Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Elecrtonic Supporting Information for

Theoretical study on mechanism and enantioselectivity of NHC-catalyzed intramolecular S_N2' nucleophilic substitution: what are roles of NHC and DBU

Huimin Zhang, Hao Xu, Huining Bai, Donghui Wei, Yanyan Zhu, and Wenjing Zhang*
College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou, Henan Province 450001, P. R. China

Content

* Corresponding author: zhangwj@zzu.edu.cn (W.-J. Zhang)

Part 1: The absolute energies of all structures involved in this study.

Table S1. Thermal correction to Gibbs free energies (G_{Thermo}) calculated at Level A, Born-Oppenheimer energies calculated at Level A (E_A) and Level B (E_B) of all structures involved in this study (Unit: a.u.)

	G_{Thermo}	E_A	E_B
R	0.16897	-8329.40606	-8336.77183
NHC	0.22399	-1429.98877	-1430.48420
DBU	0.22290	-461.89648	-462.03444
DBU-H$^+$	0.23826	-462.37024	-462.50283
***Si*-TS1**	0.41710	-9759.40975	-9767.25540
***Re*-TS1**	0.41747	-9759.40919	-9767.25232
***Si*-Int1**	0.41711	-9759.41171	-9767.25923
***Re*-Int1**	0.41863	-9759.41774	-9767.26363
***Re*-TS6'**	0.41131	-9759.37542	-9767.21406
***Si*-TS6'**	0.41289	-9759.37470	-9767.22166
***Re*-Int6'**	0.41500	-9759.43256	-9767.27921
***Si*-Int6'**	0.41713	-9759.44929	-9767.29437
TS2	0.41328	-9759.34617	-9767.19593
Int2	0.41861	-9759.43316	-9767.27965
TS3	0.65534	-10221.28678	-10229.26849
Int3	0.66308	-10221.33033	-10229.31225
Int4	0.67244	-10221.82644	-10229.79688
TS4	0.67340	-10221.82814	-10229.79714
Int5	0.67237	-10221.82644	-10229.79645
TS5	0.67055	-10221.78553	-10229.75830
TS6*R*	0.41787	-9759.38898	-9767.23802
TS6*S*	0.41931	-9759.38903	-9767.23596
Int6*R*	0.42355	-9759.46727	-9767.31729
Int6*S*	0.42393	-9759.44207	-9767.29251
TS7*R*	0.41930	-9759.44375	-9767.29096
P*R*	0.41516	-9759.45647	-9767.30442
HBr	0.16239	-5757.04604	-5762.02175

Part 2: The scanning curve to the N9–H5 bond in the DBPT pathway.

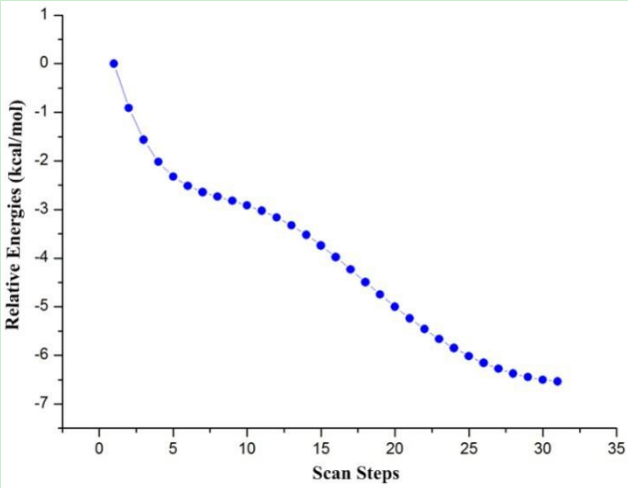

Fig. S1 The flexible scanning curve to the bond of N9–H5. We start with the optimized structure of **Int3** and scan the N9–H5 bond by taking 30 steps of size 0.02 angstroms.

Part 2: List of Cartesian coordinates of all structures involved in this work

R

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.619218	1.035618	-0.283553
2	6	0	-0.588281	0.088688	-0.373097
3	6	0	-0.930842	-1.270826	-0.302396
4	6	0	-2.251028	-1.661470	-0.061422
5	6	0	-3.239018	-0.703137	0.061197
6	6	0	-2.934347	0.649349	-0.070384
7	1	0	-3.712269	1.399954	0.001159
8	35	0	-5.027170	-1.217984	0.377301
9	35	0	-1.232808	2.868674	-0.466685
10	8	0	0.681997	0.529240	-0.553201
11	6	0	1.716193	0.006634	0.289183
12	1	0	1.258313	-0.568399	1.107407
13	1	0	2.344111	-0.667913	-0.301999
14	6	0	3.798406	0.843846	1.306839
15	1	0	4.415011	1.653516	1.687149
16	6	0	4.400001	-0.519867	1.332703
17	1	0	5.242023	-0.587654	2.016976
18	1	0	3.686586	-1.310349	1.561886
19	35	0	5.142352	-1.029029	-0.430385
20	6	0	2.573828	1.121802	0.846194
21	6	0	2.000254	2.505158	0.869472
22	1	0	1.769030	2.845608	-0.143372
23	1	0	1.054229	2.527484	1.420613
24	1	0	2.700012	3.200946	1.335346
25	6	0	0.050007	-2.354871	-0.597522
26	1	0	0.994825	-2.042956	-1.076246
27	8	0	-0.184191	-3.520806	-0.386191
28	1	0	-2.473142	-2.721365	-0.005138

DBU

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

1	6	0	-0.919461	-1.553239	-0.108294
2	6	0	0.365004	-0.740366	-0.174017
3	6	0	-2.003018	-1.009966	0.824363
4	6	0	-0.847780	1.509421	-0.042523
5	6	0	-2.901666	0.008547	0.119975
6	6	0	-2.088849	0.972214	-0.746603
7	1	0	-1.322929	-1.673740	-1.121765
8	1	0	-1.108503	1.811677	0.986166
9	1	0	-1.525935	-0.549610	1.697955
10	1	0	-3.476210	0.575016	0.861688
11	1	0	-0.586760	-2.544156	0.202331
12	1	0	-2.611177	-1.835177	1.206386
13	1	0	-0.529251	2.425833	-0.556942
14	1	0	-3.629756	-0.513933	-0.510903
15	1	0	-2.712887	1.825137	-1.031357
16	1	0	-1.778666	0.492385	-1.680977
17	6	0	1.546609	1.382771	0.259097
18	1	0	1.791356	2.020505	-0.603761
19	1	0	1.349943	2.054662	1.106261
20	6	0	2.683895	-0.687578	-0.433671
21	1	0	3.513088	-1.379991	-0.263124
22	1	0	2.810352	-0.279147	-1.448576
23	6	0	2.708142	0.456238	0.574240
24	1	0	3.646538	1.016996	0.545332
25	1	0	2.593491	0.039284	1.580186
26	7	0	1.437520	-1.425219	-0.343545
27	7	0	0.322487	0.637507	-0.028498

DBU-H$^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.919461	-1.553239	-0.108294
2	6	0	0.365004	-0.740366	-0.174017
3	6	0	-2.003018	-1.009966	0.824363
4	6	0	-0.847780	1.509421	-0.042523
5	6	0	-2.901666	0.008547	0.119975
6	6	0	-2.088849	0.972214	-0.746603

7	1	0	-1.322929	-1.673740	-1.121765
8	1	0	-1.108503	1.811677	0.986166
9	1	0	-1.525935	-0.549610	1.697955
10	1	0	-3.476210	0.575016	0.861688
11	1	0	-0.586760	-2.544156	0.202331
12	1	0	-2.611177	-1.835177	1.206386
13	1	0	-0.529251	2.425833	-0.556942
14	1	0	-3.629756	-0.513933	-0.510903
15	1	0	-2.712887	1.825137	-1.031357
16	1	0	-1.778666	0.492385	-1.680977
17	6	0	1.546609	1.382771	0.259097
18	1	0	1.791356	2.020505	-0.603761
19	1	0	1.349943	2.054662	1.106261
20	6	0	2.683895	-0.687578	-0.433671
21	1	0	3.513088	-1.379991	-0.263124
22	1	0	2.810352	-0.279147	-1.448576
23	6	0	2.708142	0.456238	0.574240
24	1	0	3.646538	1.016996	0.545332
25	1	0	2.593491	0.039284	1.580186
26	7	0	1.437520	-1.425219	-0.343545
27	7	0	0.322487	0.637507	-0.028498
28	1	0	1.415045	-2.422721	-0.410517

NHC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.272594	2.568990	-1.169682
2	6	0	-3.957400	2.987022	-0.974534
3	6	0	-3.017911	2.137983	-0.385934
4	6	0	-3.433458	0.869674	-0.012905
5	6	0	-4.754036	0.434604	-0.212729
6	6	0	-5.681657	1.288144	-0.791558
7	1	0	-5.986689	3.244238	-1.630126
8	1	0	-3.659403	3.982974	-1.285486
9	1	0	-1.986747	2.437700	-0.231100
10	1	0	-6.704224	0.964074	-0.960972
11	6	0	2.707364	0.787986	0.947180
12	6	0	4.040089	1.145250	0.789009

13	6	0	4.801686	0.553003	-0.209297
14	6	0	4.228690	-0.388359	-1.054466
15	6	0	2.890818	-0.725799	-0.904326
16	6	0	2.116515	-0.145785	0.098473
17	9	0	2.353714	-1.603231	-1.741715
18	9	0	4.956680	-0.947165	-2.015870
19	9	0	6.077796	0.886226	-0.356454
20	9	0	4.594108	2.037389	1.603690
21	9	0	2.012574	1.342350	1.930154
22	6	0	-3.470845	-1.466475	0.177859
23	1	0	-3.204068	-1.605018	-0.884253
24	8	0	-3.108535	-2.610673	0.912723
25	6	0	-1.780557	-2.990194	0.586621
26	1	0	-1.434385	-3.675238	1.362087
27	1	0	-1.764251	-3.519161	-0.377115
28	6	0	-0.845532	-1.805041	0.490036
29	7	0	-1.295400	-0.498676	0.460890
30	7	0	0.440393	-1.841995	0.356544
31	7	0	0.762282	-0.499471	0.251800
32	6	0	-0.266770	0.385407	0.321446
33	6	0	-2.704413	-0.244627	0.683504
34	1	0	-2.868693	-0.169846	1.768351
35	6	0	-4.924772	-1.005628	0.248839
36	1	0	-5.599641	-1.592174	-0.377180
37	1	0	-5.279690	-1.058220	1.285914

***Si*-TS1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.600279	1.094605	-2.101721
2	6	0	3.319193	1.527713	-2.445536
3	6	0	2.248622	0.637363	-2.442719
4	6	0	2.484001	-0.679248	-2.068540
5	6	0	3.772808	-1.128937	-1.752343
6	6	0	4.837227	-0.234804	-1.758943
7	1	0	5.419098	1.806237	-2.089774
8	1	0	3.145291	2.571163	-2.682630
9	1	0	1.247270	0.982880	-2.686076

10	1	0	5.837985	-0.568536	-1.501734
11	6	0	-3.909978	-0.918157	-0.847961
12	6	0	-5.095952	-0.506191	-0.256188
13	6	0	-5.289875	-0.723799	1.099717
14	6	0	-4.306528	-1.343094	1.868159
15	6	0	-3.122897	-1.734281	1.271201
16	6	0	-2.922466	-1.512575	-0.084456
17	9	0	-2.154374	-2.279801	1.996340
18	9	0	-4.509653	-1.537529	3.167657
19	9	0	-6.424745	-0.344288	1.674172
20	9	0	-6.036534	0.086926	-0.980093
21	9	0	-3.711778	-0.709158	-2.144532
22	6	0	2.331546	-2.941680	-1.301955
23	1	0	2.088099	-2.774968	-0.242191
24	8	0	1.938359	-4.238264	-1.695591
25	6	0	0.533655	-4.399569	-1.881659
26	1	0	0.347246	-4.600014	-2.944230
27	1	0	0.185889	-5.261092	-1.306034
28	6	0	-0.278529	-3.205718	-1.459909
29	7	0	0.208721	-1.921548	-1.587494
30	7	0	-1.452644	-3.203587	-0.911936
31	7	0	-1.684629	-1.877403	-0.675136
32	6	0	-0.676382	-1.062385	-1.033883
33	6	0	1.579165	-1.874819	-2.116287
34	1	0	1.500933	-2.221122	-3.157219
35	6	0	3.808988	-2.627124	-1.513435
36	1	0	4.416700	-2.916585	-0.652730
37	1	0	4.181579	-3.157173	-2.397989
38	6	0	1.656061	1.557813	0.331916
39	6	0	0.761549	0.485380	0.413792
40	6	0	1.108781	-0.636335	1.165933
41	6	0	2.375762	-0.742638	1.715947
42	6	0	3.297700	0.291539	1.614743
43	6	0	2.911572	1.442430	0.943837
44	1	0	0.384981	-1.437339	1.297060
45	1	0	4.290881	0.204381	2.037078
46	35	0	2.894821	-2.363553	2.545749
47	35	0	4.142788	2.862701	0.782791
48	8	0	1.367728	2.663778	-0.416165
49	6	0	0.879164	3.800313	0.331780
50	1	0	1.578645	4.019273	1.146190

51	1	0	0.904680	4.621757	-0.387048
52	6	0	-1.514698	3.700115	-0.047916
53	1	0	-1.297246	4.120146	-1.028860
54	6	0	-2.918262	3.247485	0.164569
55	1	0	-3.636907	4.061725	0.263281
56	1	0	-2.997262	2.525189	0.974321
57	35	0	-3.495053	2.273268	-1.441231
58	6	0	-0.520255	3.541273	0.830877
59	6	0	-0.698806	2.988124	2.223197
60	1	0	-1.473163	3.533076	2.770995
61	1	0	-0.993021	1.933547	2.165777
62	1	0	0.229802	3.064616	2.794998
63	6	0	-0.630706	0.526994	-0.243304
64	8	0	-1.606836	0.561321	0.582654
65	1	0	-0.635766	1.217236	-1.109627

***Re*-TS1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.015817	-0.028057	-1.392641
2	6	0	-3.922709	-0.428852	-2.159791
3	6	0	-2.777911	0.364008	-2.247251
4	6	0	-2.756153	1.556701	-1.534766
5	6	0	-3.865301	1.985985	-0.790100
6	6	0	-4.997865	1.186262	-0.707766
7	1	0	-5.883175	-0.676099	-1.317535
8	1	0	-3.936734	-1.392291	-2.657935
9	1	0	-1.902079	0.011613	-2.791155
10	1	0	-5.853378	1.502788	-0.118529
11	6	0	3.509840	0.493193	-1.554151
12	6	0	4.650497	-0.212626	-1.199813
13	6	0	5.257979	0.022627	0.026278
14	6	0	4.704626	0.930703	0.918184
15	6	0	3.526832	1.584412	0.586459
16	6	0	2.931190	1.385849	-0.656500
17	9	0	2.950349	2.375055	1.480962
18	9	0	5.264785	1.122004	2.105144
19	9	0	6.347283	-0.651710	0.360173

20	9	0	5.160391	-1.119078	-2.027898
21	9	0	2.940556	0.264705	-2.727417
22	6	0	-2.134540	3.489408	-0.280950
23	1	0	-1.701179	2.970305	0.589843
24	8	0	-1.650746	4.814669	-0.352799
25	6	0	-0.350176	4.948907	-0.919165
26	1	0	-0.443739	5.386541	-1.921779
27	1	0	0.241850	5.627739	-0.301569
28	6	0	0.382689	3.643571	-1.026682
29	7	0	-0.289876	2.490411	-1.387390
30	7	0	1.628274	3.400082	-0.769820
31	7	0	1.715792	2.042210	-0.964451
32	6	0	0.554889	1.445960	-1.305023
33	6	0	-1.744119	2.672125	-1.525361
34	1	0	-1.881231	3.295902	-2.420666
35	6	0	-3.651723	3.369092	-0.206269
36	1	0	-4.030365	3.480603	0.812025
37	1	0	-4.115035	4.139373	-0.834836
38	6	0	-1.640929	-1.635530	-0.358092
39	6	0	-0.626772	-0.671888	-0.272794
40	6	0	-0.572651	0.145731	0.860326
41	6	0	-1.586567	0.135872	1.799332
42	6	0	-2.651142	-0.749453	1.691561
43	6	0	-2.636686	-1.644317	0.636412
44	1	0	0.247230	0.847991	0.986962
45	1	0	-3.458944	-0.755682	2.412328
46	35	0	-1.564830	1.413865	3.196868
47	35	0	-4.031256	-2.904099	0.496027
48	8	0	-1.815032	-2.529998	-1.360201
49	6	0	-0.736809	-3.361778	-1.824175
50	1	0	-1.224947	-4.316817	-2.050947
51	1	0	-0.317979	-2.920826	-2.726959
52	6	0	1.583245	-3.190105	-1.037163
53	1	0	1.804539	-2.701270	-1.984235
54	6	0	2.684465	-3.298724	-0.044349
55	1	0	3.675708	-3.214684	-0.485390
56	1	0	2.622755	-4.183215	0.587424
57	35	0	2.582744	-1.789548	1.253465
58	6	0	0.324660	-3.564489	-0.778104
59	6	0	-0.115542	-4.141954	0.544129
60	1	0	0.268729	-3.538914	1.373712

61	1	0	-1.206697	-4.166382	0.613565
62	1	0	0.251801	-5.166927	0.669560
63	6	0	0.384554	-0.444031	-1.415738
64	8	0	0.126386	-0.812320	-2.584353
65	1	0	1.403016	-0.595481	-1.000934

***Si*-Int1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.725180	0.853585	-2.042373
2	6	0	3.483004	1.378481	-2.402109
3	6	0	2.349685	0.570694	-2.405799
4	6	0	2.482050	-0.756626	-2.018170
5	6	0	3.731237	-1.301759	-1.695535
6	6	0	4.859685	-0.488895	-1.696449
7	1	0	5.593918	1.503330	-2.023340
8	1	0	3.388668	2.431110	-2.644010
9	1	0	1.379695	0.991542	-2.656065
10	1	0	5.830723	-0.896682	-1.432332
11	6	0	-4.042202	-0.933838	-0.724873
12	6	0	-5.223014	-0.520294	-0.122056
13	6	0	-5.342870	-0.598033	1.256593
14	6	0	-4.288737	-1.071842	2.036880
15	6	0	-3.112075	-1.463271	1.428599
16	6	0	-2.985493	-1.373369	0.048811
17	9	0	-2.087668	-1.884982	2.156696
18	9	0	-4.424437	-1.133688	3.358282
19	9	0	-6.472094	-0.221958	1.845025
20	9	0	-6.230824	-0.070677	-0.859540
21	9	0	-3.915706	-0.869918	-2.046317
22	6	0	2.159374	-3.012349	-1.270395
23	1	0	1.921265	-2.844893	-0.209483
24	8	0	1.674402	-4.275120	-1.680939
25	6	0	0.289690	-4.299427	-2.022233
26	1	0	0.191462	-4.345547	-3.114775
27	1	0	-0.165054	-5.197068	-1.598600
28	6	0	-0.465143	-3.104738	-1.512598
29	7	0	0.109658	-1.850643	-1.545333

30	7	0	-1.628290	-3.072361	-0.942278
31	7	0	-1.771007	-1.764926	-0.582141
32	6	0	-0.713054	-0.999995	-0.896539
33	6	0	1.489142	-1.880325	-2.069944
34	1	0	1.379539	-2.201233	-3.115690
35	6	0	3.658266	-2.799276	-1.462089
36	1	0	4.230476	-3.130680	-0.592190
37	1	0	4.007325	-3.351563	-2.342387
38	6	0	1.704864	1.536902	0.311341
39	6	0	0.814750	0.462391	0.414185
40	6	0	1.169216	-0.642882	1.187043
41	6	0	2.439238	-0.738566	1.731335
42	6	0	3.354191	0.299682	1.616137
43	6	0	2.959316	1.438052	0.928257
44	1	0	0.452296	-1.447143	1.333824
45	1	0	4.350649	0.222824	2.032596
46	35	0	2.973435	-2.359117	2.553053
47	35	0	4.190844	2.852810	0.724389
48	8	0	1.430256	2.611232	-0.486184
49	6	0	0.931882	3.785437	0.193981
50	1	0	1.609838	4.035648	1.017534
51	1	0	0.989914	4.570928	-0.562474
52	6	0	-1.446240	3.653544	-0.263999
53	1	0	-1.191457	3.992166	-1.267405
54	6	0	-2.856706	3.215863	-0.064463
55	1	0	-3.579073	4.032786	-0.049752
56	1	0	-2.955827	2.549687	0.789362
57	35	0	-3.388177	2.119621	-1.608255
58	6	0	-0.485463	3.567594	0.661392
59	6	0	-0.711117	3.121030	2.083411
60	1	0	-1.559148	3.642937	2.535660
61	1	0	-0.926534	2.045476	2.090068
62	1	0	0.169789	3.319891	2.699635
63	6	0	-0.576697	0.466276	-0.257659
64	8	0	-1.560930	0.628667	0.591990
65	1	0	-0.539591	1.154512	-1.133805

***Re*-Int1**

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-5.127660	-0.034007	-1.290844
2	6	0	-4.057083	-0.495736	-2.056576
3	6	0	-2.890633	0.257154	-2.186105
4	6	0	-2.823362	1.469159	-1.510270
5	6	0	-3.913158	1.968776	-0.783064
6	6	0	-5.069421	1.208200	-0.660312
7	1	0	-6.013629	-0.651633	-1.181949
8	1	0	-4.106966	-1.475593	-2.519419
9	1	0	-2.017132	-0.118594	-2.719530
10	1	0	-5.911488	1.576591	-0.082075
11	6	0	3.569802	0.446294	-1.455202
12	6	0	4.737287	-0.190308	-1.061913
13	6	0	5.310788	0.109163	0.167123
14	6	0	4.706942	1.023797	1.019664
15	6	0	3.511342	1.618909	0.644697
16	6	0	2.946883	1.348433	-0.598031
17	9	0	2.890537	2.431993	1.487350
18	9	0	5.242549	1.282722	2.204606
19	9	0	6.421766	-0.505019	0.539207
20	9	0	5.295458	-1.108125	-1.846096
21	9	0	3.022221	0.150109	-2.622316
22	6	0	-2.141650	3.455837	-0.369145
23	1	0	-1.717751	2.984871	0.533301
24	8	0	-1.623233	4.763286	-0.524927
25	6	0	-0.373669	4.841051	-1.201569
26	1	0	-0.540608	5.144005	-2.243887
27	1	0	0.244161	5.599009	-0.716598
28	6	0	0.371292	3.538997	-1.187527
29	7	0	-0.311616	2.358543	-1.397974
30	7	0	1.624144	3.331903	-0.926877
31	7	0	1.722924	1.965794	-0.952191
32	6	0	0.552067	1.351429	-1.196012
33	6	0	-1.771869	2.546653	-1.556350
34	1	0	-1.875422	3.107674	-2.495536
35	6	0	-3.660702	3.375940	-0.278568
36	1	0	-4.027109	3.554849	0.734529
37	1	0	-4.111023	4.120047	-0.946715
38	6	0	-1.606955	-1.592191	-0.334765
39	6	0	-0.660803	-0.564529	-0.198889

40	6	0	-0.689409	0.222674	0.955985
41	6	0	-1.708612	0.111178	1.884215
42	6	0	-2.693087	-0.854672	1.740987
43	6	0	-2.600927	-1.708878	0.654449
44	1	0	0.069128	0.987122	1.113344
45	1	0	-3.506351	-0.947499	2.449238
46	35	0	-1.806301	1.363184	3.301526
47	35	0	-3.914726	-3.045490	0.448580
48	8	0	-1.748576	-2.436631	-1.383487
49	6	0	-0.628208	-3.101325	-1.991115
50	1	0	-1.063426	-4.031747	-2.373995
51	1	0	-0.246643	-2.475937	-2.797500
52	6	0	1.690006	-2.953490	-1.216712
53	1	0	1.870458	-2.338257	-2.097372
54	6	0	2.809930	-3.140648	-0.257752
55	1	0	3.790680	-2.954060	-0.691375
56	1	0	2.797647	-4.101037	0.254729
57	35	0	2.652808	-1.817444	1.227877
58	6	0	0.451308	-3.405941	-0.990311
59	6	0	0.051385	-4.170902	0.246011
60	1	0	0.468316	-3.702040	1.142989
61	1	0	-1.037246	-4.198631	0.346759
62	1	0	0.410254	-5.205750	0.202842
63	6	0	0.354562	-0.169461	-1.309944
64	8	0	0.072800	-0.420001	-2.575824
65	1	0	1.324575	-0.563533	-0.925677

***Re*-TS6'**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.742229	1.866649	-2.942295
2	6	0	-5.756059	2.576421	-2.256600
3	6	0	-5.163850	2.039202	-1.113224
4	6	0	-5.554707	0.772987	-0.696557
5	6	0	-6.580806	0.075314	-1.353812
6	6	0	-7.172501	0.619176	-2.487025
7	1	0	-7.191455	2.296879	-3.831365
8	1	0	-5.453696	3.556910	-2.608669

9	1	0	-4.426639	2.602665	-0.549312
10	1	0	-7.960182	0.084466	-3.008879
11	6	0	-0.090555	1.553721	2.089227
12	6	0	1.241514	1.871206	2.304609
13	6	0	2.183369	0.861615	2.426081
14	6	0	1.781534	-0.463585	2.337552
15	6	0	0.453693	-0.775401	2.087756
16	6	0	-0.504507	0.230513	1.959283
17	9	0	0.142761	-2.055315	1.900833
18	9	0	2.687798	-1.439708	2.384644
19	9	0	3.467962	1.162915	2.579430
20	9	0	1.612474	3.147738	2.371379
21	9	0	-0.968781	2.548417	2.006220
22	6	0	-5.660464	-1.429442	0.192094
23	1	0	-4.890424	-1.902383	-0.443291
24	8	0	-5.807573	-2.161199	1.387948
25	6	0	-4.544830	-2.392811	1.994856
26	1	0	-4.717902	-2.611878	3.049280
27	1	0	-4.058084	-3.260845	1.528428
28	6	0	-3.580034	-1.237133	1.841129
29	7	0	-3.801953	-0.171693	0.990529
30	7	0	-2.381316	-1.189166	2.320581
31	7	0	-1.851778	-0.074456	1.706388
32	6	0	-2.676263	0.591155	0.849209
33	6	0	-5.177256	-0.013389	0.526568
34	1	0	-5.764681	0.350394	1.380932
35	6	0	-6.928992	-1.210436	-0.624206
36	1	0	-7.167287	-2.045007	-1.285438
37	1	0	-7.778897	-1.049468	0.050402
38	6	0	3.668733	0.903829	-0.674691
39	6	0	2.664532	-0.071693	-0.640366
40	6	0	3.037650	-1.413998	-0.786612
41	6	0	4.372064	-1.766596	-0.996588
42	6	0	5.334678	-0.774491	-1.052097
43	6	0	4.998539	0.567368	-0.880845
44	1	0	5.761518	1.336324	-0.898665
45	35	0	7.147109	-1.234239	-1.336284
46	35	0	3.184610	2.695217	-0.370838
47	8	0	1.380133	0.277444	-0.380478
48	6	0	0.529368	0.572292	-1.530757
49	1	0	1.149510	1.112257	-2.259830

50	1	0	0.230347	-0.385777	-1.969955
51	6	0	-1.912996	0.977096	-1.013846
52	6	0	-2.378434	-0.313258	-1.666091
53	1	0	-3.463662	-0.399943	-1.645703
54	1	0	-2.034649	-0.374497	-2.696940
55	35	0	-1.733117	-1.976200	-0.832625
56	6	0	-0.623872	1.425839	-1.132747
57	6	0	-0.321107	2.884812	-0.906159
58	1	0	0.291005	3.067106	-0.016016
59	1	0	0.242638	3.300617	-1.751243
60	1	0	-1.243971	3.460989	-0.793006
61	6	0	2.015495	-2.485640	-0.664774
62	1	0	0.987189	-2.146721	-0.462056
63	8	0	2.286682	-3.662183	-0.773715
64	1	0	4.627108	-2.815413	-1.101335
65	1	0	-2.667645	1.746480	-1.105707

***Si*-TS6'**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.514625	5.770534	-2.595099
2	6	0	-1.000354	4.487521	-2.843318
3	6	0	-1.163469	3.575590	-1.797092
4	6	0	-0.832647	3.984124	-0.515024
5	6	0	-0.360529	5.281507	-0.252491
6	6	0	-0.195447	6.179538	-1.297081
7	1	0	-0.395197	6.466046	-3.419352
8	1	0	-1.258663	4.196259	-3.855954
9	1	0	-1.555415	2.577701	-1.973036
10	1	0	0.161099	7.187861	-1.110030
11	6	0	-3.209280	-1.882329	1.582726
12	6	0	-3.766510	-3.108256	1.255489
13	6	0	-4.729061	-3.176279	0.256337
14	6	0	-5.129526	-2.026803	-0.411198
15	6	0	-4.569083	-0.804456	-0.072637
16	6	0	-3.611307	-0.718495	0.933161
17	9	0	-4.941446	0.282770	-0.736199
18	9	0	-6.039436	-2.104195	-1.376417

19	9	0	-5.260643	-4.347307	-0.068815
20	9	0	-3.369458	-4.216187	1.872058
21	9	0	-2.242877	-1.825340	2.493713
22	6	0	-1.071543	4.396096	1.775800
23	1	0	-2.112356	4.735600	1.643579
24	8	0	-0.886107	3.952686	3.099089
25	6	0	-1.961374	3.098807	3.463388
26	1	0	-1.678956	2.581750	4.381197
27	1	0	-2.866352	3.690633	3.656298
28	6	0	-2.269036	2.083784	2.385410
29	7	0	-1.784880	2.207450	1.096339
30	7	0	-3.015592	1.031864	2.496033
31	7	0	-2.978512	0.505228	1.215568
32	6	0	-2.174690	1.149850	0.325576
33	6	0	-0.831035	3.248624	0.794427
34	1	0	0.175799	2.839876	0.976614
35	6	0	-0.144200	5.485809	1.240387
36	1	0	-0.403064	6.487851	1.585357
37	1	0	0.892235	5.271853	1.529781
38	6	0	3.131059	-1.521933	-0.649463
39	6	0	3.232674	-0.206658	-1.121568
40	6	0	4.394967	0.520975	-0.829024
41	6	0	5.415239	-0.038158	-0.056833
42	6	0	5.278014	-1.333934	0.406999
43	6	0	4.145599	-2.089577	0.109602
44	1	0	4.052432	-3.107677	0.468298
45	35	0	6.649747	-2.112259	1.450803
46	35	0	1.584043	-2.523904	-1.034507
47	8	0	2.244913	0.342980	-1.875136
48	6	0	1.341758	1.240569	-1.153588
49	1	0	1.945639	2.061969	-0.741766
50	1	0	0.715317	1.650739	-1.947108
51	6	0	-0.677273	0.014519	-0.329301
52	6	0	-1.116931	-0.338734	-1.734749
53	1	0	-1.941411	0.272711	-2.095660
54	1	0	-0.284200	-0.359741	-2.436355
55	35	0	-1.824884	-2.174956	-1.754390
56	6	0	0.550136	0.563241	-0.080372
57	6	0	1.132476	0.460845	1.310255
58	1	0	1.487072	-0.558520	1.513599
59	1	0	1.981771	1.137841	1.448649

60	1	0	0.388495	0.700802	2.082490
61	6	0	4.587820	1.885715	-1.386670
62	1	0	3.827535	2.220157	-2.113125
63	8	0	5.530600	2.587209	-1.091417
64	1	0	6.300969	0.551791	0.151061
65	1	0	-1.013028	-0.691015	0.429515

***Re*-Int6'**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.509424	-0.642994	3.651923
2	6	0	5.677561	0.471040	3.542921
3	6	0	5.186295	0.849415	2.298118
4	6	0	5.503643	0.061474	1.200639
5	6	0	6.384065	-1.026429	1.295573
6	6	0	6.877186	-1.382620	2.528069
7	1	0	6.888806	-0.926123	4.628125
8	1	0	5.435729	1.053563	4.422314
9	1	0	4.594194	1.760448	2.200455
10	1	0	7.550306	-2.228954	2.631171
11	6	0	0.051094	2.498808	-1.007803
12	6	0	-1.269320	2.862230	-1.117910
13	6	0	-2.144005	2.024073	-1.796157
14	6	0	-1.703675	0.851840	-2.397132
15	6	0	-0.382847	0.482981	-2.273886
16	6	0	0.470881	1.283870	-1.544069
17	9	0	0.038146	-0.679573	-2.765872
18	9	0	-2.555226	0.037383	-2.992006
19	9	0	-3.430689	2.342495	-1.852476
20	9	0	-1.688320	3.989412	-0.557681
21	9	0	0.941780	3.287059	-0.406557
22	6	0	5.536673	-1.095329	-0.899145
23	1	0	4.661756	-1.759067	-0.756876
24	8	0	5.790738	-0.935553	-2.278347
25	6	0	4.946513	0.011019	-2.924391
26	1	0	5.539374	0.892237	-3.191865
27	1	0	4.534324	-0.415913	-3.839232
28	6	0	3.744692	0.462151	-2.078823

29	7	0	3.786809	0.541350	-0.691942
30	7	0	2.546491	0.720999	-2.504149
31	7	0	1.814797	0.909435	-1.385293
32	6	0	2.468279	0.608699	-0.219411
33	6	0	5.173000	0.253790	-0.236001
34	1	0	5.766072	1.068297	-0.674615
35	6	0	6.702989	-1.602039	-0.074189
36	1	0	6.783627	-2.690115	-0.078961
37	1	0	7.642376	-1.182886	-0.453798
38	6	0	-3.704207	0.381223	0.952031
39	6	0	-2.673887	-0.402000	0.303132
40	6	0	-3.091350	-1.724733	-0.068490
41	6	0	-4.415216	-2.157857	0.064422
42	6	0	-5.346378	-1.311426	0.622564
43	6	0	-4.998749	-0.025018	1.080382
44	1	0	-5.756775	0.613139	1.516699
45	35	0	-7.146072	-1.870162	0.787323
46	35	0	-3.180000	2.128560	1.494801
47	8	0	-1.570423	0.001812	0.074729
48	6	0	-0.154513	-0.124891	1.811146
49	1	0	-1.149000	0.106440	2.341419
50	1	0	-0.148817	-1.197008	1.395453
51	6	0	2.222254	0.543859	0.796378
52	6	0	2.380167	-1.059873	1.190943
53	1	0	3.427521	-1.374299	1.313657
54	1	0	1.754611	-1.310342	2.097911
55	35	0	1.729432	-2.053282	-0.358168
56	6	0	0.662286	0.777264	1.600319
57	6	0	0.392964	2.123971	2.225180
58	1	0	-0.099645	2.882868	1.592415
59	1	0	-0.286537	1.982966	3.077544
60	1	0	1.295943	2.612681	2.621776
61	6	0	-2.101376	-2.576927	-0.700014
62	1	0	-1.096678	-2.133242	-0.775388
63	8	0	-2.322824	-3.710747	-1.119781
64	1	0	-4.687281	-3.144226	-0.282277
65	1	0	2.838007	0.879484	1.745917

***Si*-Int6'**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.534138	5.837489	-2.403862
2	6	0	-1.724530	4.491678	-2.710878
3	6	0	-1.718642	3.528194	-1.699310
4	6	0	-1.522362	3.950136	-0.391718
5	6	0	-1.377800	5.309001	-0.072155
6	6	0	-1.366211	6.251982	-1.079974
7	1	0	-1.532540	6.573958	-3.200588
8	1	0	-1.875360	4.188759	-3.741494
9	1	0	-1.863632	2.493014	-1.951187
10	1	0	-1.246256	7.304752	-0.843515
11	6	0	-2.112822	-2.454072	1.394232
12	6	0	-2.327154	-3.769064	1.045029
13	6	0	-3.472980	-4.105506	0.322355
14	6	0	-4.395456	-3.127289	-0.053930
15	6	0	-4.160537	-1.801908	0.284815
16	6	0	-3.011146	-1.472676	0.989594
17	9	0	-5.001859	-0.860526	-0.118577
18	9	0	-5.470402	-3.471602	-0.742939
19	9	0	-3.676474	-5.361227	-0.010355
20	9	0	-1.462399	-4.693877	1.394757
21	9	0	-1.025070	-2.090767	2.059754
22	6	0	-1.998732	4.212206	1.864924
23	1	0	-3.062988	4.313883	1.631672
24	8	0	-1.853291	3.774890	3.198050
25	6	0	-2.792536	2.746622	3.407779
26	1	0	-2.538808	2.212417	4.325833
27	1	0	-3.817072	3.138619	3.490185
28	6	0	-2.731843	1.708621	2.282159
29	7	0	-1.971892	1.883257	1.126664
30	7	0	-3.185316	0.489030	2.345842
31	7	0	-2.659211	-0.133925	1.256001
32	6	0	-1.669639	0.620724	0.596762
33	6	0	-1.359454	3.204984	0.899847
34	1	0	-0.293963	3.037503	1.082167
35	6	0	-1.294303	5.491784	1.433061
36	1	0	-1.794751	6.400842	1.783830
37	1	0	-0.266085	5.501344	1.787098
38	6	0	3.119771	-1.051492	-0.700616

39	6	0	3.189200	0.276044	-1.263656
40	6	0	4.322122	1.032529	-0.830272
41	6	0	5.329127	0.489648	-0.021438
42	6	0	5.214347	-0.813346	0.423564
43	6	0	4.107378	-1.591751	0.087512
44	1	0	4.030698	-2.615981	0.452839
45	35	0	6.578410	-1.573487	1.484208
46	35	0	1.598065	-2.103527	-1.141043
47	8	0	2.299066	0.736667	-2.005910
48	6	0	0.988062	1.750312	-0.899776
49	1	0	1.874959	2.405162	-0.615882
50	1	0	0.571743	2.058396	-1.893722
51	6	0	-1.106271	0.332140	-0.260849
52	6	0	-1.085556	-0.033038	-1.813479
53	1	0	-1.659343	0.634067	-2.509389
54	1	0	0.010431	-0.108353	-2.114327
55	35	0	-1.818516	-1.832015	-2.162171
56	6	0	0.340079	1.141037	0.007706
57	6	0	0.973973	0.739590	1.323680
58	1	0	1.178633	-0.351421	1.456009
59	1	0	1.938212	1.243382	1.434832
60	1	0	0.376750	1.032672	2.242807
61	6	0	4.484502	2.393154	-1.338340
62	1	0	3.709119	2.713123	-2.051394
63	8	0	5.393682	3.146986	-1.016110
64	1	0	6.182430	1.101086	0.237610
65	1	0	-0.564279	-0.822477	-0.026343

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.799770	0.314878	-1.600728
2	6	0	-3.676938	-0.487113	-1.820174
3	6	0	-2.398424	0.056875	-1.740262
4	6	0	-2.268116	1.397777	-1.406794
5	6	0	-3.387237	2.220793	-1.243376
6	6	0	-4.662965	1.673196	-1.325167
7	1	0	-5.789554	-0.127400	-1.648963

8	1	0	-3.807140	-1.548366	-2.014685
9	1	0	-1.509042	-0.548632	-1.883286
10	1	0	-5.538657	2.295680	-1.168839
11	6	0	4.461154	0.740493	0.281552
12	6	0	5.489305	0.111557	0.965887
13	6	0	5.240883	-0.444869	2.215746
14	6	0	3.976586	-0.366562	2.785041
15	6	0	2.956302	0.272989	2.098611
16	6	0	3.195604	0.829572	0.848050
17	9	0	1.760992	0.405000	2.659378
18	9	0	3.755365	-0.895981	3.983856
19	9	0	6.224050	-1.049794	2.872441
20	9	0	6.703258	0.023476	0.428541
21	9	0	4.684291	1.238309	-0.931257
22	6	0	-1.527204	3.532434	-0.637888
23	1	0	-1.492884	3.320455	0.442230
24	8	0	-0.703541	4.644104	-0.933701
25	6	0	0.635185	4.335442	-1.315527
26	1	0	0.709353	4.311481	-2.411242
27	1	0	1.286556	5.129259	-0.947002
28	6	0	1.117214	3.024133	-0.762590
29	7	0	0.248494	1.955129	-0.711425
30	7	0	2.277763	2.743488	-0.273943
31	7	0	2.145953	1.435095	0.133333
32	6	0	0.898991	0.926545	-0.074606
33	6	0	-1.040875	2.263256	-1.352095
34	1	0	-0.779739	2.518108	-2.390011
35	6	0	-2.994181	3.671166	-1.042801
36	1	0	-3.591743	4.180171	-0.283269
37	1	0	-3.071330	4.232210	-1.981860
38	6	0	-1.499796	-1.865247	0.653919
39	6	0	-0.838127	-0.630126	0.799467
40	6	0	-1.528298	0.430468	1.386990
41	6	0	-2.883324	0.328593	1.666301
42	6	0	-3.573640	-0.853683	1.459333
43	6	0	-2.854713	-1.943514	0.974012
44	1	0	-1.013253	1.365634	1.578569
45	1	0	-4.637178	-0.930051	1.646284
46	35	0	-3.806962	1.878290	2.239065
47	35	0	-3.779701	-3.543275	0.590051
48	8	0	-0.838044	-2.973395	0.217744

49	6	0	-0.902899	-3.316137	-1.171150
50	1	0	-1.140133	-4.385777	-1.207987
51	1	0	-1.713359	-2.771424	-1.669804
52	6	0	0.514384	-2.237107	-2.887273
53	1	0	-0.386974	-1.764557	-3.273584
54	6	0	1.787524	-1.880301	-3.571578
55	1	0	1.636378	-1.527994	-4.589054
56	1	0	2.524728	-2.679554	-3.558652
57	35	0	2.687363	-0.369653	-2.645194
58	6	0	0.432557	-3.048445	-1.823393
59	6	0	1.612040	-3.717813	-1.175238
60	1	0	2.545461	-3.203177	-1.409059
61	1	0	1.488898	-3.675950	-0.091776
62	1	0	1.677619	-4.764885	-1.494730
63	6	0	0.517809	-0.418472	0.237668
64	8	0	1.581067	-1.299459	0.571071
65	1	0	0.910350	-1.132656	-0.605443

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.474016	-0.355059	2.092132
2	6	0	4.287501	-0.921249	1.628819
3	6	0	3.184738	-0.121484	1.334764
4	6	0	3.282713	1.260846	1.463371
5	6	0	4.454644	1.815363	2.005001
6	6	0	5.553469	1.018754	2.304717
7	1	0	6.328579	-0.987931	2.308119
8	1	0	4.212895	-1.995511	1.493234
9	1	0	2.269569	-0.585319	0.995110
10	1	0	6.457177	1.466843	2.706195
11	6	0	-3.025236	2.710627	-0.936154
12	6	0	-4.200642	2.210240	-1.467638
13	6	0	-4.151410	1.365684	-2.568821
14	6	0	-2.937772	1.073630	-3.170226
15	6	0	-1.764312	1.577819	-2.632966
16	6	0	-1.797266	2.394972	-1.509042
17	9	0	-0.605123	1.296770	-3.215869

18	9	0	-2.893718	0.239790	-4.210589
19	9	0	-5.273789	0.834432	-3.043594
20	9	0	-5.367907	2.457528	-0.869046
21	9	0	-3.080067	3.423567	0.190209
22	6	0	3.144586	3.630761	1.355618
23	1	0	3.526798	3.755968	0.328388
24	8	0	2.418639	4.769741	1.743634
25	6	0	1.506591	5.111683	0.723340
26	1	0	0.785813	5.824658	1.124170
27	1	0	2.037283	5.580363	-0.117894
28	6	0	0.768691	3.909980	0.195004
29	7	0	1.275760	2.614836	0.235263
30	7	0	-0.358628	3.986142	-0.424996
31	7	0	-0.602945	2.697533	-0.830913
32	6	0	0.357326	1.814227	-0.427582
33	6	0	2.246699	2.374628	1.347543
34	1	0	1.637545	2.363623	2.262342
35	6	0	4.303630	3.291887	2.271706
36	1	0	5.198553	3.879323	2.059662
37	1	0	4.012480	3.467902	3.314603
38	6	0	1.186783	-1.767080	-1.456455
39	6	0	1.308813	-0.387868	-1.150013
40	6	0	2.529516	0.229350	-1.445819
41	6	0	3.628434	-0.494983	-1.870982
42	6	0	3.554291	-1.858777	-2.100942
43	6	0	2.319236	-2.462639	-1.901853
44	1	0	2.649708	1.294699	-1.287333
45	1	0	4.414006	-2.434574	-2.418237
46	35	0	5.292962	0.395728	-2.030451
47	35	0	2.169632	-4.323074	-2.230906
48	8	0	0.027822	-2.475915	-1.433556
49	6	0	-0.714144	-2.605865	-0.230390
50	1	0	-0.519910	-3.615606	0.161516
51	1	0	-0.391572	-1.867630	0.505773
52	6	0	-3.036280	-2.479808	0.554426
53	1	0	-2.633186	-2.592603	1.560295
54	6	0	-4.507232	-2.349858	0.444286
55	1	0	-5.038205	-2.715068	1.320383
56	1	0	-4.927796	-2.789495	-0.456775
57	35	0	-5.079989	-0.426963	0.312775
58	6	0	-2.196184	-2.419064	-0.487859

59	6	0	-2.635042	-2.189620	-1.902762
60	1	0	-3.658319	-1.809175	-1.947433
61	1	0	-1.964304	-1.447911	-2.338415
62	1	0	-2.568554	-3.111887	-2.491120
63	6	0	0.164136	0.369020	-0.522646
64	8	0	-1.054292	-0.003431	-0.889913
65	1	0	0.069654	0.250868	0.913232
66	6	0	0.611749	-1.466772	3.156945
67	6	0	-0.722624	-0.786891	2.894620
68	6	0	0.809519	-2.043649	4.559756
69	6	0	-2.049542	-2.387794	4.340058
70	6	0	0.236505	-3.454086	4.691246
71	6	0	-1.129756	-3.559222	4.015807
72	1	0	0.786069	-2.241683	2.397957
73	1	0	-2.013516	-2.154646	5.413262
74	1	0	0.342450	-1.373716	5.290803
75	1	0	0.147246	-3.718629	5.750137
76	1	0	1.351559	-0.687546	2.975496
77	1	0	1.878850	-2.051450	4.787910
78	1	0	-3.080729	-2.685739	4.118047
79	1	0	0.920815	-4.178642	4.237322
80	1	0	-1.633466	-4.476114	4.334538
81	1	0	-1.021054	-3.634535	2.926856
82	6	0	-3.069361	-0.354816	3.473913
83	1	0	-3.775049	-0.853460	2.796864
84	1	0	-3.518652	-0.336837	4.472415
85	6	0	-1.901386	0.960594	1.749000
86	1	0	-1.594519	1.963209	1.434909
87	1	0	-2.419225	0.494303	0.902848
88	6	0	-2.788790	1.048997	2.976765
89	1	0	-3.733588	1.536930	2.722095
90	1	0	-2.297873	1.636353	3.759759
91	7	0	-0.687730	0.202370	2.040417
92	7	0	-1.840783	-1.154500	3.563360

Int3

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

1	6	0	5.281473	-0.872036	2.121447
2	6	0	4.041518	-1.265646	1.616066
3	6	0	3.055504	-0.319950	1.347204
4	6	0	3.323534	1.031271	1.548045
5	6	0	4.541204	1.411890	2.131461
6	6	0	5.527147	0.469235	2.403451
7	1	0	6.047819	-1.615784	2.314387
8	1	0	3.840141	-2.314397	1.421182
9	1	0	2.102165	-0.640253	0.943160
10	1	0	6.473335	0.779382	2.836800
11	6	0	-3.035999	2.945362	-0.207869
12	6	0	-4.255224	2.596614	-0.760204
13	6	0	-4.306894	2.013260	-2.020889
14	6	0	-3.131104	1.778567	-2.711036
15	6	0	-1.912392	2.120698	-2.146141
16	6	0	-1.830822	2.681234	-0.867797
17	9	0	-0.809963	1.960514	-2.874613
18	9	0	-3.169885	1.218466	-3.923287
19	9	0	-5.480531	1.657277	-2.542829
20	9	0	-5.380337	2.733453	-0.049638
21	9	0	-3.018704	3.433249	1.039415
22	6	0	3.434686	3.408848	1.601881
23	1	0	3.827139	3.596524	0.588067
24	8	0	2.814183	4.567875	2.103163
25	6	0	1.829373	5.021156	1.190697
26	1	0	1.181063	5.726786	1.710837
27	1	0	2.311838	5.536302	0.346725
28	6	0	0.991898	3.899969	0.635872
29	7	0	1.549085	2.649565	0.340259
30	7	0	-0.246294	4.030402	0.331336
31	7	0	-0.605053	2.819100	-0.234824
32	6	0	0.479751	1.896217	-0.241855
33	6	0	2.421782	2.253971	1.472108
34	1	0	1.795754	2.240705	2.382977
35	6	0	4.552709	2.880307	2.483969
36	1	0	5.508986	3.376806	2.308750
37	1	0	4.281300	3.019757	3.538091
38	6	0	1.345436	-1.453411	-1.807526
39	6	0	1.471103	-0.124090	-1.324041
40	6	0	2.741904	0.469562	-1.402344
41	6	0	3.858127	-0.260742	-1.751388

42	6	0	3.774330	-1.592801	-2.136576
43	6	0	2.502127	-2.149843	-2.176985
44	1	0	2.863676	1.505047	-1.108013
45	1	0	4.651121	-2.173925	-2.390414
46	35	0	5.559349	0.549164	-1.541984
47	35	0	2.327151	-3.955099	-2.730797
48	8	0	0.152746	-2.080025	-2.025070
49	6	0	-0.621784	-2.481733	-0.905302
50	1	0	-0.427892	-3.550573	-0.731517
51	1	0	-0.326336	-1.915175	-0.019511
52	6	0	-2.979917	-2.560495	-0.196069
53	1	0	-2.623422	-2.916337	0.770911
54	6	0	-4.451238	-2.476622	-0.363493
55	1	0	-4.998391	-3.054144	0.378096
56	1	0	-4.793487	-2.733720	-1.362849
57	35	0	-5.161043	-0.609413	-0.127245
58	6	0	-2.099435	-2.252069	-1.159848
59	6	0	-2.501553	-1.696097	-2.493241
60	1	0	-3.518401	-1.298210	-2.468031
61	1	0	-1.814690	-0.883640	-2.732695
62	1	0	-2.430312	-2.458296	-3.277627
63	6	0	0.318955	0.621080	-0.771501
64	8	0	-0.883376	0.156283	-0.912892
65	1	0	-0.255074	-0.074607	1.389665
66	6	0	0.276065	-2.046119	2.874766
67	6	0	-1.076517	-1.390216	2.698595
68	6	0	0.520037	-2.683235	4.245213
69	6	0	-2.349529	-3.078941	4.048023
70	6	0	-0.028504	-4.107126	4.325805
71	6	0	-1.406463	-4.216407	3.674802
72	1	0	0.426741	-2.781774	2.074526
73	1	0	-2.296312	-2.855447	5.120742
74	1	0	0.070203	-2.051021	5.018754
75	1	0	-0.086752	-4.416109	5.374111
76	1	0	1.006934	-1.251074	2.710455
77	1	0	1.595990	-2.683968	4.436253
78	1	0	-3.374736	-3.392904	3.836004
79	1	0	0.658585	-4.797734	3.826438
80	1	0	-1.885541	-5.151062	3.978756
81	1	0	-1.322343	-4.262467	2.582453
82	6	0	-3.458180	-1.079303	3.152014

83	1	0	-4.059700	-1.569270	2.377242
84	1	0	-3.985066	-1.176357	4.104665
85	6	0	-2.270940	0.491171	1.643925
86	1	0	-1.926307	1.516548	1.519859
87	1	0	-2.702438	0.151629	0.700614
88	6	0	-3.240699	0.381041	2.803847
89	1	0	-4.197993	0.823789	2.517889
90	1	0	-2.856575	0.921847	3.673962
91	7	0	-1.092979	-0.310160	1.941246
92	7	0	-2.186825	-1.818450	3.292788

Int4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.373456	2.040372	-1.406732
2	6	0	4.057262	2.248029	-1.825700
3	6	0	3.217859	1.161302	-2.073844
4	6	0	3.709472	-0.121786	-1.867568
5	6	0	5.043141	-0.334479	-1.498818
6	6	0	5.877905	0.751674	-1.249239
7	1	0	6.005641	2.894889	-1.199345
8	1	0	3.675194	3.253050	-1.940832
9	1	0	2.195039	1.326603	-2.399900
10	1	0	6.909843	0.594820	-0.951291
11	6	0	-2.488986	-2.622320	-1.617639
12	6	0	-3.818843	-2.770296	-1.245508
13	6	0	-4.132889	-2.985552	0.082637
14	6	0	-3.119820	-3.080214	1.032790
15	6	0	-1.795668	-2.912714	0.664051
16	6	0	-1.475835	-2.664858	-0.667420
17	9	0	-0.846606	-2.968124	1.575536
18	9	0	-3.436799	-3.269299	2.312107
19	9	0	-5.401286	-3.063458	0.465534
20	9	0	-4.782171	-2.643743	-2.153418
21	9	0	-2.191959	-2.372420	-2.886833
22	6	0	4.044778	-2.471584	-1.531423
23	1	0	3.714390	-2.575726	-0.487701
24	8	0	3.972450	-3.727255	-2.180130

25	6	0	2.689688	-4.063103	-2.714710
26	1	0	2.690542	-3.896933	-3.797671
27	1	0	2.503855	-5.121291	-2.526122
28	6	0	1.576795	-3.267054	-2.098863
29	7	0	1.761978	-1.925830	-1.830487
30	7	0	0.419006	-3.670717	-1.682186
31	7	0	-0.126439	-2.560875	-1.105261
32	6	0	0.686929	-1.492530	-1.149532
33	6	0	3.109912	-1.452212	-2.205914
34	1	0	3.144581	-1.585175	-3.294953
35	6	0	5.417689	-1.805354	-1.525401
36	1	0	6.023755	-2.121063	-0.678494
37	1	0	5.958064	-2.046389	-2.452696
38	6	0	2.123721	1.366939	0.705750
39	6	0	1.638529	0.063560	0.516393
40	6	0	2.269710	-1.004971	1.139281
41	6	0	3.448580	-0.808659	1.835139
42	6	0	3.994262	0.454618	1.981071
43	6	0	3.317337	1.535214	1.420587
44	1	0	1.849708	-2.006173	1.051697
45	1	0	4.932001	0.608368	2.491609
46	35	0	4.384293	-2.314785	2.492298
47	35	0	4.121555	3.236952	1.542685
48	8	0	1.486905	2.381681	0.057780
49	6	0	1.070616	3.549626	0.796849
50	1	0	1.201213	3.372504	1.870235
51	1	0	1.707730	4.391705	0.502470
52	6	0	-0.694174	4.886542	-0.267018
53	1	0	0.092660	5.518231	-0.676974
54	6	0	-2.089481	5.277026	-0.598163
55	1	0	-2.174506	6.299210	-0.961642
56	1	0	-2.793936	5.108273	0.211440
57	35	0	-2.805126	4.171673	-2.095068
58	6	0	-0.372701	3.827522	0.480426
59	6	0	-1.359341	2.845733	1.031795
60	1	0	-2.343322	2.935173	0.562755
61	1	0	-0.990090	1.821081	0.860057
62	1	0	-1.468019	2.980160	2.119109
63	6	0	0.401618	-0.179892	-0.359881
64	8	0	-0.712374	-0.321229	0.353954
65	1	0	0.394704	0.618563	-1.135304

66	6	0	-3.269595	0.038211	2.107253
67	6	0	-3.942541	0.127981	0.751682
68	6	0	-3.969840	0.909032	3.160751
69	6	0	-6.292806	-0.039035	1.612895
70	6	0	-5.087733	0.134950	3.863685
71	6	0	-5.883348	-0.744491	2.897183
72	1	0	-3.243314	-1.000619	2.439476
73	1	0	-6.715687	0.952757	1.831460
74	1	0	-4.365112	1.811510	2.684134
75	1	0	-5.766080	0.843470	4.360453
76	1	0	-2.230031	0.327730	1.949993
77	1	0	-3.225566	1.241656	3.892113
78	1	0	-7.074650	-0.625836	1.125084
79	1	0	-4.661084	-0.498650	4.647288
80	1	0	-6.801992	-1.082441	3.381081
81	1	0	-5.331906	-1.657799	2.641791
82	6	0	-5.808477	0.314293	-0.780631
83	1	0	-5.946083	-0.673988	-1.233602
84	1	0	-6.791544	0.776206	-0.659761
85	6	0	-3.513064	0.579102	-1.651319
86	1	0	-2.776645	1.284882	-2.041867
87	1	0	-3.504061	-0.315220	-2.276547
88	6	0	-4.902451	1.195817	-1.619583
89	1	0	-5.303590	1.283595	-2.631671
90	1	0	-4.847525	2.198605	-1.188799
91	7	0	-3.129341	0.259300	-0.287374
92	7	0	-5.252451	0.124949	0.579004
93	1	0	-2.235152	0.161227	-0.121044

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.418397	1.976072	-1.528660
2	6	0	4.090271	2.181190	-1.910003
3	6	0	3.235846	1.099156	-2.096826
4	6	0	3.725566	-0.181192	-1.864552
5	6	0	5.069095	-0.397823	-1.533660
6	6	0	5.918823	0.688822	-1.349237

7	1	0	6.067295	2.831428	-1.372285
8	1	0	3.715713	3.190009	-2.046867
9	1	0	2.203089	1.263342	-2.390408
10	1	0	6.958896	0.532733	-1.080539
11	6	0	-2.463853	-2.669800	-1.495642
12	6	0	-3.801364	-2.806632	-1.152848
13	6	0	-4.147285	-2.961521	0.180072
14	6	0	-3.158430	-3.015250	1.158727
15	6	0	-1.823162	-2.876011	0.812074
16	6	0	-1.477574	-2.681939	-0.520093
17	9	0	-0.892534	-2.909081	1.746689
18	9	0	-3.509101	-3.146299	2.436127
19	9	0	-5.424582	-3.032770	0.528050
20	9	0	-4.741893	-2.727193	-2.089395
21	9	0	-2.134095	-2.468625	-2.765398
22	6	0	4.051546	-2.528643	-1.477275
23	1	0	3.753630	-2.609279	-0.421305
24	8	0	3.958299	-3.795788	-2.095091
25	6	0	2.660217	-4.136267	-2.581241
26	1	0	2.627224	-3.991869	-3.667723
27	1	0	2.468331	-5.188358	-2.366239
28	6	0	1.568194	-3.318647	-1.951338
29	7	0	1.757059	-1.972553	-1.711931
30	7	0	0.416240	-3.715302	-1.508132
31	7	0	-0.121566	-2.595071	-0.945005
32	6	0	0.692473	-1.527716	-1.025394
33	6	0	3.101605	-1.516493	-2.144535
34	1	0	3.095313	-1.679150	-3.230090
35	6	0	5.427934	-1.871524	-1.531480
36	1	0	6.056111	-2.165294	-0.687677
37	1	0	5.940184	-2.144413	-2.460884
38	6	0	2.186673	1.394640	0.679124
39	6	0	1.707252	0.082747	0.553422
40	6	0	2.369973	-0.966247	1.180432
41	6	0	3.576852	-0.739238	1.825165
42	6	0	4.109698	0.537673	1.908560
43	6	0	3.402796	1.594861	1.346220
44	1	0	1.961327	-1.972378	1.143341
45	1	0	5.069138	0.714856	2.378861
46	35	0	4.558021	-2.211217	2.487651
47	35	0	4.202246	3.301590	1.385250

48	8	0	1.517337	2.379763	0.026642
49	6	0	1.121611	3.572875	0.741098
50	1	0	1.301986	3.429006	1.812591
51	1	0	1.737646	4.403256	0.390200
52	6	0	-0.703840	4.850575	-0.292107
53	1	0	0.054282	5.476149	-0.756568
54	6	0	-2.122948	5.201846	-0.570780
55	1	0	-2.243800	6.215391	-0.943276
56	1	0	-2.786346	5.027200	0.273359
57	35	0	-2.866460	4.053904	-2.013510
58	6	0	-0.336242	3.821835	0.478926
59	6	0	-1.295180	2.859231	1.117196
60	1	0	-2.246169	2.807959	0.580175
61	1	0	-0.862541	1.853355	1.120309
62	1	0	-1.490370	3.141702	2.159316
63	6	0	0.451077	-0.201185	-0.270176
64	8	0	-0.623220	-0.338403	0.558406
65	1	0	0.348428	0.588928	-1.032386
66	6	0	-3.484601	0.191645	2.022361
67	6	0	-4.057563	0.196387	0.617488
68	6	0	-4.263383	1.088513	2.993293
69	6	0	-6.460542	-0.033176	1.392688
70	6	0	-5.389185	0.318750	3.689346
71	6	0	-6.095298	-0.646959	2.737370
72	1	0	-3.446260	-0.829156	2.414835
73	1	0	-6.939815	0.944750	1.537315
74	1	0	-4.668472	1.947259	2.445062
75	1	0	-6.114922	1.024089	4.106925
76	1	0	-2.449613	0.520126	1.927914
77	1	0	-3.573320	1.496073	3.736452
78	1	0	-7.195247	-0.682018	0.906374
79	1	0	-4.979788	-0.251764	4.529536
80	1	0	-7.029410	-0.989109	3.192336
81	1	0	-5.497406	-1.548077	2.569265
82	6	0	-5.892786	0.234888	-0.976663
83	1	0	-6.016714	-0.772300	-1.393619
84	1	0	-6.880635	0.697683	-0.918755
85	6	0	-3.561209	0.491782	-1.748767
86	1	0	-2.829353	1.162719	-2.205702
87	1	0	-3.517818	-0.460170	-2.291908
88	6	0	-4.961489	1.075105	-1.831709

89	1	0	-5.314504	1.088316	-2.864902
90	1	0	-4.947908	2.104899	-1.461673
91	7	0	-3.182928	0.311744	-0.354111
92	7	0	-5.381121	0.118800	0.398389
93	1	0	-1.864473	0.036243	0.027709

Int5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.372825	2.026968	-1.397102
2	6	0	4.058075	2.242022	-1.816869
3	6	0	3.213686	1.169985	-2.068473
4	6	0	3.698860	-0.115981	-1.854827
5	6	0	5.031087	-0.346035	-1.485286
6	6	0	5.870862	0.735460	-1.242241
7	1	0	6.018943	2.877890	-1.197007
8	1	0	3.691029	3.259149	-1.939920
9	1	0	2.192008	1.341036	-2.395140
10	1	0	6.901728	0.572880	-0.943651
11	6	0	-2.521989	-2.626978	-1.627174
12	6	0	-3.852897	-2.759403	-1.256710
13	6	0	-4.169296	-2.966366	0.080608
14	6	0	-3.157676	-3.078245	1.031520
15	6	0	-1.832377	-2.926264	0.654490
16	6	0	-1.520035	-2.686710	-0.676074
17	9	0	-0.874486	-2.978513	1.566796
18	9	0	-3.476851	-3.268892	2.310059
19	9	0	-5.438434	-3.039034	0.452057
20	9	0	-4.814688	-2.625977	-2.165265
21	9	0	-2.222482	-2.375446	-2.895461
22	6	0	4.012412	-2.478150	-1.534078
23	1	0	3.680452	-2.593218	-0.490952
24	8	0	3.944677	-3.721891	-2.195888
25	6	0	2.660834	-4.050227	-2.722554
26	1	0	2.653604	-3.871413	-3.805100
27	1	0	2.459688	-5.107918	-2.546727
28	6	0	1.551191	-3.250296	-2.095879
29	7	0	1.722601	-1.910604	-1.814071

30	7	0	0.390998	-3.669335	-1.691356
31	7	0	-0.169663	-2.568214	-1.112299
32	6	0	0.638939	-1.493711	-1.143160
33	6	0	3.083196	-1.442635	-2.197004
34	1	0	3.108313	-1.573098	-3.286334
35	6	0	5.388530	-1.818604	-1.525076
36	1	0	5.992203	-2.139314	-0.668338
37	1	0	5.928655	-2.060020	-2.442417
38	6	0	2.097726	1.354247	0.700493
39	6	0	1.606405	0.053688	0.517489
40	6	0	2.231754	-1.029387	1.128392
41	6	0	3.420863	-0.840509	1.825898
42	6	0	3.962547	0.429786	1.965448
43	6	0	3.291427	1.514996	1.416919
44	1	0	1.816985	-2.028361	1.047964
45	1	0	4.910507	0.577722	2.477291
46	35	0	4.358627	-2.342769	2.480340
47	35	0	4.123738	3.202463	1.543947
48	8	0	1.456459	2.363648	0.064342
49	6	0	1.085179	3.561729	0.785890
50	1	0	1.233864	3.391324	1.858992
51	1	0	1.736605	4.371431	0.464158
52	6	0	-0.672040	4.909766	-0.276475
53	1	0	0.118221	5.518647	-0.704139
54	6	0	-2.075133	5.297829	-0.598071
55	1	0	-2.154841	6.321279	-0.949149
56	1	0	-2.771239	5.120496	0.220415
57	35	0	-2.784632	4.199557	-2.088361
58	6	0	-0.356440	3.857366	0.488724
59	6	0	-1.358334	2.909005	1.086759
60	1	0	-2.301622	2.894365	0.526850
61	1	0	-0.953937	1.892703	1.072929
62	1	0	-1.567112	3.171612	2.134395
63	6	0	0.389189	-0.191672	-0.370602
64	8	0	-0.736254	-0.339405	0.421765
65	1	0	0.296949	0.628846	-1.094109
66	6	0	-3.243344	0.068109	2.133469
67	6	0	-3.814486	0.154245	0.727490
68	6	0	-3.990423	0.929918	3.158349
69	6	0	-6.226479	-0.043273	1.555887
70	6	0	-5.112781	0.149577	3.848278

71	6	0	-5.861720	-0.743746	2.858854
72	1	0	-3.222442	-0.971663	2.483192
73	1	0	-6.664784	0.940087	1.766420
74	1	0	-4.400871	1.815541	2.653500
75	1	0	-5.808221	0.840246	4.326060
76	1	0	-2.202196	0.382866	2.057979
77	1	0	-3.285162	1.307238	3.901294
78	1	0	-7.000688	-0.635102	1.055870
79	1	0	-4.689976	-0.477995	4.640774
80	1	0	-6.802462	-1.078323	3.311009
81	1	0	-5.294447	-1.649180	2.631813
82	6	0	-5.707987	0.343383	-0.796242
83	1	0	-5.879860	-0.622996	-1.291739
84	1	0	-6.678871	0.829753	-0.685195
85	6	0	-3.390529	0.579032	-1.594021
86	1	0	-2.650348	1.252248	-2.042160
87	1	0	-3.395288	-0.333792	-2.211441
88	6	0	-4.766892	1.212437	-1.612148
89	1	0	-5.136555	1.314553	-2.634390
90	1	0	-4.717541	2.213911	-1.168879
91	7	0	-2.939656	0.283894	-0.230407
92	7	0	-5.164314	0.118097	0.543439
93	1	0	-1.546718	-0.040282	0.056550

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.194218	1.773497	-0.938746
2	6	0	3.975971	1.898172	-0.269999
3	6	0	2.839673	1.249372	-0.742876
4	6	0	2.934536	0.433731	-1.866848
5	6	0	4.141008	0.378890	-2.581678
6	6	0	5.274600	1.033785	-2.113906
7	1	0	6.076696	2.271189	-0.551381
8	1	0	3.910158	2.494217	0.634732
9	1	0	1.908041	1.352002	-0.203651
10	1	0	6.209303	0.964260	-2.661151
11	6	0	-3.277010	-2.431081	-1.103540

12	6	0	-4.399579	-2.748845	-0.352369
13	6	0	-4.241186	-3.324438	0.903896
14	6	0	-2.970046	-3.582145	1.410886
15	6	0	-1.855777	-3.264999	0.651253
16	6	0	-2.007307	-2.686865	-0.601673
17	9	0	-0.637450	-3.435481	1.139735
18	9	0	-2.833441	-4.111492	2.616025
19	9	0	-5.305849	-3.618386	1.626789
20	9	0	-5.611410	-2.482893	-0.817101
21	9	0	-3.421091	-1.833250	-2.283224
22	6	0	2.764267	-1.218070	-3.577094
23	1	0	3.072747	-2.095147	-2.980526
24	8	0	2.033421	-1.621327	-4.706212
25	6	0	1.050014	-2.560412	-4.345366
26	1	0	0.308989	-2.611062	-5.144576
27	1	0	1.493752	-3.558420	-4.217749
28	6	0	0.363783	-2.208903	-3.045921
29	7	0	0.853589	-1.284101	-2.134782
30	7	0	-0.688027	-2.811549	-2.591099
31	7	0	-0.868982	-2.281892	-1.348026
32	6	0	0.050710	-1.351347	-1.046455
33	6	0	1.891328	-0.331955	-2.664107
34	1	0	1.315135	0.371571	-3.278935
35	6	0	3.996716	-0.386250	-3.875615
36	1	0	4.863648	-0.996581	-4.133585
37	1	0	3.791983	0.293484	-4.711493
38	6	0	1.433814	-0.048250	2.257624
39	6	0	1.309871	-0.683435	1.006778
40	6	0	2.415728	-1.379368	0.521703
41	6	0	3.646768	-1.310098	1.156817
42	6	0	3.806591	-0.612383	2.342487
43	6	0	2.679930	-0.007177	2.889087
44	1	0	2.364984	-1.934057	-0.405844
45	1	0	4.769922	-0.536892	2.831286
46	35	0	5.136689	-2.069513	0.287958
47	35	0	2.826264	0.940640	4.508065
48	8	0	0.354306	0.451534	2.916076
49	6	0	-0.105227	1.766199	2.624296
50	1	0	0.262959	2.440655	3.409586
51	1	0	0.283111	2.112307	1.656465
52	6	0	-2.301941	2.366320	1.664092

53	1	0	-1.767420	2.932422	0.907622
54	6	0	-3.779417	2.302364	1.506089
55	1	0	-4.168178	3.058595	0.826362
56	1	0	-4.338764	2.316175	2.438710
57	35	0	-4.279320	0.557609	0.672875
58	6	0	-1.614173	1.712977	2.609516
59	6	0	-2.236178	0.816983	3.638593
60	1	0	-3.318492	0.929390	3.701502
61	1	0	-2.005859	-0.220835	3.376527
62	1	0	-1.798163	0.998980	4.624029
63	6	0	0.069309	-0.485627	0.160514
64	8	0	-1.113288	-0.683058	0.889384
65	1	0	-0.052544	0.723147	-0.535195
66	6	0	0.213645	3.681411	-0.943161
67	6	0	-0.980411	2.869889	-1.415479
68	6	0	0.401779	5.029633	-1.650699
69	6	0	-2.488363	4.914612	-1.564239
70	6	0	-0.349400	6.159270	-0.945878
71	6	0	-1.742806	5.713854	-0.502018
72	1	0	0.156946	3.837906	0.142429
73	1	0	-2.385704	5.397935	-2.546224
74	1	0	0.066291	4.938370	-2.690258
75	1	0	-0.431756	7.020361	-1.616558
76	1	0	1.076421	3.042818	-1.126283
77	1	0	1.468717	5.261672	-1.695728
78	1	0	-3.555110	4.929098	-1.319147
79	1	0	0.216882	6.494993	-0.071071
80	1	0	-2.352270	6.591252	-0.267213
81	1	0	-1.696845	5.126717	0.422506
82	6	0	-3.264976	2.708001	-2.274109
83	1	0	-3.936077	2.369481	-1.473990
84	1	0	-3.827243	3.375899	-2.931815
85	6	0	-1.810778	0.734876	-2.129295
86	1	0	-1.323220	-0.053800	-2.713039
87	1	0	-2.405336	0.247671	-1.346670
88	6	0	-2.734990	1.517157	-3.043308
89	1	0	-3.560201	0.883799	-3.376843
90	1	0	-2.186827	1.860972	-3.926572
91	7	0	-0.774444	1.578956	-1.532290
92	7	0	-2.155956	3.481848	-1.695819
93	1	0	-1.677601	0.101147	0.826926

Int2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.427177	0.226657	-0.298533
2	6	0	5.760666	0.031286	-0.652219
3	6	0	6.766913	0.655893	0.075181
4	6	0	6.409372	1.466040	1.153358
5	6	0	5.070160	1.642998	1.503924
6	6	0	4.057113	1.016580	0.779213
7	6	0	3.518945	-0.524003	-1.245172
8	6	0	4.475547	-1.556578	-1.926386
9	6	0	5.863483	-0.888488	-1.845561
10	1	0	7.811418	0.510461	-0.184036
11	1	0	7.184452	1.959002	1.731596
12	1	0	4.806966	2.274307	2.345597
13	1	0	3.013358	1.119971	1.060904
14	1	0	4.170164	-1.754925	-2.955729
15	1	0	6.640922	-1.651901	-1.756168
16	1	0	3.055577	0.147058	-1.969101
17	1	0	6.059979	-0.318931	-2.761525
18	6	0	2.724951	-2.353952	0.163461
19	6	0	1.103887	-1.012703	-0.465350
20	7	0	1.655085	-2.881435	0.673283
21	7	0	2.437372	-1.222483	-0.544773
22	7	0	0.649026	-2.038143	0.278395
23	6	0	4.122417	-2.871943	0.073353
24	1	0	4.803958	-2.275524	0.692343
25	1	0	4.154224	-3.913341	0.393378
26	8	0	4.472573	-2.836504	-1.298839
27	6	0	-0.694808	-2.412105	0.638196
28	6	0	-1.423665	-3.175180	-0.278989
29	6	0	-1.156059	-2.119928	1.926415
30	6	0	-2.708109	-3.573599	0.091780
31	6	0	-2.443693	-2.548385	2.248299
32	6	0	-3.235676	-3.261409	1.345765
33	1	0	-3.301875	-4.152364	-0.610770
34	1	0	-2.834808	-2.323150	3.237338

35	6	0	-0.826882	-3.567348	-1.605135
36	1	0	0.105148	-4.121529	-1.455875
37	1	0	-1.517475	-4.199667	-2.164668
38	1	0	-0.595184	-2.689258	-2.217683
39	6	0	-4.628398	-3.686227	1.732944
40	1	0	-4.604270	-4.363315	2.591711
41	1	0	-5.232342	-2.819641	2.017850
42	1	0	-5.132514	-4.198023	0.910944
43	6	0	-0.282372	-1.421923	2.931302
44	1	0	0.079619	-0.461356	2.554068
45	1	0	-0.831221	-1.258153	3.860012
46	1	0	0.593367	-2.040201	3.153930
47	6	0	0.429566	0.093871	-1.227128
48	8	0	1.151637	1.067365	-1.528780
49	6	0	-0.952455	0.026942	-1.497836
50	1	0	-1.480960	-0.886825	-1.255792
51	6	0	-1.447125	0.799288	-2.693022
52	1	0	-1.378233	0.183625	-3.597440
53	1	0	-2.492546	1.102110	-2.584539
54	1	0	-0.824880	1.682969	-2.841496
55	6	0	0.489761	2.186627	0.812958
56	8	0	0.830326	1.132155	1.377142
57	6	0	-0.739075	2.394828	0.120731
58	6	0	-1.581269	1.276675	0.153803
59	1	0	-1.281041	0.529751	0.885234
60	6	0	-3.046304	1.249876	-0.087564
61	6	0	-3.694463	0.004078	-0.019798
62	6	0	-3.829055	2.391365	-0.307642
63	6	0	-5.060444	-0.116867	-0.203203
64	1	0	-3.104804	-0.883974	0.182079
65	6	0	-5.204383	2.290887	-0.491837
66	1	0	-3.373936	3.372501	-0.308358
67	6	0	-5.795515	1.038050	-0.446301
68	1	0	-5.562235	-1.075946	-0.162166
69	1	0	-5.820690	3.164971	-0.661157
70	7	0	-7.245750	0.927133	-0.644572
71	8	0	-7.739254	-0.185297	-0.581296
72	8	0	-7.867404	1.951537	-0.860295
73	6	0	1.484680	3.361159	0.910298
74	9	0	2.341798	3.169984	1.921179
75	9	0	2.204698	3.509015	-0.208717

76	9	0	0.862297	4.528356	1.146198
77	6	0	-0.958005	3.624157	-0.730219
78	1	0	-1.377885	4.464918	-0.166033
79	1	0	-0.015227	3.960531	-1.166574
80	1	0	-1.630614	3.400394	-1.560121

TS6*R*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.282571	1.944367	0.254579
2	6	0	-4.795489	0.960382	-0.604426
3	6	0	-3.515390	1.062914	-1.143871
4	6	0	-2.710487	2.134170	-0.773514
5	6	0	-3.248874	3.186132	-0.017452
6	6	0	-4.524076	3.080330	0.524503
7	1	0	-6.276717	1.845561	0.677918
8	1	0	-5.408544	0.102517	-0.863508
9	1	0	-3.172134	0.323371	-1.859287
10	1	0	-4.931633	3.887572	1.125411
11	6	0	4.247119	0.713383	-0.410285
12	6	0	5.361962	0.446949	0.367916
13	6	0	5.224760	0.348353	1.743523
14	6	0	3.986819	0.556580	2.345649
15	6	0	2.890516	0.878646	1.564838
16	6	0	3.005467	0.916273	0.177467
17	9	0	1.729300	1.170827	2.143024
18	9	0	3.877871	0.501917	3.668725
19	9	0	6.276617	0.055687	2.495199
20	9	0	6.534638	0.213693	-0.205388
21	9	0	4.361847	0.726431	-1.733380
22	6	0	-1.060422	3.878565	-0.581686
23	1	0	-0.431170	3.592344	0.276668
24	8	0	-0.356669	4.772800	-1.420232
25	6	0	0.543731	4.103333	-2.304136
26	1	0	0.088039	4.008158	-3.296958
27	1	0	1.455687	4.695399	-2.389121
28	6	0	0.913401	2.761100	-1.748262
29	7	0	-0.064895	1.841652	-1.368213

30	7	0	2.088173	2.458344	-1.328154
31	7	0	1.913897	1.285922	-0.638184
32	6	0	0.595505	0.878605	-0.598656
33	6	0	-1.385218	2.571931	-1.344015
34	1	0	-1.554127	2.809146	-2.401443
35	6	0	-2.382611	4.424779	-0.064681
36	1	0	-2.279926	4.939365	0.893056
37	1	0	-2.792290	5.136653	-0.790403
38	6	0	-2.049860	-1.423415	-0.714912
39	6	0	-1.178370	-0.771303	0.161299
40	6	0	-1.567019	-0.560458	1.489848
41	6	0	-2.803595	-0.986774	1.937193
42	6	0	-3.670928	-1.663055	1.084901
43	6	0	-3.286955	-1.869966	-0.226910
44	1	0	-0.869600	-0.074352	2.163748
45	1	0	-4.642407	-1.997905	1.427634
46	35	0	-3.334785	-0.650725	3.718640
47	35	0	-4.513166	-2.644640	-1.427944
48	8	0	-1.830872	-1.620749	-2.036293
49	6	0	-0.634261	-1.145235	-2.646255
50	1	0	-0.670614	-1.574427	-3.652226
51	1	0	-0.663929	-0.051472	-2.743844
52	6	0	1.872168	-1.180339	-2.422785
53	1	0	1.986836	-0.161749	-2.787191
54	6	0	3.012105	-2.003607	-2.403365
55	1	0	3.919444	-1.609847	-2.847060
56	1	0	2.890527	-3.074067	-2.509934
57	35	0	3.919933	-2.430825	-0.278286
58	6	0	0.618562	-1.612318	-1.953418
59	6	0	0.524000	-3.018869	-1.400232
60	1	0	1.419570	-3.293572	-0.842202
61	1	0	-0.341620	-3.160440	-0.754267
62	1	0	0.416478	-3.710080	-2.245947
63	6	0	0.234765	-0.433731	-0.190916
64	8	0	1.094784	-1.025498	0.719500
65	1	0	1.889668	-1.412712	0.297402

TS6*S*

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-5.000909	1.632102	-0.424804
2	6	0	-4.219953	0.713102	-1.125200
3	6	0	-2.870983	0.967215	-1.347952
4	6	0	-2.289014	2.119879	-0.840276
5	6	0	-3.095112	3.076068	-0.207190
6	6	0	-4.444917	2.829274	0.015542
7	1	0	-6.047583	1.419193	-0.234361
8	1	0	-4.647351	-0.225319	-1.467833
9	1	0	-2.268873	0.245057	-1.867972
10	1	0	-5.053831	3.564471	0.532560
11	6	0	4.334455	0.225166	0.851202
12	6	0	5.176993	-0.579251	1.608907
13	6	0	4.652586	-1.481151	2.522991
14	6	0	3.277325	-1.578536	2.688331
15	6	0	2.441273	-0.765743	1.941709
16	6	0	2.948926	0.103049	0.977695
17	9	0	1.134790	-0.816889	2.167761
18	9	0	2.770261	-2.414637	3.587563
19	9	0	5.463417	-2.240477	3.246657
20	9	0	6.493481	-0.466736	1.473821
21	9	0	4.888921	1.104438	0.039048
22	6	0	-0.901934	3.834459	0.055977
23	1	0	-0.673488	3.371434	1.031286
24	8	0	0.029093	4.838473	-0.244512
25	6	0	1.302292	4.316555	-0.601385
26	1	0	1.473694	4.494730	-1.670566
27	1	0	2.085025	4.824840	-0.034312
28	6	0	1.415068	2.848534	-0.334331
29	7	0	0.408873	1.956100	-0.670246
30	7	0	2.415259	2.275049	0.235601
31	7	0	2.078887	0.954608	0.251085
32	6	0	0.875000	0.704091	-0.341460
33	6	0	-0.879999	2.673474	-0.979108
34	1	0	-0.741365	3.084046	-1.988392
35	6	0	-2.332266	4.340182	0.092438
36	1	0	-2.588271	4.801675	1.048166
37	1	0	-2.478695	5.083526	-0.700148
38	6	0	-1.748609	-1.969286	-0.394443
39	6	0	-0.953032	-0.910658	0.061911

40	6	0	-1.416792	-0.132703	1.124783
41	6	0	-2.667706	-0.366108	1.673447
42	6	0	-3.470638	-1.404170	1.224575
43	6	0	-2.999310	-2.192951	0.180563
44	1	0	-0.812622	0.678708	1.516090
45	1	0	-4.457166	-1.571006	1.638863
46	35	0	-3.325828	0.824174	2.986053
47	35	0	-4.133545	-3.492278	-0.576812
48	8	0	-1.352776	-2.713360	-1.458544
49	6	0	-1.229300	-1.926406	-2.644477
50	1	0	-1.219086	-2.653738	-3.458617
51	1	0	-2.131741	-1.318168	-2.769413
52	6	0	1.179721	-1.906274	-3.046422
53	1	0	1.199184	-2.922474	-2.659653
54	6	0	2.284159	-1.418078	-3.736626
55	1	0	2.166607	-0.606135	-4.443344
56	1	0	3.094189	-2.099377	-3.972796
57	35	0	3.519880	0.075716	-2.381886
58	6	0	0.057187	-1.104714	-2.727717
59	6	0	-0.028532	0.242931	-3.411162
60	1	0	-0.145181	0.107746	-4.493586
61	1	0	-0.874510	0.841652	-3.069070
62	1	0	0.896338	0.803089	-3.239187
63	6	0	0.341645	-0.636066	-0.628379
64	8	0	1.283329	-1.611486	-0.335315
65	1	0	1.925046	-1.614879	-1.071742

Int6*R*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.523608	-0.102466	-1.485784
2	6	0	-4.549259	-0.774511	-2.228046
3	6	0	-3.257539	-0.272570	-2.312428
4	6	0	-2.935173	0.892588	-1.617181
5	6	0	-3.936569	1.622696	-0.966598
6	6	0	-5.228484	1.109363	-0.873591
7	1	0	-6.522157	-0.519908	-1.409578
8	1	0	-4.796147	-1.702168	-2.731908

9	1	0	-2.522598	-0.791572	-2.915200
10	1	0	-5.997696	1.666511	-0.347206
11	6	0	4.068820	0.423680	-1.336645
12	6	0	5.360709	0.224716	-0.879936
13	6	0	5.696999	0.606675	0.410568
14	6	0	4.747584	1.170921	1.254262
15	6	0	3.454295	1.347079	0.799665
16	6	0	3.104625	0.935430	-0.482039
17	9	0	2.536056	1.894421	1.583671
18	9	0	5.080495	1.520498	2.486814
19	9	0	6.928178	0.415380	0.848985
20	9	0	6.274509	-0.308283	-1.681845
21	9	0	3.768860	0.157858	-2.606514
22	6	0	-1.982703	2.960472	-0.783286
23	1	0	-1.502286	2.727207	0.177812
24	8	0	-1.428418	4.147396	-1.321306
25	6	0	-0.258859	3.943746	-2.105900
26	1	0	-0.519121	3.937364	-3.172170
27	1	0	0.431360	4.769603	-1.925825
28	6	0	0.448319	2.672118	-1.735816
29	7	0	-0.247052	1.495958	-1.500326
30	7	0	1.699354	2.552910	-1.438072
31	7	0	1.812446	1.282035	-0.978607
32	6	0	0.637420	0.621132	-0.949557
33	6	0	-1.716375	1.769931	-1.734184
34	1	0	-1.708229	2.136188	-2.767288
35	6	0	-3.492374	3.014689	-0.578174
36	1	0	-3.754690	3.282138	0.447988
37	1	0	-3.931317	3.754615	-1.256599
38	6	0	-1.956542	-1.592067	0.017669
39	6	0	-1.002127	-0.655295	0.412465
40	6	0	-1.325384	0.315471	1.361033
41	6	0	-2.607436	0.371509	1.873007
42	6	0	-3.545141	-0.612578	1.565498
43	6	0	-3.202267	-1.604950	0.665457
44	1	0	-0.557078	1.010143	1.688939
45	1	0	-4.534198	-0.597541	2.007237
46	35	0	-3.109643	1.824706	2.972651
47	35	0	-4.430896	-2.969916	0.267562
48	8	0	-1.748685	-2.481970	-0.975539
49	6	0	-0.583146	-2.251873	-1.756577

50	1	0	-0.460448	-3.140885	-2.376895
51	1	0	-0.749773	-1.385191	-2.416637
52	6	0	1.826988	-1.901787	-1.864360
53	1	0	1.686558	-1.187167	-2.678951
54	6	0	2.967918	-2.580472	-1.794401
55	1	0	3.749035	-2.408228	-2.528836
56	1	0	3.191617	-3.269105	-0.988245
57	35	0	3.896237	-2.013210	1.387105
58	6	0	0.664819	-2.024176	-0.908437
59	6	0	0.795698	-3.198155	0.071189
60	1	0	1.715287	-3.147918	0.655308
61	1	0	-0.049439	-3.227901	0.761855
62	1	0	0.795895	-4.128177	-0.505254
63	6	0	0.435451	-0.698682	-0.107848
64	8	0	1.261763	-0.536582	0.982127
65	1	0	2.122653	-1.095055	1.001956

Int6*S*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.047163	3.195354	0.030390
2	6	0	-4.493329	1.924698	-0.093937
3	6	0	-3.112180	1.735842	-0.003844
4	6	0	-2.295885	2.837800	0.197579
5	6	0	-2.860725	4.112429	0.387732
6	6	0	-4.231273	4.297426	0.291450
7	1	0	-6.121780	3.325361	-0.042923
8	1	0	-5.137239	1.065721	-0.252248
9	1	0	-2.696357	0.739163	-0.073589
10	1	0	-4.664731	5.281000	0.445553
11	6	0	4.060575	0.017868	0.418246
12	6	0	5.128909	-0.860232	0.263078
13	6	0	4.918285	-2.229151	0.296730
14	6	0	3.634667	-2.726075	0.485535
15	6	0	2.575853	-1.848898	0.650773
16	6	0	2.759473	-0.468352	0.572275
17	9	0	1.371637	-2.355137	0.867484
18	9	0	3.431256	-4.038707	0.537750

19	9	0	5.938458	-3.064380	0.154672
20	9	0	6.359487	-0.382272	0.110268
21	9	0	4.334068	1.309247	0.443319
22	6	0	-0.805652	4.103671	1.412589
23	1	0	-1.271543	3.657862	2.308478
24	8	0	0.468686	4.565289	1.743434
25	6	0	1.093612	3.534797	2.479651
26	1	0	2.137047	3.805165	2.639820
27	1	0	0.598146	3.404947	3.452548
28	6	0	1.072060	2.249506	1.693820
29	7	0	0.137215	1.949043	0.702124
30	7	0	1.971110	1.343430	1.798166
31	7	0	1.682123	0.433398	0.807287
32	6	0	0.722690	0.951449	-0.064064
33	6	0	-0.790522	3.014976	0.317578
34	1	0	-0.374253	3.461663	-0.596842
35	6	0	-1.800564	5.102039	0.830322
36	1	0	-2.163049	5.827179	1.560764
37	1	0	-1.342128	5.640978	-0.007705
38	6	0	-1.756361	-1.779170	-1.049847
39	6	0	-0.958316	-0.908281	-0.295538
40	6	0	-1.025483	-0.981163	1.096559
41	6	0	-1.842317	-1.923094	1.705892
42	6	0	-2.598561	-2.820223	0.964774
43	6	0	-2.556922	-2.733050	-0.418813
44	1	0	-0.435017	-0.332134	1.728480
45	1	0	-3.224706	-3.558644	1.450063
46	35	0	-1.909190	-1.998681	3.593001
47	35	0	-3.616726	-3.883158	-1.462660
48	8	0	-1.808348	-1.657896	-2.396770
49	6	0	-1.894850	-0.281309	-2.750466
50	1	0	-2.121979	-0.255410	-3.818100
51	1	0	-2.728630	0.175907	-2.202719
52	6	0	0.331120	-0.014776	-3.627711
53	1	0	0.281228	-1.088274	-3.797763
54	6	0	1.089019	0.738382	-4.416935
55	1	0	1.203464	1.806695	-4.271080
56	1	0	1.648807	0.288467	-5.230732
57	35	0	2.193159	2.201706	-1.533954
58	6	0	-0.578908	0.478546	-2.503422
59	6	0	-0.937113	1.954118	-2.710726

60	1	0	-1.330479	2.054122	-3.727228
61	1	0	-1.724579	2.277056	-2.032309
62	1	0	-0.072184	2.605865	-2.619442
63	6	0	0.043317	-0.033430	-1.077759
64	8	0	1.084347	-0.924391	-1.412127
65	1	0	1.720969	-0.392084	-1.928781

TS7*R*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.410345	-0.244919	-1.640398
2	6	0	-4.363825	-0.817102	-2.368304
3	6	0	-3.110729	-0.216195	-2.391265
4	6	0	-2.902059	0.943780	-1.647847
5	6	0	-3.973945	1.568816	-0.998647
6	6	0	-5.226920	0.960367	-0.971368
7	1	0	-6.378169	-0.734915	-1.617283
8	1	0	-4.526350	-1.738382	-2.916875
9	1	0	-2.321609	-0.642569	-2.998280
10	1	0	-6.052873	1.437286	-0.452515
11	6	0	3.979547	0.502058	-1.446573
12	6	0	5.279494	0.243476	-1.041783
13	6	0	5.680530	0.587499	0.239584
14	6	0	4.784271	1.164220	1.129896
15	6	0	3.480328	1.387738	0.731108
16	6	0	3.063989	1.031823	-0.548895
17	9	0	2.608151	1.918606	1.576600
18	9	0	5.171524	1.456146	2.364041
19	9	0	6.917132	0.327901	0.632612
20	9	0	6.139138	-0.317446	-1.886203
21	9	0	3.627938	0.253599	-2.703933
22	6	0	-2.113275	2.989811	-0.639035
23	1	0	-1.686105	2.670212	0.322630
24	8	0	-1.571458	4.246503	-1.001086
25	6	0	-0.369595	4.174026	-1.763096
26	1	0	-0.596934	4.259988	-2.832508
27	1	0	0.273510	5.007593	-1.478313
28	6	0	0.377230	2.897793	-1.509850

29	7	0	-0.288261	1.683323	-1.435890
30	7	0	1.634025	2.765809	-1.240644
31	7	0	1.767557	1.435781	-0.971154
32	6	0	0.609546	0.751071	-1.035569
33	6	0	-1.750064	1.912065	-1.683864
34	1	0	-1.754333	2.363604	-2.682856
35	6	0	-3.633672	2.966021	-0.530237
36	1	0	-3.977823	3.182870	0.483183
37	1	0	-4.066392	3.706058	-1.212706
38	6	0	-1.939871	-1.651949	0.020233
39	6	0	-0.985874	-0.726435	0.449947
40	6	0	-1.324233	0.249204	1.388821
41	6	0	-2.617756	0.312164	1.869447
42	6	0	-3.559191	-0.657956	1.527270
43	6	0	-3.204358	-1.648308	0.629787
44	1	0	-0.566472	0.952455	1.721204
45	1	0	-4.560423	-0.631896	1.940586
46	35	0	-3.130255	1.755822	2.975071
47	35	0	-4.435253	-2.999562	0.192500
48	8	0	-1.704624	-2.555776	-0.952082
49	6	0	-0.533970	-2.323496	-1.731347
50	1	0	-0.400538	-3.216388	-2.342717
51	1	0	-0.698713	-1.463922	-2.392542
52	6	0	1.870833	-1.900430	-1.807095
53	1	0	1.714515	-1.158447	-2.590858
54	6	0	3.026050	-2.554977	-1.752727
55	1	0	3.810096	-2.339001	-2.472736
56	1	0	3.250608	-3.279976	-0.979356
57	35	0	3.988198	-2.004256	1.518572
58	6	0	0.702582	-2.084634	-0.870382
59	6	0	0.865265	-3.274229	0.090195
60	1	0	1.765120	-3.186378	0.699802
61	1	0	0.001705	-3.360037	0.753407
62	1	0	0.931613	-4.189770	-0.503693
63	6	0	0.439035	-0.817395	-0.031707
64	8	0	1.285055	-0.587419	0.987705
65	1	0	2.171330	-1.072050	0.949104

P*R*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.455922	0.625137	-0.110272
2	6	0	-0.503262	-0.775417	-0.122318
3	6	0	0.674300	-1.526805	-0.082708
4	6	0	1.891861	-0.878287	-0.016307
5	6	0	1.958602	0.515799	0.018252
6	6	0	0.791646	1.259525	-0.029791
7	1	0	0.599097	-2.608543	-0.093431
8	1	0	2.916733	1.018524	0.074783
9	35	0	3.497551	-1.872268	0.037659
10	35	0	0.872233	3.138044	0.001472
11	8	0	-1.564104	1.390743	-0.160783
12	6	0	-2.729300	0.743977	-0.669092
13	1	0	-3.545885	1.455448	-0.535284
14	1	0	-2.587400	0.558451	-1.743260
15	6	0	-4.241721	-1.205590	-0.586623
16	1	0	-4.071190	-1.597755	-1.588245
17	6	0	-5.453052	-1.296705	-0.050153
18	1	0	-6.271169	-1.749083	-0.599593
19	1	0	-5.674614	-0.941618	0.951178
20	6	0	-3.037205	-0.569608	0.061789
21	6	0	-3.210698	-0.309619	1.564084
22	1	0	-3.436245	-1.244099	2.082698
23	1	0	-2.303291	0.123361	1.991960
24	1	0	-4.028660	0.396584	1.732777
25	6	0	-1.818571	-1.478059	-0.112949
26	8	0	-1.903384	-2.683184	-0.192544

HBr

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	0.000000	0.000000	0.039190
2	1	0	0.000000	0.000000	-1.371653