136	5.768315	0.271681
34	1	0	-0.828957	4.486861	1.490788
35	6	0	-2.482635	3.167782	-0.056196

36	1	0	-2.923067	4.151861	0.135815
37	1	0	-3.272433	2.518893	-0.449386
38	1	0	-2.142381	2.743853	0.889510
39	6	0	-1.847488	3.842457	-2.361644
40	1	0	-2.706316	3.259744	-2.708209
41	1	0	-2.173311	4.880042	-2.230232
42	1	0	-1.089162	3.814402	-3.146901
43	5	0	-1.008494	-1.290120	-0.970619
44	5	0	-1.760177	-0.833101	-2.530563
45	5	0	-1.060952	-2.440480	-2.343166
46	5	0	-1.468289	-3.008243	-0.734907
47	6	0	-2.407783	-1.786721	-0.104133
48	6	0	-2.563201	-0.563840	-1.108028
49	5	0	-2.577468	-2.229184	-3.237810
50	5	0	-3.512522	-0.974868	-2.426134
51	1	0	-1.361744	0.099804	-3.123737
52	5	0	-2.403901	-3.580564	-2.121189
53	1	0	-0.071424	-2.774030	-2.899275
54	5	0	-3.229747	-3.151166	-0.626746
55	1	0	-0.806248	-3.637842	0.010780
56	5	0	-3.927258	-1.543146	-0.814835
57	1	0	-2.599027	0.417338	-0.644898
58	5	0	-3.922296	-2.670860	-2.172586
59	1	0	-2.623647	-2.359976	-4.415651
60	1	0	-4.188009	-0.126921	-2.904732
61	1	0	-2.328033	-4.708020	-2.477948
62	1	0	-3.694374	-3.863830	0.195213
63	1	0	-4.947840	-3.118693	-2.560429
64	77	0	1.401447	-0.089820	-0.963788
65	6	0	3.409167	-1.198050	-1.763947
66	6	0	2.321771	1.315522	-2.627371
67	6	0	1.185761	0.734509	-3.181569
68	6	0	2.371429	-1.769093	-2.471371
69	6	0	4.382007	-0.214138	-2.341912
70	1	0	3.731228	-1.684489	-0.851136
71	6	0	3.730250	0.973582	-3.061847
72	1	0	2.211935	2.282258	-2.143626
73	6	0	1.189785	-0.350556	-4.219994
74	1	0	0.256545	1.290992	-3.097783
75	6	0	2.166598	-1.492081	-3.937768
76	1	0	1.885008	-2.637693	-2.039703

77	1	0	5.013331	0.160753	-1.535149
78	1	0	5.047991	-0.750636	-3.035764
79	1	0	4.358022	1.856651	-2.913015
80	1	0	3.706575	0.790110	-4.144222
81	1	0	0.178676	-0.759477	-4.292835
82	1	0	1.397613	0.093321	-5.206597
83	1	0	3.142786	-1.283778	-4.394148
84	1	0	1.798109	-2.403704	-4.419469
85	5	0	1.963962	-1.550969	0.547486
86	5	0	-0.096778	-0.470631	0.501062
87	8	0	1.767891	-2.863846	0.152900
88	8	0	2.927954	-1.472958	1.548474
89	8	0	-0.940582	0.582242	1.015526
90	6	0	3.453680	-2.802099	1.804094
91	6	0	2.423165	-3.746660	1.088180
92	8	0	0.036902	-1.395368	1.599672
93	6	0	-1.113420	0.517218	2.442280
94	6	0	-0.434025	-0.850958	2.846650
95	6	0	3.047293	-4.876851	0.289271
96	1	0	3.605035	-5.560289	0.938611
97	1	0	2.259354	-5.450467	-0.206202
98	1	0	3.723991	-4.502096	-0.482627
99	6	0	1.361417	-4.304155	2.024616
100	1	0	0.596410	-4.816722	1.436118
101	1	0	1.788492	-5.019576	2.734847
102	1	0	0.869344	-3.502022	2.576841
103	6	0	3.565330	-3.006148	3.305806
104	1	0	4.010165	-3.982526	3.526782
105	1	0	4.215551	-2.236880	3.732964
106	1	0	2.603097	-2.952356	3.813011
107	6	0	4.865594	-2.876200	1.228364
108	1	0	5.494995	-2.121682	1.708203
109	1	0	5.313913	-3.855601	1.420852
110	1	0	4.902348	-2.705114	0.150429
111	1	0	-2.351004	-1.530488	0.945956
112	6	0	-1.387084	-1.873944	3.459067
113	1	0	-0.849719	-2.809278	3.636677
114	1	0	-1.773865	-1.524144	4.421748
115	1	0	-2.242839	-2.111167	2.821878
116	6	0	0.754891	-0.683383	3.782351
117	1	0	1.150671	-1.668320	4.040333

118	1	0	1.554942	-0.112243	3.309881
119	1	0	0.454988	-0.196324	4.715820
120	6	0	-2.607090	0.578096	2.736386
121	1	0	-3.178457	-0.217092	2.252442
122	1	0	-2.794698	0.522252	3.814312
123	1	0	-3.020944	1.522225	2.370318
124	6	0	-0.446716	1.743658	3.051970
125	1	0	0.604076	1.797052	2.767129
126	1	0	-0.942848	2.646372	2.681798
127	1	0	-0.533973	1.742959	4.143338
128	5	0	-5.199260	-0.796052	-0.023649
129	8	0	-5.064558	0.463372	0.523996
130	8	0	-6.484117	-1.268456	0.041489
131	6	0	-6.324850	0.780914	1.178441
132	6	0	-7.326371	-0.145217	0.423703
133	6	0	-6.175448	0.412217	2.647301
134	1	0	-5.342433	0.969258	3.083079
135	1	0	-7.079629	0.653374	3.214270
136	1	0	-5.969788	-0.656058	2.767357
137	6	0	-6.576757	2.266620	1.024684
138	1	0	-7.549831	2.544215	1.443710
139	1	0	-5.806408	2.830379	1.559529
140	1	0	-6.550040	2.573687	-0.022686
141	6	0	-8.475136	-0.664286	1.262593
142	1	0	-9.089138	0.163313	1.633975
143	1	0	-9.114829	-1.312114	0.658259
144	1	0	-8.121864	-1.243990	2.117212
145	6	0	-7.839114	0.470302	-0.870194
146	1	0	-8.356056	-0.295254	-1.453168
147	1	0	-8.539025	1.289385	-0.678273
148	1	0	-7.014570	0.855278	-1.477992

TS8u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-2.359085	1.125961	-0.739536
2	8	0	-2.922365	1.752205	-1.842316
3	8	0	-3.108664	1.362691	0.394741
4	6	0	-3.884256	2.717836	-1.350026
5	6	0	-4.294580	2.107821	0.024807
6	6	0	-5.455548	1.132219	-0.089584
7	1	0	-5.558684	0.572647	0.844582
8	1	0	-6.396251	1.659350	-0.280739
9	1	0	-5.278559	0.408030	-0.886095
10	6	0	-4.563447	3.127756	1.115945
11	1	0	-5.367469	3.813097	0.825280
12	1	0	-4.875281	2.620039	2.034252
13	1	0	-3.666385	3.710011	1.342384
14	6	0	-5.004041	2.840084	-2.362981
15	1	0	-5.789850	3.511183	-1.999333
16	1	0	-4.615819	3.255366	-3.297682
17	1	0	-5.453869	1.870416	-2.586131
18	6	0	-3.142016	4.039642	-1.203760
19	1	0	-2.727981	4.335604	-2.172777
20	1	0	-3.801151	4.842797	-0.858783
21	1	0	-2.316477	3.928570	-0.494108
22	5	0	-2.143757	-1.454833	-0.508863
23	8	0	-1.832998	-2.793717	-0.634528
24	8	0	-3.505166	-1.243628	-0.647998
25	6	0	-4.120386	-2.495551	-1.048640
26	6	0	-3.058690	-3.558766	-0.616045
27	6	0	-4.319551	-2.429794	-2.556563
28	1	0	-4.878176	-3.293834	-2.929845
29	1	0	-4.879652	-1.523238	-2.807663
30	1	0	-3.362382	-2.391992	-3.084986
31	6	0	-5.461596	-2.617869	-0.351189
32	1	0	-6.153501	-1.856577	-0.722824
33	1	0	-5.909895	-3.598993	-0.542132
34	1	0	-5.365260	-2.485710	0.728675
35	6	0	-3.268728	-4.076814	0.797564

36	1	0	-4.146301	-4.728405	0.858614
37	1	0	-2.388488	-4.647485	1.104851
38	1	0	-3.390020	-3.251116	1.499179
39	6	0	-2.891358	-4.726306	-1.570977
40	1	0	-2.105142	-5.389686	-1.199858
41	1	0	-3.816679	-5.307863	-1.646671
42	1	0	-2.605584	-4.399059	-2.573098
43	5	0	0.831101	-1.639907	0.613441
44	5	0	1.281794	-3.108665	-0.316429
45	5	0	3.045986	-3.269463	-0.373933
46	5	0	2.108011	-4.279958	0.717242
47	1	0	0.684272	-3.370996	-1.296633
48	5	0	3.759461	-1.945479	0.549960
49	1	0	2.373153	-1.094837	-1.116578
50	5	0	3.232952	-2.134445	2.213378
51	1	0	2.472223	-0.048748	1.195121
52	5	0	2.221185	-3.576779	2.321395
53	1	0	-0.286765	-3.756892	1.624637
54	5	0	3.637537	-3.557497	1.256187
55	1	0	3.552476	-3.557697	-1.404965
56	1	0	1.991235	-5.442626	0.519456
57	1	0	3.870440	-1.618606	3.066897
58	1	0	4.621327	-4.183924	1.462412
59	77	0	-0.557872	-0.006178	-0.801851
60	6	0	0.376065	1.781468	-2.014116
61	6	0	-1.268724	-0.305112	-2.959762
62	6	0	-0.313252	-1.304602	-2.702603
63	6	0	1.378577	0.814953	-1.916990
64	6	0	-0.383845	2.078082	-3.273785
65	1	0	0.410798	2.605951	-1.310859
66	6	0	-1.013707	0.842003	-3.916611
67	1	0	-2.315996	-0.570521	-2.844073
68	6	0	1.063529	-1.305857	-3.307340
69	1	0	-0.683445	-2.283640	-2.413338
70	6	0	1.813189	0.016953	-3.130904
71	1	0	2.101997	0.949388	-1.115337
72	1	0	-1.166946	2.800669	-3.039301
73	1	0	0.299080	2.575111	-3.981647
74	1	0	-1.963713	1.126882	-4.377270
75	1	0	-0.377449	0.467911	-4.730710
76	1	0	1.635665	-2.126019	-2.861500

77	1	0	0.991883	-1.563674	-4.375976
78	1	0	1.690247	0.646698	-4.021664
79	1	0	2.891557	-0.175659	-3.065464
80	5	0	-0.046868	1.577551	0.611629
81	5	0	-0.772995	-0.505253	1.287677
82	8	0	1.319142	1.691199	0.840091
83	8	0	-0.695796	2.759665	0.940251
84	8	0	-1.801873	-1.361701	1.699205
85	6	0	0.286740	3.747559	1.352251
86	6	0	1.590635	2.900318	1.579972
87	8	0	-0.423608	0.311761	2.389849
88	6	0	-2.202640	-1.119119	3.063250
89	6	0	-1.384391	0.164661	3.469446
90	6	0	2.859409	3.499390	0.999885
91	1	0	3.111435	4.450363	1.481610
92	1	0	3.688404	2.803532	1.159098
93	1	0	2.770433	3.666480	-0.077683
94	6	0	1.822784	2.504024	3.030648
95	1	0	2.648742	1.787297	3.080271
96	1	0	2.084030	3.368463	3.649238
97	1	0	0.941044	2.016582	3.447875
98	6	0	-0.226957	4.460236	2.591214
99	1	0	0.464627	5.255075	2.891081
100	1	0	-1.195038	4.921054	2.373279
101	1	0	-0.356899	3.788637	3.439401
102	6	0	0.410994	4.781232	0.236967
103	1	0	-0.560575	5.253371	0.067752
104	1	0	1.123232	5.566469	0.508094
105	1	0	0.741121	4.350055	-0.710827
106	1	0	1.037839	-1.411588	3.182429
107	6	0	-0.635396	0.027281	4.787163
108	1	0	-0.055421	0.933635	4.982594
109	1	0	-1.349031	-0.086202	5.610416
110	1	0	0.047394	-0.822071	4.808883
111	6	0	-2.214594	1.438868	3.516725
112	1	0	-1.567515	2.276232	3.787199
113	1	0	-2.656924	1.658752	2.546327
114	1	0	-2.999778	1.370852	4.276181
115	6	0	-1.851008	-2.363002	3.867825
116	1	0	-0.783471	-2.588972	3.823901
117	1	0	-2.142560	-2.253072	4.917218

118	1	0	-2.385078	-3.223765	3.456887
119	6	0	-3.708986	-0.906398	3.066011
120	1	0	-3.990097	-0.113896	2.368506
121	1	0	-4.215521	-1.826965	2.760507
122	1	0	-4.069075	-0.651432	4.068256
123	6	0	2.387223	-1.132393	1.159307
124	6	0	2.290324	-1.777402	-0.287712
125	5	0	1.479197	-1.983104	2.257655
126	5	0	0.764263	-3.295509	1.339340
127	1	0	2.176474	-4.211455	3.322099
128	5	0	5.001858	-0.943755	0.044195
129	8	0	4.815276	0.424525	-0.041361
130	8	0	6.249047	-1.336195	-0.362825
131	6	0	5.954427	0.957595	-0.775690
132	6	0	7.043467	-0.129899	-0.529310
133	6	0	7.802012	0.076896	0.773695
134	1	0	8.387764	-0.818210	0.994931
135	1	0	8.485665	0.929170	0.712626
136	1	0	7.115130	0.244128	1.608592
137	6	0	8.004206	-0.336078	-1.681767
138	1	0	8.565472	0.581931	-1.887292
139	1	0	8.723077	-1.120630	-1.433105
140	1	0	7.483590	-0.635055	-2.593426
141	6	0	5.523001	1.050276	-2.231912
142	1	0	4.621275	1.666948	-2.299341
143	1	0	6.297148	1.504853	-2.857633
144	1	0	5.291722	0.060327	-2.638279
145	6	0	6.299270	2.330292	-0.235624
146	1	0	7.218676	2.705598	-0.697934
147	1	0	5.498518	3.039465	-0.462815
148	1	0	6.441079	2.314174	0.846989
