Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

Understanding the *Z* selectivity of the metal-free intermolecular aminoarylation of alkynes: A DFT study

Huining Bai,[a] Huimin Zhang,[a] Yuen Guo,[a] Hui Chen,[b] Donghui Wei,[a] Shijun Li,[a] Yanyan Zhu[a] and Wenjing Zhang *[a]

[a] College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou, Henan Province 450001, P. R. China

[b] Institute of Chemistry Henan Academy of Sciences, Zhengzhou 450002, P.R. China

Contents

Part 1: Flexible scanning results from **CP1**, **Int5** and **Int8**.

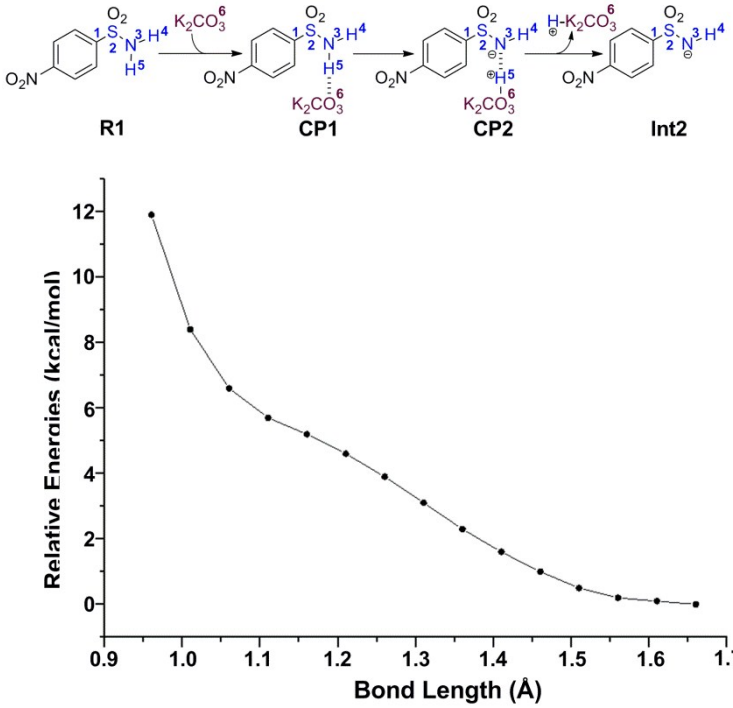


Figure S1 The flexible scanning curve to the bond length of H5–O6 from the optimized structure of **CP1**.

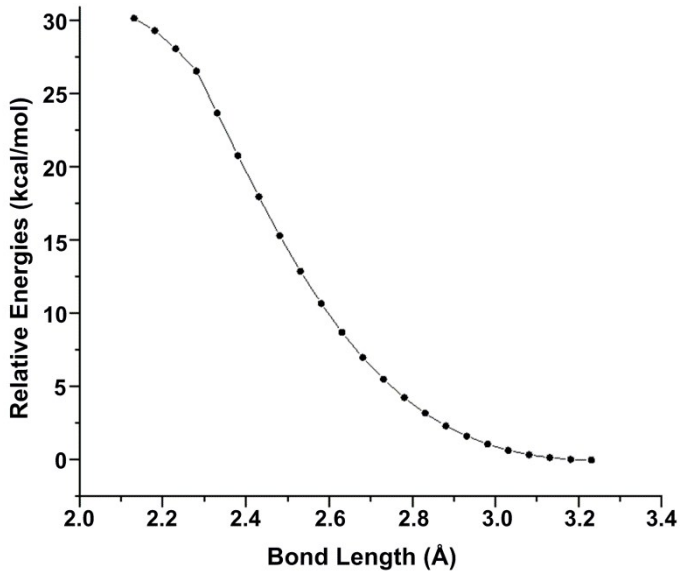


Figure S2 The flexible scanning curve to the bond length of C1–S2 from the optimized structure of **Int5**

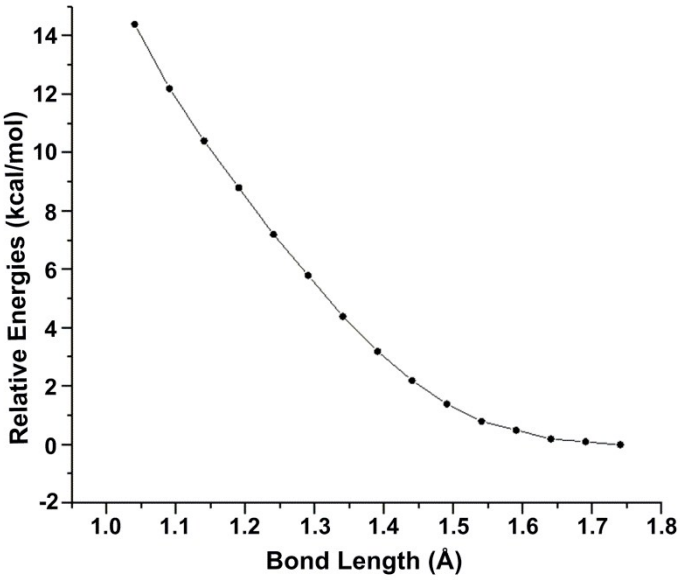


Figure S3 The flexible scanning curve to the bond length of H4–O6' from the optimized structure of **Int8**

Part 2: Optimized geometries of all structures involved in Mechanisms I and II.

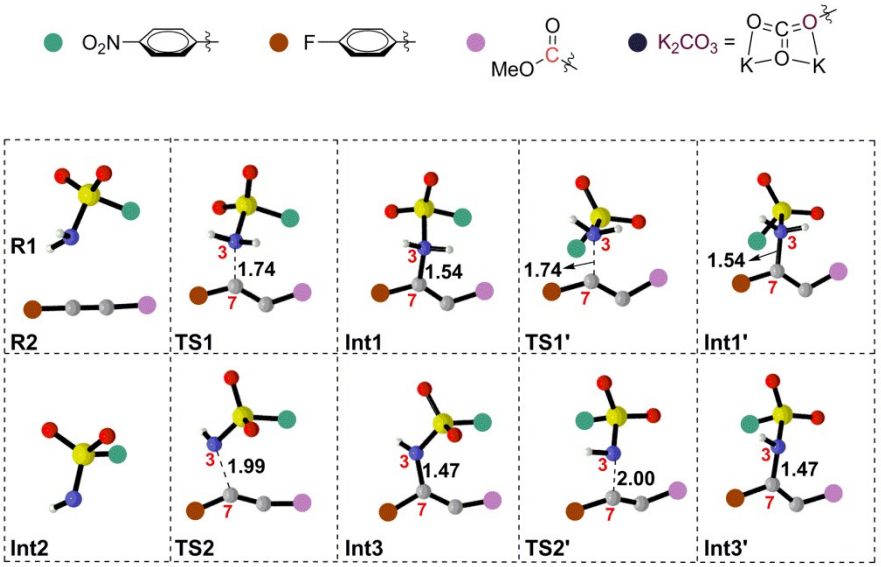


Figure S4 Optimized geometries of all structures involved in Stage I. All three-dimensional structures are represented using CYLView.[1] Bond lengths in Å. All hydrogen atoms except for these in the reactive center are omitted for brevity.

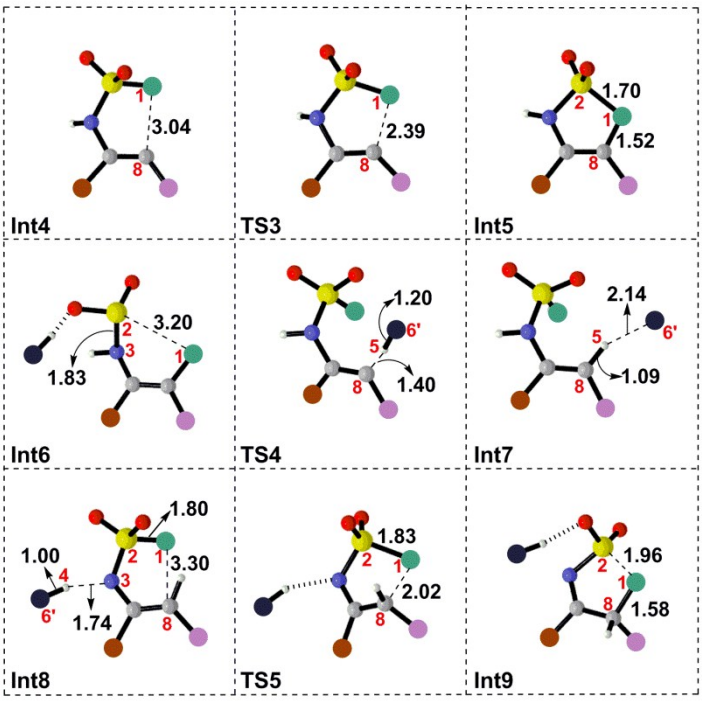


Figure S5 Optimized geometries of all structures involved in Stage II. All three-dimensional structures are represented using CYLView. Bond lengths in Å. All hydrogen atoms except for these in the reactive center are omitted for brevity.

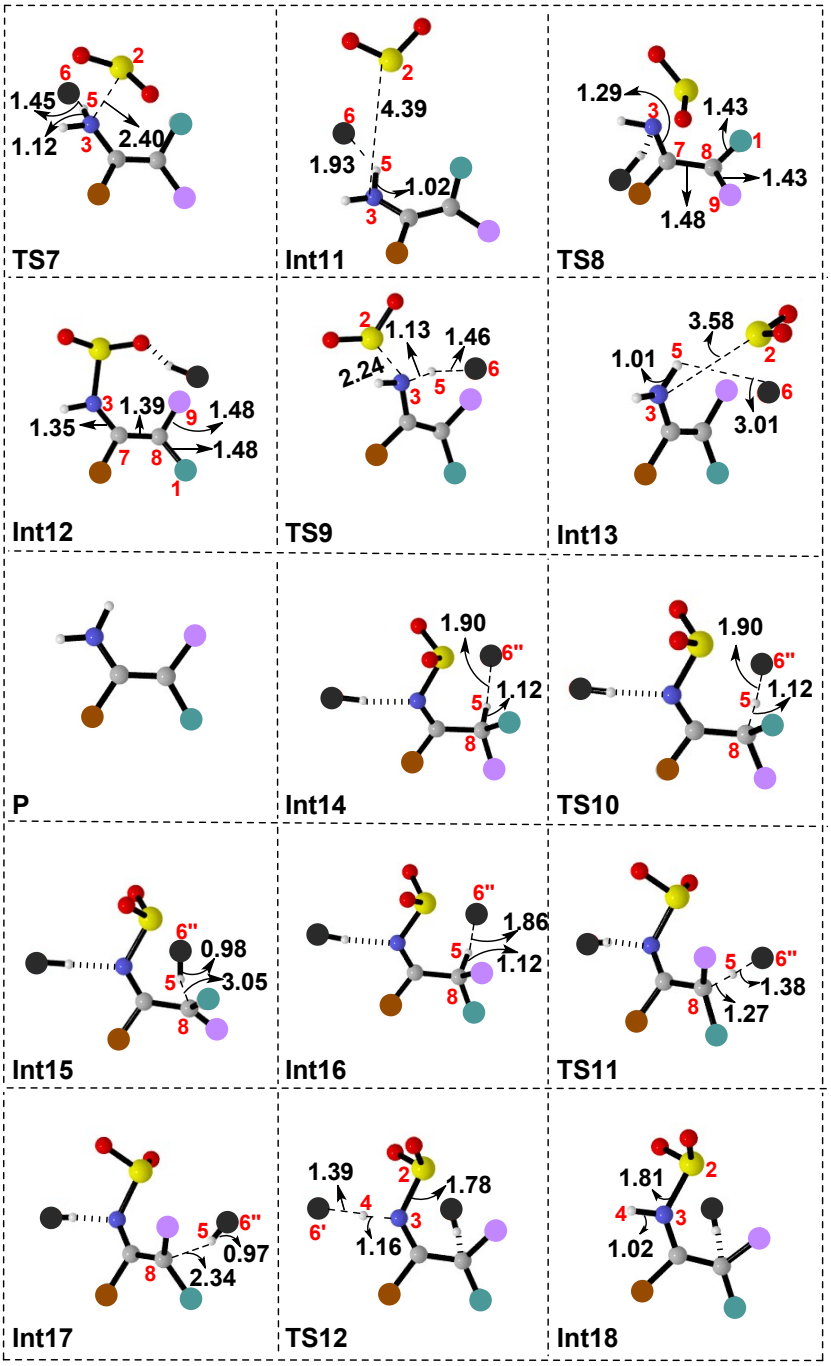
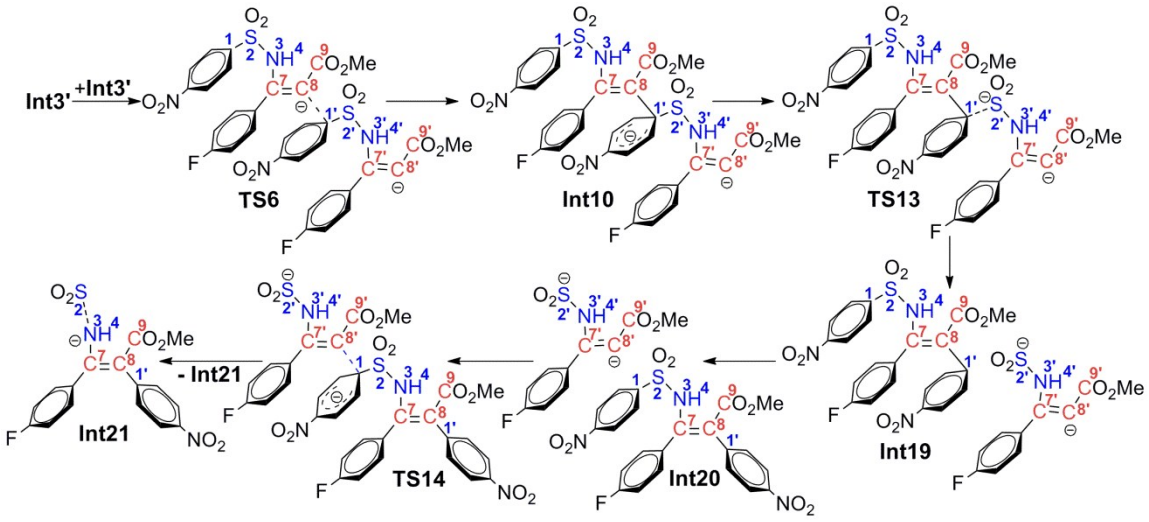


Figure S6 Optimized geometries of all structures involved in Stage III. All three-dimensional structures are represented using CYLView. Bond lengths in Å. All hydrogen atoms except for these in the reactive center are omitted for brevity.

References:

1. C. Y. Legault *Cylview*, 1.0b; (http://www.cylview.org/); Université de Sherbrooke, 2009.

Part 3: Mechanism of Path b3.



Scheme S1 Proposed mechanism of Path b3.

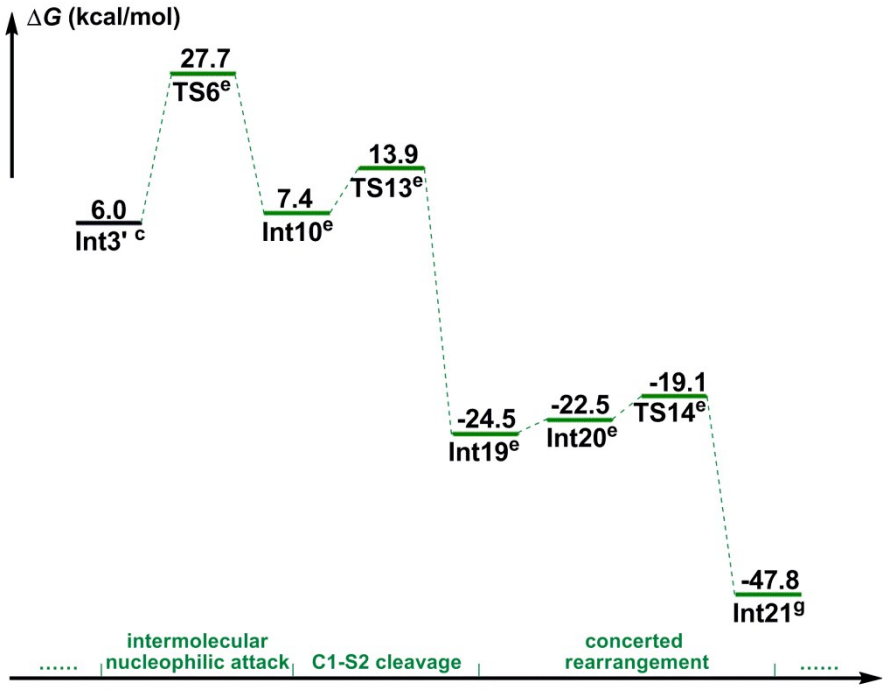


Figure S7 Gibbs free energy profiles of Path b3. Energies **R1**+**R2**+K_2CO_3+**Int3'** were set as 0.0 kcal/mol. The superscripts represent adding energies of (b) **R2** + K_2CO_3 + K_2CO_3-H^+, (c) K_2CO_3-H^+ + K_2CO_3, (d) K_2CO_3, (e) K_2CO_3-H^+, (f) SO_2 + 2 × K_2CO_3, (g) K_2CO_3-H^+ + **Int3.**

Part 4: The calculated Gibbs free energy profiles of the possible direct cleavage of the C1-S2 bond.

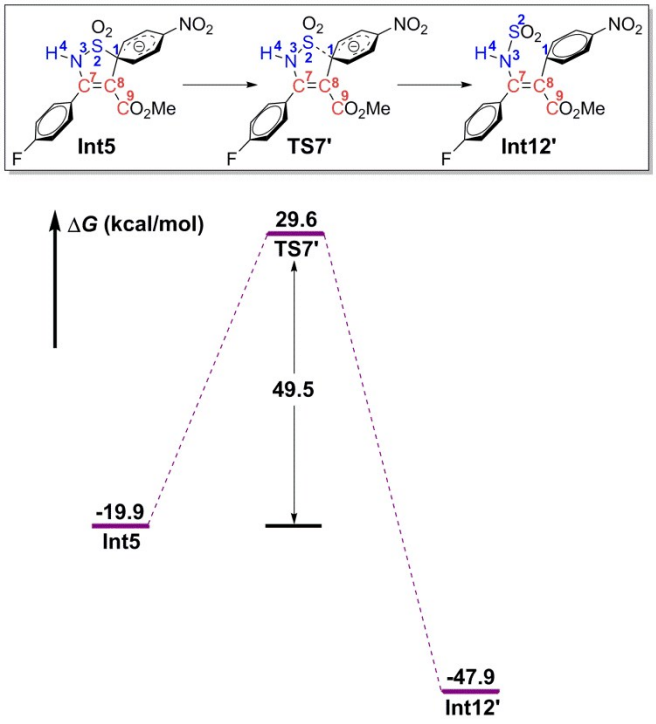


Figure S8 The calculated Gibbs free energy profiles of the possible direct cleavage of the **C1-S2** bond.

Part 5: The Gibbs free energy profiles of the whole reaction going through Mechanism I and Mechanism II.

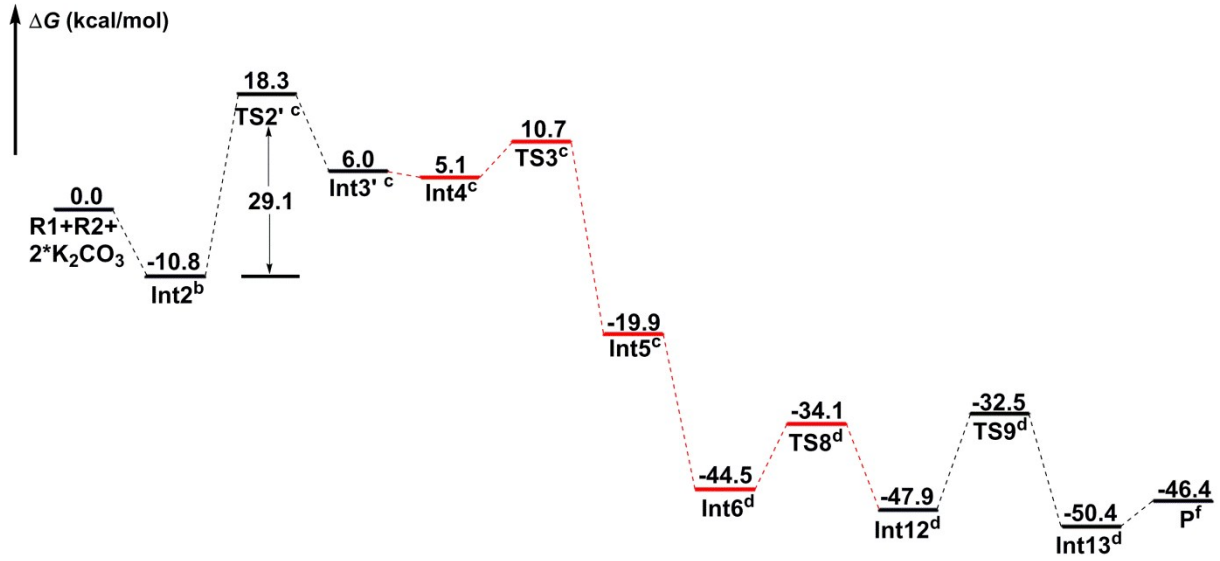


Figure S9 Gibbs free energy profiles of the whole reaction going through Mechanism I. The superscripts represent adding energies of (b) **R2** + K_2CO_3 + K_2CO_3-H^+, (c) K_2CO_3-H^+ + K_2CO_3, (d) K_2CO_3, (e) K_2CO_3-H^+, (f) SO_2 + 2 × K_2CO_3.

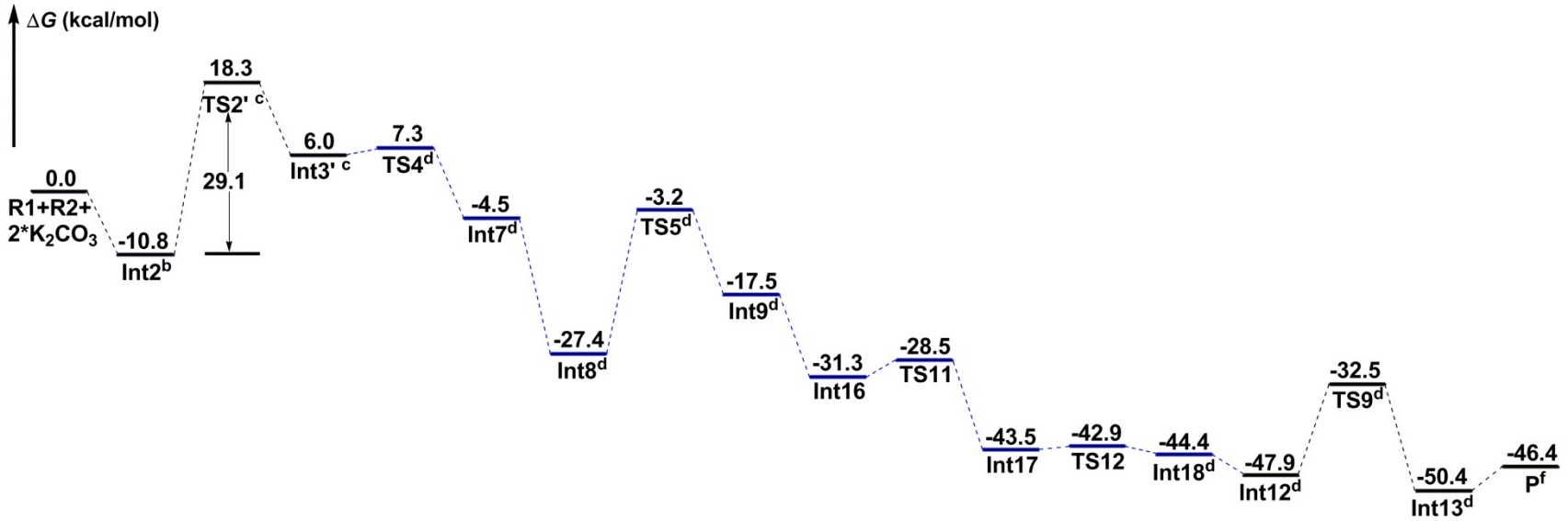
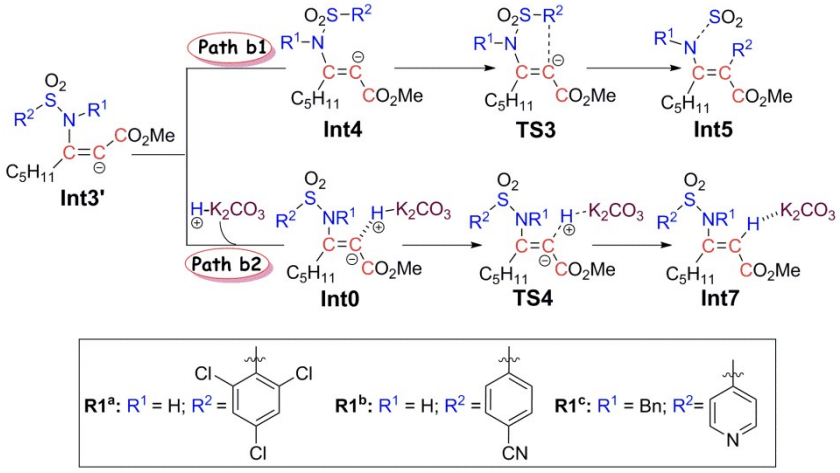


Figure S10 Gibbs free energy profiles of the whole reaction going through Mechanism II. The superscripts represent adding energies of (b) **R2** + K_2CO_3 + K_2CO_3-H^+, (c) K_2CO_3-H^+ + K_2CO_3, (d) K_2CO_3, (e) K_2CO_3-H^+, (f) SO_2 + 2 × K_2CO_3**.**

Part 6: Substituent effect studies.

Based on the experimental results, we selected three sulfonamides (denoted as **R1[a]**, **R1[b]**, **R1[c]**, as shown in Scheme S2) to check whether the novel mechanism we newly proposed or the Similes rearrangement mechanism is more favorable. Accordingly, the transformation of the anionic adduct **Int3'** through Paths b1 and b2 was calculated. All calculated results were listed in Table S1. As we can see, the energy barriers of the nucleophilic attack reaction via **TS3[a]**, **TS3[b]** and **TS3[c]** are 5.9, 6.8, and 6.9 kcal/mol, respectively, while the protonation of the carbon anion via **TS4**s are all barrierless since the ΔG are all negative. That's to say, for no matter the triply chlorinated sulfonamide (**R1[a]**), the electron-deficient group (**R1[b]**), or even the heteroaryl substrate (**R1[c]**), Path b2 is always more favorable over Path b1. Therefore, we have one more reason to believe that the conclusion that the title reaction is more likely to occur through the novel mechanism we proposed should be reliable to be extrapolated to other groups, at least those reported by Greaney (*Angew. Chem. Int. Ed.*, 2017, **56**, 4183).



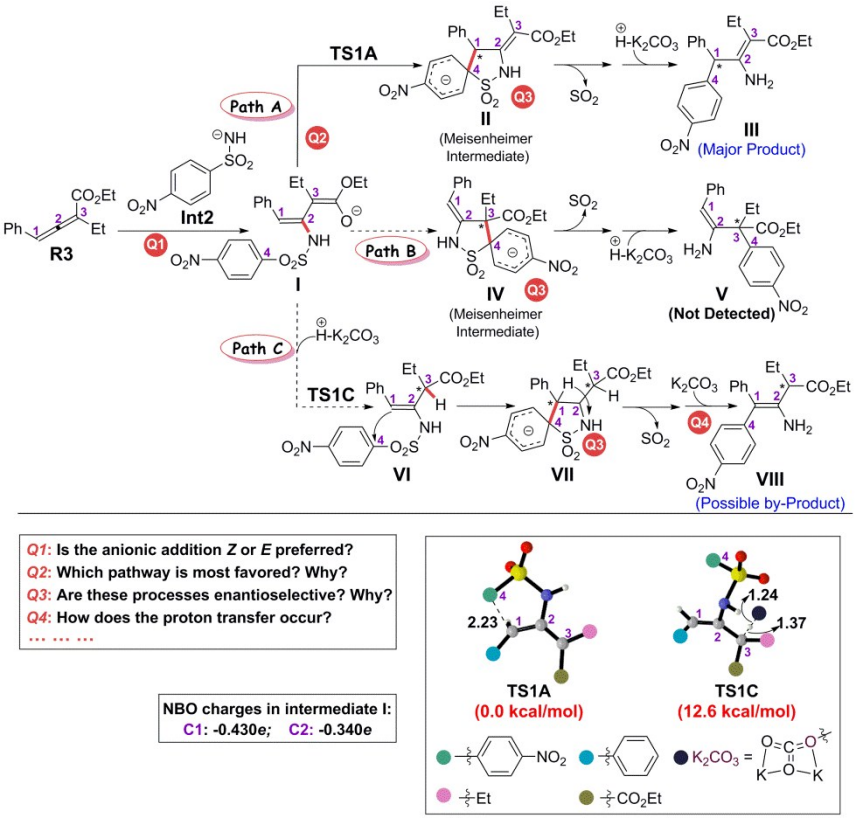
Scheme S2 Details of further transformation of **Int3'** through Paths b1 and b2 with the sulfonamides being **R1[a]**, **R1[b]** and **R1[c]**.

Table S1 The relative Gibbs free energies and corresponding barriers of reactions of selected substrates through Paths b1 and b2. (Unit: kcal/mol)

Sulfonamide substrates	Path b1					Path b2				
	Int3'	**Int4**	**TS3**	**Int5'**	ΔG	**Int3'**	**Int0**	**TS4**	**Int7**	ΔG
R1[a]	0.0	-3.2	2.7	-70.9	5.9	0.0	-0.6	-0.8	-11.7	-0.2
R1[b]	0.0	-1.4	5.4	-57.0	6.8	0.0	-2.1	-3.1	-11.8	-1.0
R1[c]	0.0	-5.2	1.7	-60.5	6.9	0.0	-1.5	-2.8	-12.3	-1.3

Part 7: Possible reaction mechanisms of allene.

Although the basic processes are similar, there are much more detailed issues that need to be addressed for the reaction of allene before we can get thorough understanding to the mechanism and stereoselectivities. As shown in the Scheme S3, for example, does the anionic addition prefer to give intermediate **I** in *Z* or in *E* geometry? Will the nucleophilic attack (Paths A & B, Smiles rearrangement) or the protonation of the C3 atom (Path C, the novel mechanism we proposed) follows up? Whether the reaction is enantioselective or not? If yes, what's the origin of the selectivity? How should the proton transfer being accomplished in Path C? Therefore, to absolutely make clear the mechanism and the stereoselectivity of the aminoarylation of allene is really a complicated work which is far beyond the scope of our current study. Nonetheless, we have carried out some brief calculations to address whether the Similes rearrangement or the novel mechanism we proposed is more possible to occur.



Scheme S3 Possible reaction mechanisms of allene, NBO charges in intermediate **I**, and the optimized geometries of **TS1A** and **TS1C**.

As it is shown, given the anionic adduct **I**, the Meisenheimer intermediate is possible to be formed by nucleophilic attack of the C1 (Path A) or the C3 atom (Path A) to the C4 atom, determined by which one is more nucleophilic. The NBO analysis disclosed that the C1 atom (-0.430 *e*) is obviously more negative than the C3 atom (-0.340 *e*), which helps to reasonably exclude Path B. In regarding Path A and Path C, we have calculated the transition states **TS1A** and **TS1C** which corresponds to formation of Meisenheimer intermediate **II** and the protonation of the C3 atom, respectively. The results reveal that the energy barrier via **TS1A** is 12.6 kcal/mol higher than that via **TS1C**, indicating the Smiles rearrangement mechanism is more favorable for the reaction of allene. All these results are in good agreement with the experimental fact that **III** is the main product. However, for the tentative by-product **VIII**, we still have no idea about whether it is formed through Path C or the isomerization of the major product **III**.

Part 8: List of Cartesian coordinates of all structures involved in this work

R1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.320987	-1.219482	-0.038432
2	6	0	0.067395	-1.202248	-0.073960
3	6	0	0.725096	0.026467	-0.073854
4	6	0	0.045823	1.239381	-0.043145
5	6	0	-1.346097	1.228079	-0.006754
6	6	0	-1.991246	-0.000913	-0.004028
7	1	0	-1.874280	-2.149966	-0.039621
8	1	0	0.630031	-2.129022	-0.106764
9	1	0	0.593518	2.174743	-0.055398
10	1	0	-1.916602	2.147842	0.016030
11	7	0	-3.465330	-0.015798	0.031528
12	8	0	-4.044730	1.055629	0.063079
13	8	0	-4.023104	-1.099106	0.027857
14	16	0	2.509542	0.033042	-0.115398
15	8	0	2.925382	1.390698	-0.453635
16	8	0	2.954373	-1.091764	-0.932546
17	7	0	2.907168	-0.351603	1.444638
18	1	0	3.735880	-0.942669	1.466855
19	1	0	3.010636	0.470843	2.035096

R2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.687398	0.224242	0.000089
2	6	0	0.478493	0.154135	-0.000017
3	6	0	-0.950058	0.066731	-0.000004
4	6	0	-1.576761	-1.189808	-0.000068
5	6	0	-1.725756	1.237138	0.000053
6	6	0	-2.963301	-1.279771	-0.000074
7	1	0	-0.973382	-2.090921	-0.000115
8	6	0	-3.112956	1.156711	0.000051
9	1	0	-1.237495	2.205497	0.000098
10	6	0	-3.697383	-0.102059	-0.000013

11	1	0	-3.472751	-2.236407	-0.000125
12	1	0	-3.735747	2.043756	0.000096
13	9	0	-5.042497	-0.184875	-0.000018
14	6	0	3.129204	0.365786	0.000166
15	8	0	3.704733	1.433439	-0.000214
16	8	0	3.740493	-0.818760	0.000337
17	6	0	5.176945	-0.774113	-0.000175
18	1	0	5.498069	-1.812650	-0.002175
19	1	0	5.533200	-0.256727	-0.892069
20	1	0	5.533827	-0.260065	0.893424

SO_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000000	0.379682	0.000000
2	8	0	1.235298	-0.379677	0.000000
3	8	0	-1.235298	-0.379687	0.000000

K_2CO_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000001	0.857837	0.000406
2	8	0	1.125009	1.488414	0.014873
3	8	0	-0.000139	-0.449329	0.001498
4	8	0	-1.124865	1.488585	-0.015239
5	19	0	2.616168	-0.667596	-0.003028
6	19	0	-2.616170	-0.667582	0.002423

K_2CO_3-H^+

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.927010	2.444378	0.000254
2	6	0	0.101614	0.823635	0.000225
3	8	0	-1.109976	1.494881	0.000664
4	8	0	-0.013268	-0.425283	0.001126

5	8	0	1.141567	1.510243	-0.000982
6	19	0	-2.677182	-0.750515	-0.000361
7	19	0	2.686168	-0.724481	-0.000064

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.594863	-0.616599	-0.092139
2	6	0	-2.475255	-1.406961	0.144040
3	6	0	-1.205531	-0.093824	-1.493871
4	6	0	-2.325197	0.694684	-1.727020
5	6	0	-3.485355	0.411471	-1.017912
6	1	0	-4.528321	-0.793141	0.427148
7	1	0	-2.511778	-2.230969	0.848705
8	1	0	-0.279051	0.082438	-2.029376
9	1	0	-2.300625	1.510033	-2.438516
10	7	0	-4.670944	1.259204	-1.258200
11	8	0	-5.679334	1.016814	-0.619965
12	8	0	-4.571436	2.152428	-2.079644
13	6	0	-1.306701	-1.121382	-0.557626
14	6	0	0.546771	1.323986	1.074229
15	6	0	1.417718	0.454053	0.688934
16	6	0	-0.759838	1.118699	1.647437
17	8	0	-1.798962	1.653023	1.300478
18	8	0	-0.730023	0.244916	2.699003
19	6	0	-1.951518	0.108908	3.438465
20	1	0	-2.237007	1.071294	3.867116
21	1	0	-2.752303	-0.252062	2.790308
22	1	0	-1.740520	-0.612439	4.225238
23	6	0	2.809315	0.528925	0.211057
24	6	0	3.463533	-0.480137	-0.504676
25	6	0	3.508015	1.715315	0.496326
26	6	0	4.782940	-0.318210	-0.926449
27	1	0	2.951035	-1.394830	-0.778700
28	6	0	4.821545	1.890876	0.082679
29	6	0	5.433866	0.863310	-0.621575
30	1	0	5.294699	-1.092878	-1.486073
31	1	0	5.369129	2.800255	0.303486
32	9	0	6.713285	1.026151	-1.024813
33	7	0	1.012655	-1.246388	0.916355
34	16	0	0.104154	-2.155422	-0.288997

35	8	0	0.945363	-2.161856	-1.469556
36	8	0	-0.306378	-3.387629	0.357157
37	1	0	3.003303	2.498999	1.050197
38	1	0	1.855695	-1.796722	1.130127
39	1	0	0.447230	-1.208549	1.779336

Int1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.564100	0.636903	-0.196302
2	6	0	2.439823	1.439897	-0.048902
3	6	0	1.166559	-0.087690	-1.501978
4	6	0	2.297998	-0.886893	-1.636191
5	6	0	3.456299	-0.499361	-0.984219
6	1	0	4.502937	0.884028	0.281909
7	1	0	2.475282	2.347813	0.543237
8	1	0	0.241463	-0.336874	-1.998121
9	1	0	2.279743	-1.785035	-2.233234
10	7	0	4.647576	-1.355882	-1.132973
11	8	0	5.661617	-1.018358	-0.551722
12	8	0	4.545388	-2.349262	-1.827567
13	6	0	1.278899	1.051513	-0.712209
14	6	0	-0.569258	-1.194868	1.208903
15	6	0	-1.315131	-0.044447	0.769352
16	6	0	0.757257	-0.890406	1.715110
17	8	0	1.811252	-1.439868	1.428346
18	8	0	0.760604	0.048809	2.746830
19	6	0	2.004521	0.240705	3.421717
20	1	0	2.330737	-0.687488	3.889780
21	1	0	2.776953	0.566146	2.718368
22	1	0	1.828523	1.009647	4.172715
23	6	0	-2.742606	-0.427650	0.301412
24	6	0	-3.534489	0.548074	-0.326619
25	6	0	-3.334391	-1.695788	0.487204
26	6	0	-4.841407	0.306035	-0.735054
27	1	0	-3.139553	1.537638	-0.545936
28	6	0	-4.645117	-1.961990	0.085248
29	6	0	-5.383856	-0.946833	-0.513824
30	1	0	-5.433916	1.073079	-1.215053
31	1	0	-5.093821	-2.932652	0.236056
32	9	0	-6.655621	-1.180484	-0.904359

33	7	0	-1.010253	1.068907	0.883309
34	16	0	-0.144315	2.062525	-0.557606
35	8	0	-1.057923	1.886157	-1.648617
36	8	0	0.187151	3.352829	-0.001960
37	1	0	-2.730476	-2.469598	0.957140
38	1	0	-1.865610	1.623973	1.095476
39	1	0	-0.366421	1.224049	1.700573

TS1'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.077438	-2.161309	-0.679017
2	6	0	-0.159893	-1.793698	-0.160418
3	6	0	0.959297	-0.705446	1.730433
4	6	0	2.196145	-1.056654	1.201855
5	6	0	2.218260	-1.772205	0.010699
6	1	0	1.157208	-2.719203	-1.603355
7	1	0	-1.081252	-2.049614	-0.672749
8	1	0	0.892792	-0.154209	2.662533
9	1	0	3.119051	-0.783603	1.697747
10	7	0	3.532825	-2.119404	-0.566901
11	8	0	3.545670	-2.770339	-1.595850
12	8	0	4.527647	-1.727185	0.015560
13	6	0	-0.187360	-1.071779	1.029108
14	6	0	-2.040376	1.086541	-1.531845
15	6	0	-1.217876	1.353383	-0.571928
16	6	0	-3.393092	0.631044	-1.298198
17	8	0	-4.218125	1.211359	-0.592169
18	8	0	-3.683316	-0.509487	-1.939113
19	6	0	0.196821	1.734706	-0.450094
20	6	0	1.094027	1.200857	-1.387338
21	6	0	0.687007	2.599528	0.538152
22	6	0	2.450849	1.502246	-1.333224
23	1	0	0.715237	0.534697	-2.155576
24	6	0	2.042431	2.907507	0.610104
25	6	0	2.896594	2.342283	-0.324014
26	1	0	3.154931	1.087277	-2.046577
27	1	0	2.432484	3.575991	1.368987
28	9	0	4.213639	2.627529	-0.252729
29	7	0	-1.847161	1.104128	1.064727
30	16	0	-1.761935	-0.546289	1.651293

31	8	0	-1.721460	-0.471401	3.098755
32	8	0	-2.822960	-1.233212	0.941402
33	1	0	0.020576	3.071596	1.253355
34	1	0	-1.454536	1.727577	1.775765
35	6	0	-4.961881	-1.083306	-1.642005
36	1	0	-5.761690	-0.411503	-1.958281
37	1	0	-5.002124	-2.014238	-2.203773
38	1	0	-5.043684	-1.276502	-0.570603
39	1	0	-2.850430	1.331458	0.939308

Int1'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.888910	-2.220881	-0.344418
2	6	0	-0.327587	-1.729909	0.124169
3	6	0	0.879656	-0.412376	1.821361
4	6	0	2.083402	-0.883614	1.328201
5	6	0	2.051192	-1.773797	0.263435
6	1	0	0.933503	-2.915498	-1.173103
7	1	0	-1.268677	-2.006349	-0.339872
8	1	0	0.844425	0.288814	2.647184
9	1	0	3.028653	-0.572380	1.753374
10	7	0	3.336413	-2.240671	-0.286788
11	8	0	3.308974	-3.153671	-1.090033
12	8	0	4.346487	-1.675430	0.088846
13	6	0	-0.287289	-0.846001	1.194843
14	6	0	-1.825482	0.773863	-1.718782
15	6	0	-1.252370	1.262134	-0.476598
16	6	0	-3.201933	0.400906	-1.434424
17	8	0	-4.121254	1.117374	-0.982751
18	8	0	-3.472723	-0.883382	-1.803821
19	6	0	0.253793	1.628716	-0.634031
20	6	0	1.134808	0.975638	-1.518854
21	6	0	0.823741	2.556715	0.245569
22	6	0	2.515464	1.201189	-1.483758
23	1	0	0.710345	0.250421	-2.209977
24	6	0	2.191515	2.801065	0.304686
25	6	0	3.024138	2.100465	-0.553184
26	1	0	3.198164	0.675882	-2.146794
27	1	0	2.615788	3.521052	1.002236
28	9	0	4.352063	2.310194	-0.472837

29	7	0	-1.768448	1.390691	0.488143
30	16	0	-1.809459	-0.147428	1.701124
31	8	0	-1.757000	0.359678	3.054598
32	8	0	-2.943637	-0.865806	1.187798
33	1	0	0.205873	3.152873	0.919829
34	1	0	-1.351346	2.181115	1.023911
35	6	0	-4.763296	-1.373556	-1.453208
36	1	0	-5.546944	-0.823157	-1.976337
37	1	0	-4.782026	-2.424192	-1.759590
38	1	0	-4.926294	-1.294869	-0.374572
39	1	0	-2.821979	1.593801	0.404251

Int2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.102416	-0.438725	-1.187445
2	6	0	-0.268394	-0.614279	-1.063924
3	6	0	0.091721	-2.577582	0.320583
4	6	0	1.465955	-2.436364	0.178244
5	6	0	1.936804	-1.349760	-0.548857
6	1	0	1.520089	0.376487	-1.766688
7	1	0	-0.960064	0.065090	-1.548538
8	1	0	-0.323431	-3.394309	0.900790
9	1	0	2.163262	-3.127726	0.635428
10	7	0	3.381517	-1.140775	-0.623046
11	8	0	3.777465	0.003169	-0.826063
12	8	0	4.114602	-2.095576	-0.466223
13	6	0	-0.763087	-1.657177	-0.283170
14	7	0	-2.748087	-0.779562	1.347355
15	16	0	-2.524759	-1.706711	0.093042
16	8	0	-2.807591	-3.135450	0.337912
17	8	0	-3.172262	-1.100370	-1.083837
18	1	0	-2.439963	-1.291618	2.174464

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.609002	0.448681	0.295305

2	6	0	2.484940	1.197935	0.629065
3	6	0	1.438760	0.579833	-1.476826
4	6	0	2.553511	-0.173838	-1.819253
5	6	0	3.615441	-0.218929	-0.922428
6	1	0	4.461263	0.380871	0.960308
7	1	0	2.430171	1.724524	1.575569
8	1	0	0.589099	0.626344	-2.150995
9	1	0	2.601836	-0.720331	-2.752626
10	7	0	4.793628	-1.022898	-1.273303
11	8	0	5.709310	-1.081962	-0.468542
12	8	0	4.798815	-1.592728	-2.352487
13	6	0	1.414977	1.258759	-0.259938
14	6	0	-0.658615	-0.960229	0.847423
15	6	0	-1.608702	-0.305433	0.368638
16	6	0	0.613003	-1.394121	1.284404
17	8	0	1.409304	-2.057973	0.627595
18	8	0	0.869221	-1.041936	2.571067
19	6	0	2.097879	-1.532996	3.108695
20	1	0	2.105360	-2.625378	3.113790
21	1	0	2.946066	-1.170777	2.523467
22	1	0	2.147440	-1.149304	4.126268
23	6	0	-3.023684	-0.434992	0.009407
24	6	0	-3.456349	-1.663220	-0.513185
25	6	0	-3.962595	0.583464	0.218976
26	6	0	-4.796711	-1.877635	-0.821456
27	1	0	-2.730622	-2.453163	-0.676556
28	6	0	-5.308028	0.381562	-0.077806
29	6	0	-5.693659	-0.845520	-0.594203
30	1	0	-5.143630	-2.819458	-1.231749
31	1	0	-6.048325	1.156874	0.085581
32	9	0	-6.999381	-1.043484	-0.891501
33	7	0	-1.344837	1.569712	-0.237042
34	16	0	0.006950	2.318229	0.128603
35	8	0	0.218522	3.511937	-0.720997
36	8	0	0.072263	2.522462	1.584450
37	1	0	-3.627857	1.534187	0.614930
38	1	0	-1.523610	1.649273	-1.239316

Int3

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

1	6	0	3.610780	0.426331	0.289647
2	6	0	2.504963	1.185956	0.636314
3	6	0	1.420068	0.568496	-1.451746
4	6	0	2.519760	-0.200592	-1.802947
5	6	0	3.593294	-0.249908	-0.922221
6	1	0	4.473341	0.348049	0.939911
7	1	0	2.461739	1.716056	1.582895
8	1	0	0.557486	0.615279	-2.112589
9	1	0	2.552747	-0.757144	-2.730523
10	7	0	4.752013	-1.067502	-1.283592
11	8	0	5.679336	-1.125179	-0.494016
12	8	0	4.732630	-1.647394	-2.355938
13	6	0	1.428013	1.251422	-0.238144
14	6	0	-0.683998	-0.906746	0.804896
15	6	0	-1.539356	-0.053699	0.285272
16	6	0	0.579011	-1.334694	1.221288
17	8	0	1.391160	-2.018474	0.586068
18	8	0	0.855118	-1.008801	2.540183
19	6	0	2.074530	-1.535325	3.045315
20	1	0	2.076283	-2.631928	3.034563
21	1	0	2.932837	-1.185529	2.464230
22	1	0	2.151125	-1.176810	4.072704
23	6	0	-2.995910	-0.351812	0.000057
24	6	0	-3.434924	-1.652559	-0.296313
25	6	0	-3.953652	0.670178	0.006979
26	6	0	-4.773597	-1.920023	-0.588910
27	1	0	-2.707111	-2.459408	-0.302208
28	6	0	-5.294681	0.423579	-0.272952
29	6	0	-5.684049	-0.869134	-0.579499
30	1	0	-5.114586	-2.921066	-0.832868
31	1	0	-6.030881	1.218601	-0.263166
32	9	0	-6.978828	-1.106146	-0.871853
33	7	0	-1.309024	1.451586	-0.182868
34	16	0	0.051566	2.304356	0.174344
35	8	0	0.179728	3.485585	-0.692867
36	8	0	0.092769	2.521223	1.617641
37	1	0	-3.647760	1.680393	0.246908
38	1	0	-1.541178	1.554041	-1.172224

TS2'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.094787	-2.259990	-0.629473
2	6	0	-0.108675	-1.879396	-0.039715
3	6	0	1.113010	-0.663569	1.677160
4	6	0	2.318036	-1.026817	1.092050
5	6	0	2.278376	-1.817553	-0.053262
6	1	0	1.117089	-2.873267	-1.521799
7	1	0	-1.058368	-2.184689	-0.464794
8	1	0	1.106740	-0.045839	2.570086
9	1	0	3.266951	-0.704917	1.502784
10	7	0	3.549284	-2.184954	-0.692557
11	8	0	3.510945	-2.916737	-1.668293
12	8	0	4.579812	-1.734740	-0.218758
13	6	0	-0.087298	-1.086635	1.103178
14	6	0	-2.247769	1.093630	-1.293663
15	6	0	-1.319059	1.397905	-0.504052
16	6	0	-3.589027	0.597076	-1.304066
17	8	0	-4.582023	1.215558	-0.942086
18	8	0	-3.672008	-0.644158	-1.829234
19	6	0	0.077707	1.821888	-0.447127
20	6	0	0.990494	1.211886	-1.319025
21	6	0	0.536348	2.807301	0.437192
22	6	0	2.338713	1.558867	-1.301254
23	1	0	0.635587	0.450307	-2.005921
24	6	0	1.880197	3.166951	0.467570
25	6	0	2.753334	2.525275	-0.399018
26	1	0	3.057771	1.086716	-1.962399
27	1	0	2.250561	3.928567	1.144534
28	9	0	4.062571	2.862329	-0.364443
29	7	0	-1.714275	1.076709	1.460131
30	16	0	-1.630463	-0.477049	1.808213
31	8	0	-1.507022	-0.717752	3.261455
32	8	0	-2.704963	-1.187286	1.100527
33	1	0	-0.162078	3.307606	1.100483
34	1	0	-1.069917	1.563933	2.086162
35	6	0	-4.966226	-1.246049	-1.782414
36	1	0	-5.683253	-0.664636	-2.365744
37	1	0	-4.845285	-2.238838	-2.212229
38	1	0	-5.312201	-1.319090	-0.748980

Int3'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.577828	-2.401574	-0.574721
2	6	0	-0.495449	-1.717625	-0.026198
3	6	0	0.929087	-0.935691	1.807562
4	6	0	2.010058	-1.606409	1.252103
5	6	0	1.807072	-2.324314	0.079563
6	1	0	0.485377	-2.968282	-1.485560
7	1	0	-1.468335	-1.696625	-0.527030
8	1	0	1.033003	-0.365750	2.720029
9	1	0	2.987305	-1.590313	1.717024
10	7	0	2.945055	-3.045420	-0.504253
11	8	0	2.754551	-3.682782	-1.525603
12	8	0	4.021878	-2.968058	0.061814
13	6	0	-0.299511	-1.004003	1.150083
14	6	0	-1.810592	1.058741	-1.420293
15	6	0	-1.191823	1.443816	-0.088717
16	6	0	-3.143107	0.569377	-1.378262
17	8	0	-4.240974	1.158566	-1.375624
18	8	0	-3.181639	-0.816111	-1.695096
19	6	0	0.291974	1.977496	-0.501019
20	6	0	1.298674	1.219135	-1.113525
21	6	0	0.692397	3.215553	0.045738
22	6	0	2.644704	1.624908	-1.116807
23	1	0	1.027775	0.253515	-1.556556
24	6	0	2.012574	3.646521	0.054305
25	6	0	2.974203	2.828972	-0.504367
26	1	0	3.425859	1.015154	-1.553841
27	1	0	2.299691	4.598377	0.493188
28	9	0	4.263254	3.229292	-0.455963
29	7	0	-1.392320	1.456291	0.891200
30	16	0	-1.664375	-0.057623	1.752245
31	8	0	-1.516219	0.101571	3.206464
32	8	0	-2.902954	-0.561562	1.224209
33	1	0	-0.063143	3.857025	0.498571
34	1	0	-0.623852	1.970148	1.344491
35	6	0	-4.450934	-1.429156	-1.541008
36	1	0	-5.189740	-1.001045	-2.216676
37	1	0	-4.304107	-2.491054	-1.776786
38	1	0	-4.816340	-1.332385	-0.517680

Int4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.787190	0.056084	0.559079
2	6	0	2.789052	0.969093	0.961887
3	6	0	1.811948	0.912757	-1.257774
4	6	0	2.803820	-0.008890	-1.677967
5	6	0	3.756542	-0.339433	-0.757041
6	1	0	4.546820	-0.324623	1.245015
7	1	0	2.708000	1.306261	1.992908
8	1	0	1.009134	1.193349	-1.933288
9	1	0	2.819537	-0.445867	-2.685544
10	7	0	4.904294	-1.209282	-1.229587
11	8	0	5.737139	-1.491033	-0.414432
12	8	0	4.892276	-1.525971	-2.387377
13	6	0	1.939713	1.481807	0.001696
14	6	0	-0.569376	-0.331893	0.971196
15	6	0	-1.335952	0.494470	0.270968
16	6	0	-0.445020	-1.661418	1.149731
17	8	0	0.106305	-2.512263	0.414782
18	8	0	-0.825311	-2.030398	2.454699
19	6	0	-0.580416	-3.381709	2.773533
20	1	0	-1.101813	-4.063786	2.093044
21	1	0	0.491330	-3.637585	2.743052
22	1	0	-0.958817	-3.534752	3.796773
23	6	0	-2.680884	0.194973	-0.298872
24	6	0	-2.943689	-1.124473	-0.672957
25	6	0	-3.728680	1.133724	-0.343888
26	6	0	-4.218608	-1.522748	-1.084478
27	1	0	-2.132197	-1.845581	-0.630533
28	6	0	-5.011693	0.749493	-0.736012
29	6	0	-5.222522	-0.564962	-1.097264
30	1	0	-4.436251	-2.537500	-1.374624
31	1	0	-5.832433	1.457057	-0.768054
32	9	0	-6.459188	-0.946154	-1.489290
33	7	0	-0.976638	1.934867	0.101014
34	16	0	0.495221	2.461642	0.595295
35	8	0	0.720054	3.707576	-0.164884
36	8	0	0.566725	2.531943	2.047560
37	1	0	-3.542456	2.156741	-0.038085
38	1	0	-1.161336	2.326220	-0.825554

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.692892	0.007500	0.604222
2	6	0	2.619638	0.753205	1.049934
3	6	0	1.710088	0.791702	-1.218915
4	6	0	2.777776	0.037835	-1.661878
5	6	0	3.753409	-0.364219	-0.743331
6	1	0	4.487553	-0.282857	1.280561
7	1	0	2.543193	1.049110	2.089881
8	1	0	0.952231	1.125165	-1.920968
9	1	0	2.876375	-0.227983	-2.707195
10	7	0	4.874049	-1.145687	-1.207183
11	8	0	5.735482	-1.474699	-0.396534
12	8	0	4.922948	-1.454039	-2.394645
13	6	0	1.576269	1.073323	0.158055
14	6	0	-0.344253	-0.189543	0.734696
15	6	0	-1.304991	0.561226	0.215901
16	6	0	-0.266261	-1.569826	1.058805
17	8	0	0.305712	-2.439448	0.395066
18	8	0	-0.792257	-1.866899	2.283356
19	6	0	-0.642372	-3.219911	2.712961
20	1	0	-1.147042	-3.902796	2.025432
21	1	0	0.413753	-3.491399	2.776802
22	1	0	-1.104030	-3.270019	3.698057
23	6	0	-2.662463	0.180790	-0.247527
24	6	0	-2.912931	-1.133900	-0.669941
25	6	0	-3.714817	1.106558	-0.264871
26	6	0	-4.182094	-1.523697	-1.083826
27	1	0	-2.100600	-1.854379	-0.687493
28	6	0	-4.992977	0.732569	-0.677646
29	6	0	-5.196798	-0.577259	-1.077022
30	1	0	-4.386914	-2.534960	-1.417564
31	1	0	-5.816935	1.437554	-0.687619
32	9	0	-6.434031	-0.949856	-1.482967
33	7	0	-1.026110	1.979871	0.076312
34	16	0	0.477744	2.425355	0.616370
35	8	0	0.841081	3.616518	-0.160792
36	8	0	0.475075	2.536542	2.071904
37	1	0	-3.541735	2.125616	0.065658
38	1	0	-1.214069	2.388777	-0.839213

Int5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.423610	-0.460841	0.993289
2	6	0	2.108903	-0.220324	1.211468
3	6	0	1.781108	0.054620	-1.239582
4	6	0	3.099854	-0.195619	-1.430454
5	6	0	3.975075	-0.408622	-0.324223
6	1	0	4.071721	-0.736825	1.817428
7	1	0	1.689577	-0.303325	2.209039
8	1	0	1.112480	0.180174	-2.085971
9	1	0	3.502385	-0.269086	-2.434542
10	7	0	5.311673	-0.650357	-0.530503
11	8	0	6.068081	-0.872098	0.448316
12	8	0	5.778244	-0.643273	-1.697421
13	6	0	1.199393	0.198537	0.117235
14	6	0	-0.243742	-0.280429	0.221423
15	6	0	-1.231912	0.635937	0.054731
16	6	0	-0.456655	-1.724649	0.435777
17	8	0	0.320021	-2.588628	0.075337
18	8	0	-1.582280	-1.996736	1.110569
19	6	0	-1.905061	-3.384952	1.250802
20	1	0	-2.008882	-3.847397	0.266735
21	1	0	-1.127183	-3.899892	1.816865
22	1	0	-2.850959	-3.411941	1.787423
23	6	0	-2.672274	0.395538	-0.165461
24	6	0	-3.098060	-0.624430	-1.025609
25	6	0	-3.618506	1.221958	0.450809
26	6	0	-4.452216	-0.839048	-1.249948
27	1	0	-2.365360	-1.244619	-1.533628
28	6	0	-4.979579	1.015534	0.242014
29	6	0	-5.362319	-0.013591	-0.603483
30	1	0	-4.804448	-1.618300	-1.916096
31	1	0	-5.730664	1.634508	0.719223
32	9	0	-6.679319	-0.217211	-0.817815
33	7	0	-0.849366	1.981794	0.074340
34	16	0	0.814075	2.122465	0.405346
35	8	0	1.380809	3.040467	-0.591567
36	8	0	0.968048	2.479762	1.820319
37	1	0	-3.288602	2.018008	1.110467
38	1	0	-1.216635	2.600431	-0.646154

Int6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.355607	0.112382	1.167716
2	6	0	3.013135	-0.219248	1.198482
3	6	0	3.047146	-0.663041	-1.170391
4	6	0	4.395993	-0.348357	-1.223740
5	6	0	5.027169	0.045163	-0.051427
6	1	0	4.888221	0.408846	2.062320
7	1	0	2.473173	-0.183056	2.139041
8	1	0	2.531646	-0.968630	-2.074916
9	1	0	4.957913	-0.413759	-2.146690
10	7	0	6.445557	0.382121	-0.092612
11	8	0	6.990042	0.717326	0.948486
12	8	0	7.025149	0.313891	-1.165984
13	6	0	2.324068	-0.572717	0.026639
14	6	0	0.921745	-1.069018	0.073101
15	6	0	-0.003632	-0.505617	-0.782585
16	6	0	0.692917	-2.171887	1.001140
17	8	0	1.578038	-2.813371	1.537905
18	8	0	-0.613050	-2.458256	1.260750
19	6	0	-0.821897	-3.690587	1.959045
20	1	0	-0.331548	-4.512393	1.434762
21	1	0	-0.432291	-3.628422	2.976165
22	1	0	-1.899988	-3.850891	1.972261
23	6	0	-1.332805	-1.069552	-1.134312
24	6	0	-1.489114	-2.432957	-1.412087
25	6	0	-2.436961	-0.217271	-1.251909
26	6	0	-2.729239	-2.947936	-1.763917
27	1	0	-0.628917	-3.092000	-1.354288
28	6	0	-3.689962	-0.718997	-1.594641
29	6	0	-3.810484	-2.078590	-1.840158
30	1	0	-2.868514	-3.999393	-1.986701
31	1	0	-4.558617	-0.075559	-1.675501
32	9	0	-5.012458	-2.572306	-2.172369
33	7	0	0.331219	0.649462	-1.402255
34	16	0	1.295335	1.868166	-0.469198
35	8	0	2.459630	2.187811	-1.335638
36	8	0	0.291415	3.013846	-0.581690
37	1	0	-2.320560	0.846157	-1.064763
38	1	0	-0.347819	1.066976	-2.032643
39	1	0	-1.117262	2.891892	0.035614

40	6	0	-2.267656	1.797080	1.154441
41	8	0	-2.089380	2.862641	0.323815
42	8	0	-3.462934	1.588328	1.505936
43	8	0	-1.265530	1.109945	1.452114
44	19	0	-4.648908	3.590263	0.262502
45	19	0	-2.818425	-0.965060	1.923812

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.722873	0.162849	2.463555
2	6	0	-0.625522	-0.395827	1.813514
3	6	0	-2.080774	-2.080552	0.805054
4	6	0	-3.179703	-1.522602	1.445834
5	6	0	-2.970119	-0.410120	2.254121
6	1	0	-1.617686	1.030292	3.102974
7	1	0	0.366605	0.027441	1.925631
8	1	0	-2.199510	-2.943513	0.157838
9	1	0	-4.174902	-1.929568	1.318632
10	7	0	-4.139680	0.206761	2.906269
11	8	0	-3.946359	1.162054	3.637892
12	8	0	-5.237167	-0.268729	2.672768
13	6	0	-0.826309	-1.503422	0.996120
14	6	0	0.854252	0.896888	-1.428972
15	6	0	-0.067747	-0.063006	-1.550564
16	6	0	0.461274	2.304424	-1.531892
17	8	0	0.350465	2.929953	-2.575779
18	8	0	0.316581	2.903651	-0.329954
19	6	0	-1.549014	0.102373	-1.694253
20	6	0	-2.242327	1.030247	-0.904120
21	6	0	-2.284530	-0.693150	-2.584445
22	6	0	-3.626879	1.158336	-0.986093
23	1	0	-1.697062	1.639372	-0.190343
24	6	0	-3.668919	-0.577688	-2.685291
25	6	0	-4.311117	0.344410	-1.874344
26	1	0	-4.170190	1.860895	-0.362758
27	1	0	-4.242016	-1.186349	-3.375753
28	9	0	-5.657210	0.453378	-1.953810
29	7	0	0.369238	-1.457515	-1.480540
30	16	0	0.540991	-2.126138	0.034449
31	8	0	0.390243	-3.569003	-0.147491

32	8	0	1.767813	-1.611885	0.635626
33	1	0	-1.783568	-1.409179	-3.230649
34	1	0	-0.193752	-2.102694	-2.032666
35	6	0	-0.000967	4.298645	-0.360968
36	1	0	-0.957548	4.459276	-0.863885
37	1	0	-0.062637	4.610337	0.679945
38	1	0	2.226389	0.599044	-1.323101
39	6	0	4.050005	0.590580	-0.238591
40	8	0	3.365064	0.211720	-1.315376
41	8	0	5.031937	-0.151972	0.112538
42	8	0	3.716455	1.641072	0.386740
43	19	0	4.004283	-2.349022	-0.956562
44	19	0	5.631784	1.367562	2.213431
45	1	0	0.780087	4.856278	-0.881072

Int7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.864249	2.449802	-0.319855
2	6	0	0.116469	1.550173	0.087236
3	6	0	-1.174988	1.089193	2.119992
4	6	0	-2.148119	1.994421	1.714617
5	6	0	-1.966615	2.647116	0.501990
6	1	0	-0.784493	2.981235	-1.259498
7	1	0	0.998947	1.353220	-0.536688
8	1	0	-1.272347	0.547679	3.054427
9	1	0	-3.027973	2.189443	2.313442
10	7	0	-3.004939	3.595727	0.061486
11	8	0	-2.840748	4.162138	-1.003401
12	8	0	-3.968849	3.758373	0.787041
13	6	0	-0.065690	0.890400	1.302526
14	6	0	0.484258	-1.317193	-1.304865
15	6	0	-0.110579	-1.675192	-0.161159
16	6	0	-0.370043	-1.169660	-2.518759
17	8	0	-0.754460	-2.071243	-3.226973
18	8	0	-0.622061	0.122565	-2.788377
19	6	0	-1.574787	-1.896615	0.065635
20	6	0	-2.512192	-0.950660	-0.363767
21	6	0	-2.032918	-3.036758	0.742524
22	6	0	-3.872688	-1.133543	-0.138167
23	1	0	-2.171056	-0.050290	-0.872520

24	6	0	-3.389614	-3.237292	0.974452
25	6	0	-4.284849	-2.276789	0.528689
26	1	0	-4.606766	-0.403304	-0.459541
27	1	0	-3.752637	-4.119411	1.485840
28	9	0	-5.597256	-2.460065	0.754598
29	7	0	0.684903	-1.773195	1.052559
30	16	0	1.125366	-0.331713	1.798087
31	8	0	1.023537	-0.566413	3.236372
32	8	0	2.419970	0.079000	1.251444
33	1	0	-1.328307	-3.795227	1.074624
34	1	0	0.228352	-2.332689	1.774207
35	6	0	-1.423939	0.352112	-3.948121
36	1	0	-2.396638	-0.133805	-3.835492
37	1	0	-1.546915	1.431313	-4.017245
38	1	0	1.407022	-1.166032	-1.391281
39	6	0	3.516197	0.104217	-1.324325
40	8	0	3.051404	-1.076067	-1.579747
41	8	0	4.674672	0.198990	-0.755828
42	8	0	2.824430	1.156925	-1.592862
43	19	0	4.115326	-2.020437	0.614918
44	19	0	3.837590	2.328033	0.534139
45	1	0	-0.925487	-0.036715	-4.836184

Int8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.594945	-0.871676	0.791044
2	6	0	-3.334756	-1.534355	0.634412
3	6	0	-2.846376	-0.237184	-1.308101
4	6	0	-4.069788	0.459309	-1.184007
5	6	0	-4.861651	0.036268	-0.171113
6	1	0	-5.273602	-1.072349	1.603837
7	1	0	-3.020227	-2.297931	1.339769
8	1	0	-2.142795	0.005890	-2.100826
9	1	0	-4.360964	1.280731	-1.855347
10	7	0	-6.259056	0.719545	-0.088115
11	8	0	-6.955302	0.357693	0.797433
12	8	0	-6.484715	1.541161	-0.910288
13	6	0	-2.717538	-1.344638	-0.553378
14	6	0	-0.352818	0.038027	1.039336
15	6	0	0.190293	-0.233853	-0.150981

16	6	0	-1.306126	1.054999	1.251895
17	8	0	-2.085590	1.210656	2.242706
18	8	0	-1.386005	2.028461	0.238778
19	6	0	1.185694	0.786336	-0.586809
20	6	0	1.652713	1.621668	0.433150
21	6	0	1.768949	0.848693	-1.840666
22	6	0	2.648064	2.566909	0.193570
23	1	0	1.233541	1.502712	1.426937
24	6	0	2.779303	1.776311	-2.111574
25	6	0	3.181109	2.615119	-1.083548
26	1	0	3.017562	3.230560	0.962696
27	1	0	3.244341	1.871923	-3.085748
28	9	0	4.154737	3.523645	-1.332689
29	7	0	0.194818	-1.394630	-0.956384
30	16	0	-1.071942	-2.279311	-0.761861
31	8	0	-1.492638	-2.897892	-2.045197
32	8	0	-0.990701	-3.235158	0.362781
33	1	0	1.424940	0.176535	-2.619507
34	1	0	2.059529	-1.909066	-0.739510
35	6	0	-2.183558	3.161857	0.521234
36	1	0	-1.897325	3.642369	1.460545
37	1	0	-2.024960	3.849139	-0.313770
38	1	0	-3.249230	2.901981	0.586085
39	1	0	-1.079370	-1.143348	1.411240
40	6	0	3.232896	-1.394857	0.687015
41	8	0	2.282620	-1.464962	1.476824
42	8	0	4.398747	-0.956508	0.918357
43	8	0	3.044069	-1.846363	-0.604528
44	19	0	3.620811	-0.164816	3.354491
45	19	0	5.286242	-0.712957	-1.552109

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.607697	-0.966367	0.787960
2	6	0	-3.341188	-1.497493	0.776675
3	6	0	-2.832467	-0.208486	-1.246999
4	6	0	-4.093167	0.325462	-1.220192
5	6	0	-4.985877	-0.027418	-0.187741
6	1	0	-5.325404	-1.273787	1.539487
7	1	0	-3.042595	-2.222089	1.526727

8	1	0	-2.152002	0.050204	-2.052997
9	1	0	-4.420738	1.001427	-2.001315
10	7	0	-6.291202	0.523131	-0.167574
11	8	0	-7.072712	0.184383	0.728763
12	8	0	-6.615069	1.332424	-1.044865
13	6	0	-2.368810	-1.046609	-0.174270
14	6	0	-0.850262	-0.106480	0.827691
15	6	0	0.164999	-0.225487	-0.200212
16	6	0	-1.465147	1.147474	1.237315
17	8	0	-2.061303	1.307080	2.293380
18	8	0	-1.445750	2.080952	0.268529
19	6	0	1.143387	0.831650	-0.527466
20	6	0	1.604635	1.699997	0.470028
21	6	0	1.658615	0.932637	-1.825096
22	6	0	2.568002	2.659655	0.183076
23	1	0	1.225329	1.605862	1.483322
24	6	0	2.614959	1.894652	-2.133944
25	6	0	3.048556	2.733324	-1.117562
26	1	0	2.947628	3.335791	0.940635
27	1	0	3.018491	2.001627	-3.134497
28	9	0	3.981235	3.665102	-1.405728
29	7	0	0.223910	-1.332984	-0.910506
30	16	0	-1.106343	-2.293604	-0.652312
31	8	0	-1.462495	-2.922487	-1.927137
32	8	0	-0.900138	-3.188320	0.495722
33	1	0	1.296763	0.257148	-2.593340
34	1	0	2.120667	-1.923050	-0.746207
35	6	0	-2.180469	3.277233	0.538081
36	1	0	-1.798111	3.766642	1.435944
37	1	0	-2.038046	3.913407	-0.333193
38	1	0	-3.239796	3.044567	0.671732
39	1	0	-0.799822	-0.852412	1.615639
40	6	0	3.321526	-1.330207	0.640082
41	8	0	2.389794	-1.387628	1.468240
42	8	0	4.489450	-0.897529	0.818643
43	8	0	3.081636	-1.787514	-0.638190
44	19	0	3.845451	-0.122430	3.344105
45	19	0	5.466347	-1.017400	-1.680214

Int9

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

1	6	0	-4.543345	-0.923276	0.765244
2	6	0	-3.308956	-1.482755	0.737612
3	6	0	-2.781876	-0.146884	-1.269401
4	6	0	-4.018188	0.407709	-1.209807
5	6	0	-4.926151	0.087868	-0.158213
6	1	0	-5.273602	-1.252949	1.500637
7	1	0	-3.033127	-2.246331	1.455869
8	1	0	-2.116995	0.109090	-2.087926
9	1	0	-4.348064	1.087231	-1.984347
10	7	0	-6.168756	0.680845	-0.088115
11	8	0	-6.968202	0.344793	0.810333
12	8	0	-6.484715	1.554061	-0.923188
13	6	0	-2.227338	-0.957638	-0.140578
14	6	0	-0.946218	-0.232873	0.691036
15	6	0	0.203193	-0.298353	-0.292881
16	6	0	-1.460926	1.080799	1.187395
17	8	0	-2.033990	1.210656	2.242706
18	8	0	-1.386005	2.028461	0.251678
19	6	0	1.211494	0.747636	-0.548109
20	6	0	1.639813	1.621668	0.458950
21	6	0	1.781849	0.835793	-1.827766
22	6	0	2.635164	2.554009	0.206470
23	1	0	1.207741	1.554312	1.452737
24	6	0	2.766403	1.776311	-2.098674
25	6	0	3.181109	2.615119	-1.070648
26	1	0	2.991762	3.230560	0.975596
27	1	0	3.205641	1.871923	-3.085748
28	9	0	4.141837	3.510745	-1.319789
29	7	0	0.246418	-1.368830	-1.007984
30	16	0	-1.136442	-2.318011	-0.761861
31	8	0	-1.505538	-2.872092	-2.058097
32	8	0	-0.913301	-3.248058	0.349881
33	1	0	1.437840	0.163635	-2.606607
34	1	0	2.111129	-2.012266	-0.752410
35	6	0	-2.183558	3.187657	0.508334
36	1	0	-1.884425	3.655269	1.447645
37	1	0	-2.012060	3.862039	-0.326670
38	1	0	-3.236330	2.901981	0.560285
39	1	0	-0.666570	-0.872448	1.578940
40	6	0	3.232896	-1.394857	0.687015
41	8	0	2.256820	-1.452062	1.463924
42	8	0	4.385847	-0.956508	0.918357
43	8	0	3.056969	-1.846363	-0.604528

44	19	0	3.620811	-0.164816	3.354491
45	19	0	5.286242	-0.712957	-1.552109

TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.438488	-0.903282	-1.460691
2	6	0	0.944407	0.270524	-0.957780
3	6	0	0.899530	-0.706497	1.284298
4	6	0	0.358957	-1.864720	0.780351
5	6	0	0.066681	-1.942104	-0.587507
6	1	0	0.348951	-1.055753	-2.529489
7	1	0	1.256972	1.081884	-1.606991
8	1	0	1.165384	-0.629663	2.331557
9	1	0	0.166696	-2.723557	1.412455
10	7	0	-0.535059	-3.130343	-1.102522
11	8	0	-0.755209	-3.206320	-2.315332
12	8	0	-0.838644	-4.031829	-0.322788
13	6	0	1.004858	0.443991	0.455962
14	6	0	4.326367	1.350912	-1.541843
15	6	0	4.208437	0.720339	-0.375850
16	6	0	3.881662	2.666697	-1.858550
17	8	0	4.493798	3.724542	-1.781973
18	8	0	2.639929	2.628677	-2.477172
19	6	0	4.747983	-0.657162	-0.183489
20	6	0	5.713141	-1.134278	-1.088684
21	6	0	4.355396	-1.518089	0.849890
22	6	0	6.270596	-2.396628	-0.962838
23	1	0	5.987483	-0.463409	-1.897371
24	6	0	4.902790	-2.795520	0.989010
25	6	0	5.858421	-3.211633	0.084701
26	1	0	7.018701	-2.763549	-1.658681
27	1	0	4.584416	-3.465854	1.780471
28	9	0	6.410405	-4.445008	0.215806
29	7	0	3.617232	1.249123	0.858890
30	16	0	2.061655	1.766398	1.068037
31	8	0	1.914680	1.830749	2.528118
32	8	0	1.829842	2.947286	0.254286
33	1	0	3.574805	-1.213827	1.540147
34	1	0	3.946765	0.846045	1.728642
35	6	0	2.034553	3.891770	-2.649691

36	1	0	2.499556	4.448829	-3.473380
37	1	0	0.981229	3.695008	-2.861264
38	1	0	2.123696	4.484646	-1.734811
39	6	0	-2.702231	-1.023870	-2.538854
40	6	0	-2.840054	0.129595	-1.769318
41	6	0	-4.777841	-0.867711	-0.663853
42	6	0	-4.617111	-2.029166	-1.406305
43	6	0	-3.594653	-2.068223	-2.346141
44	1	0	-1.912805	-1.134242	-3.270920
45	1	0	-2.147192	0.965725	-1.875173
46	1	0	-5.591273	-0.757391	0.045360
47	1	0	-5.273325	-2.882922	-1.295343
48	7	0	-3.504933	-3.249515	-3.218838
49	8	0	-2.900028	-3.133475	-4.265511
50	8	0	-4.090881	-4.258707	-2.861942
51	6	0	-3.899241	0.196046	-0.866553
52	6	0	-0.860119	1.688416	0.825078
53	6	0	-1.878406	1.218758	1.536788
54	6	0	-0.937248	2.714362	-0.193212
55	8	0	-0.843934	2.547280	-1.402365
56	8	0	-1.043256	3.952258	0.345340
57	6	0	-1.732628	0.238047	2.649182
58	6	0	-2.570138	-0.879222	2.746110
59	6	0	-0.749394	0.430652	3.625784
60	6	0	-2.434735	-1.794528	3.785073
61	1	0	-3.314990	-1.055467	1.972956
62	6	0	-0.605964	-0.472610	4.675203
63	6	0	-1.453390	-1.567724	4.736814
64	1	0	-3.059166	-2.678054	3.857391
65	1	0	0.155391	-0.341984	5.436627
66	9	0	-1.321491	-2.443498	5.758135
67	7	0	-3.279426	1.616770	1.426437
68	16	0	-4.188085	1.701976	0.056404
69	8	0	-5.570472	1.651847	0.537618
70	8	0	-3.747411	2.798229	-0.784609
71	1	0	-0.072569	1.275195	3.520804
72	1	0	-3.871686	1.318477	2.194116
73	6	0	-1.032769	4.996621	-0.611015
74	1	0	-1.841451	4.860846	-1.334934
75	1	0	-1.175949	5.920412	-0.047276
76	1	0	-0.077048	5.022059	-1.140924

Int10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.489160	0.893570	-1.419767
2	6	0	-0.808506	-0.338449	-0.980601
3	6	0	-0.640245	0.464250	1.336861
4	6	0	-0.259572	1.679288	0.874668
5	6	0	-0.021412	1.904599	-0.511472
6	1	0	-0.595079	1.154125	-2.478619
7	1	0	-1.223721	-1.069319	-1.667806
8	1	0	-0.896461	0.346996	2.384854
9	1	0	-0.196366	2.542018	1.561444
10	7	0	0.458096	3.088176	-0.961069
11	8	0	0.493437	3.345374	-2.192258
12	8	0	0.924212	3.930870	-0.147451
13	6	0	-0.494503	-0.805739	0.464198
14	6	0	-4.246743	-1.156920	-1.532849
15	6	0	-4.042262	-0.572639	-0.356456
16	6	0	-3.973152	-2.493014	-1.900609
17	8	0	-4.678633	-3.492369	-1.737287
18	8	0	-2.843725	-2.592313	-2.697017
19	6	0	-4.483305	0.827041	-0.060264
20	6	0	-5.401576	1.443315	-0.934226
21	6	0	-4.027018	1.565118	1.029640
22	6	0	-5.829033	2.750835	-0.737020
23	1	0	-5.747341	0.873610	-1.780219
24	6	0	-4.452335	2.873168	1.255103
25	6	0	-5.349722	3.442737	0.368351
26	1	0	-6.528257	3.228809	-1.407727
27	1	0	-4.091309	3.455505	2.102465
28	9	0	-5.753670	4.714224	0.569466
29	7	0	-3.436257	-1.207545	0.824239
30	16	0	-1.946836	-1.919712	0.944062
31	8	0	-1.815203	-2.191906	2.386335
32	8	0	-1.877061	-3.048351	0.017887
33	1	0	-3.276148	1.154268	1.696536
34	1	0	-3.677903	-0.811358	1.720940
35	6	0	-2.465433	-3.918558	-3.022200
36	1	0	-3.221014	-4.417552	-3.622440
37	1	0	-1.538650	-3.840521	-3.592654
38	1	0	-2.292401	-4.502787	-2.113760
39	6	0	2.628767	1.302868	-2.512409

40	6	0	2.834836	0.082123	-1.884956
41	6	0	4.537125	1.103284	-0.462814
42	6	0	4.303900	2.332297	-1.072045
43	6	0	3.372703	2.392513	-2.092077
44	1	0	1.888022	1.424207	-3.302809
45	1	0	2.263699	-0.788856	-2.177855
46	1	0	5.298210	1.001744	0.303435
47	1	0	4.852942	3.225057	-0.781583
48	7	0	3.192843	3.669952	-2.793097
49	8	0	2.773999	3.631027	-3.940708
50	8	0	3.497339	4.689485	-2.210661
51	6	0	3.800274	-0.000060	-0.894301
52	6	0	0.732704	-1.595878	0.506683
53	6	0	1.796845	-1.347633	1.337127
54	6	0	0.920064	-2.656365	-0.588906
55	8	0	0.864593	-2.431899	-1.778333
56	8	0	1.120680	-3.895285	-0.112174
57	6	0	1.645276	-0.580961	2.602149
58	6	0	2.353213	0.609256	2.806443
59	6	0	0.808802	-1.075738	3.601616
60	6	0	2.145285	1.349282	3.959723
61	1	0	3.004870	0.991356	2.035159
62	6	0	0.593856	-0.353688	4.766845
63	6	0	1.250973	0.858322	4.915156
64	1	0	2.631400	2.305456	4.126217
65	1	0	-0.070670	-0.700782	5.547201
66	9	0	1.028458	1.593278	6.008417
67	7	0	3.171562	-1.784901	1.189587
68	16	0	4.146954	-1.593108	-0.171692
69	8	0	5.516185	-1.570780	0.348534
70	8	0	3.750724	-2.604328	-1.141233
71	1	0	0.273399	-2.009104	3.437550
72	1	0	3.729949	-1.598641	2.027193
73	6	0	1.189756	-4.906878	-1.134763
74	1	0	2.046499	-4.708658	-1.783743
75	1	0	1.315533	-5.855378	-0.607380
76	1	0	0.277331	-4.906661	-1.728917

TS7

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

1	6	0	1.914679	-2.951902	0.000699
2	6	0	0.576472	-2.614495	-0.130118
3	6	0	1.196520	-0.486594	-1.092920
4	6	0	2.542282	-0.791398	-0.941360
5	6	0	2.874166	-2.017958	-0.384238
6	1	0	2.222244	-3.899727	0.424790
7	1	0	-0.191894	-3.299122	0.204990
8	1	0	0.915779	0.469750	-1.516598
9	1	0	3.302179	-0.079377	-1.242211
10	7	0	4.283539	-2.331634	-0.173820
11	8	0	4.595724	-3.486278	0.043578
12	8	0	5.092017	-1.408698	-0.221285
13	6	0	0.202571	-1.365351	-0.653922
14	6	0	-1.221479	-0.951000	-0.702907
15	6	0	-1.669061	0.134038	-0.000296
16	6	0	-2.128449	-1.842699	-1.461723
17	8	0	-1.980125	-3.045361	-1.564564
18	8	0	-3.121410	-1.188532	-2.084858
19	6	0	-3.122335	0.406281	0.199046
20	6	0	-3.963237	-0.592745	0.700571
21	6	0	-3.641196	1.680626	-0.044882
22	6	0	-5.309856	-0.336936	0.929155
23	1	0	-3.549857	-1.571874	0.924359
24	6	0	-4.988696	1.951409	0.171700
25	6	0	-5.796613	0.932904	0.653184
26	1	0	-5.977459	-1.094974	1.322147
27	1	0	-5.414547	2.928521	-0.024581
28	9	0	-7.098315	1.187309	0.869540
29	7	0	-0.813204	0.944211	0.730542
30	16	0	0.113709	-0.208525	2.385781
31	8	0	-0.137139	0.823036	3.406829
32	8	0	-0.838097	-1.331334	2.436751
33	1	0	-2.990387	2.464046	-0.422421
34	1	0	-1.353103	1.589059	1.307409
35	6	0	-4.106003	-2.019462	-2.701769
36	1	0	-4.832440	-1.340550	-3.143705
37	1	0	-4.585772	-2.655092	-1.953528
38	1	0	0.135128	1.647691	0.186617
39	1	0	-3.651939	-2.648343	-3.469160
40	6	0	2.214960	2.129623	0.126869
41	8	0	2.292139	1.589872	1.264677
42	8	0	3.231856	2.391388	-0.607139
43	8	0	1.014491	2.435699	-0.372475
44	19	0	4.846146	1.081429	1.039906

45	19	0	1.948655	3.551633	-2.561388

Int11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.700142	-2.942642	0.566083
2	6	0	0.363085	-2.617779	0.427977
3	6	0	0.913975	-1.101009	-1.386220
4	6	0	2.261381	-1.402285	-1.249209
5	6	0	2.633818	-2.317501	-0.267193
6	1	0	2.038334	-3.647936	1.309343
7	1	0	-0.370631	-3.067066	1.076510
8	1	0	0.639793	-0.360838	-2.147832
9	1	0	2.987882	-0.894368	-1.893632
10	7	0	4.050461	-2.603212	-0.081510
11	8	0	4.359923	-3.558660	0.609782
12	8	0	4.867156	-1.882081	-0.631522
13	6	0	-0.051171	-1.671085	-0.550037
14	6	0	-1.466763	-1.243614	-0.602941
15	6	0	-1.849589	0.066211	-0.546051
16	6	0	-2.493378	-2.325661	-0.635411
17	8	0	-2.400019	-3.387791	-0.053791
18	8	0	-3.532366	-2.016513	-1.417579
19	6	0	-3.229459	0.496990	-0.224277
20	6	0	-3.929313	-0.083398	0.840906
21	6	0	-3.822439	1.527784	-0.960026
22	6	0	-5.212367	0.347836	1.156269
23	1	0	-3.458588	-0.853632	1.441371
24	6	0	-5.108806	1.966383	-0.661880
25	6	0	-5.777936	1.370053	0.393610
26	1	0	-5.776347	-0.067159	1.978440
27	1	0	-5.586054	2.750378	-1.234923
28	9	0	-7.008696	1.790235	0.690760
29	7	0	-0.962549	1.133591	-0.585793
30	16	0	0.544059	0.833935	1.654931
31	8	0	0.470202	2.230555	2.039162
32	8	0	-0.437503	-0.038574	2.269557
33	1	0	-3.275354	1.976531	-1.793719
34	1	0	-1.358870	2.057813	-0.481538
35	6	0	-4.631225	-2.939949	-1.368719
36	1	0	-5.374424	-2.555305	-2.045701

37	1	0	-5.021299	-2.991286	-0.350097
38	1	0	-0.315130	1.044001	-1.075901
39	1	0	-4.302741	-3.935012	-1.676550
40	6	0	2.406854	1.972059	0.168673
41	8	0	2.119281	0.895696	0.838422
42	8	0	3.612264	2.060393	-0.387580
43	8	0	1.546497	2.915530	0.004412
44	19	0	4.403563	-0.241873	0.446661
45	19	0	3.009439	4.400471	-1.389116

TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.993880	0.354499	0.647928
2	6	0	-3.712964	0.392465	1.154660
3	6	0	-2.830102	0.210408	-1.095885
4	6	0	-4.108845	0.172550	-1.603763
5	6	0	-5.198317	0.240931	-0.730383
6	1	0	-5.850913	0.408172	1.308645
7	1	0	-3.561524	0.477447	2.220686
8	1	0	-2.002172	0.164606	-1.794688
9	1	0	-4.281970	0.096014	-2.670250
10	7	0	-6.532519	0.198898	-1.253421
11	8	0	-7.476076	0.259791	-0.468613
12	8	0	-6.686543	0.103158	-2.468956
13	6	0	-2.570450	0.311246	0.304184
14	6	0	-1.227904	0.348944	0.797789
15	6	0	-0.107475	0.115771	-0.141161
16	6	0	-0.884207	0.428472	2.180512
17	8	0	-1.624988	0.511816	3.154523
18	8	0	0.483387	0.341776	2.374840
19	6	0	0.863380	0.001769	3.706852
20	1	0	0.758712	0.855398	4.380463
21	1	0	0.252572	-0.822873	4.077213
22	1	0	1.904569	-0.319156	3.655089
23	6	0	0.798564	1.226737	-0.534770
24	6	0	0.528484	2.517929	-0.056616
25	6	0	1.908387	1.028414	-1.372782
26	6	0	1.351979	3.587572	-0.385013
27	1	0	-0.338114	2.674534	0.576124

28	6	0	2.737942	2.088436	-1.713384
29	6	0	2.441531	3.351493	-1.213947
30	1	0	1.158232	4.589787	-0.021539
31	1	0	3.603147	1.950149	-2.351132
32	9	0	3.238737	4.373102	-1.537840
33	7	0	0.031128	-1.066842	-0.631757
34	16	0	-0.779338	-2.638643	0.195556
35	8	0	-0.399220	-3.616705	-0.842331
36	8	0	0.117564	-2.668148	1.391562
37	1	0	2.153257	0.040928	-1.749386
38	1	0	0.821096	-1.321564	-1.234788
39	1	0	1.689852	-1.935360	1.250120
40	6	0	3.166079	-1.434193	0.080960
41	8	0	2.520754	-1.401568	1.281589
42	8	0	4.184277	-0.702375	0.014343
43	8	0	2.679895	-2.136794	-0.841934
44	19	0	3.143941	1.196445	1.622119
45	19	0	4.917015	-1.886464	-2.287905

Int12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.059304	-1.345512	-2.228642
2	6	0	-1.717409	-0.987251	-2.219282
3	6	0	-1.903126	-0.327952	0.103584
4	6	0	-3.245596	-0.687685	0.112860
5	6	0	-3.796059	-1.182461	-1.065229
6	1	0	-3.529049	-1.735502	-3.119609
7	1	0	-1.127323	-1.099988	-3.117300
8	1	0	-1.422187	0.031991	1.005366
9	1	0	-3.850105	-0.591942	1.000728
10	7	0	-5.211433	-1.556977	-1.067441
11	8	0	-5.690794	-1.991036	-2.103454
12	8	0	-5.844084	-1.418891	-0.038097
13	6	0	-1.121697	-0.464878	-1.057487
14	6	0	0.316955	-0.127758	-1.033335
15	6	0	0.814859	0.985269	-0.371944
16	6	0	1.211866	-1.217072	-1.475470
17	8	0	0.943221	-2.411066	-1.395284
18	8	0	2.371928	-0.773543	-1.984354
19	6	0	3.386103	-1.734655	-2.226274

20	1	0	3.829231	-2.064636	-1.269943
21	1	0	2.989220	-2.584331	-2.783393
22	1	0	4.159878	-1.208599	-2.794604
23	6	0	-0.089731	2.113938	-0.011308
24	6	0	-0.937528	2.664968	-0.977542
25	6	0	-0.064973	2.660731	1.274678
26	6	0	-1.760847	3.742286	-0.661389
27	1	0	-0.959006	2.247144	-1.972761
28	6	0	-0.890195	3.732343	1.606217
29	6	0	-1.724931	4.247876	0.623621
30	1	0	-2.422951	4.189885	-1.403097
31	1	0	-0.893514	4.160595	2.605044
32	9	0	-2.520357	5.286697	0.937429
33	7	0	2.141851	1.045253	0.025150
34	16	0	3.415594	1.729069	-1.334639
35	8	0	3.579051	3.092495	-0.746785
36	8	0	4.604863	0.865984	-1.091371
37	1	0	0.565197	2.198041	2.030697
38	1	0	2.241433	1.872698	0.612547
39	1	0	2.332418	-0.227964	0.710099
40	6	0	1.468253	-1.051080	2.005478
41	8	0	2.415533	-0.884492	1.021329
42	8	0	1.270134	-2.252543	2.415450
43	8	0	0.883394	-0.021580	2.435484
44	19	0	2.324674	-3.668320	0.541466
45	19	0	-0.744583	-1.416941	3.996170

TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.986858	-1.138605	-2.346158
2	6	0	-1.634584	-0.834243	-2.277181
3	6	0	-1.857406	-0.308819	0.072794
4	6	0	-3.210732	-0.605584	0.022513
5	6	0	-3.752316	-1.012119	-1.192657
6	1	0	-3.449897	-1.462363	-3.269538
7	1	0	-1.019758	-0.924718	-3.166875
8	1	0	-1.385558	-0.015355	1.006784
9	1	0	-3.840289	-0.540970	0.901082
10	7	0	-5.178357	-1.330982	-1.255946
11	8	0	-5.639659	-1.693571	-2.325901

12	8	0	-5.837837	-1.218626	-0.235027
13	6	0	-1.056053	-0.401625	-1.076377
14	6	0	0.393575	-0.106313	-0.983289
15	6	0	0.867979	0.980751	-0.298166
16	6	0	1.280936	-1.201379	-1.428545
17	8	0	0.952680	-2.377828	-1.478414
18	8	0	2.485251	-0.780544	-1.817781
19	6	0	3.458845	-1.781875	-2.108493
20	1	0	3.754359	-2.286925	-1.185220
21	1	0	3.065490	-2.504830	-2.823952
22	1	0	4.314285	-1.245566	-2.511158
23	6	0	-0.022069	2.119597	0.057149
24	6	0	-0.810474	2.730669	-0.923536
25	6	0	-0.047285	2.610310	1.368137
26	6	0	-1.614898	3.819583	-0.607963
27	1	0	-0.787390	2.352477	-1.940900
28	6	0	-0.854590	3.692530	1.699535
29	6	0	-1.620924	4.277244	0.701535
30	1	0	-2.225965	4.314739	-1.353595
31	1	0	-0.902761	4.081671	2.710187
32	9	0	-2.399220	5.326358	1.015106
33	7	0	2.189768	1.074962	0.123356
34	16	0	3.648731	1.746822	-1.285065
35	8	0	3.823427	3.086070	-0.689290
36	8	0	4.742059	0.814517	-0.962835
37	1	0	0.531586	2.092931	2.127676
38	1	0	2.280109	1.852678	0.775997
39	1	0	2.432176	-0.071850	0.685631
40	6	0	1.277818	-1.287192	1.986650
41	8	0	2.331926	-1.274896	1.167945
42	8	0	0.803582	-2.429231	2.305667
43	8	0	0.794844	-0.191760	2.406534
44	19	0	1.966883	-3.872956	0.514656
45	19	0	-0.974723	-1.417928	3.929251

Int13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.778100	3.126663	1.336892
2	6	0	-0.132838	1.949599	1.679141
3	6	0	-1.465757	0.739545	0.072051

4	6	0	-2.122135	1.907616	-0.280899
5	6	0	-1.768500	3.089351	0.360847
6	1	0	-0.532429	4.063949	1.819985
7	1	0	0.619101	1.955141	2.456931
8	1	0	-1.727939	-0.182386	-0.434187
9	1	0	-2.885236	1.915129	-1.048671
10	7	0	-2.453599	4.323632	-0.002302
11	8	0	-2.109500	5.358256	0.548745
12	8	0	-3.339772	4.266204	-0.841546
13	6	0	-0.466124	0.728988	1.062996
14	6	0	0.260407	-0.518185	1.391597
15	6	0	-0.355588	-1.759258	1.361671
16	6	0	1.686526	-0.373374	1.711976
17	8	0	2.389642	0.557291	1.369283
18	8	0	2.195675	-1.382055	2.469314
19	6	0	3.620987	-1.363610	2.598536
20	1	0	4.089443	-1.391639	1.612554
21	1	0	3.945551	-0.466641	3.127323
22	1	0	3.887112	-2.256329	3.163021
23	6	0	-1.740008	-1.978486	0.863546
24	6	0	-2.742750	-1.037502	1.132636
25	6	0	-2.067120	-3.150855	0.171200
26	6	0	-4.042591	-1.242255	0.694612
27	1	0	-2.499499	-0.144330	1.700141
28	6	0	-3.366179	-3.364425	-0.283659
29	6	0	-4.327968	-2.403897	-0.012333
30	1	0	-4.833361	-0.529734	0.898488
31	1	0	-3.636482	-4.255957	-0.837813
32	9	0	-5.581673	-2.603764	-0.442347
33	7	0	0.238939	-2.856980	1.874846
34	16	0	4.001824	-0.598960	-0.602948
35	8	0	4.590711	-1.226333	-1.815261
36	8	0	4.735435	0.636623	-0.197979
37	1	0	-1.289836	-3.877182	-0.061594
38	1	0	-0.264568	-3.730454	1.899536
39	6	0	1.437102	-0.438353	-1.533552
40	8	0	2.580183	0.263028	-1.292184
41	8	0	0.454869	0.288098	-1.864579
42	8	0	1.436481	-1.682709	-1.396333
43	19	0	1.651924	2.644019	-1.016923
44	19	0	-1.002426	-1.881900	-2.428757
45	1	0	1.250198	-2.925744	1.893450

P

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.282735	0.034259	-0.990749
2	6	0	-0.898088	-0.096654	-1.004472
3	6	0	-1.022595	-1.741599	0.766053
4	6	0	-2.402304	-1.634126	0.778905
5	6	0	-3.008532	-0.740549	-0.099412
6	1	0	-2.790162	0.702974	-1.669881
7	1	0	-0.305184	0.489721	-1.691451
8	1	0	-0.537962	-2.428933	1.446930
9	1	0	-3.018077	-2.214831	1.460360
10	7	0	-4.469527	-0.610108	-0.079042
11	8	0	-4.979779	0.181945	-0.849338
12	8	0	-5.100416	-1.304922	0.701215
13	6	0	-0.254688	-0.968994	-0.117590
14	6	0	1.232844	-1.096567	-0.109810
15	6	0	2.048545	-0.026138	-0.162861
16	6	0	1.750000	-2.497955	-0.145153
17	8	0	1.123415	-3.434521	-0.619065
18	8	0	2.911816	-2.643787	0.486344
19	6	0	1.601648	1.376181	0.011295
20	6	0	0.883476	1.756336	1.148276
21	6	0	1.906474	2.315174	-0.981007
22	6	0	0.476190	3.076659	1.301539
23	1	0	0.665279	1.024824	1.913463
24	6	0	1.495854	3.632616	-0.833774
25	6	0	0.783286	3.986262	0.307406
26	1	0	-0.067950	3.408091	2.182913
27	1	0	1.705601	4.394624	-1.587214
28	9	0	0.390877	5.271035	0.452420
29	7	0	3.441842	-0.132645	-0.277922
30	1	0	2.431239	1.976802	-1.874684
31	6	0	3.555093	-3.907731	0.309643
32	1	0	4.455883	-3.880093	0.933139
33	1	0	3.830409	-4.016371	-0.744921
34	1	0	2.895128	-4.723558	0.623920
35	1	0	3.854856	0.690319	-0.714345
36	1	0	3.729751	-0.856378	-0.674238

Ps

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.525113	0.455582	1.094641
2	6	0	-2.147814	0.603720	1.011492
3	6	0	-2.136127	-0.591965	-1.091402
4	6	0	-3.514278	-0.757667	-1.019643
5	6	0	-4.180322	-0.227294	0.076234
6	1	0	-4.088830	0.850944	1.929961
7	1	0	-1.605497	1.119127	1.794440
8	1	0	-1.594253	-0.975344	-1.950923
9	1	0	-4.066039	-1.273593	-1.794808
10	7	0	-5.634754	-0.393655	0.162258
11	8	0	-6.210553	0.093596	1.120171
12	8	0	-6.193730	-1.011222	-0.728260
13	6	0	-1.439222	0.078553	-0.077638
14	6	0	0.038955	0.234839	-0.160484
15	6	0	0.860580	-0.842216	-0.039654
16	6	0	0.522726	1.627985	-0.301178
17	8	0	-0.096007	2.595510	0.095102
18	8	0	1.688971	1.731945	-0.950835
19	6	0	2.342897	-0.777151	0.083567
20	6	0	2.929304	-0.004086	1.090904
21	6	0	3.150646	-1.533488	-0.768533
22	6	0	4.310059	0.032088	1.234683
23	1	0	2.293462	0.555574	1.769982
24	6	0	4.535961	-1.501914	-0.639899
25	6	0	5.086327	-0.716557	0.360633
26	1	0	4.788493	0.619715	2.009433
27	1	0	5.183815	-2.069084	-1.297739
28	9	0	6.421768	-0.682805	0.494190
29	7	0	0.354609	-2.109026	0.183916
30	1	0	2.700754	-2.135035	-1.553166
31	1	0	1.000870	-2.878201	0.060041
32	6	0	2.242599	3.048797	-1.007144
33	1	0	3.188923	2.948589	-1.534445
34	1	0	2.406078	3.434150	0.001430
35	1	0	-0.587898	-2.308288	-0.128888
36	1	0	1.572699	3.721469	-1.545140

Int14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.803008	-0.870689	-0.980014
2	6	0	-2.436481	-0.677885	-0.839304
3	6	0	-2.707679	-0.335866	1.541781
4	6	0	-4.080357	-0.513211	1.416703
5	6	0	-4.598476	-0.781779	0.156961
6	1	0	-4.253060	-1.076648	-1.942908
7	1	0	-1.778520	-0.686266	-1.703511
8	1	0	-2.280767	-0.130392	2.517990
9	1	0	-4.740133	-0.453380	2.272786
10	7	0	-6.043673	-0.988218	0.021988
11	8	0	-6.481420	-1.264880	-1.082153
12	8	0	-6.734572	-0.874158	1.020266
13	6	0	-1.882141	-0.410916	0.416564
14	6	0	-0.376938	-0.281025	0.514458
15	6	0	0.246164	1.093249	0.781438
16	6	0	0.117554	-1.281739	1.549879
17	8	0	0.449784	-2.423645	1.288909
18	8	0	0.112199	-0.787409	2.781344
19	6	0	1.740715	1.037306	0.931242
20	6	0	2.496746	0.020684	0.339249
21	6	0	2.402121	2.031190	1.663540
22	6	0	3.886628	0.014765	0.430323
23	1	0	2.040321	-0.783131	-0.232060
24	6	0	3.786638	2.031490	1.780138
25	6	0	4.506105	1.023730	1.150326
26	1	0	4.464241	-0.760077	-0.062849
27	1	0	4.310608	2.790945	2.349322
28	9	0	5.845354	1.027689	1.249317
29	7	0	-0.267199	2.253804	0.854934
30	16	0	-1.973937	2.759485	0.840121
31	8	0	-1.713380	4.245835	0.847855
32	8	0	-2.486819	2.320219	-0.520295
33	1	0	1.815253	2.802135	2.151918
34	1	0	-1.403446	2.773818	-1.662398
35	6	0	0.526978	-1.679544	3.828117
36	1	0	0.413108	-1.118823	4.752086
37	1	0	1.569319	-1.966442	3.680325
38	1	0	0.036344	-0.612773	-0.448972
39	6	0	0.360981	2.175239	-2.161608

40	8	0	-0.049429	0.994645	-2.220173
41	8	0	1.554444	2.573987	-2.166174
42	8	0	-0.581666	3.170808	-2.070335
43	19	0	2.290771	-0.088930	-2.773174
44	19	0	0.803078	4.567961	-0.303281
45	1	0	-0.105092	-2.568310	3.832348
46	6	0	1.751922	-2.878716	-1.583011
47	8	0	2.943927	-2.383100	-1.466992
48	8	0	1.528960	-4.106410	-1.246082
49	8	0	0.778287	-2.123174	-1.979834
50	19	0	2.990237	-3.645577	0.865785
51	19	0	-0.985382	-3.649779	-0.812473

TS10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.644125	-0.713318	0.692450
2	6	0	-2.274831	-0.526067	0.566431
3	6	0	-2.609698	0.460818	-1.620797
4	6	0	-3.983423	0.288593	-1.504746
5	6	0	-4.474841	-0.294173	-0.342158
6	1	0	-4.072734	-1.168677	1.576432
7	1	0	-1.593266	-0.855193	1.347966
8	1	0	-2.211371	0.907612	-2.527391
9	1	0	-4.663006	0.594230	-2.289928
10	7	0	-5.922376	-0.460809	-0.198699
11	8	0	-6.341661	-0.972722	0.825871
12	8	0	-6.636685	-0.075713	-1.109868
13	6	0	-1.743034	0.067023	-0.589436
14	6	0	-0.268933	0.362669	-0.626968
15	6	0	0.699447	-0.777064	-0.748128
16	6	0	0.020537	1.532484	-1.522932
17	8	0	-0.265826	2.684599	-1.223274
18	8	0	0.591411	1.218995	-2.682781
19	6	0	2.150548	-0.378245	-0.810586
20	6	0	2.635079	0.791001	-0.218014
21	6	0	3.043443	-1.190517	-1.521295
22	6	0	3.989711	1.114437	-0.275411
23	1	0	1.982774	1.470984	0.325889
24	6	0	4.394528	-0.876835	-1.601834
25	6	0	4.846229	0.270076	-0.962680

26	1	0	4.374959	2.008556	0.203141
27	1	0	5.092270	-1.494466	-2.155933
28	9	0	6.152785	0.575694	-1.026673
29	7	0	0.508114	-2.043330	-0.739079
30	16	0	-0.982303	-2.920800	-1.105930
31	8	0	-0.302996	-4.122641	-1.717134
32	8	0	-1.534462	-3.278734	0.268158
33	1	0	2.658344	-2.060695	-2.042611
34	1	0	-0.447079	-3.578320	1.378015
35	6	0	0.956987	2.313830	-3.533086
36	1	0	1.323661	1.863107	-4.452029
37	1	0	1.745331	2.903535	-3.060026
38	1	0	-0.116439	0.896773	0.516124
39	6	0	0.920240	-2.501870	2.206220
40	8	0	0.086571	-1.626495	2.537307
41	8	0	2.172324	-2.387052	2.170146
42	8	0	0.433089	-3.734021	1.841557
43	19	0	1.839535	0.302491	2.781459
44	19	0	2.153052	-4.162495	-0.089189
45	1	0	0.090582	2.945962	-3.730517
46	6	0	0.296132	2.794090	1.764796
47	8	0	1.574126	2.847102	1.802819
48	8	0	-0.424879	3.845884	1.764998
49	8	0	-0.292142	1.608691	1.680605
50	19	0	1.252711	4.758419	-0.068118
51	19	0	-2.514632	2.794342	0.693326

Int15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.568216	-0.925133	0.629285
2	6	0	-2.210985	-0.664300	0.506317
3	6	0	-2.604571	0.370305	-1.647971
4	6	0	-3.966853	0.124951	-1.534432
5	6	0	-4.424749	-0.517851	-0.389190
6	1	0	-3.968696	-1.427936	1.500677
7	1	0	-1.522459	-0.986287	1.281290
8	1	0	-2.233376	0.866011	-2.540323
9	1	0	-4.663654	0.418468	-2.309179
10	7	0	-5.860050	-0.763349	-0.248083
11	8	0	-6.248245	-1.334385	0.757632

12	8	0	-6.597932	-0.382044	-1.142340
13	6	0	-1.696610	-0.002063	-0.624431
14	6	0	-0.258907	0.342335	-0.714061
15	6	0	0.752266	-0.703476	-0.762671
16	6	0	-0.020844	1.562562	-1.486109
17	8	0	-0.465568	2.688617	-1.198771
18	8	0	0.706559	1.385244	-2.600215
19	6	0	2.204131	-0.261420	-0.800472
20	6	0	2.638906	0.928717	-0.210401
21	6	0	3.137731	-1.047182	-1.488336
22	6	0	3.982997	1.295842	-0.244655
23	1	0	1.950233	1.585354	0.293812
24	6	0	4.479612	-0.690478	-1.545802
25	6	0	4.881035	0.474474	-0.906835
26	1	0	4.330271	2.207060	0.230703
27	1	0	5.207159	-1.288736	-2.082624
28	9	0	6.178011	0.822923	-0.946417
29	7	0	0.641145	-2.004568	-0.731736
30	16	0	-0.773485	-2.937121	-1.156846
31	8	0	-0.021217	-4.089062	-1.786301
32	8	0	-1.340393	-3.378008	0.194701
33	1	0	2.790923	-1.931444	-2.012645
34	1	0	-0.271283	-3.618819	1.306755
35	6	0	1.074370	2.553071	-3.342593
36	1	0	1.550304	2.188307	-4.249766
37	1	0	1.782417	3.158915	-2.763854
38	1	0	-0.283594	1.287653	1.184505
39	6	0	1.015500	-2.497386	2.212659
40	8	0	0.131836	-1.673858	2.549202
41	8	0	2.260195	-2.313547	2.199060
42	8	0	0.601194	-3.744548	1.815274
43	19	0	1.780428	0.351554	2.743623
44	19	0	2.378618	-4.042252	-0.085287
45	1	0	0.192589	3.148327	-3.580850
46	6	0	0.083369	2.799475	1.750084
47	8	0	1.320787	2.884023	1.751770
48	8	0	-0.735297	3.733804	1.829007
49	8	0	-0.456061	1.503236	1.622867
50	19	0	0.812325	4.884953	-0.001703
51	19	0	-2.749834	2.609205	0.674425

Int16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.908203	1.067315	-1.512271
2	6	0	-2.834191	0.304699	-1.074426
3	6	0	-3.839057	0.126944	1.114097
4	6	0	-4.929645	0.874369	0.688506
5	6	0	-4.937435	1.341111	-0.620398
6	1	0	-3.963392	1.436768	-2.528844
7	1	0	-2.007468	0.037074	-1.738782
8	1	0	-3.829657	-0.242084	2.136230
9	1	0	-5.756164	1.106767	1.353657
10	7	0	-6.082244	2.135286	-1.074329
11	8	0	-6.070392	2.549489	-2.223680
12	8	0	-6.985016	2.351306	-0.284893
13	6	0	-2.786367	-0.152482	0.248624
14	6	0	-1.597011	-0.997625	0.655168
15	6	0	-0.227176	-0.320867	0.553548
16	6	0	-1.835727	-1.737431	1.952745
17	8	0	-2.660995	-2.614288	2.065306
18	8	0	-1.058436	-1.325903	2.955579
19	6	0	-0.148512	1.126509	0.220811
20	6	0	-0.633379	2.043938	1.146248
21	6	0	0.510474	1.567747	-0.928099
22	6	0	-0.400619	3.404679	0.978241
23	1	0	-1.167218	1.694392	2.028870
24	6	0	0.738279	2.926859	-1.122425
25	6	0	0.297993	3.807526	-0.148003
26	1	0	-0.736041	4.140191	1.700688
27	1	0	1.253504	3.303144	-1.999916
28	9	0	0.599726	5.124413	-0.287043
29	7	0	0.879072	-0.920657	0.739040
30	16	0	0.940294	-2.621807	1.249463
31	8	0	1.752864	-3.182924	0.092475
32	8	0	1.787673	-2.494847	2.481916
33	1	0	0.806165	0.836191	-1.672890
34	1	0	2.430557	-0.075363	0.518658
35	6	0	-1.111917	-2.133341	4.136153
36	1	0	-0.401385	-1.693550	4.828109
37	1	0	-0.818187	-3.153268	3.886689
38	1	0	-1.568055	-1.596306	0.100450
39	6	0	3.386864	1.616580	0.474210

40	8	0	2.685559	2.031308	1.415038
41	8	0	4.255099	2.259890	-0.178510
42	8	0	3.235573	0.306528	0.076960
43	19	0	3.222931	4.544511	0.771576
44	19	0	5.802070	0.278226	-0.922265
45	1	0	-2.118485	-2.130924	4.553293
46	6	0	-0.451348	-2.357646	-2.103625
47	8	0	-0.278460	-1.074353	-2.248611
48	8	0	0.280789	-3.181770	-2.787398
49	8	0	-1.301273	-2.823023	-1.269028
50	19	0	2.306518	-1.586217	-1.919286
51	19	0	0.087101	-5.015512	-0.927028

TS11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.904990	1.077035	-1.511284
2	6	0	-2.832787	0.316519	-1.073243
3	6	0	-3.845113	0.128577	1.113872
4	6	0	-4.929375	0.882892	0.688009
5	6	0	-4.939389	1.351413	-0.620321
6	1	0	-3.958460	1.447968	-2.527417
7	1	0	-2.014623	0.053004	-1.741425
8	1	0	-3.832973	-0.237432	2.135485
9	1	0	-5.751792	1.115851	1.352477
10	7	0	-6.073247	2.148117	-1.074511
11	8	0	-6.063425	2.564746	-2.222971
12	8	0	-6.981525	2.363954	-0.286177
13	6	0	-2.778324	-0.160639	0.249290
14	6	0	-1.595586	-0.981231	0.665295
15	6	0	-0.247086	-0.334685	0.552001
16	6	0	-1.837308	-1.736460	1.934079
17	8	0	-2.671079	-2.609797	2.062959
18	8	0	-1.062251	-1.331071	2.955726
19	6	0	-0.146900	1.121918	0.220625
20	6	0	-0.629665	2.043981	1.151454
21	6	0	0.512766	1.567133	-0.923643
22	6	0	-0.393899	3.404405	0.984675
23	1	0	-1.164301	1.690194	2.029207
24	6	0	0.743559	2.925952	-1.116749
25	6	0	0.305442	3.806555	-0.141313

26	1	0	-0.727606	4.140034	1.707770
27	1	0	1.259446	3.301985	-1.993949
28	9	0	0.610540	5.123008	-0.278969
29	7	0	0.880572	-0.923135	0.742640
30	16	0	0.934937	-2.620712	1.247749
31	8	0	1.747365	-3.183915	0.084931
32	8	0	1.781786	-2.503885	2.481050
33	1	0	0.810903	0.839915	-1.669133
34	1	0	2.420567	-0.084631	0.517546
35	6	0	-1.118762	-2.141343	4.129698
36	1	0	-0.403944	-1.708183	4.825917
37	1	0	-0.832437	-3.167110	3.886027
38	1	0	-1.504145	-1.863548	-0.247707
39	6	0	3.389560	1.609318	0.478227
40	8	0	2.689371	2.025231	1.419372
41	8	0	4.258763	2.251112	-0.174351
42	8	0	3.235635	0.299589	0.080429
43	19	0	3.234002	4.537724	0.774443
44	19	0	5.804718	0.275343	-0.927667
45	1	0	-2.124498	-2.133514	4.553268
46	6	0	-0.437398	-2.336971	-2.117558
47	8	0	-0.280019	-1.076528	-2.248408
48	8	0	0.261243	-3.180565	-2.778633
49	8	0	-1.311008	-2.796175	-1.237859
50	19	0	2.303783	-1.587930	-1.921935
51	19	0	0.078098	-5.014234	-0.926182

Int17

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.908015	1.072239	-1.508011
2	6	0	-2.834606	0.319879	-1.070836
3	6	0	-3.850139	0.119746	1.118129
4	6	0	-4.928620	0.879922	0.693209
5	6	0	-4.948029	1.346956	-0.615589
6	1	0	-3.963289	1.441966	-2.524480
7	1	0	-2.031481	0.063024	-1.747134
8	1	0	-3.829144	-0.238015	2.140176
9	1	0	-5.743074	1.113058	1.358798
10	7	0	-6.069201	2.142440	-1.068816
11	8	0	-6.068950	2.556880	-2.218082

12	8	0	-6.982867	2.359267	-0.278903
13	6	0	-2.763674	-0.183646	0.252087
14	6	0	-1.586483	-0.961143	0.680895
15	6	0	-0.273524	-0.354796	0.544281
16	6	0	-1.825417	-1.735466	1.909427
17	8	0	-2.663059	-2.611455	2.068197
18	8	0	-1.058697	-1.324977	2.957983
19	6	0	-0.147452	1.115537	0.211801
20	6	0	-0.630886	2.044789	1.149161
21	6	0	0.511473	1.567811	-0.925828
22	6	0	-0.396748	3.405316	0.981332
23	1	0	-1.164691	1.684129	2.020463
24	6	0	0.740642	2.926719	-1.119975
25	6	0	0.301762	3.807651	-0.145158
26	1	0	-0.731038	4.141033	1.704092
27	1	0	1.255855	3.302638	-1.997630
28	9	0	0.604841	5.124243	-0.284064
29	7	0	0.889693	-0.921346	0.740608
30	16	0	0.937840	-2.611162	1.250647
31	8	0	1.749250	-3.184404	0.081655
32	8	0	1.785932	-2.496871	2.482724
33	1	0	0.817533	0.847589	-1.670916
34	1	0	2.407468	-0.089148	0.508179
35	6	0	-1.112488	-2.132607	4.126912
36	1	0	-0.401154	-1.693724	4.830123
37	1	0	-0.819971	-3.164296	3.900093
38	1	0	-1.398128	-2.284316	-0.782525
39	6	0	3.388577	1.613265	0.475128
40	8	0	2.688164	2.028545	1.416376
41	8	0	4.257192	2.255782	-0.177868
42	8	0	3.235694	0.303459	0.077673
43	19	0	3.227924	4.541307	0.773189
44	19	0	5.801686	0.272618	-0.922774
45	1	0	-2.118852	-2.129200	4.556029
46	6	0	-0.409094	-2.310328	-2.136237
47	8	0	-0.280926	-1.084662	-2.246524
48	8	0	0.241322	-3.181043	-2.763011
49	8	0	-1.316584	-2.763438	-1.186320
50	19	0	2.303665	-1.587867	-1.918531
51	19	0	0.081044	-5.014991	-0.925946

TS12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.026002	0.984460	-1.275553
2	6	0	-2.860905	0.456380	-0.748219
3	6	0	-3.980616	0.064362	1.359262
4	6	0	-5.152481	0.581697	0.837363
5	6	0	-5.165822	1.046480	-0.477153
6	1	0	-4.075281	1.324736	-2.304018
7	1	0	-1.989287	0.349171	-1.385442
8	1	0	-3.973054	-0.295107	2.378608
9	1	0	-6.053868	0.645151	1.437938
10	7	0	-6.390555	1.592680	-1.024432
11	8	0	-6.376387	2.015669	-2.174312
12	8	0	-7.387133	1.612838	-0.314348
13	6	0	-2.795060	-0.001217	0.591043
14	6	0	-1.549371	-0.529167	1.147002
15	6	0	-0.281104	-0.057130	0.702546
16	6	0	-1.660468	-1.488972	2.242764
17	8	0	-2.578573	-2.273033	2.427327
18	8	0	-0.642222	-1.387756	3.130693
19	6	0	-0.153671	1.357089	0.221345
20	6	0	-0.661777	2.379836	1.025880
21	6	0	0.559459	1.680620	-0.933637
22	6	0	-0.423033	3.713289	0.717450
23	1	0	-1.227093	2.123040	1.917418
24	6	0	0.798180	3.011024	-1.265747
25	6	0	0.315087	3.995939	-0.420620
26	1	0	-0.786340	4.521142	1.341899
27	1	0	1.350544	3.287063	-2.158003
28	9	0	0.610245	5.286989	-0.701594
29	7	0	0.860820	-0.715633	0.749881
30	16	0	0.997950	-2.450147	1.120234
31	8	0	1.682061	-2.913287	-0.162419
32	8	0	1.977489	-2.446854	2.255527
33	1	0	0.898171	0.886310	-1.584344
34	1	0	1.876913	-0.235941	0.467917
35	6	0	-0.573154	-2.422959	4.105067
36	1	0	0.349763	-2.251534	4.654385
37	1	0	-0.540687	-3.400961	3.617568
38	1	0	-1.567454	-1.980328	-0.687585
39	6	0	3.346932	1.409796	0.433227

40	8	0	2.675007	1.861155	1.406143
41	8	0	4.281976	2.087171	-0.141396
42	8	0	3.099106	0.189426	-0.028068
43	19	0	3.255002	4.315148	0.798154
44	19	0	5.720735	-0.016243	-0.646609
45	1	0	-1.437600	-2.383410	4.773706
46	6	0	-0.421586	-2.174464	-2.216814
47	8	0	-0.296475	-0.930566	-2.240457
48	8	0	0.171650	-3.025569	-2.912682
49	8	0	-1.299614	-2.703651	-1.281709
50	19	0	2.369729	-1.346025	-2.124872
51	19	0	0.237758	-4.944245	-1.086842

Int18

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.984723	0.072351	-1.418716
2	6	0	-1.819834	-0.017985	-0.685508
3	6	0	-2.319356	-2.328621	-0.158192
4	6	0	-3.486635	-2.245444	-0.887713
5	6	0	-3.827213	-1.041195	-1.516662
6	1	0	-3.242250	0.989160	-1.936199
7	1	0	-1.148507	0.833766	-0.665393
8	1	0	-2.074979	-3.264910	0.325905
9	1	0	-4.149036	-3.099382	-0.967871
10	7	0	-5.036618	-0.953850	-2.277623
11	8	0	-5.329454	0.119151	-2.807410
12	8	0	-5.748199	-1.954352	-2.380408
13	6	0	-1.442910	-1.213927	-0.004233
14	6	0	-0.240945	-1.275768	0.793427
15	6	0	0.355768	-0.068203	1.371142
16	6	0	0.298096	-2.575806	1.154516
17	8	0	0.169945	-3.625249	0.527792
18	8	0	0.970663	-2.564388	2.332404
19	6	0	-0.568381	1.027257	1.821089
20	6	0	-1.736700	0.717124	2.523704
21	6	0	-0.241977	2.365646	1.587401
22	6	0	-2.563718	1.726442	3.012587
23	1	0	-1.997085	-0.323841	2.693171
24	6	0	-1.063632	3.389219	2.052215
25	6	0	-2.203007	3.041472	2.762577

26	1	0	-3.466943	1.508168	3.571545
27	1	0	-0.837967	4.434709	1.871193
28	9	0	-3.003845	4.031825	3.227297
29	7	0	1.609080	0.178388	1.606149
30	16	0	2.881685	-0.880005	1.014086
31	8	0	3.644189	0.114641	0.138877
32	8	0	3.656758	-1.138692	2.289970
33	1	0	0.647712	2.589358	1.008658
34	6	0	1.717046	-3.738365	2.638446
35	1	0	2.261500	-3.512221	3.553249
36	1	0	2.421380	-3.961482	1.832258
37	1	0	0.766362	-0.681167	-1.150861
38	1	0	1.051940	-4.591998	2.786893
39	6	0	1.543725	0.841431	-2.051599
40	8	0	0.860385	1.612781	-1.347227
41	8	0	2.423074	1.144543	-2.898244
42	8	0	1.339971	-0.516729	-1.921262
43	19	0	2.286130	3.741779	-2.202316
44	19	0	4.052819	-0.914157	-2.275185
45	1	0	1.855972	0.989476	2.136414

TS13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.240135	1.344482	-1.062335
2	6	0	-0.922335	0.038615	-0.862654
3	6	0	0.079484	0.635881	1.293195
4	6	0	-0.233207	1.941536	1.059741
5	6	0	-0.844891	2.349918	-0.146105
6	1	0	-1.813928	1.632669	-1.936255
7	1	0	-1.256503	-0.698825	-1.576431
8	1	0	0.508489	0.380328	2.249146
9	1	0	-0.018676	2.689598	1.814941
10	7	0	-1.188124	3.677289	-0.360777
11	8	0	-1.747110	3.998947	-1.425216
12	8	0	-0.939012	4.527089	0.517222
13	6	0	-0.163486	-0.429814	0.310872
14	6	0	-4.426625	-1.740098	-0.610937
15	6	0	-3.966849	-0.909252	0.325962
16	6	0	-4.182450	-3.140527	-0.671718
17	8	0	-4.730861	-4.037229	-0.026826

18	8	0	-3.359382	-3.469749	-1.729624
19	6	0	-4.369658	0.531058	0.364972
20	6	0	-5.518779	0.945462	-0.327839
21	6	0	-3.631699	1.511310	1.038142
22	6	0	-5.911730	2.276096	-0.357815
23	1	0	-6.087281	0.186881	-0.855333
24	6	0	-3.998234	2.857145	1.009533
25	6	0	-5.136199	3.215128	0.311538
26	1	0	-6.800256	2.597630	-0.890581
27	1	0	-3.388767	3.619436	1.485428
28	9	0	-5.506934	4.513267	0.273549
29	7	0	-3.096983	-1.281918	1.439348
30	16	0	-1.516148	-1.847778	1.310714
31	8	0	-1.110621	-1.979859	2.734304
32	8	0	-1.555253	-3.094776	0.516015
33	1	0	-2.714815	1.240372	1.551505
34	1	0	-3.139572	-0.657048	2.240117
35	6	0	-2.968008	-4.828411	-1.775351
36	1	0	-3.831822	-5.495200	-1.842330
37	1	0	-2.350107	-4.939548	-2.668634
38	1	0	-2.385959	-5.089183	-0.885708
39	6	0	1.862409	1.990529	-2.102733
40	6	0	2.172554	0.634389	-2.118419
41	6	0	4.453327	1.151958	-1.399127
42	6	0	4.147401	2.507132	-1.393514
43	6	0	2.853780	2.886485	-1.730157
44	1	0	0.872265	2.347543	-2.355916
45	1	0	1.424623	-0.099774	-2.405247
46	1	0	5.445352	0.802565	-1.133639
47	1	0	4.883157	3.254373	-1.126531
48	7	0	2.511291	4.318745	-1.681571
49	8	0	1.350839	4.629326	-1.874118
50	8	0	3.408933	5.107465	-1.445251
51	6	0	3.457274	0.241498	-1.747797
52	6	0	0.954870	-1.421923	-0.000662
53	6	0	2.188494	-1.390267	0.573689
54	6	0	0.709806	-2.429490	-1.101283
55	8	0	0.154452	-2.226230	-2.158981
56	8	0	1.183941	-3.627735	-0.753120
57	6	0	2.543423	-0.832853	1.902712
58	6	0	3.525598	0.155713	2.033722
59	6	0	1.950034	-1.376440	3.047527
60	6	0	3.881146	0.635744	3.287383
61	1	0	3.994742	0.575934	1.149393

62	6	0	2.308237	-0.915590	4.309469
63	6	0	3.262928	0.086235	4.402403
64	1	0	4.621957	1.416533	3.412686
65	1	0	1.862235	-1.318325	5.211394
66	9	0	3.608499	0.538852	5.616746
67	7	0	3.330254	-1.925997	-0.074214
68	16	0	3.823709	-1.497122	-1.621936
69	8	0	5.266755	-1.691060	-1.600372
70	8	0	3.008189	-2.188546	-2.604392
71	1	0	1.178743	-2.131746	2.942898
72	1	0	4.149940	-2.032990	0.518081
73	6	0	1.078746	-4.633412	-1.760956
74	1	0	1.606183	-4.311498	-2.660729
75	1	0	1.541117	-5.523935	-1.339595
76	1	0	0.030431	-4.823863	-1.997119

Int19

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.622608	0.941789	-1.592206
2	6	0	-0.985113	-0.159560	-1.031278
3	6	0	0.716605	1.290669	-0.125024
4	6	0	0.079506	2.396773	-0.649517
5	6	0	-1.090607	2.201202	-1.382636
6	1	0	-2.559439	0.801720	-2.119295
7	1	0	-1.430660	-1.135720	-1.163489
8	1	0	1.660839	1.438776	0.384209
9	1	0	0.485558	3.393456	-0.529159
10	7	0	-1.791645	3.364477	-1.916555
11	8	0	-2.706550	3.181323	-2.704591
12	8	0	-1.433235	4.471884	-1.541094
13	6	0	0.184085	-0.010409	-0.277783
14	6	0	-4.288911	-0.767685	-1.051318
15	6	0	-3.971518	-0.469504	0.217548
16	6	0	-4.359511	-2.139347	-1.462224
17	8	0	-5.327584	-2.895742	-1.542398
18	8	0	-3.118062	-2.583948	-1.884651
19	6	0	-3.696592	0.944483	0.621045
20	6	0	-4.288683	2.012930	-0.062930
21	6	0	-2.744797	1.245130	1.612500
22	6	0	-3.939603	3.333420	0.201740

23	1	0	-5.011054	1.787048	-0.840567
24	6	0	-2.371607	2.559947	1.879740
25	6	0	-2.975364	3.584196	1.165674
26	1	0	-4.389354	4.162387	-0.335326
27	1	0	-1.605882	2.795766	2.612012
28	9	0	-2.617268	4.863882	1.417123
29	7	0	-3.762066	-1.456693	1.254042
30	16	0	-2.225858	-2.336763	1.255632
31	8	0	-1.677778	-1.911958	2.616956
32	8	0	-2.687910	-3.775434	1.312733
33	1	0	-2.258960	0.434383	2.153051
34	1	0	-3.815996	-1.036377	2.182330
35	6	0	-3.012003	-3.964599	-2.178847
36	1	0	-3.696947	-4.255590	-2.978999
37	1	0	-1.975397	-4.129415	-2.478124
38	1	0	-3.229199	-4.566550	-1.288736
39	6	0	2.563481	0.600144	-2.715218
40	6	0	2.786847	-0.641153	-2.134965
41	6	0	4.593639	0.304666	-0.786823
42	6	0	4.389217	1.543291	-1.387036
43	6	0	3.359997	1.661586	-2.313456
44	1	0	1.767412	0.751713	-3.435469
45	1	0	2.163203	-1.490230	-2.395176
46	1	0	5.372029	0.168268	-0.042690
47	1	0	4.991407	2.404915	-1.129635
48	7	0	3.061139	2.995330	-2.859262
49	8	0	2.006868	3.137212	-3.451125
50	8	0	3.875814	3.881088	-2.672843
51	6	0	3.771685	-0.756556	-1.156614
52	6	0	0.933540	-1.199672	0.206338
53	6	0	1.901742	-1.140496	1.171151
54	6	0	0.637911	-2.504084	-0.474321
55	8	0	0.301982	-2.633689	-1.634903
56	8	0	0.698774	-3.522584	0.383417
57	6	0	1.933231	-0.139783	2.260640
58	6	0	3.086294	0.604976	2.536857
59	6	0	0.773655	0.050890	3.028608
60	6	0	3.069518	1.588908	3.518629
61	1	0	3.991672	0.446570	1.957719
62	6	0	0.753703	1.024866	4.018720
63	6	0	1.894988	1.787385	4.229692
64	1	0	3.939320	2.198039	3.734359
65	1	0	-0.118180	1.187953	4.642585
66	9	0	1.870657	2.737123	5.176093

67	7	0	3.006902	-2.000729	1.135858
68	16	0	3.891381	-2.298991	-0.265697
69	8	0	5.252078	-2.511839	0.205752
70	8	0	3.232868	-3.312532	-1.072629
71	1	0	-0.069548	-0.631662	2.885346
72	1	0	3.598346	-2.038656	1.961666
73	6	0	0.340770	-4.798483	-0.149305
74	1	0	0.924037	-4.996325	-1.050491
75	1	0	0.590381	-5.520401	0.627613
76	1	0	-0.731868	-4.829504	-0.371511

Int20

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.939078	-2.158460	1.302552
2	6	0	4.191954	-2.097055	0.142660
3	6	0	3.117094	-0.089380	0.926811
4	6	0	3.852543	-0.136444	2.103851
5	6	0	4.762609	-1.176990	2.268706
6	1	0	5.663106	-2.956546	1.464314
7	1	0	4.313078	-2.861393	-0.615513
8	1	0	2.398829	0.714321	0.786222
9	1	0	3.717714	0.605045	2.880448
10	7	0	5.553823	-1.237657	3.496832
11	8	0	6.335689	-2.157319	3.624747
12	8	0	5.384918	-0.364259	4.332082
13	6	0	3.276604	-1.051962	-0.073083
14	6	0	-3.360448	-0.976379	-1.165823
15	6	0	-4.185971	-0.329851	-0.326185
16	6	0	-3.206290	-2.374018	-1.211753
17	8	0	-3.646327	-3.173211	-2.080083
18	8	0	-2.265269	-2.881898	-0.293481
19	6	0	-4.168027	1.172799	-0.219547
20	6	0	-3.779270	1.982329	-1.307393
21	6	0	-4.522967	1.829371	0.976369
22	6	0	-3.787968	3.371367	-1.230378
23	1	0	-3.461370	1.474709	-2.218913
24	6	0	-4.525770	3.227506	1.074364
25	6	0	-4.168045	3.972951	-0.035148
26	1	0	-3.510805	3.995419	-2.072160
27	1	0	-4.804404	3.734979	1.988362

28	9	0	-4.208691	5.329181	0.038893
29	7	0	-5.162359	-0.954019	0.586291
30	16	0	-4.499795	-1.701438	2.018675
31	8	0	-5.290163	-0.935840	3.079758
32	8	0	-4.983867	-3.132409	1.937249
33	1	0	-4.797419	1.242771	1.842826
34	1	0	-5.849631	-0.290926	0.950156
35	6	0	-1.955112	-4.257626	-0.452451
36	1	0	-1.551365	-4.463713	-1.449278
37	1	0	-1.201292	-4.496673	0.309609
38	1	0	-2.839227	-4.892036	-0.317279
39	6	0	-0.115706	-0.363593	1.675188
40	6	0	-0.172291	-0.741821	0.322417
41	6	0	-0.756236	1.551681	-0.296759
42	6	0	-0.721058	1.935981	1.052365
43	6	0	-0.343760	0.970409	1.956795
44	1	0	0.088660	-1.081971	2.478344
45	1	0	-0.065848	-1.783331	0.023518
46	1	0	-1.082468	2.251504	-1.064006
47	1	0	-0.992929	2.942698	1.393007
48	7	0	-0.184759	1.400487	3.386888
49	8	0	0.246140	0.583200	4.163224
50	8	0	-0.471281	2.543274	3.650769
51	6	0	-0.327874	0.282148	-0.623277
52	6	0	2.464734	-1.006407	-1.311926
53	6	0	2.137119	0.146995	-1.951639
54	6	0	1.992071	-2.347062	-1.804651
55	8	0	1.679215	-3.270189	-1.066535
56	8	0	2.046717	-2.452012	-3.125349
57	6	0	2.878910	1.420361	-1.760711
58	6	0	2.213739	2.643264	-1.677331
59	6	0	4.280756	1.399635	-1.728494
60	6	0	2.925912	3.833775	-1.513674
61	1	0	1.129909	2.692518	-1.723916
62	6	0	5.005474	2.569111	-1.581300
63	6	0	4.310049	3.761572	-1.471359
64	1	0	2.425274	4.785285	-1.428755
65	1	0	6.089084	2.576357	-1.565387
66	9	0	5.005334	4.904786	-1.338713
67	7	0	1.039597	0.240225	-2.805022
68	16	0	-0.563319	-0.262644	-2.335575
69	8	0	-1.352959	0.634516	-3.161760
70	8	0	-0.578599	-1.705070	-2.469751
71	1	0	4.803135	0.449359	-1.827775

72	1	0	0.975972	1.074804	-3.384613
73	6	0	1.522163	-3.661046	-3.664586
74	1	0	0.475585	-3.773511	-3.382054
75	1	0	1.619506	-3.572143	-4.743749
76	1	0	2.095018	-4.520391	-3.304166

TS14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.040413	-2.069082	1.271247
2	6	0	4.238973	-2.061768	0.139885
3	6	0	3.151653	-0.044821	0.906019
4	6	0	3.939615	-0.039373	2.045998
5	6	0	4.876997	-1.053622	2.206277
6	1	0	5.780334	-2.841923	1.435172
7	1	0	4.350933	-2.854685	-0.591530
8	1	0	2.400880	0.726527	0.773411
9	1	0	3.821282	0.719289	2.809305
10	7	0	5.711369	-1.059988	3.406713
11	8	0	6.518915	-1.965452	3.540197
12	8	0	5.560766	-0.158571	4.215341
13	6	0	3.291625	-1.046803	-0.069797
14	6	0	-2.994631	-0.886883	-0.678349
15	6	0	-4.017533	-0.221718	-0.116964
16	6	0	-3.005593	-2.332811	-0.858125
17	8	0	-3.648953	-2.933009	-1.706351
18	8	0	-2.138435	-2.993342	-0.050150
19	6	0	-4.098317	1.262048	-0.097320
20	6	0	-3.808692	2.010406	-1.242351
21	6	0	-4.488285	1.930468	1.071270
22	6	0	-3.886214	3.400336	-1.225843
23	1	0	-3.502515	1.485706	-2.143235
24	6	0	-4.556801	3.319006	1.109779
25	6	0	-4.254121	4.026865	-0.044937
26	1	0	-3.669631	3.997839	-2.104578
27	1	0	-4.840380	3.855270	2.008437
28	9	0	-4.330083	5.371919	-0.019158
29	7	0	-5.073070	-0.891906	0.544398
30	16	0	-4.615376	-1.780551	2.036364
31	8	0	-5.497826	-1.048203	3.023148
32	8	0	-5.125201	-3.169686	1.777991

33	1	0	-4.724801	1.346992	1.958692
34	1	0	-5.828003	-0.261540	0.811777
35	6	0	-1.947896	-4.366332	-0.366873
36	1	0	-1.620099	-4.475909	-1.403745
37	1	0	-1.175758	-4.728252	0.311642
38	1	0	-2.871880	-4.931498	-0.222516
39	6	0	0.039218	-0.275326	1.647244
40	6	0	-0.264479	-0.803165	0.422074
41	6	0	-0.952928	1.421391	-0.348756
42	6	0	-0.642279	1.940891	0.883896
43	6	0	-0.176970	1.094782	1.902067
44	1	0	0.488518	-0.891257	2.416743
45	1	0	-0.076176	-1.846445	0.204565
46	1	0	-1.284489	2.074229	-1.146493
47	1	0	-0.720165	3.005684	1.069626
48	7	0	0.201078	1.645668	3.154261
49	8	0	0.725514	0.909456	3.994948
50	8	0	-0.002147	2.844200	3.366242
51	6	0	-0.911929	0.009200	-0.567504
52	6	0	2.416965	-1.065389	-1.262207
53	6	0	2.003888	0.076250	-1.886901
54	6	0	1.967594	-2.424534	-1.696224
55	8	0	1.728507	-3.338563	-0.934999
56	8	0	1.973146	-2.555887	-3.024967
57	6	0	2.748164	1.359170	-1.803177
58	6	0	2.078656	2.585954	-1.722121
59	6	0	4.148969	1.348897	-1.867448
60	6	0	2.787344	3.780864	-1.674045
61	1	0	0.995759	2.608015	-1.663213
62	6	0	4.870024	2.532819	-1.824892
63	6	0	4.171675	3.729273	-1.723889
64	1	0	2.286136	4.738415	-1.596708
65	1	0	5.952119	2.544955	-1.880248
66	9	0	4.863185	4.876690	-1.682737
67	7	0	0.866844	0.124345	-2.688794
68	16	0	-0.685720	-0.471676	-2.274668
69	8	0	-1.526879	0.307301	-3.177356
70	8	0	-0.657715	-1.923586	-2.371006
71	1	0	4.671425	0.402558	-1.961442
72	1	0	0.767613	0.947203	-3.275350
73	6	0	1.484797	-3.807865	-3.510878
74	1	0	0.451642	-3.946754	-3.188914
75	1	0	1.543880	-3.747787	-4.595742
76	1	0	2.102505	-4.627378	-3.139003

Int21

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.065613	-0.227161	-0.155875
2	6	0	1.691960	-0.115261	-0.005719
3	6	0	1.374762	-0.588566	-2.352274
4	6	0	2.746424	-0.706846	-2.523354
5	6	0	3.570346	-0.518968	-1.418893
6	1	0	3.740302	-0.105668	0.682473
7	1	0	1.258232	0.091514	0.968617
8	1	0	0.715748	-0.731013	-3.202364
9	1	0	3.180478	-0.932996	-3.489009
10	7	0	5.016220	-0.643655	-1.588163
11	8	0	5.726312	-0.480069	-0.608302
12	8	0	5.445740	-0.905752	-2.700269
13	6	0	0.825868	-0.278842	-1.099224
14	6	0	-0.642736	-0.180508	-0.908973
15	6	0	-1.208508	0.837742	-0.167625
16	6	0	-1.383702	-1.372518	-1.334787
17	8	0	-0.868558	-2.459993	-1.578192
18	8	0	-2.701456	-1.189218	-1.441422
19	6	0	-0.389776	2.043155	0.172784
20	6	0	0.244868	2.761686	-0.845604
21	6	0	-0.311627	2.505203	1.491011
22	6	0	0.958356	3.920273	-0.558725
23	1	0	0.172205	2.411175	-1.870467
24	6	0	0.408288	3.655978	1.794527
25	6	0	1.029214	4.341294	0.760778
26	1	0	1.450306	4.495692	-1.334386
27	1	0	0.495304	4.023839	2.810629
28	9	0	1.722990	5.456529	1.047976
29	7	0	-2.497415	0.842821	0.302955
30	16	0	-3.995334	1.217947	-0.973522
31	8	0	-4.594581	2.301883	-0.149029
32	8	0	-3.261711	1.726664	-2.157005
33	1	0	-0.782376	1.924678	2.277736
34	6	0	-3.488909	-2.325128	-1.788707
35	1	0	-4.492127	-1.939837	-1.962090
36	1	0	-3.509640	-3.043983	-0.965950
37	1	0	-3.097683	-2.806638	-2.685596

38	1	0	-2.631140	1.668883	0.885911

CP1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.191042	-0.199464	-1.049908
2	6	0	-0.149985	-0.530176	-0.921600
3	6	0	0.459039	-2.636491	0.143915
4	6	0	1.805863	-2.331616	-0.013637
5	6	0	2.133052	-1.106024	-0.580878
6	1	0	1.491670	0.745558	-1.484896
7	1	0	-0.920003	0.166588	-1.230611
8	1	0	0.147433	-3.561661	0.614943
9	1	0	2.586589	-3.003576	0.320458
10	7	0	3.547269	-0.725049	-0.638552
11	8	0	3.805306	0.472342	-0.654242
12	8	0	4.381623	-1.606308	-0.650834
13	6	0	-0.495572	-1.724075	-0.298168
14	7	0	-2.588938	-1.068037	1.349559
15	16	0	-2.222265	-2.006547	0.070332
16	8	0	-2.348374	-3.408242	0.464854
17	8	0	-2.984095	-1.508244	-1.071610
18	1	0	-1.817079	-1.054528	1.985209
19	6	0	0.103809	3.412925	0.335278
20	8	0	-1.159826	3.196878	0.073532
21	8	0	0.750269	4.248287	-0.417853
22	8	0	0.681454	2.790994	1.286279
23	19	0	-1.338996	4.993671	-1.776502
24	19	0	3.023636	3.788774	0.742917
25	1	0	-2.779376	-0.137548	1.036633

CP2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.110215	-0.429723	-1.191997
2	6	0	-0.259025	-0.616345	-1.068473
3	6	0	0.117580	-2.575825	0.318190
4	6	0	1.490698	-2.424022	0.174501

5	6	0	1.951786	-1.333538	-0.552761
6	1	0	1.521387	0.388197	-1.771930
7	1	0	-0.956424	0.056801	-1.553399
8	1	0	-0.290992	-3.394414	0.900409
9	1	0	2.193879	-3.109111	0.632171
10	7	0	3.394493	-1.110056	-0.625037
11	8	0	3.778400	0.039740	-0.816703
12	8	0	4.136785	-2.059189	-0.477630
13	6	0	-0.743973	-1.662050	-0.285638
14	7	0	-2.730834	-0.779771	1.338825
15	16	0	-2.503749	-1.721984	0.092892
16	8	0	-2.777645	-3.147217	0.360777
17	8	0	-3.160206	-1.132168	-1.086507
18	1	0	-2.409304	-1.273360	2.171854
19	1	0	-2.061933	0.642339	1.074335
20	6	0	-0.368132	1.703097	0.915600
21	8	0	-1.705636	1.560872	0.713383
22	8	0	0.167512	2.642127	0.251574
23	8	0	0.214691	0.925791	1.702445
24	19	0	-1.938242	3.408854	-1.146215
25	19	0	2.590435	1.899614	0.989823

Int3'[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.845618	-2.206900	-1.063564
2	6	0	-0.278784	-1.654590	-0.460138
3	6	0	0.906917	-1.594779	1.676448
4	6	0	2.028010	-2.155747	1.077452
5	6	0	1.968345	-2.442012	-0.280391
6	1	0	0.857949	-2.456317	-2.116627
7	1	0	2.926952	-2.369220	1.640648
8	6	0	-0.223426	-1.352337	0.900149
9	6	0	-1.855013	1.323274	-1.144782
10	6	0	-1.133714	1.490455	-0.038408
11	6	0	-3.152108	0.733504	-1.205665
12	8	0	-4.236166	1.257144	-0.958957
13	8	0	-3.111136	-0.521841	-1.776047
14	7	0	-1.533003	1.031241	1.302591
15	16	0	-1.636109	-0.573182	1.662681
16	8	0	-1.487770	-0.672733	3.114635

17	8	0	-2.816790	-1.141805	1.027067
18	1	0	-1.103901	1.520307	2.084672
19	6	0	-4.347694	-1.218533	-1.769353
20	1	0	-5.103511	-0.688630	-2.354107
21	1	0	-4.149837	-2.193716	-2.215228
22	1	0	-4.711518	-1.343805	-0.746311
23	6	0	0.217432	2.217448	-0.170639
24	1	0	0.741982	1.842748	-1.024657
25	1	0	0.801558	2.047461	0.709589
26	6	0	-0.027087	3.728384	-0.340592
27	1	0	-0.388794	3.922223	-1.328769
28	1	0	-0.752289	4.055057	0.375136
29	6	0	1.292731	4.490171	-0.118422
30	1	0	2.035779	4.120869	-0.793993
31	1	0	1.622987	4.345222	0.888962
32	6	0	1.067795	5.992097	-0.373813
33	1	0	0.738168	6.137106	-1.381393
34	1	0	0.324276	6.361253	0.301318
35	6	0	2.387389	6.754006	-0.150726
36	1	0	3.130209	6.386559	-0.827558
37	1	0	2.230509	7.797871	-0.325755
38	1	0	2.718309	6.606967	0.856136
39	17	0	-1.744623	-1.332111	-1.379336
40	17	0	0.898369	-1.205311	3.392794
41	17	0	3.389955	-3.139228	-1.048841

Int3'[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.845618	-2.206900	-1.063564
2	6	0	-0.278784	-1.654590	-0.460138
3	6	0	0.906917	-1.594779	1.676448
4	6	0	2.028010	-2.155747	1.077452
5	6	0	1.968345	-2.442012	-0.280391
6	1	0	0.857949	-2.456317	-2.116627
7	1	0	2.926952	-2.369220	1.640648
8	6	0	-0.223426	-1.352337	0.900149
9	6	0	-1.855013	1.323274	-1.144782
10	6	0	-1.133714	1.490455	-0.038408
11	6	0	-3.152108	0.733504	-1.205665
12	8	0	-4.236166	1.257144	-0.958957

13	8	0	-3.111136	-0.521841	-1.776047
14	7	0	-1.533003	1.031241	1.302591
15	16	0	-1.636109	-0.573182	1.662681
16	8	0	-1.487770	-0.672733	3.114635
17	8	0	-2.816790	-1.141805	1.027067
18	1	0	-1.103901	1.520307	2.084672
19	6	0	-4.347694	-1.218533	-1.769353
20	1	0	-5.103511	-0.688630	-2.354107
21	1	0	-4.149837	-2.193716	-2.215228
22	1	0	-4.711518	-1.343805	-0.746311
23	6	0	0.217432	2.217448	-0.170639
24	1	0	0.741982	1.842748	-1.024657
25	1	0	0.801558	2.047461	0.709589
26	6	0	-0.027087	3.728384	-0.340592
27	1	0	-0.388794	3.922223	-1.328769
28	1	0	-0.752289	4.055057	0.375136
29	6	0	1.292731	4.490171	-0.118422
30	1	0	2.035779	4.120869	-0.793993
31	1	0	1.622987	4.345222	0.888962
32	6	0	1.067795	5.992097	-0.373813
33	1	0	0.738168	6.137106	-1.381393
34	1	0	0.324276	6.361253	0.301318
35	6	0	2.387389	6.754006	-0.150726
36	1	0	3.130209	6.386559	-0.827558
37	1	0	2.230509	7.797871	-0.325755
38	1	0	2.718309	6.606967	0.856136
39	1	0	-1.166567	-1.465728	-1.026770
40	1	0	0.911996	-1.352667	2.718684
41	6	0	3.212254	-3.052076	-0.952784
42	7	0	4.138400	-3.506297	-1.453412

Int3’[c]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.627523	-1.993356	0.856046
2	6	0	-0.592757	-1.240646	0.513463
3	6	0	-2.736035	-2.371739	0.052637
4	8	0	-2.802399	-3.271800	-0.786025
5	8	0	-3.897684	-1.724597	0.442921
6	7	0	-0.433596	-0.550338	-0.795051
7	16	0	-1.495442	0.625107	-1.248694

8	8	0	-0.803438	1.435933	-2.251641
9	8	0	-2.778915	0.023883	-1.585407
10	6	0	-5.022155	-1.974754	-0.382616
11	1	0	-5.290700	-3.034209	-0.379747
12	1	0	-5.841602	-1.384545	0.029768
13	1	0	-4.823211	-1.663689	-1.411851
14	6	0	0.599999	-0.948961	1.400229
15	1	0	0.377517	-1.361354	2.388309
16	1	0	0.725265	0.139577	1.519403
17	6	0	1.920904	-1.547953	0.899291
18	1	0	1.795214	-2.632487	0.787912
19	1	0	2.169435	-1.165370	-0.101187
20	6	0	3.093120	-1.258771	1.833894
21	1	0	2.862504	-1.649475	2.834508
22	1	0	3.207936	-0.171906	1.947643
23	6	0	4.411814	-1.857583	1.349339
24	1	0	4.292841	-2.941995	1.232646
25	1	0	4.640358	-1.463821	0.350970
26	6	0	5.572727	-1.565425	2.296377
27	1	0	5.375065	-1.975537	3.291821
28	1	0	6.507990	-1.999793	1.933688
29	1	0	5.723073	-0.486735	2.406288
30	6	0	-1.765484	1.648279	0.189488
31	6	0	-2.701412	1.263280	1.142090
32	6	0	-0.998274	2.791990	0.368549
33	6	0	-2.822312	2.076716	2.267785
34	1	0	-3.300349	0.366842	1.009098
35	6	0	-1.215137	3.528156	1.530928
36	1	0	-0.270822	3.102324	-0.372729
37	7	0	-2.102952	3.184720	2.468379
38	1	0	-3.536362	1.819442	3.045819
39	1	0	-0.647046	4.436792	1.711654
40	6	0	0.919439	-0.028426	-1.035472
41	6	0	1.701397	-0.562891	-2.059855
42	6	0	1.421512	1.001166	-0.239600
43	6	0	2.985381	-0.068275	-2.287808
44	1	0	1.305574	-1.375119	-2.686633
45	6	0	2.705495	1.496718	-0.468127
46	1	0	0.805275	1.422645	0.567702
47	6	0	3.487502	0.962107	-1.491940
48	1	0	3.602024	-0.489923	-3.094815
49	1	0	3.100938	2.308791	0.159278
50	6	0	4.905248	1.508077	-1.743956
51	1	0	5.557061	0.700820	-2.005442

52	1	0	4.877180	2.217477	-2.544496
53	1	0	5.266560	1.985277	-0.857033

Int4[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.620250	0.582652	0.337949
2	6	0	-2.495634	0.102451	1.025922
3	6	0	-1.935511	-1.285324	-0.847375
4	6	0	-3.046289	-0.811476	-1.559758
5	6	0	-3.900944	0.068761	-0.918566
6	1	0	-4.261457	1.337836	0.777652
7	1	0	-3.215475	-1.126047	-2.586435
8	6	0	-1.743918	-0.964436	0.494040
9	6	0	0.727489	0.976386	0.294695
10	6	0	1.417869	-0.110424	-0.072294
11	6	0	0.610948	2.230867	-0.289026
12	8	0	-0.137104	2.572430	-1.229214
13	8	0	1.304427	3.218144	0.430772
14	6	0	1.020831	4.542517	0.028835
15	1	0	1.273070	4.713256	-1.027679
16	1	0	-0.036109	4.804945	0.160881
17	1	0	1.641538	5.192457	0.660281
18	7	0	1.141682	-1.420020	0.585076
19	16	0	-0.278008	-1.655385	1.370043
20	8	0	-0.558223	-3.098763	1.269214
21	8	0	-0.233471	-1.083678	2.706054
22	1	0	1.283920	-2.227649	-0.020494
23	6	0	2.649616	-0.264885	-0.960520
24	1	0	2.643628	0.555841	-1.690543
25	1	0	2.658859	-1.217403	-1.527905
26	6	0	3.920717	-0.176352	-0.103860
27	1	0	3.866229	0.762666	0.475387
28	1	0	3.918798	-0.995824	0.628334
29	6	0	5.208791	-0.207403	-0.907883
30	1	0	5.219267	0.615210	-1.630964
31	1	0	5.248441	-1.131005	-1.502806
32	6	0	6.467620	-0.122778	-0.029463
33	1	0	6.415210	0.791262	0.571752
34	1	0	6.463144	-0.962863	0.674187
35	6	0	7.749665	-0.137213	-0.853027

36	1	0	7.783108	0.708098	-1.545760
37	1	0	8.636912	-0.074458	-0.210085
38	1	0	7.824126	-1.056901	-1.439407
39	17	0	-2.181558	0.924841	2.512994
40	17	0	-0.834346	-2.271900	-1.751137
41	17	0	-5.340444	0.577750	-1.725106

Int4[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.008637	0.090085	0.722339
2	6	0	-2.890639	-0.660011	1.132585
3	6	0	-2.242486	-0.973660	-1.185878
4	6	0	-3.355909	-0.223941	-1.610648
5	6	0	-4.227204	0.243860	-0.636850
6	1	0	-4.702771	0.534741	1.447628
7	1	0	-2.648487	-0.803904	2.175934
8	1	0	-1.528439	-1.356355	-1.912306
9	1	0	-3.540863	-0.006238	-2.666889
10	6	0	-2.126984	-1.273760	0.166677
11	6	0	0.317249	0.680056	0.410322
12	6	0	1.033710	-0.209107	-0.271805
13	6	0	0.148426	2.023178	0.340887
14	8	0	-0.631558	2.691075	-0.375140
15	8	0	0.835063	2.672455	1.381042
16	6	0	0.571383	4.056703	1.497215
17	1	0	0.833137	4.599170	0.579253
18	1	0	-0.480491	4.255313	1.718140
19	1	0	1.202176	4.422370	2.313482
20	7	0	0.765921	-1.673373	-0.091236
21	16	0	-0.600722	-2.123893	0.699806
22	8	0	-0.886001	-3.483124	0.196239
23	8	0	-0.465907	-1.949071	2.144946
24	1	0	0.852270	-2.241288	-0.929229
25	6	0	2.295128	-0.024445	-1.100327
26	1	0	2.291946	1.016313	-1.479692
27	1	0	2.374521	-0.692184	-1.982084
28	6	0	3.536919	-0.220592	-0.218266
29	1	0	3.443620	0.419481	0.676053
30	1	0	3.562904	-1.255425	0.153126
31	6	0	4.840810	0.093332	-0.947350
32	1	0	4.835319	1.137528	-1.266789

33	1	0	4.905683	-0.507996	-1.862836
34	6	0	6.093460	-0.163624	-0.100658
35	1	0	6.035735	0.437587	0.812763
36	1	0	6.106020	-1.206428	0.217875
37	6	0	7.380356	0.163443	-0.860440
38	1	0	7.397962	1.217713	-1.164374
39	1	0	8.263507	-0.023335	-0.251712
40	1	0	7.448503	-0.436403	-1.773543
41	6	0	-5.449869	0.904468	-1.068021
42	7	0	-6.431314	1.391235	-1.409775

Int4[c]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.517283	-1.312670	1.072523
2	6	0	0.812706	-0.110929	0.594915
3	6	0	1.408143	-1.986957	1.963165
4	8	0	1.411117	-1.963689	3.194316
5	8	0	2.260049	-2.845117	1.298785
6	6	0	3.077316	-3.648134	2.137325
7	1	0	3.731009	-3.034020	2.762803
8	1	0	2.472565	-4.281042	2.792472
9	1	0	3.678336	-4.269542	1.473042
10	7	0	-0.106011	0.586727	-0.338671
11	16	0	-0.546341	-0.193008	-1.724604
12	8	0	-1.219260	0.785534	-2.578416
13	8	0	0.615640	-0.904280	-2.242651
14	6	0	2.038666	0.748612	0.820533
15	1	0	2.540536	0.412986	1.736078
16	1	0	1.734337	1.793244	0.986501
17	6	0	3.020293	0.699927	-0.353741
18	1	0	3.364412	-0.335435	-0.477265
19	1	0	2.484931	0.958402	-1.276371
20	6	0	4.221025	1.625024	-0.174043
21	1	0	4.743025	1.370550	0.759179
22	1	0	3.869596	2.659640	-0.055598
23	6	0	5.209348	1.559520	-1.336639
24	1	0	5.557648	0.525643	-1.453847
25	1	0	4.686463	1.814897	-2.266910
26	6	0	6.406157	2.487788	-1.146445
27	1	0	6.956691	2.230548	-0.235892

28	1	0	7.101785	2.427865	-1.987688
29	1	0	6.080136	3.528660	-1.053258
30	6	0	-1.795528	-1.408906	-1.321600
31	6	0	-1.439106	-2.728877	-1.078525
32	6	0	-3.124727	-1.015145	-1.246580
33	6	0	-2.464863	-3.620581	-0.780317
34	1	0	-0.402950	-3.039857	-1.113951
35	6	0	-4.064708	-1.992909	-0.922038
36	1	0	-3.420796	0.008284	-1.446709
37	7	0	-3.753440	-3.270617	-0.695858
38	1	0	-2.236572	-4.666907	-0.595593
39	1	0	-5.116655	-1.729463	-0.849331
40	6	0	-1.100680	1.451429	0.238410
41	6	0	-1.274393	2.740752	-0.265105
42	6	0	-1.878354	1.008499	1.307990
43	6	0	-2.229537	3.581250	0.305574
44	1	0	-0.662074	3.073296	-1.093559
45	6	0	-2.821373	1.858695	1.871270
46	1	0	-1.710782	0.004450	1.685643
47	6	0	-3.017019	3.150830	1.377067
48	1	0	-2.358190	4.585960	-0.082407
49	1	0	-3.421864	1.511514	2.712209
50	6	0	-4.069234	4.057170	1.968597
51	1	0	-3.742477	5.134026	1.919147
52	1	0	-5.030950	3.961974	1.391874
53	1	0	-4.269405	3.783786	3.034512

TS3[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.604044	0.568301	0.386907
2	6	0	-2.416599	0.214973	1.009476
3	6	0	-1.825952	-1.120742	-0.878044
4	6	0	-2.999938	-0.763071	-1.524714
5	6	0	-3.897359	0.067304	-0.874069
6	1	0	-4.286306	1.247101	0.884216
7	1	0	-3.207983	-1.143666	-2.517389
8	6	0	-1.457391	-0.629903	0.397494
9	6	0	0.489142	0.732940	0.161347
10	6	0	1.390959	-0.207142	-0.062292
11	6	0	0.398835	2.059744	-0.340526

12	8	0	-0.391743	2.472828	-1.187225
13	8	0	1.219211	2.941371	0.323366
14	6	0	1.041230	4.306579	-0.030206
15	1	0	1.248649	4.471139	-1.090626
16	1	0	0.019887	4.637237	0.176644
17	1	0	1.746136	4.872494	0.578645
18	7	0	1.186773	-1.493215	0.598542
19	16	0	-0.275310	-1.639648	1.364680
20	8	0	-0.686486	-3.039955	1.233321
21	8	0	-0.172356	-1.098596	2.710857
22	1	0	1.326334	-2.302579	-0.005505
23	6	0	2.657641	-0.194368	-0.881875
24	1	0	2.634014	0.688730	-1.528657
25	1	0	2.691187	-1.074500	-1.542187
26	6	0	3.923897	-0.168168	-0.018046
27	1	0	3.897618	0.730164	0.612002
28	1	0	3.917508	-1.028512	0.662895
29	6	0	5.205766	-0.180106	-0.846251
30	1	0	5.200775	0.673240	-1.538456
31	1	0	5.226749	-1.083094	-1.471999
32	6	0	6.470793	-0.128597	0.007981
33	1	0	6.447631	0.775253	0.629428
34	1	0	6.471306	-0.978988	0.701269
35	6	0	7.746507	-0.145674	-0.829984
36	1	0	7.774918	0.709753	-1.512377
37	1	0	8.641077	-0.105177	-0.203066
38	1	0	7.801539	-1.055334	-1.436357
39	17	0	-2.094660	1.041663	2.505441
40	17	0	-0.742952	-2.135897	-1.803093
41	17	0	-5.394353	0.504588	-1.651106

TS3[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.953141	0.081189	0.736852
2	6	0	-2.780888	-0.526175	1.143420
3	6	0	-2.143853	-0.840846	-1.185453
4	6	0	-3.309667	-0.222599	-1.588653
5	6	0	-4.219806	0.256582	-0.630834
6	1	0	-4.677521	0.414091	1.472402
7	1	0	-2.562491	-0.665941	2.195553

8	1	0	-1.446869	-1.225746	-1.923138
9	1	0	-3.537139	-0.122408	-2.644432
10	6	0	-1.825115	-0.908754	0.185522
11	6	0	0.082724	0.522875	0.298158
12	6	0	0.994626	-0.263024	-0.248376
13	6	0	0.027666	1.946908	0.298843
14	8	0	-0.653929	2.660949	-0.433749
15	8	0	0.742003	2.505860	1.331433
16	6	0	0.602087	3.914167	1.464892
17	1	0	0.960691	4.434328	0.572796
18	1	0	-0.442028	4.192352	1.629615
19	1	0	1.204174	4.198621	2.327667
20	7	0	0.801228	-1.700261	-0.095830
21	16	0	-0.593569	-2.111573	0.693864
22	8	0	-0.978415	-3.425599	0.164350
23	8	0	-0.416148	-1.992045	2.137963
24	1	0	0.910664	-2.263727	-0.937698
25	6	0	2.268064	0.060581	-0.989794
26	1	0	2.232714	1.115453	-1.281821
27	1	0	2.324611	-0.525902	-1.919649
28	6	0	3.526685	-0.204691	-0.156025
29	1	0	3.481738	0.412514	0.750370
30	1	0	3.527193	-1.250200	0.176699
31	6	0	4.815542	0.091096	-0.918119
32	1	0	4.806470	1.135584	-1.259171
33	1	0	4.852100	-0.527888	-1.825286
34	6	0	6.072886	-0.157284	-0.087485
35	1	0	6.034287	0.462416	0.817028
36	1	0	6.077742	-1.200047	0.253692
37	6	0	7.355512	0.138199	-0.860490
38	1	0	7.381119	1.182717	-1.186815
39	1	0	8.244481	-0.045350	-0.251409
40	1	0	7.424402	-0.490079	-1.754201
41	6	0	-5.434771	0.887809	-1.049647
42	7	0	-6.418174	1.400956	-1.388581

TS3[c]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.151171	1.115569	-0.482600
2	6	0	0.104680	0.731006	-0.337142

3	6	0	-1.670253	2.237013	-1.190835
4	8	0	-2.099899	2.258444	-2.342560
5	8	0	-1.793739	3.344576	-0.388214
6	6	0	-2.442088	4.454896	-0.994370
7	1	0	-1.887232	4.808968	-1.867090
8	1	0	-3.454737	4.193659	-1.311924
9	1	0	-2.478791	5.236246	-0.235543
10	7	0	0.342185	-0.409686	0.551747
11	16	0	-0.948247	-0.664340	1.583601
12	8	0	-0.815342	-2.022961	2.113113
13	8	0	-1.018630	0.434414	2.542536
14	6	0	1.385759	1.358199	-0.837895
15	1	0	1.112220	2.192199	-1.493167
16	1	0	1.954540	0.645746	-1.451342
17	6	0	2.284389	1.854742	0.298925
18	1	0	1.708938	2.541150	0.934094
19	1	0	2.564625	1.003904	0.933154
20	6	0	3.544414	2.551562	-0.207348
21	1	0	3.261858	3.403724	-0.840821
22	1	0	4.106463	1.862322	-0.852881
23	6	0	4.453068	3.040755	0.918579
24	1	0	3.889010	3.726242	1.563340
25	1	0	4.735575	2.187953	1.548438
26	6	0	5.708576	3.736806	0.399705
27	1	0	5.446689	4.607082	-0.210422
28	1	0	6.346870	4.080124	1.218056
29	1	0	6.298589	3.059245	-0.225641
30	6	0	-2.419992	-0.616121	0.557711
31	6	0	-3.583286	-0.041988	1.096089
32	6	0	-2.574221	-1.617094	-0.417374
33	6	0	-4.796680	-0.354527	0.507485
34	1	0	-3.519308	0.667953	1.912008
35	6	0	-3.841808	-1.834946	-0.932143
36	1	0	-1.721842	-2.175638	-0.789141
37	7	0	-4.954373	-1.220561	-0.505456
38	1	0	-5.705095	0.112337	0.883019
39	1	0	-3.973649	-2.567196	-1.726279
40	6	0	1.077770	-1.538057	0.067840
41	6	0	1.905440	-2.252765	0.934621
42	6	0	1.017501	-1.897618	-1.279706
43	6	0	2.644289	-3.328997	0.457334
44	1	0	1.960585	-1.956564	1.976652
45	6	0	1.778075	-2.964199	-1.749394
46	1	0	0.380279	-1.329110	-1.951864

47	6	0	2.595596	-3.702488	-0.889911
48	1	0	3.283899	-3.881551	1.140289
49	1	0	1.731430	-3.229564	-2.801991
50	6	0	3.389922	-4.880052	-1.393657
51	1	0	4.339855	-4.972190	-0.861684
52	1	0	2.838054	-5.813780	-1.243752
53	1	0	3.599433	-4.788038	-2.461626

Int5[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.585770	0.522382	0.403750
2	6	0	-2.355949	0.283067	0.989728
3	6	0	-1.705420	-1.012374	-0.894772
4	6	0	-2.921661	-0.759442	-1.505322
5	6	0	-3.864500	0.034055	-0.867745
6	1	0	-4.313113	1.132748	0.940681
7	1	0	-3.148377	-1.205151	-2.467499
8	6	0	-1.198159	-0.354549	0.319424
9	6	0	0.261159	0.523181	0.067789
10	6	0	1.361555	-0.270328	-0.036082
11	6	0	0.185135	1.913158	-0.367524
12	8	0	-0.631665	2.377565	-1.149002
13	8	0	1.090428	2.717608	0.262471
14	6	0	0.987624	4.118162	-0.051055
15	1	0	1.174147	4.282381	-1.109625
16	1	0	-0.013357	4.489783	0.201141
17	1	0	1.743923	4.623092	0.553627
18	7	0	1.244019	-1.535942	0.632471
19	16	0	-0.252102	-1.624374	1.383155
20	8	0	-0.755113	-2.995690	1.235645
21	8	0	-0.109745	-1.099321	2.734286
22	1	0	1.394725	-2.346785	0.033277
23	6	0	2.648506	-0.094623	-0.810079
24	1	0	2.588438	0.840546	-1.387883
25	1	0	2.705821	-0.912764	-1.550723
26	6	0	3.922726	-0.102344	0.042481
27	1	0	3.919333	0.762421	0.714410
28	1	0	3.934561	-0.996354	0.682268
29	6	0	5.187721	-0.084331	-0.825903
30	1	0	5.144563	0.792152	-1.496326

31	1	0	5.196675	-0.973404	-1.473319
32	6	0	6.468815	-0.036192	-0.012083
33	1	0	6.466920	0.863294	0.621512
34	1	0	6.497750	-0.890157	0.678765
35	6	0	7.728086	-0.041635	-0.879789
36	1	0	7.728084	0.818023	-1.559864
37	1	0	8.636945	-0.002009	-0.280156
38	1	0	7.772151	-0.946098	-1.498646
39	17	0	-2.067273	1.102159	2.508943
40	17	0	-0.633559	-2.072944	-1.813084
41	17	0	-5.391763	0.416634	-1.652536

Int5[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.869744	0.061832	0.750651
2	6	0	-2.627356	-0.366191	1.149638
3	6	0	-2.020577	-0.685688	-1.197193
4	6	0	-3.258508	-0.238540	-1.570307
5	6	0	-4.212266	0.241514	-0.624423
6	1	0	-4.624314	0.264432	1.501799
7	1	0	-2.422277	-0.490564	2.210225
8	1	0	-1.344585	-1.066940	-1.953062
9	1	0	-3.544964	-0.281169	-2.627118
10	6	0	-1.464269	-0.490223	0.198681
11	6	0	-0.167052	0.335248	0.177070
12	6	0	0.974298	-0.316083	-0.220964
13	6	0	-0.188399	1.835601	0.319069
14	8	0	-0.935713	2.569890	-0.280298
15	8	0	0.695798	2.313485	1.227705
16	6	0	0.620430	3.732727	1.453740
17	1	0	0.875973	4.276478	0.546450
18	1	0	-0.393355	4.016357	1.762620
19	1	0	1.330822	3.947743	2.253305
20	7	0	0.878685	-1.723847	-0.109612
21	16	0	-0.563443	-2.102710	0.656465
22	8	0	-1.059121	-3.354141	0.067567
23	8	0	-0.346309	-2.076280	2.102057
24	1	0	1.028222	-2.272855	-0.959557
25	6	0	2.250308	0.192920	-0.861453
26	1	0	2.177662	1.276196	-0.998064

27	1	0	2.271729	-0.253595	-1.872808
28	6	0	3.536710	-0.188149	-0.109677
29	1	0	3.540678	0.331895	0.855717
30	1	0	3.532251	-1.267665	0.099205
31	6	0	4.796200	0.172943	-0.893819
32	1	0	4.761113	1.242910	-1.170886
33	1	0	4.804191	-0.388641	-1.841268
34	6	0	6.072668	-0.109553	-0.115327
35	1	0	6.051822	0.451848	0.830078
36	1	0	6.094811	-1.178220	0.160886
37	6	0	7.335238	0.244515	-0.890318
38	1	0	7.343361	1.304601	-1.152166
39	1	0	8.241245	0.033172	-0.307629
40	1	0	7.406702	-0.335512	-1.815887
41	6	0	-5.440430	0.800166	-1.021631
42	7	0	-6.446791	1.305423	-1.350953

Int5[c]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.348126	0.819837	-0.317794
2	6	0	-0.001034	0.706373	-0.229578
3	6	0	-1.980886	1.978007	-1.050102
4	8	0	-2.451918	1.902998	-2.165688
5	8	0	-2.018106	3.104607	-0.342930
6	6	0	-2.748867	4.198787	-0.937948
7	1	0	-2.257381	4.513126	-1.866972
8	1	0	-3.773141	3.883573	-1.161772
9	1	0	-2.735988	4.997596	-0.208269
10	7	0	0.417532	-0.345410	0.642417
11	16	0	-0.946759	-0.722356	1.584999
12	8	0	-0.829711	-2.131798	1.994643
13	8	0	-1.037639	0.291663	2.645573
14	6	0	1.141780	1.540336	-0.806441
15	1	0	0.725220	2.433418	-1.289316
16	1	0	1.631816	0.947619	-1.596642
17	6	0	2.181523	1.918091	0.267548
18	1	0	1.684324	2.490629	1.063562
19	1	0	2.558522	0.999193	0.741078
20	6	0	3.357832	2.717774	-0.281251
21	1	0	2.990842	3.621783	-0.787633

22	1	0	3.879794	2.126167	-1.049570
23	6	0	4.361722	3.122556	0.807715
24	1	0	3.827117	3.707708	1.576494
25	1	0	4.729895	2.227932	1.308590
26	6	0	5.530837	3.936143	0.268854
27	1	0	5.184055	4.857963	-0.211345
28	1	0	6.224817	4.220006	1.060967
29	1	0	6.091826	3.368872	-0.483034
30	6	0	-2.224082	-0.287734	0.236012
31	6	0	-3.541906	-0.099555	0.948916
32	6	0	-2.407056	-1.533551	-0.595988
33	6	0	-4.719877	-0.644919	0.473675
34	1	0	-3.579174	0.595283	1.787805
35	6	0	-3.657885	-1.989827	-0.973265
36	1	0	-1.533668	-2.026570	-1.008136
37	7	0	-4.867637	-1.538745	-0.537281
38	1	0	-5.660985	-0.361027	0.970706
39	1	0	-3.715244	-2.815493	-1.698116
40	6	0	1.228593	-1.405018	0.114002
41	6	0	2.089587	-2.070773	0.984704
42	6	0	1.185063	-1.765462	-1.233304
43	6	0	2.910114	-3.087924	0.499485
44	1	0	2.122159	-1.774237	2.028154
45	6	0	2.026632	-2.763150	-1.701778
46	1	0	0.503378	-1.254522	-1.898201
47	6	0	2.890837	-3.449697	-0.850391
48	1	0	3.580189	-3.597577	1.184717
49	1	0	1.996030	-3.030506	-2.754595
50	6	0	3.797624	-4.545487	-1.359018
51	1	0	4.822724	-4.397711	-1.008565
52	1	0	3.466441	-5.522154	-0.982649
53	1	0	3.799767	-4.572895	-2.450291

Int0[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.429925	3.294512	0.338101
2	6	0	-0.275686	2.157212	-0.046852
3	6	0	1.523591	1.555272	-1.526390
4	6	0	2.234538	2.686677	-1.150829
5	6	0	1.666892	3.553821	-0.228212

6	1	0	0.010457	3.958887	1.083151
7	1	0	3.217876	2.873736	-1.563449
8	6	0	0.240140	1.279816	-1.017698
9	6	0	-0.375456	-1.121732	1.470846
10	6	0	0.545514	-1.277344	0.532637
11	6	0	0.030672	-0.803960	2.796370
12	8	0	-0.080082	-1.493757	3.809143
13	8	0	0.487143	0.488688	2.899292
14	7	0	0.119163	-1.472500	-0.880399
15	16	0	-0.625024	-0.197834	-1.610457
16	8	0	-0.423204	-0.315949	-3.045082
17	8	0	-2.017013	-0.152234	-1.152996
18	1	0	0.853738	-1.802255	-1.507990
19	6	0	0.806775	0.923737	4.209953
20	1	0	1.617381	0.330246	4.637372
21	1	0	1.124241	1.961935	4.117061
22	1	0	-2.272699	-1.645595	1.397922
23	6	0	-3.855038	-1.168679	0.820183
24	8	0	-2.852839	-2.056385	1.197809
25	8	0	-4.539572	-1.565796	-0.148988
26	8	0	-3.959609	-0.105052	1.445038
27	19	0	-2.584834	-3.013733	-1.205151
28	19	0	-4.494023	0.978201	-0.917382
29	1	0	-0.057563	0.852820	4.877178
30	6	0	2.049159	-1.193280	0.664434
31	1	0	2.277060	-1.062339	1.727134
32	1	0	2.431765	-0.292499	0.159537
33	6	0	2.816320	-2.404099	0.146193
34	1	0	2.637484	-2.551470	-0.929333
35	1	0	2.452696	-3.310882	0.645454
36	6	0	4.321926	-2.261850	0.358071
37	1	0	4.521749	-2.127379	1.428711
38	1	0	4.670262	-1.346949	-0.141200
39	6	0	5.111636	-3.456925	-0.163620
40	1	0	4.759082	-4.368553	0.334460
41	1	0	4.903254	-3.588413	-1.232805
42	6	0	6.614317	-3.298854	0.052650
43	1	0	6.844979	-3.192440	1.117269
44	1	0	7.172825	-4.161480	-0.326702
45	1	0	6.989032	-2.406757	-0.459022
46	17	0	-1.770340	1.897876	0.782057
47	17	0	2.366186	0.471627	-2.598660
48	17	0	2.538328	4.974336	0.247469

Int0[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.348402	3.020204	0.377035
2	6	0	-0.714467	1.742042	-0.030749
3	6	0	0.462279	2.104030	-2.148432
4	6	0	0.815374	3.382637	-1.738216
5	6	0	0.409860	3.829999	-0.475084
6	1	0	-0.644578	3.387437	1.353093
7	1	0	-1.285524	1.086469	0.621798
8	1	0	0.761946	1.725808	-3.119602
9	1	0	1.398521	4.028414	-2.384010
10	6	0	-0.297755	1.312424	-1.290579
11	6	0	0.274339	-1.066723	1.282351
12	6	0	1.018884	-0.985808	0.192610
13	6	0	0.814330	-0.631600	2.532434
14	8	0	1.188063	-1.339818	3.466574
15	8	0	0.793690	0.729920	2.674181
16	7	0	0.458030	-1.348291	-1.127243
17	16	0	-0.676734	-0.348205	-1.801452
18	8	0	-0.517078	-0.460588	-3.248199
19	8	0	-1.993324	-0.668909	-1.229436
20	1	0	1.159627	-1.511399	-1.847308
21	6	0	1.233104	1.227424	3.930550
22	1	0	2.270993	0.944101	4.124253
23	1	0	1.143797	2.311104	3.874030
24	1	0	-1.505264	-1.743151	1.512729
25	6	0	-3.129522	-1.115795	1.285615
26	8	0	-2.162469	-2.087514	1.470889
27	8	0	-4.171027	-1.529351	0.720486
28	8	0	-2.874293	0.045257	1.652147
29	19	0	-2.826601	-3.254155	-0.777586
30	19	0	-4.214711	0.820139	-0.500055
31	1	0	0.609520	0.841144	4.744303
32	6	0	0.780947	5.154068	-0.044103
33	7	0	1.077607	6.217395	0.302627
34	6	0	2.445367	-0.510548	0.073893
35	1	0	2.730966	-0.036381	1.020854
36	1	0	2.523200	0.270072	-0.703563
37	6	0	3.443930	-1.630270	-0.240048
38	1	0	3.160489	-2.144116	-1.169604

39	1	0	3.389715	-2.379869	0.555319
40	6	0	4.870175	-1.116521	-0.378728
41	1	0	5.162131	-0.604145	0.548070
42	1	0	4.908651	-0.360214	-1.174594
43	6	0	5.877172	-2.223286	-0.683901
44	1	0	5.836518	-2.976192	0.112909
45	1	0	5.580060	-2.735195	-1.607781
46	6	0	7.302599	-1.695376	-0.822936
47	1	0	7.626840	-1.203542	0.099558
48	1	0	8.009899	-2.499469	-1.041720
49	1	0	7.367932	-0.960401	-1.631434

Int0[c]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.517283	-1.312670	1.072523
2	6	0	0.812706	-0.110929	0.594915
3	6	0	1.408143	-1.986957	1.963165
4	8	0	1.411117	-1.963689	3.194316
5	8	0	2.260049	-2.845117	1.298785
6	6	0	3.077316	-3.648134	2.137325
7	1	0	3.731009	-3.034020	2.762803
8	1	0	2.472565	-4.281042	2.792472
9	1	0	3.678336	-4.269542	1.473042
10	7	0	-0.106011	0.586727	-0.338671
11	16	0	-0.546341	-0.193008	-1.724604
12	8	0	-1.219260	0.785534	-2.578416
13	8	0	0.615640	-0.904280	-2.242651
14	6	0	2.038666	0.748612	0.820533
15	1	0	2.540536	0.412986	1.736078
16	1	0	1.734337	1.793244	0.986501
17	6	0	3.020293	0.699927	-0.353741
18	1	0	3.364412	-0.335435	-0.477265
19	1	0	2.484931	0.958402	-1.276371
20	6	0	4.221025	1.625024	-0.174043
21	1	0	4.743025	1.370550	0.759179
22	1	0	3.869596	2.659640	-0.055598
23	6	0	5.209348	1.559520	-1.336639
24	1	0	5.557648	0.525643	-1.453847
25	1	0	4.686463	1.814897	-2.266910

26	6	0	6.406157	2.487788	-1.146445
27	1	0	6.956691	2.230548	-0.235892
28	1	0	7.101785	2.427865	-1.987688
29	1	0	6.080136	3.528660	-1.053258
30	6	0	-1.795528	-1.408906	-1.321600
31	6	0	-1.439106	-2.728877	-1.078525
32	6	0	-3.124727	-1.015145	-1.246580
33	6	0	-2.464863	-3.620581	-0.780317
34	1	0	-0.402950	-3.039857	-1.113951
35	6	0	-4.064708	-1.992909	-0.922038
36	1	0	-3.420796	0.008284	-1.446709
37	7	0	-3.753440	-3.270617	-0.695858
38	1	0	-2.236572	-4.666907	-0.595593
39	1	0	-5.116655	-1.729463	-0.849331
40	6	0	-1.100680	1.451429	0.238410
41	6	0	-1.274393	2.740752	-0.265105
42	6	0	-1.878354	1.008499	1.307990
43	6	0	-2.229537	3.581250	0.305574
44	1	0	-0.662074	3.073296	-1.093559
45	6	0	-2.821373	1.858695	1.871270
46	1	0	-1.710782	0.004450	1.685643
47	6	0	-3.017019	3.150830	1.377067
48	1	0	-2.358190	4.585960	-0.082407
49	1	0	-3.421864	1.511514	2.712209
50	6	0	-4.069234	4.057170	1.968597
51	1	0	-3.742477	5.134026	1.919147
52	1	0	-5.030950	3.961974	1.391874
53	1	0	-4.269405	3.783786	3.034512

TS4[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.436541	3.278888	0.333103
2	6	0	-0.269505	2.142985	-0.054871
3	6	0	1.532645	1.540587	-1.531089
4	6	0	2.243788	2.670881	-1.152681
5	6	0	1.674818	3.537829	-0.230613
6	1	0	0.016534	3.942368	1.078658
7	1	0	3.228659	2.856858	-1.562127
8	6	0	0.247249	1.266795	-1.026486
9	6	0	-0.418709	-1.142350	1.443814

10	6	0	0.528346	-1.280656	0.512471
11	6	0	-0.010347	-0.765162	2.801089
12	8	0	-0.176269	-1.428885	3.809097
13	8	0	0.513507	0.484734	2.856873
14	7	0	0.118680	-1.489261	-0.878436
15	16	0	-0.624039	-0.203933	-1.622608
16	8	0	-0.403142	-0.337532	-3.054794
17	8	0	-2.007944	-0.159799	-1.171284
18	1	0	0.854872	-1.830055	-1.495807
19	6	0	0.832172	0.954494	4.165805
20	1	0	1.604542	0.331508	4.622620
21	1	0	1.195638	1.973036	4.038417
22	1	0	-1.770656	-1.481699	1.330026
23	6	0	-3.824261	-1.170916	0.838988
24	8	0	-2.848025	-2.005442	1.219987
25	8	0	-4.538181	-1.538821	-0.157478
26	8	0	-3.980205	-0.070637	1.439356
27	19	0	-2.599620	-3.016112	-1.160702
28	19	0	-4.488759	0.978633	-0.925131
29	1	0	-0.053194	0.944253	4.805049
30	6	0	2.029737	-1.191049	0.681770
31	1	0	2.249867	-1.070721	1.746404
32	1	0	2.409658	-0.286899	0.184773
33	6	0	2.805699	-2.403442	0.152195
34	1	0	2.640115	-2.536049	-0.926642
35	1	0	2.435842	-3.314211	0.639387
36	6	0	4.308779	-2.263661	0.383076
37	1	0	4.501004	-2.140813	1.457359
38	1	0	4.662821	-1.343599	-0.102440
39	6	0	5.108816	-3.453351	-0.142420
40	1	0	4.749677	-4.370308	0.340925
41	1	0	4.913540	-3.572449	-1.215503
42	6	0	6.608786	-3.298633	0.094109
43	1	0	6.826394	-3.204570	1.162621
44	1	0	7.166632	-4.157217	-0.288299
45	1	0	6.990174	-2.400990	-0.402704
46	17	0	-1.764630	1.881332	0.772352
47	17	0	2.378215	0.454526	-2.598302
48	17	0	2.546751	4.956675	0.248613

TS4[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.351359	3.020634	0.370437
2	6	0	-0.719032	1.743856	-0.040244
3	6	0	0.483102	2.098483	-2.145213
4	6	0	0.837757	3.375687	-1.732026
5	6	0	0.420413	3.825951	-0.473765
6	1	0	-0.656614	3.390312	1.342784
7	1	0	-1.318984	1.096085	0.601779
8	1	0	0.791680	1.718108	-3.112761
9	1	0	1.431099	4.018144	-2.371811
10	6	0	-0.290132	1.311384	-1.295006
11	6	0	0.229965	-1.077529	1.267841
12	6	0	1.003659	-0.993512	0.185155
13	6	0	0.769744	-0.619855	2.552168
14	8	0	1.071289	-1.330888	3.494543
15	8	0	0.817540	0.732438	2.645521
16	7	0	0.461255	-1.349849	-1.122980
17	16	0	-0.675086	-0.348191	-1.807484
18	8	0	-0.498345	-0.462524	-3.252809
19	8	0	-1.988599	-0.667887	-1.239696
20	1	0	1.172017	-1.516526	-1.834024
21	6	0	1.235604	1.242654	3.911053
22	1	0	2.253736	0.920293	4.140435
23	1	0	1.194134	2.327408	3.825019
24	1	0	-1.072959	-1.572337	1.383695
25	6	0	-3.102312	-1.139357	1.283821
26	8	0	-2.165198	-2.066899	1.481471
27	8	0	-4.173589	-1.511777	0.697331
28	8	0	-2.878191	0.058573	1.636002
29	19	0	-2.809698	-3.256854	-0.756930
30	19	0	-4.212627	0.818638	-0.513989
31	1	0	0.569117	0.899199	4.705028
32	6	0	0.793312	5.148423	-0.039395
33	7	0	1.091448	6.210397	0.310172
34	6	0	2.436972	-0.520264	0.099416
35	1	0	2.721061	-0.068929	1.055323
36	1	0	2.510918	0.273672	-0.659357
37	6	0	3.432202	-1.637863	-0.240772
38	1	0	3.154716	-2.130173	-1.183587
39	1	0	3.374453	-2.409274	0.537198

40	6	0	4.865768	-1.126266	-0.357865
41	1	0	5.153291	-0.636906	0.582606
42	1	0	4.912231	-0.351688	-1.135496
43	6	0	5.870666	-2.229355	-0.682416
44	1	0	5.821474	-3.001093	0.095679
45	1	0	5.578326	-2.717637	-1.620479
46	6	0	7.298949	-1.703660	-0.798486
47	1	0	7.618655	-1.236152	0.138114
48	1	0	8.004722	-2.504818	-1.032388
49	1	0	7.372642	-0.949101	-1.588020

TS4[c]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.298207	0.864616	-1.390846
2	6	0	-0.542728	0.494113	-0.423793
3	6	0	0.122819	2.207903	-1.956687
4	8	0	-0.373665	2.465499	-3.039865
5	8	0	0.657001	3.178638	-1.176807
6	7	0	-0.384929	-0.804129	0.230247
7	16	0	0.894998	-1.030824	1.248783
8	8	0	0.508344	-2.007423	2.262778
9	8	0	2.119858	-1.315676	0.487011
10	6	0	0.577168	4.500612	-1.709453
11	1	0	-0.464825	4.794831	-1.853822
12	1	0	1.054176	5.148444	-0.975780
13	1	0	1.348819	0.135831	-1.957375
14	6	0	3.366061	-0.333693	-1.828481
15	8	0	2.210196	-0.535709	-2.461559
16	8	0	4.175896	-1.319109	-1.766611
17	8	0	3.591519	0.789757	-1.284897
18	19	0	2.181366	-3.036156	-1.662480
19	19	0	4.774399	-0.507963	0.670243
20	1	0	1.098188	4.563362	-2.667068
21	6	0	-1.695669	1.311041	0.129603
22	1	0	-1.379615	2.360714	0.174525
23	1	0	-1.911587	1.002634	1.160623
24	6	0	-2.976658	1.215080	-0.710876
25	1	0	-3.296894	0.167284	-0.777167
26	1	0	-2.745979	1.540837	-1.733424
27	6	0	-4.112105	2.059023	-0.139482

28	1	0	-3.786983	3.106037	-0.063314
29	1	0	-4.328036	1.727988	0.886130
30	6	0	-5.390427	1.985665	-0.971681
31	1	0	-5.171971	2.313594	-1.995598
32	1	0	-5.711167	0.938883	-1.045051
33	6	0	-6.519529	2.831573	-0.389044
34	1	0	-6.226640	3.884739	-0.331946
35	1	0	-7.426094	2.767480	-0.996434
36	1	0	-6.769434	2.501690	0.624343
37	6	0	-1.529578	-1.669983	0.301402
38	6	0	-1.898194	-2.341926	-0.863456
39	6	0	-2.329272	-1.765514	1.439970
40	6	0	-3.062256	-3.102961	-0.888795
41	1	0	-1.282778	-2.233105	-1.751475
42	6	0	-3.483827	-2.540209	1.406705
43	1	0	-2.047952	-1.236202	2.344407
44	6	0	-3.870521	-3.218059	0.245943
45	1	0	-3.348723	-3.612787	-1.804443
46	1	0	-4.104492	-2.608800	2.295663
47	6	0	-5.114852	-4.067447	0.225987
48	1	0	-5.564021	-4.085859	-0.769436
49	1	0	-4.881805	-5.100831	0.502266
50	1	0	-5.857615	-3.695902	0.935284
51	6	0	1.156286	0.555854	2.019356
52	6	0	1.909236	1.526468	1.368095
53	6	0	0.584124	0.797660	3.260361
54	6	0	2.043988	2.748114	2.026951
55	1	0	2.351481	1.349158	0.386398
56	6	0	0.799984	2.055837	3.819692
57	1	0	0.006726	0.038512	3.776227
58	7	0	1.509144	3.016649	3.221962
59	1	0	2.610345	3.549950	1.560574
60	1	0	0.381138	2.294898	4.793190

Int7[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.426742	3.294943	0.336624
2	6	0	-0.278490	2.157142	-0.047543
3	6	0	1.520359	1.555535	-1.527738
4	6	0	2.230925	2.687439	-1.152962

5	6	0	1.663300	3.554654	-0.230398
6	1	0	0.007309	3.959394	1.081626
7	1	0	3.213965	2.874831	-1.566139
8	6	0	0.237297	1.279631	-1.018307
9	6	0	-0.449668	-1.182791	1.434596
10	6	0	0.520104	-1.276792	0.495966
11	6	0	0.006158	-0.778180	2.833565
12	8	0	-0.091460	-1.492251	3.797459
13	8	0	0.486628	0.465529	2.886569
14	7	0	0.117770	-1.484989	-0.867589
15	16	0	-0.639723	-0.186380	-1.610071
16	8	0	-0.413946	-0.329542	-3.044751
17	8	0	-2.006905	-0.153596	-1.151945
18	1	0	0.852206	-1.826914	-1.483113
19	6	0	0.818987	0.925847	4.209196
20	1	0	1.630100	0.320624	4.624146
21	1	0	1.123581	1.964161	4.091153
22	1	0	-1.116793	-1.313812	1.251683
23	6	0	-3.769630	-1.231683	0.847124
24	8	0	-2.816030	-2.008057	1.199985
25	8	0	-4.540571	-1.555742	-0.170749
26	8	0	-3.972849	-0.094096	1.434732
27	19	0	-2.597917	-3.015401	-1.190415
28	19	0	-4.496659	0.963390	-0.903237
29	1	0	-0.057292	0.854746	4.852279
30	6	0	2.023786	-1.179612	0.688485
31	1	0	2.252148	-1.060448	1.751026
32	1	0	2.393392	-0.278836	0.183058
33	6	0	2.803594	-2.402549	0.145731
34	1	0	2.624298	-2.538123	-0.929653
35	1	0	2.440669	-3.309322	0.645519
36	6	0	4.309232	-2.259466	0.356811
37	1	0	4.521816	-2.124481	1.427298
38	1	0	4.656864	-1.344583	-0.142983
39	6	0	5.111583	-3.454343	-0.164814
40	1	0	4.759731	-4.365956	0.333790
41	1	0	4.902739	-3.586347	-1.233845
42	6	0	6.614291	-3.295438	0.050654
43	1	0	6.845424	-3.188500	1.115118
44	1	0	7.160743	-4.157932	-0.328639
45	1	0	6.988307	-2.403350	-0.461545
46	17	0	-1.772604	1.897377	0.782202
47	17	0	2.362967	0.471899	-2.600007
48	17	0	2.534259	4.975787	0.244308

Int7[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.358724	3.018281	0.377749
2	6	0	-0.721483	1.738970	-0.029383
3	6	0	0.451724	2.104055	-2.148499
4	6	0	0.801514	3.383774	-1.738919
5	6	0	0.396149	3.830162	-0.475395
6	1	0	-0.654849	3.384812	1.354086
7	1	0	-1.341471	1.094635	0.611078
8	1	0	0.751378	1.726546	-3.119950
9	1	0	1.381997	4.031155	-2.385505
10	6	0	-0.304968	1.310359	-1.289622
11	6	0	0.199801	-1.105465	1.257316
12	6	0	0.994390	-0.996652	0.166657
13	6	0	0.804410	-0.616803	2.571144
14	8	0	1.181308	-1.336649	3.453374
15	8	0	0.792820	0.718895	2.661068
16	7	0	0.458879	-1.348080	-1.113798
17	16	0	-0.692530	-0.351498	-1.799753
18	8	0	-0.508425	-0.463621	-3.246683
19	8	0	-1.994599	-0.675967	-1.226157
20	1	0	1.173049	-1.522118	-1.821758
21	6	0	1.232208	1.230822	3.929736
22	1	0	2.271146	0.950603	4.109381
23	1	0	1.139623	2.314223	3.860229
24	1	0	-0.353091	-1.307628	1.192301
25	6	0	-3.048997	-1.203019	1.303143
26	8	0	-2.143577	-2.055858	1.474601
27	8	0	-4.180434	-1.516717	0.713557
28	8	0	-2.874355	0.049008	1.643423
29	19	0	-2.819694	-3.263583	-0.759983
30	19	0	-4.219529	0.806638	-0.494453
31	1	0	0.610707	0.842846	4.731383
32	6	0	0.763821	5.155399	-0.045079
33	7	0	1.057738	6.219661	0.301119
34	6	0	2.432235	-0.504272	0.097786
35	1	0	2.717556	-0.041993	1.044332
36	1	0	2.481064	0.276389	-0.666979
37	6	0	3.433721	-1.621095	-0.242919

38	1	0	3.150719	-2.135943	-1.172054
39	1	0	3.395570	-2.383585	0.552634
40	6	0	4.871178	-1.103133	-0.383358
41	1	0	5.162695	-0.589730	0.543009
42	1	0	4.906491	-0.346859	-1.179402
43	6	0	5.881087	-2.206971	-0.689508
44	1	0	5.843586	-2.959851	0.107481
45	1	0	5.584416	-2.719923	-1.612952
46	6	0	7.304784	-1.674875	-0.830295
47	1	0	7.628642	-1.181919	0.091734
48	1	0	8.014203	-2.476912	-1.049760
49	1	0	7.367003	-0.939855	-1.638998

Int7[c]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.314208	0.848741	-1.393307
2	6	0	-0.544766	0.484854	-0.419418
3	6	0	0.128742	2.228250	-1.964418
4	8	0	-0.390335	2.462775	-3.030335
5	8	0	0.654399	3.173973	-1.183947
6	7	0	-0.386238	-0.800428	0.224766
7	16	0	0.902108	-1.028365	1.244886
8	8	0	0.512249	-2.005494	2.259722
9	8	0	2.118988	-1.313993	0.480029
10	6	0	0.578975	4.501654	-1.717081
11	1	0	-0.463584	4.798828	-1.851260
12	1	0	1.065115	5.142884	-0.982809
13	1	0	0.895186	0.399981	-1.668281
14	6	0	3.332663	-0.342815	-1.855576
15	8	0	2.224100	-0.532995	-2.462987
16	8	0	4.190842	-1.322249	-1.760075
17	8	0	3.600988	0.792280	-1.281242
18	19	0	2.186627	-3.036884	-1.664055
19	19	0	4.773359	-0.509309	0.670235
20	1	0	1.090347	4.556093	-2.680049
21	6	0	-1.691969	1.313184	0.122494
22	1	0	-1.377850	2.363714	0.163637
23	1	0	-1.898118	1.001408	1.155137
24	6	0	-2.981345	1.212949	-0.707855
25	1	0	-3.300029	0.164488	-0.771022

26	1	0	-2.760030	1.536930	-1.737835
27	6	0	-4.116766	2.056114	-0.135219
28	1	0	-3.793155	3.103795	-0.061772
29	1	0	-4.329639	1.726634	0.891544
30	6	0	-5.397065	1.979218	-0.964078
31	1	0	-5.181586	2.305336	-1.989207
32	1	0	-5.716465	0.931823	-1.034513
33	6	0	-6.525979	2.824697	-0.380460
34	1	0	-6.234557	3.878435	-0.326469
35	1	0	-7.434003	2.757867	-0.985379
36	1	0	-6.772794	2.496720	0.634305
37	6	0	-1.528890	-1.668787	0.301634
38	6	0	-1.895683	-2.342545	-0.862689
39	6	0	-2.328602	-1.764843	1.440129
40	6	0	-3.058381	-3.105727	-0.887605
41	1	0	-1.280003	-2.233527	-1.750487
42	6	0	-3.481799	-2.541569	1.407277
43	1	0	-2.048232	-1.234006	2.343966
44	6	0	-3.866880	-3.221104	0.246950
45	1	0	-3.343681	-3.617057	-1.802779
46	1	0	-4.102662	-2.610508	2.296070
47	6	0	-5.109725	-4.072658	0.227302
48	1	0	-5.558028	-4.093492	-0.768483
49	1	0	-4.875177	-5.105203	0.505514
50	1	0	-5.853783	-3.701234	0.935339
51	6	0	1.159354	0.557620	2.016156
52	6	0	1.910253	1.529460	1.364530
53	6	0	0.589860	0.797706	3.258797
54	6	0	2.046075	2.750317	2.024707
55	1	0	2.368766	1.347580	0.381614
56	6	0	0.806444	2.055193	3.819271
57	1	0	0.013928	0.037681	3.774973
58	7	0	1.513905	3.017112	3.221244
59	1	0	2.611053	3.552929	1.558004
60	1	0	0.389664	2.292799	4.794007

R3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.399632	1.653913	0.300355
2	1	0	-1.771525	2.634690	0.583315

3	6	0	-0.036946	1.577742	0.077021
4	6	0	-2.428352	0.666515	0.043708
5	6	0	-3.748876	0.918837	0.478256
6	6	0	-2.226480	-0.502586	-0.724936
7	6	0	-4.792700	0.047791	0.192937
8	1	0	-3.943791	1.823470	1.050072
9	6	0	-3.273683	-1.370507	-1.009572
10	1	0	-1.234523	-0.705944	-1.116628
11	6	0	-4.565462	-1.112391	-0.548661
12	1	0	-5.792701	0.276255	0.551070
13	1	0	-3.080246	-2.257252	-1.607116
14	1	0	-5.378581	-1.795880	-0.769968
15	6	0	0.829019	0.452589	0.092718
16	6	0	2.135354	0.518013	-0.476012
17	6	0	0.448285	-0.785861	0.878638
18	1	0	-0.605840	-0.725920	1.152685
19	1	0	0.553875	-1.692523	0.269444
20	6	0	1.266670	-0.943762	2.166505
21	1	0	0.972330	-1.843180	2.718004
22	1	0	2.334170	-1.013446	1.943700
23	1	0	1.110924	-0.080022	2.820638
24	8	0	2.770177	-0.699157	-0.460925
25	8	0	2.734204	1.499189	-0.960782
26	6	0	4.137698	-0.708625	-0.868148
27	1	0	4.349203	-1.750267	-1.120959
28	1	0	4.258857	-0.094763	-1.763086
29	6	0	5.048852	-0.223388	0.246210
30	1	0	6.095278	-0.279892	-0.065643
31	1	0	4.813633	0.813797	0.493386
32	1	0	4.921405	-0.839061	1.140617

I

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.415089	1.025872	-0.074444
2	6	0	-2.309648	1.806998	-0.509845
3	6	0	-0.981092	1.002245	1.330258
4	6	0	-2.061052	0.204870	1.779062
5	6	0	-3.219510	0.328753	1.080199
6	1	0	-4.343716	0.944744	-0.649239
7	1	0	-2.364114	2.362675	-1.440623

8	1	0	-0.011070	0.925946	1.817414
9	1	0	-1.965303	-0.506033	2.612844
10	7	0	-4.404335	-0.471137	1.593677
11	8	0	-5.432477	-0.380303	0.980151
12	8	0	-4.225011	-1.123008	2.586096
13	6	0	-1.234992	1.937891	0.352305
14	6	0	0.331057	-0.086677	-1.845420
15	6	0	1.332783	0.321690	-0.984476
16	7	0	1.526763	1.719768	-0.650890
17	16	0	0.270269	2.728038	-0.394509
18	8	0	0.634538	3.628197	0.706439
19	8	0	-0.155359	3.349865	-1.652640
20	1	0	2.329336	1.882881	-0.016807
21	6	0	-0.735907	-0.960003	-1.437643
22	6	0	-1.931902	-1.082541	-2.237657
23	6	0	-0.718050	-1.828267	-0.275427
24	6	0	-2.925652	-2.008409	-1.965122
25	1	0	-2.006821	-0.437838	-3.106208
26	6	0	-1.731350	-2.735437	-0.018096
27	1	0	0.109262	-1.733293	0.409318
28	6	0	-2.843509	-2.871126	-0.862485
29	1	0	-3.780658	-2.072884	-2.635949
30	1	0	-1.657073	-3.367986	0.867656
31	1	0	-3.615695	-3.604519	-0.673046
32	6	0	2.370308	-0.561711	-0.516788
33	6	0	3.541836	-0.097884	0.091193
34	8	0	3.790311	1.033537	0.590528
35	8	0	4.554175	-1.031766	0.061573
36	6	0	5.776151	-0.693545	0.691447
37	1	0	6.518873	-1.365676	0.256678
38	1	0	6.054476	0.339177	0.439220
39	6	0	5.697896	-0.880064	2.195446
40	1	0	6.659826	-0.679196	2.656861
41	1	0	4.960524	-0.181443	2.612907
42	1	0	5.393060	-1.900633	2.430454
43	6	0	2.377907	-1.952819	-1.123146
44	1	0	1.485643	-2.048586	-1.746031
45	1	0	3.235404	-2.082517	-1.790857
46	6	0	2.418723	-3.111721	-0.117138
47	1	0	2.348757	-4.078199	-0.616174
48	1	0	3.351521	-3.084968	0.440950
49	1	0	1.592548	-3.049162	0.606828
50	1	0	-0.238957	0.987626	-2.254073

TS1A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.231350	1.091272	0.313646
2	6	0	-2.206071	1.832067	-0.237232
3	6	0	-0.626702	0.796441	1.313734
4	6	0	-1.650977	0.054418	1.859735
5	6	0	-2.945310	0.188153	1.341157
6	1	0	-4.249028	1.192104	-0.042071
7	1	0	-2.394535	2.527220	-1.047372
8	1	0	0.385281	0.704887	1.697982
9	1	0	-1.472224	-0.629440	2.680049
10	7	0	-3.996668	-0.636759	1.864734
11	8	0	-5.136683	-0.484121	1.432832
12	8	0	-3.716259	-1.467461	2.725657
13	6	0	-0.882662	1.603438	0.184019
14	6	0	0.016709	0.364941	-1.648836
15	6	0	1.303112	0.459502	-1.061418
16	7	0	1.631032	1.803580	-0.741583
17	16	0	0.373374	2.786780	-0.279544
18	8	0	0.845709	3.548548	0.879806
19	8	0	-0.132893	3.554140	-1.416819
20	1	0	2.452632	1.896582	-0.130035
21	6	0	-0.937984	-0.710977	-1.588222
22	6	0	-2.106009	-0.642653	-2.380426
23	6	0	-0.882067	-1.734350	-0.617236
24	6	0	-3.152076	-1.539841	-2.209841
25	1	0	-2.186605	0.145443	-3.125661
26	6	0	-1.931109	-2.626869	-0.445496
27	1	0	-0.024546	-1.774545	0.042123
28	6	0	-3.078944	-2.535362	-1.233933
29	1	0	-4.037875	-1.454369	-2.832766
30	1	0	-1.863035	-3.386961	0.328410
31	1	0	-3.900196	-3.231129	-1.094962
32	6	0	2.230610	-0.539704	-0.741693
33	6	0	3.409663	-0.205037	0.026969
34	8	0	3.647594	0.849933	0.634352
35	8	0	4.328668	-1.200548	0.033405
36	6	0	5.511896	-0.982386	0.810967
37	1	0	6.242468	-1.683321	0.402966
38	1	0	5.865673	0.038091	0.651403

39	6	0	5.257156	-1.250041	2.283107
40	1	0	6.185890	-1.144512	2.849621
41	1	0	4.526881	-0.539403	2.674550
42	1	0	4.878089	-2.265114	2.426090
43	6	0	2.179856	-1.896095	-1.422470
44	1	0	1.294194	-1.921507	-2.060391
45	1	0	3.042850	-1.974100	-2.097412
46	6	0	2.191603	-3.138762	-0.520325
47	1	0	2.023139	-4.038679	-1.119802
48	1	0	3.152072	-3.242486	-0.014834
49	1	0	1.414532	-3.103009	0.246759
50	1	0	-0.255350	1.195153	-2.295103

II

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.345224	1.157771	-0.049847
2	6	0	-2.276306	1.699053	-0.636304
3	6	0	-0.864836	0.801728	1.217548
4	6	0	-1.968282	0.284164	1.777292
5	6	0	-3.270121	0.274337	1.107497
6	1	0	-4.356269	1.396764	-0.418599
7	1	0	-2.390475	2.355109	-1.493857
8	1	0	0.067790	0.805524	1.777858
9	1	0	-1.932719	-0.126570	2.797098
10	7	0	-4.298975	-0.385838	1.571176
11	8	0	-5.429934	-0.331923	0.985756
12	8	0	-4.200160	-1.120784	2.607965
13	6	0	-0.779356	1.143355	-0.363124
14	6	0	-0.236402	0.506295	-1.042535
15	6	0	1.391202	0.467785	-0.743028
16	7	0	1.639718	1.776930	-0.481048
17	16	0	0.253806	2.752466	-0.335350
18	8	0	0.512860	3.585204	0.842619
19	8	0	-0.013107	3.444856	-1.597269
20	1	0	2.487679	2.059542	0.012416
21	6	0	-0.912547	-0.903540	-1.231710
22	6	0	-1.914677	-1.017347	-2.187588
23	6	0	-0.816486	-1.816469	-0.208975
24	6	0	-2.896000	-1.998950	-2.049629
25	1	0	-1.988224	-0.293553	-3.001143

26	6	0	-1.777382	-2.819151	-0.066043
27	1	0	-0.024086	-1.704277	0.533047
28	6	0	-2.835528	-2.866021	-0.966248
29	1	0	-3.715603	-2.060824	-2.756784
30	1	0	-1.724185	-3.511083	0.765150
31	1	0	-3.613637	-3.615893	-0.828228
32	6	0	2.321910	-0.512306	-0.681053
33	6	0	3.621262	-0.113643	0.009274
34	8	0	3.823062	0.944436	0.551216
35	8	0	4.524550	-1.075757	-0.026498
36	6	0	5.793239	-0.782911	0.623005
37	1	0	6.486924	-1.492163	0.169198
38	1	0	6.079683	0.232540	0.371385
39	6	0	5.682004	-0.981109	2.123277
40	1	0	6.668353	-0.819306	2.582993
41	1	0	4.973661	-0.284969	2.560109
42	1	0	5.368987	-2.003790	2.357974
43	6	0	2.232983	-1.930281	-1.217473
44	1	0	1.316205	-2.044412	-1.797148
45	1	0	3.065416	-2.013088	-1.932647
46	6	0	2.348950	-3.071622	-0.196949
47	1	0	2.286969	-4.026310	-0.736389
48	1	0	3.305203	-3.045584	0.336081
49	1	0	1.547442	-3.057188	0.532828
50	1	0	-0.083779	0.777330	-2.311283

TS1C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.169569	-0.026891	1.913924
2	6	0	0.073695	-0.757320	1.587973
3	6	0	-1.291258	-0.307047	1.272313
4	6	0	-2.310873	-1.337200	1.098614
5	6	0	-1.825053	0.940180	1.997987
6	1	0	-1.333631	1.844861	1.637834
7	1	0	-2.875274	1.055534	1.722525
8	6	0	-1.704260	0.853146	3.521717
9	1	0	-2.137199	1.737589	3.999886
10	1	0	-2.229679	-0.029482	3.903906
11	1	0	-0.657975	0.781063	3.832627
12	8	0	-3.435916	-0.832045	0.499767

13	8	0	-2.269239	-2.541461	1.356325
14	6	0	-4.624011	-1.633456	0.589737
15	1	0	-5.295800	-1.217890	-0.164003
16	1	0	-4.387876	-2.667694	0.329401
17	6	0	-5.228690	-1.541291	1.978463
18	1	0	-6.162223	-2.107631	2.022449
19	1	0	-4.539084	-1.953006	2.719229
20	1	0	-5.440460	-0.499616	2.232420
21	7	0	0.369647	-2.182709	1.479779
22	16	0	0.740946	-2.738824	-0.048690
23	8	0	-0.290730	-2.418404	-1.042314
24	8	0	1.110611	-4.143629	0.105028
25	6	0	2.180808	-1.789179	-0.488328
26	6	0	2.002106	-0.560803	-1.121738
27	6	0	3.432974	-2.302252	-0.169650
28	6	0	3.128523	0.190513	-1.433188
29	1	0	1.000895	-0.193712	-1.342819
30	6	0	4.561230	-1.554487	-0.487410
31	1	0	3.521394	-3.267631	0.315877
32	6	0	4.377007	-0.325828	-1.107116
33	1	0	3.048551	1.158222	-1.911436
34	1	0	5.559138	-1.907943	-0.263622
35	7	0	5.569864	0.471911	-1.437932
36	8	0	5.400395	1.546993	-1.983804
37	8	0	6.659432	0.012279	-1.147211
38	1	0	-1.178330	0.159859	-0.090269
39	6	0	-2.007233	1.389125	-1.575250
40	8	0	-1.114239	0.434860	-1.231668
41	8	0	-2.687067	1.156921	-2.627508
42	8	0	-2.114952	2.415480	-0.857795
43	19	0	-2.477663	-1.509067	-2.292972
44	19	0	-4.020546	3.418622	-2.355432
45	1	0	2.041669	-0.612430	2.197251
46	6	0	1.386638	1.425043	1.886939
47	6	0	2.240226	2.004141	2.841037
48	6	0	0.858754	2.252316	0.881796
49	6	0	2.529287	3.363971	2.817700
50	1	0	2.674991	1.371675	3.610949
51	6	0	1.149741	3.614536	0.861153
52	1	0	0.216424	1.829663	0.113453
53	6	0	1.980727	4.178617	1.826992
54	1	0	3.185053	3.788993	3.571386
55	1	0	0.725482	4.235786	0.077560
56	1	0	2.206464	5.240010	1.804580

57	1	0	-0.454100	-2.733966	1.758049

VI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.717478	0.460343	2.038386
2	6	0	-0.136944	-0.474101	1.594713
3	6	0	-1.426340	-0.310708	0.804646
4	6	0	-2.371055	-1.466956	1.075927
5	6	0	-2.278595	0.962195	1.065570
6	1	0	-1.800497	1.805177	0.563306
7	1	0	-3.220403	0.792211	0.529286
8	6	0	-2.560162	1.271642	2.531571
9	1	0	-3.206879	2.149858	2.610293
10	1	0	-3.060907	0.433516	3.022884
11	1	0	-1.638274	1.484554	3.078571
12	8	0	-2.965386	-1.893278	-0.054693
13	8	0	-2.656169	-1.896214	2.169434
14	6	0	-4.026202	-2.856614	0.109135
15	1	0	-4.108901	-3.349730	-0.860807
16	1	0	-3.722387	-3.586937	0.861093
17	6	0	-5.316578	-2.160519	0.495170
18	1	0	-6.124404	-2.891863	0.574093
19	1	0	-5.203969	-1.661061	1.460019
20	1	0	-5.591060	-1.419895	-0.260043
21	7	0	0.228970	-1.855849	1.831444
22	16	0	0.890328	-2.707292	0.561832
23	8	0	-0.088296	-2.669335	-0.521568
24	8	0	1.323165	-3.982970	1.111812
25	6	0	2.322008	-1.803384	0.012688
26	6	0	2.130257	-0.672747	-0.780578
27	6	0	3.576981	-2.218077	0.452309
28	6	0	3.249466	0.067378	-1.147987
29	1	0	1.141799	-0.356139	-1.122491
30	6	0	4.693560	-1.481989	0.075832
31	1	0	3.675719	-3.105194	1.067286
32	6	0	4.498376	-0.355333	-0.713020
33	1	0	3.154597	0.955348	-1.760047
34	1	0	5.691391	-1.767997	0.381448
35	7	0	5.680488	0.429215	-1.109394
36	8	0	5.502096	1.411424	-1.806032

37	8	0	6.769401	0.054050	-0.714095
38	1	0	-1.172200	-0.291756	-0.259868
39	6	0	-1.342385	1.347289	-2.163956
40	8	0	-0.306357	0.563358	-2.142285
41	8	0	-2.523504	0.821833	-2.305319
42	8	0	-1.209552	2.616715	-2.032712
43	19	0	-1.656829	-1.632153	-2.468397
44	19	0	-3.728301	3.008313	-1.647866
45	1	0	1.584089	0.093788	2.590509
46	6	0	0.687264	1.922011	1.840974
47	6	0	0.960583	2.779804	2.915179
48	6	0	0.477640	2.462813	0.567650
49	6	0	0.981669	4.158118	2.727701
50	1	0	1.147008	2.360889	3.900624
51	6	0	0.495802	3.843454	0.385101
52	1	0	0.289694	1.816675	-0.289402
53	6	0	0.745897	4.693594	1.460258
54	1	0	1.184148	4.814158	3.568300
55	1	0	0.299885	4.230037	-0.609356
56	1	0	0.764560	5.769280	1.314306
57	1	0	-0.612480	-2.332806	2.085359