Supporting information

A DFT Study on the Mechanism of Gold (III)-Catalyzed Synthesis of Highly Substituted Furans via [3, 3]-Sigmatropic Rearrangements and/or [1, 2]-Acyloxy Migration Based on Propargyl Ketones

Ran Fang [a*], Lizi Yang [a], Yongcheng Wang [b]

[a] *College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou 730000, P. R. China;*

fangr@lzu.edu.cn

[b] *College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou 730070, P. R. China;*

Table of contents

1. Complete List of Authors for References with more than 10 Authors

[24] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision E.01; Gaussian, Inc.: Wallingford CT, **2004**.

2. The detail basis set for Au atom

[29] The detail basis set for Au

```
 S   3 1.00       0.000000000000
      0.2011529900D+02 -0.1597614021D+00
      0.1219347700D+02  0.7893559105D+00
      0.6039626000D+01 -0.1571405721D+01
 S   1 1.00       0.000000000000
      0.1373721000D+01  0.1000000000D+01
 S   1 1.00       0.000000000000
      0.6500100000D+00  0.1000000000D+01
 S   1 1.00       0.000000000000
      0.1458160000D+00  0.1000000000D+01
 S   1 1.00       0.000000000000
      0.5148400000D-01  0.1000000000D+01
 S   1 1.00       0.000000000000
      0.1500000000D-01  0.1000000000D+01
 P   2 1.00       0.000000000000
      0.8609665000D+01  0.2098223171D+01
      0.7335326000D+01 -0.3045867103D+01
 P   2 1.00       0.000000000000
      0.1912970000D+01  0.3791451975D+00
      0.1057695000D+01  0.6456427958D+00
 P   1 1.00       0.000000000000
      0.4430600000D+00  0.1000000000D+01
 P   1 1.00       0.000000000000
      0.9011400000D-01  0.1000000000D+01
 P   1 1.00       0.000000000000
      0.2681100000D-01  0.1000000000D+01
 D   4 1.00       0.000000000000
      0.4143949000D+01 -0.4058457876D+00
      0.3568257000D+01  0.4275069869D+00
      0.1344324000D+01  0.4755404855D+00
      0.5552890000D+00  0.5610971828D+00
```

D 1 1.00 0.000000000000
0.1896750000D+00 0.1000000000D+01
D 1 1.00 0.000000000000
0.6000000000D-01 0.1000000000D+01
D 1 1.00 0.000000000000
0.6000000000D-01 0.1000000000D+01

3. IRC plots for selected transition states

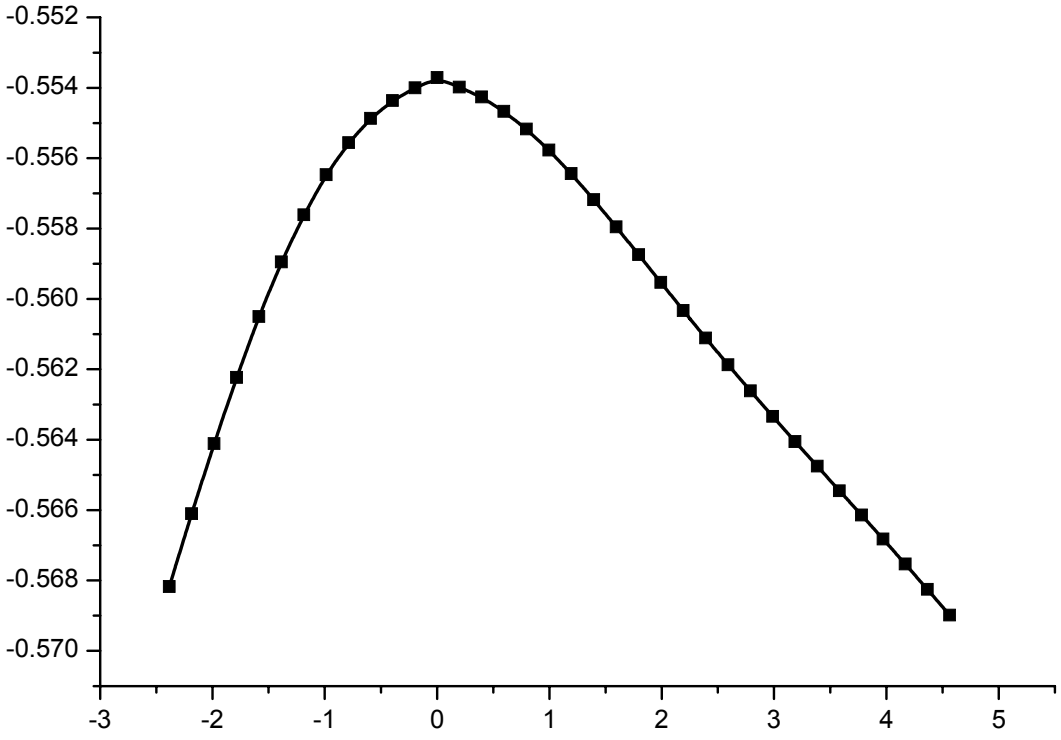

Figure S1 IRC results for TSa5

4. Thermodynamic Properties of the Structures in Figure 5 and 6

Table S1. Thermodynamic Properties (Relative Free Energies and Activation Free Energies in Gas Phase) of the Structures in Figure 5 and 6.[a]

System	ΔE^{rel}_{gas}	$\Delta E^{\neq}_{gas}$	ΔG^{rel}_{gas}	$\Delta G^{\neq}_{gas}$	ΔE^{rel}_{sol}	$\Delta E^{\neq}_{sol}$	ΔG^{rel}_{sol}	$\Delta G^{\neq}_{sol}$
1d	0.0	0.0	0.0	0.0	0	0	0	0
TSd1	3.7	4.8	3.7	4.8	3.6	3.6	3.4	3.4
2d	-13.6	-11.5			-15.4		-14.8	
TSd2	-8.5	-6.7	5.1	4.8	-8.7	6.8	-9.3	5.5
3d	-12.4	-11.9			-12.9		-13.9	
4d	-14.3	-14.2			-13.7		-13.3	
TSd3	-5.2	-4.6	9.0	9.6	-4.3	9.3	-7.0	6.4
5d	-11.9	-10.5			-11.1		-12.8	
TSd4	11.7	13.1	23.6	23.6	13.5	24.6	10.6	23.4
TSe1	5.2	6.2	5.2	6.2	5.2	5.2	4.9	4.9
2e	-5.6	-4.1			-9.2		-10.0	
TSe2	2.1	3.6	7.6	7.7	0.7	9.9	-0.8	9.1
3e	-10.7	-10.1			-11.6		-12.2	
TSe3	-2.4	-0.5	8.3	9.6	-2.6	9.0	-2.8	9.4
2e	-45.5	-43.4			-45.8		-46.2	
3d	-45.5	-43.4			-45.8		-46.2	

[a] These values, in kcal/mol, were calculated at the BHandHLYP/6-31G** (SDD for Au) level of theory and included the zero-point energy correction, using single-point PCM calculations at the BHandHLYP /PCM/6-311++G (d, p)// BHandHLYP /6-31G (d, p) (SDD for Au) level of theory to model the effect of the solvent .

5. The Cartesian coordinates of the stationary points discussed in the text

Propargyl Ketones

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.724009	1.591909	-0.162331
2	6	0	0.981836	0.697966	0.123674
3	6	0	2.597084	2.709883	-0.485965
4	1	0	3.351896	2.842312	0.284166
5	1	0	3.106561	2.550503	-1.432215
6	1	0	2.026291	3.631467	-0.558607
7	6	0	0.153322	-0.460698	0.464251
8	8	0	-1.118219	-0.417933	-0.211111
9	6	0	-1.957541	0.611207	-0.009496
10	8	0	-1.745983	1.517972	0.738503
11	6	0	0.853564	-1.693350	-0.157451
12	8	0	1.503698	-2.425510	0.533350
13	6	0	0.697090	-1.894576	-1.638260
14	1	0	0.825145	-0.958045	-2.171032
15	1	0	1.422498	-2.625317	-1.972593
16	1	0	-0.305886	-2.253339	-1.849617
17	6	0	-3.186261	0.454045	-0.854816
18	1	0	-3.870270	1.265071	-0.645990
19	1	0	-2.911581	0.461506	-1.905313
20	1	0	-3.660960	-0.499725	-0.647274
21	6	0	-0.018755	-0.638755	1.963069
22	1	0	0.947247	-0.839877	2.407761
23	1	0	-0.448212	0.253623	2.395926
24	1	0	-0.664774	-1.490205	2.152805

Sum of electronic and zero-point Energies= -575.286036
Zero-point correction= 0.199341 (Hartree/Particle)
No imaginary frequency

$AuCl_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-0.000172	-0.237328	-0.000035
2	17	0	-2.266804	-0.459302	0.000074
3	17	0	0.001266	2.022787	0.000015
4	17	0	2.266336	-0.460610	0.000074

Sum of electronic and zero-point Energies= -1516.111735
Zero-point correction= 0.003293 (Hartree/Particle)
No imaginary frequency

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.505885	1.708400	-0.207438
2	6	0	-0.944410	0.690801	0.302142
3	6	0	-0.118439	2.987192	-0.776712
4	1	0	-0.998840	3.625174	-0.762406
5	1	0	0.667150	3.439880	-0.181072
6	1	0	0.218759	2.872397	-1.801697
7	6	0	-1.948895	-0.233854	0.880731
8	8	0	-3.012327	-0.444397	-0.043070
9	6	0	-3.703518	0.595151	-0.549660
10	8	0	-3.491766	1.736377	-0.259486
11	6	0	-1.350406	-1.627626	1.172836
12	8	0	-0.253671	-1.685189	1.653519
13	6	0	-2.196275	-2.829959	0.899125
14	1	0	-2.262942	-2.967592	-0.176931
15	1	0	-1.726138	-3.693694	1.350722
16	1	0	-3.207838	-2.702405	1.270917
17	6	0	-4.737721	0.115049	-1.517376
18	1	0	-5.335834	0.953259	-1.847221
19	1	0	-4.245968	-0.347734	-2.368103
20	1	0	-5.365911	-0.637615	-1.052138
21	6	0	-2.458481	0.321294	2.215524
22	1	0	-1.630866	0.384950	2.912395
23	1	0	-2.891120	1.301628	2.070719
24	1	0	-3.211918	-0.349908	2.617523
25	79	0	1.214759	0.051118	-0.157702
26	17	0	0.263640	-1.175332	-1.904088
27	17	0	3.247255	-0.957570	-0.504464
28	17	0	2.128621	1.360566	1.532256

Sum of electronic and zero-point Energies= -2091.441979
Zero-point correction= 0.204004 (Hartree/Particle)
No imaginary frequency

TSa1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.002017	-1.604713	-0.459190
2	6	0	0.842851	-0.502766	0.110431
3	6	0	0.824738	-2.873159	-1.125346
4	1	0	1.402915	-3.635319	-0.613819
5	1	0	-0.228171	-3.135749	-1.040481
6	1	0	1.108780	-2.826499	-2.170828
7	6	0	1.818573	0.384753	0.829446
8	8	0	3.051847	0.489172	0.100035
9	6	0	3.662566	-0.571113	-0.404980
10	8	0	3.215084	-1.694320	-0.351357
11	6	0	1.280181	1.826881	0.980055
12	8	0	0.253581	1.964245	1.581405
13	6	0	2.068522	2.967115	0.417979
14	1	0	2.110424	2.873521	-0.663661
15	1	0	1.573054	3.890288	0.687895
16	1	0	3.089373	2.959312	0.787690
17	6	0	4.954577	-0.213090	-1.062377

18	1	0	5.447338	-1.112045	-1.405705
19	1	0	4.756989	0.446487	-1.902603
20	1	0	5.588775	0.323938	-0.364723
21	6	0	2.088447	-0.170778	2.226170
22	1	0	1.156913	-0.204516	2.777644
23	1	0	2.500705	-1.170209	2.157326
24	1	0	2.788425	0.476228	2.746720
25	79	0	-1.221667	-0.065081	-0.118298
26	17	0	-0.585232	1.355192	-1.862407
27	17	0	-3.447504	0.502641	-0.373690
28	17	0	-1.743897	-1.579929	1.567644

Sum of electronic and zero-point Energies= -2091.438308
Zero-point correction= 0.203681 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.331716	-0.664802	1.273340
2	6	0	-0.765366	-0.143371	0.204336
3	6	0	-0.782642	-1.198693	2.540318
4	1	0	-0.924757	-2.274796	2.602295
5	1	0	0.275254	-0.980971	2.601842
6	1	0	-1.281721	-0.736983	3.388222
7	6	0	-1.679358	0.313504	-0.908226
8	8	0	-2.849197	-0.589715	-0.935015
9	6	0	-3.396536	-0.873676	0.172722
10	8	0	-2.765926	-0.843532	1.273823
11	6	0	-2.303385	1.683328	-0.538610
12	8	0	-3.387650	1.686518	-0.014240
13	6	0	-1.526422	2.923138	-0.832216
14	1	0	-1.396646	3.037577	-1.905450
15	1	0	-2.069505	3.773104	-0.439921
16	1	0	-0.539970	2.870766	-0.378550
17	6	0	-4.804328	-1.311326	0.173219
18	1	0	-5.031132	-1.872747	1.068873
19	1	0	-5.412390	-0.410074	0.139736
20	1	0	-5.004703	-1.890616	-0.720486
21	6	0	-1.114611	0.261623	-2.308428
22	1	0	-0.267882	0.933759	-2.385080
23	1	0	-0.766932	-0.739177	-2.531050
24	1	0	-1.871036	0.561484	-3.027207
25	79	0	1.269438	-0.078185	0.022566
26	17	0	1.295501	1.943055	1.189750
27	17	0	3.598152	-0.037263	-0.219211
28	17	0	1.121297	-2.144572	-1.055904

Sum of electronic and zero-point Energies= -2091.470658
Zero-point correction= 0.207742 (Hartree/Particle)
No imaginary frequency

TSa2

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.548173	-1.305324	0.506340
2	6	0	0.899011	-0.137888	0.365384
3	6	0	0.910923	-2.647739	0.575719
4	1	0	1.529860	-3.310973	1.170676
5	1	0	-0.077752	-2.585343	1.013012
6	1	0	0.821786	-3.068885	-0.423836
7	6	0	1.381945	1.160286	0.492731
8	8	0	3.531760	0.624607	-0.167048
9	6	0	3.767033	-0.545611	-0.092599
10	8	0	2.907436	-1.453539	0.432378
11	6	0	1.018465	2.258510	-0.504992
12	8	0	1.816059	2.523625	-1.353789
13	6	0	5.026303	-1.206725	-0.539200
14	1	0	5.397826	-1.860705	0.242795
15	1	0	4.815462	-1.820294	-1.410776
16	1	0	5.759865	-0.453372	-0.790211
17	79	0	-1.152352	-0.211835	-0.027882
18	17	0	-0.654693	-0.520454	-2.277517
19	17	0	-3.445346	-0.333677	-0.434295
20	17	0	-1.494229	0.156577	2.256963
21	6	0	1.970103	1.651546	1.762008
22	1	0	2.646410	2.481247	1.590302
23	1	0	1.127057	1.999810	2.363535
24	1	0	2.453557	0.855816	2.313506
25	6	0	-0.281648	2.988414	-0.318785
26	1	0	-1.010239	2.577055	-1.013981
27	1	0	-0.685032	2.898275	0.683972
28	1	0	-0.124311	4.030411	-0.575811

Sum of electronic and zero-point Energies= -2091.439245
Zero-point correction= 0.203400 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.458739	-0.308766	1.357860
2	6	0	0.943817	0.595778	0.387944
3	6	0	1.133452	-0.185186	2.797757
4	1	0	1.942684	0.403709	3.234428
5	1	0	0.206043	0.351479	2.946842
6	1	0	1.122362	-1.156651	3.278336
7	6	0	1.491541	1.717664	-0.062708
8	8	0	3.372982	-0.669935	-0.722286
9	6	0	2.885450	-1.575297	-0.159135
10	8	0	2.173797	-1.348639	1.085459
11	6	0	0.865532	2.662338	-1.060941
12	8	0	1.433703	3.708131	-1.250110
13	6	0	2.965971	-3.035578	-0.400996
14	1	0	3.478494	-3.507370	0.432753
15	1	0	1.966346	-3.447927	-0.471740
16	1	0	3.510856	-3.205258	-1.319369

17	79	0	-0.968571	-0.221060	0.018284
18	17	0	-0.001837	-1.656036	-1.549057
19	17	0	-3.090654	-1.056163	-0.463711
20	17	0	-1.859800	1.218651	1.614144
21	6	0	2.841518	2.181194	0.411095
22	1	0	3.523833	2.250506	-0.429685
23	1	0	2.759504	3.174947	0.838308
24	1	0	3.273268	1.508290	1.143694
25	6	0	-0.388450	2.318628	-1.809817
26	1	0	-0.321067	1.342854	-2.282297
27	1	0	-1.246641	2.320934	-1.142460
28	1	0	-0.538884	3.077440	-2.567539

Sum of electronic and zero-point Energies= -2091.455711
Zero-point correction= 0.204447 (Hartree/Particle)
No imaginary frequency

4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.554932	-0.498534	1.478825
2	6	0	1.638556	0.652048	0.867233
3	6	0	0.813549	-0.695360	2.761040
4	1	0	1.501069	-1.067168	3.516173
5	1	0	0.364506	0.229861	3.096925
6	1	0	0.028480	-1.431822	2.615010
7	6	0	1.724539	1.872761	0.386997
8	8	0	3.346820	-0.687381	-0.537295
9	6	0	2.908707	-1.685969	-0.057390
10	8	0	2.071948	-1.673458	1.015278
11	6	0	0.768675	2.321050	-0.629804
12	8	0	-0.247738	1.711687	-0.983560
13	6	0	3.160100	-3.085082	-0.508464
14	1	0	3.367646	-3.730212	0.337909
15	1	0	2.260801	-3.450147	-0.997313
16	1	0	3.983358	-3.092558	-1.209528
17	79	0	-1.129503	-0.032797	-0.271781
18	17	0	-0.100771	-1.219246	-1.985316
19	17	0	-2.213133	-1.905683	0.431241
20	17	0	-2.109228	1.231513	1.416145
21	6	0	2.869430	2.782407	0.765643
22	1	0	3.527383	2.963555	-0.080514
23	1	0	2.516517	3.743038	1.131693
24	1	0	3.457265	2.319239	1.547442
25	6	0	1.022851	3.616037	-1.331858
26	1	0	1.031074	4.429936	-0.611365
27	1	0	1.998407	3.595659	-1.810050
28	1	0	0.251183	3.786761	-2.069610

Sum of electronic and zero-point Energies= -2091.460463
Zero-point correction= 0.205363 (Hartree/Particle)
No imaginary frequency

TSa3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.226968	-0.894693	-0.649396
2	6	0	-2.923530	0.375130	-0.484093
3	6	0	-2.905637	-1.800541	-1.775230
4	1	0	-3.807379	-2.266911	-2.161771
5	1	0	-2.420884	-1.237997	-2.561968
6	1	0	-2.220361	-2.575054	-1.443648
7	6	0	-2.213771	1.451297	-0.971904
8	8	0	-3.915832	-1.473506	0.406221
9	6	0	-4.107625	-0.574713	1.336399
10	8	0	-3.673143	0.549225	1.095019
11	6	0	-0.840323	1.420676	-0.706511
12	8	0	-0.377776	0.508690	0.055561
13	6	0	0.100605	2.419818	-1.297791
14	1	0	0.723402	2.830006	-0.507876
15	1	0	0.754094	1.911302	-2.004371
16	1	0	-0.409712	3.221849	-1.813066
17	6	0	-4.791055	-0.991025	2.581184
18	1	0	-5.209436	-0.123960	3.074302
19	1	0	-5.558702	-1.723299	2.361851
20	1	0	-4.056655	-1.450024	3.238892
21	6	0	-2.905510	2.577150	-1.702757
22	1	0	-2.505781	2.724043	-2.703345
23	1	0	-3.961859	2.353886	-1.809615
24	1	0	-2.829175	3.523934	-1.172123
25	79	0	1.566342	-0.115928	0.119592
26	17	0	1.989726	1.420988	1.807222
27	17	0	3.694203	-0.930789	0.256078
28	17	0	1.044208	-1.584512	-1.614999

Sum of electronic and zero-point Energies= -2091.440869
Zero-point correction= 0.204909 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.776456	-0.210291	1.468169
2	6	0	2.003153	0.579057	0.416905
3	6	0	1.070165	-0.054162	2.752105
4	1	0	1.748130	-0.175356	3.592369
5	1	0	0.623684	0.932465	2.786792
6	1	0	0.272403	-0.787692	2.830443
7	6	0	1.689640	1.944814	0.046616
8	8	0	2.319818	-1.462166	1.173730
9	6	0	2.803043	-1.400732	-0.013009
10	8	0	2.697931	-0.237232	-0.514425
11	6	0	0.699135	2.099074	-0.868272
12	8	0	0.058546	1.069364	-1.391483
13	6	0	0.256823	3.409462	-1.436529
14	1	0	0.298496	3.344615	-2.520240
15	1	0	-0.781117	3.568709	-1.158926
16	1	0	0.850939	4.253223	-1.111223
17	6	0	3.425736	-2.540810	-0.696506
18	1	0	4.258490	-2.196944	-1.298144

19	1	0	3.747312	-3.275479	0.030159
20	1	0	2.676420	-2.981547	-1.349162
21	6	0	2.483124	3.033333	0.716299
22	1	0	2.093285	4.014082	0.477681
23	1	0	2.454954	2.934619	1.800366
24	1	0	3.531835	3.014201	0.420625
25	79	0	-1.074188	-0.183758	-0.266450
26	17	0	-0.015888	-1.985203	-1.337828
27	17	0	-2.343017	-1.649841	0.984043
28	17	0	-2.039212	1.620562	0.829760

Sum of electronic and zero-point Energies= -2091.454087
Zero-point correction= 0.207214 (Hartree/Particle)
No imaginary frequency

TSa4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.963251	-0.851647	-0.516957
2	6	0	2.678814	0.265416	-0.327878
3	6	0	1.202110	-1.992531	-1.060901
4	1	0	0.751919	-2.575732	-0.263363
5	1	0	0.426575	-1.628974	-1.720845
6	1	0	1.866425	-2.632867	-1.628868
7	6	0	2.201166	1.618604	-0.389735
8	8	0	3.487885	-1.951930	0.024116
9	6	0	4.335669	-1.114745	0.253345
10	8	0	4.001201	0.142642	0.051795
11	6	0	0.861870	1.646222	-0.565499
12	8	0	0.332788	0.450907	-0.753950
13	6	0	-0.036026	2.832795	-0.581665
14	1	0	-0.694560	2.781603	-1.444219
15	1	0	-0.651854	2.839320	0.314947
16	1	0	0.520378	3.760695	-0.617085
17	6	0	5.709399	-1.354681	0.757449
18	1	0	5.778071	-0.992088	1.779433
19	1	0	5.926923	-2.413133	0.730514
20	1	0	6.423645	-0.800573	0.158116
21	6	0	3.143974	2.768912	-0.231624
22	1	0	2.616832	3.710194	-0.325111
23	1	0	3.628053	2.758672	0.742106
24	1	0	3.928108	2.755107	-0.985324
25	79	0	-1.486352	-0.067629	0.078127
26	17	0	-2.235121	-0.538698	-2.070365
27	17	0	-3.482540	-0.725205	0.969922
28	17	0	-0.637342	0.424931	2.188253

Sum of electronic and zero-point Energies= -2091.414229
Zero-point correction= 0.205183 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

TSa5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.739736	-0.069488	1.612739
2	6	0	2.680943	0.718515	0.613744
3	6	0	2.589201	-0.776031	2.870018
4	1	0	3.302092	-0.428083	3.612216
5	1	0	1.583379	-0.552041	3.218368
6	1	0	2.674125	-1.852978	2.754392
7	6	0	2.208253	1.524425	-0.418879
8	8	0	4.092423	0.093384	0.729980
9	6	0	4.441026	-0.930323	-0.237267
10	8	0	5.531761	-0.836808	-0.663137
11	6	0	0.829013	1.498340	-0.514338
12	8	0	0.176371	0.846439	0.384933
13	6	0	0.084588	2.198626	-1.601505
14	1	0	-0.309533	1.459804	-2.297153
15	1	0	-0.756888	2.733974	-1.171424
16	1	0	0.711279	2.888692	-2.151700
17	6	0	3.398889	-1.951234	-0.530733
18	1	0	3.795690	-2.609771	-1.291184
19	1	0	3.172948	-2.528201	0.361190
20	1	0	2.469413	-1.504536	-0.870271
21	6	0	3.155742	2.328174	-1.268080
22	1	0	3.063000	3.395544	-1.082183
23	1	0	4.183683	2.054388	-1.052899
24	1	0	2.989776	2.155428	-2.327246
25	79	0	-1.590980	-0.114792	0.012508
26	17	0	-0.367928	-1.705881	-1.191267
27	17	0	-3.536351	-1.267863	-0.302534
28	17	0	-2.705154	1.549403	1.172704

Sum of electronic and zero-point Energies= -2091.352304
Zero-point correction= -2091.414229 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

TSb1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.490093	-1.201642	-0.642967
2	6	0	1.390194	-0.570646	-0.053472
3	6	0	0.328374	-2.387681	-1.516269
4	1	0	1.301295	-2.822331	-1.716672
5	1	0	-0.304225	-3.117499	-1.021260
6	1	0	-0.146559	-2.095024	-2.446724
7	6	0	2.129978	0.330525	0.847273
8	8	0	3.422893	0.598618	0.280274
9	6	0	3.962936	-0.412401	-0.392244
10	8	0	3.330439	-1.417672	-0.604875
11	6	0	1.409050	1.720799	0.901559
12	8	0	0.723808	1.958654	1.848786
13	6	0	1.641177	2.663641	-0.238084

14	1	0	1.403624	2.184199	-1.183268
15	1	0	1.003908	3.527471	-0.102401
16	1	0	2.683068	2.968218	-0.261139
17	6	0	5.364158	-0.154039	-0.826551
18	1	0	5.717634	-0.982425	-1.424054
19	1	0	5.403517	0.768678	-1.396647
20	1	0	5.994015	-0.027782	0.048830
21	6	0	2.289489	-0.262066	2.235995
22	1	0	2.856184	0.422412	2.857256
23	1	0	1.311227	-0.412139	2.675203
24	1	0	2.803050	-1.215074	2.174257
25	79	0	-1.308829	-0.161742	-0.139146
26	17	0	-1.079524	1.035513	-2.126100
27	17	0	-3.376486	0.790657	0.272038
28	17	0	-1.454523	-1.467157	1.777842

Sum of electronic and zero-point Energies= -2091.436393
Zero-point correction= 0.203862 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.486459	-0.813423	-0.899240
2	6	0	1.624860	-0.505645	-0.320733
3	6	0	0.385140	-1.646012	-2.134230
4	1	0	1.352086	-1.967457	-2.508770
5	1	0	-0.217703	-2.525092	-1.922643
6	1	0	-0.124247	-1.079734	-2.908609
7	6	0	2.050128	0.237955	0.925343
8	8	0	3.532757	0.294939	0.701867
9	6	0	3.840672	-0.439178	-0.289822
10	8	0	2.879148	-0.960238	-0.915251
11	6	0	1.580895	1.715069	0.999227
12	8	0	0.932999	2.045903	1.946923
13	6	0	1.945621	2.634087	-0.125631
14	1	0	1.306827	2.409263	-0.977073
15	1	0	1.757055	3.652728	0.187817
16	1	0	2.984168	2.526109	-0.423498
17	6	0	5.245330	-0.668696	-0.669855
18	1	0	5.297064	-1.163240	-1.629880
19	1	0	5.769154	0.280972	-0.693659
20	1	0	5.713238	-1.287781	0.091528
21	6	0	1.830506	-0.499097	2.222712
22	1	0	2.271753	0.050722	3.045566
23	1	0	0.765873	-0.597125	2.394903
24	1	0	2.255512	-1.495825	2.164542
25	79	0	-1.297051	-0.157156	-0.154193
26	17	0	-1.157192	1.599245	-1.692967
27	17	0	-3.380634	0.571026	0.640997
28	17	0	-1.306917	-2.024591	1.242914

Sum of electronic and zero-point Energies= -2091.455830
Zero-point correction= 0.206810 (Hartree/Particle)
No imaginary frequency

TSb2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.582156	-0.929275	-0.645270
2	6	0	-1.712060	-0.227622	-0.465707
3	6	0	-0.578250	-2.229047	-1.368710
4	1	0	-1.572758	-2.572835	-1.629096
5	1	0	0.010826	-2.126475	-2.277925
6	1	0	-0.080556	-2.971416	-0.750425
7	6	0	-1.873140	1.089687	0.056849
8	8	0	-3.712961	0.355454	0.857750
9	6	0	-3.901427	-0.493214	0.009200
10	8	0	-2.948358	-0.768148	-0.873990
11	6	0	-1.068626	1.619453	1.248630
12	8	0	-0.507521	2.664117	1.081779
13	6	0	-1.108947	0.858057	2.531361
14	1	0	-0.725628	-0.149139	2.398489
15	1	0	-0.503486	1.383074	3.258876
16	1	0	-2.136991	0.786359	2.876387
17	6	0	-5.143348	-1.291561	-0.154830
18	1	0	-5.431106	-1.308668	-1.200576
19	1	0	-4.942611	-2.315352	0.149587
20	1	0	-5.932611	-0.876089	0.455707
21	6	0	-2.544591	2.143656	-0.730621
22	1	0	-3.108947	2.822277	-0.102167
23	1	0	-1.709161	2.707854	-1.151841
24	1	0	-3.150528	1.750446	-1.535065
25	79	0	1.261964	-0.223870	-0.150490
26	17	0	1.249947	-1.768923	1.606177
27	17	0	3.417155	0.517978	0.376737
28	17	0	1.098453	1.209976	-1.983675

Sum of electronic and zero-point Energies= -2091.434388
Zero-point correction= 0.204174 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.698403	-0.876146	-0.208615
2	6	0	-1.801251	-0.036885	-0.427160
3	6	0	-0.907449	-2.334567	-0.131296
4	1	0	-1.835698	-2.664251	-0.579856
5	1	0	-0.063634	-2.872032	-0.548582
6	1	0	-0.926554	-2.566196	0.938500
7	6	0	-1.782863	1.326265	-0.517438
8	8	0	-3.809429	0.044842	1.328032
9	6	0	-3.952554	-0.621035	0.350838
10	8	0	-3.016836	-0.678929	-0.640033
11	6	0	-0.570345	2.217618	-0.349858
12	8	0	0.081935	2.434276	-1.331157

13	6	0	-0.385984	2.881342	0.976833
14	1	0	-0.244196	2.142056	1.759456
15	1	0	0.477127	3.533346	0.921449
16	1	0	-1.273223	3.462405	1.222171
17	6	0	-5.127547	-1.478575	0.013457
18	1	0	-5.511730	-1.216866	-0.967247
19	1	0	-4.819803	-2.519471	-0.025043
20	1	0	-5.892506	-1.349573	0.766437
21	6	0	-3.011872	2.096032	-0.847471
22	1	0	-3.538612	2.315549	0.081283
23	1	0	-2.759573	3.032085	-1.332724
24	1	0	-3.676831	1.520168	-1.480405
25	79	0	1.224558	-0.317623	0.048942
26	17	0	0.778632	-0.223468	2.347583
27	17	0	3.465919	0.238240	0.331032
28	17	0	1.444236	-0.671878	-2.245224

Sum of electronic and zero-point Energies= -2091.446072
Zero-point correction= 0.203527 (Hartree/Particle)
No imaginary frequency

TSb3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.521420	-0.447913	1.004312
2	6	0	1.820013	0.107573	0.665067
3	6	0	0.495857	-1.388477	2.127391
4	1	0	1.461268	-1.583020	2.574457
5	1	0	-0.192328	-0.935677	2.848137
6	1	0	-0.009614	-2.309063	1.841672
7	6	0	2.076422	1.407930	0.440409
8	8	0	3.573588	-0.501037	-1.348227
9	6	0	3.571336	-1.156068	-0.359807
10	8	0	2.804684	-0.850648	0.741986
11	6	0	0.894372	2.305217	0.501581
12	8	0	0.001920	2.022863	1.271485
13	6	0	0.820217	3.477491	-0.425559
14	1	0	0.733833	3.105476	-1.445270
15	1	0	-0.051480	4.070775	-0.182980
16	1	0	1.716068	4.088432	-0.373777
17	6	0	4.366575	-2.391313	-0.090984
18	1	0	4.893691	-2.303288	0.853301
19	1	0	3.695291	-3.242082	-0.017203
20	1	0	5.064329	-2.546915	-0.902050
21	6	0	3.439271	1.963022	0.210511
22	1	0	3.649585	2.002938	-0.855982
23	1	0	3.529286	2.961088	0.626074
24	1	0	4.193635	1.331223	0.664419
25	79	0	-1.193752	-0.263247	-0.102398
26	17	0	0.124233	-0.313890	-2.029232
27	17	0	-3.115768	-0.135312	-1.402511
28	17	0	-2.505617	-0.284773	1.825810

Sum of electronic and zero-point Energies= -2091.433074
Zero-point correction= 0.203513 (Hartree/Particle)

One imaginary frequency, one negative Eigenvalue

TSb4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.425937	0.569471	0.895836
2	6	0	-1.661795	-0.086408	0.547500
3	6	0	-0.375934	1.424307	2.095712
4	1	0	-1.351320	1.722397	2.461914
5	1	0	0.125496	0.811634	2.847606
6	1	0	0.265084	2.284881	1.940546
7	6	0	-1.858960	-1.383470	0.282360
8	8	0	-1.411978	2.316342	-0.177385
9	6	0	-2.542216	1.957245	0.011729
10	8	0	-2.787582	0.739034	0.530402
11	6	0	-3.268392	-1.876289	0.023348
12	8	0	-3.809545	-2.546935	0.857129
13	6	0	-3.863936	-1.566838	-1.317916
14	1	0	-3.212447	-1.936601	-2.106916
15	1	0	-4.838021	-2.034254	-1.392768
16	1	0	-3.951946	-0.493961	-1.454887
17	6	0	-3.778672	2.737374	-0.263945
18	1	0	-4.263260	2.328997	-1.146951
19	1	0	-4.469777	2.647977	0.566947
20	1	0	-3.520837	3.771833	-0.443305
21	6	0	-0.849694	-2.479949	0.329903
22	1	0	-1.230035	-3.253511	0.993017
23	1	0	-0.741846	-2.919612	-0.659931
24	1	0	0.123999	-2.173256	0.682920
25	79	0	1.306677	0.084403	-0.069113
26	17	0	0.246967	0.353455	-2.129846
27	17	0	3.295229	-0.427974	-1.164035
28	17	0	2.320360	-0.352808	1.991730

Sum of electronic and zero-point Energies= -2091.437171
Zero-point correction= 0.203951 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.764683	-0.622188	0.948978
2	6	0	-1.942971	0.035478	0.377723
3	6	0	-0.657679	-0.628330	2.464009
4	1	0	-1.615072	-0.919717	2.893526
5	1	0	0.099228	-1.337818	2.763631
6	1	0	-0.380724	0.350135	2.825719
7	6	0	-2.714371	-0.863014	-0.327768
8	8	0	-0.488958	2.178385	1.422536
9	6	0	-1.525327	2.345908	0.875891
10	8	0	-2.341235	1.292209	0.483953

11	6	0	-2.032977	-2.065260	-0.219230
12	8	0	-0.963832	-1.979368	0.516240
13	6	0	-2.309629	-3.372186	-0.847788
14	1	0	-1.750215	-3.437607	-1.779848
15	1	0	-1.977072	-4.175607	-0.200462
16	1	0	-3.362711	-3.485064	-1.073891
17	6	0	-2.162122	3.633923	0.492287
18	1	0	-3.209820	3.641556	0.772319
19	1	0	-1.630318	4.448075	0.964592
20	1	0	-2.099498	3.733488	-0.588116
21	6	0	-3.945395	-0.557766	-1.110215
22	1	0	-3.686845	-0.114956	-2.068566
23	1	0	-4.529190	-1.452685	-1.295752
24	1	0	-4.571304	0.148624	-0.575676
25	79	0	1.027479	-0.038464	-0.123532
26	17	0	2.324209	-1.126412	1.463781
27	17	0	2.978561	0.526196	-1.274951
28	17	0	-0.230663	0.969100	-1.846690

Sum of electronic and zero-point Energies= -2091.499387
Zero-point correction= 0.207486 (Hartree/Particle)
No imaginary frequency

TSb5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.602807	0.510458	1.047819
2	6	0	-1.448048	-0.391293	0.373812
3	6	0	-0.559118	0.387082	2.556193
4	1	0	-1.521098	0.695300	2.960749
5	1	0	-0.351319	-0.630498	2.853672
6	1	0	0.218525	1.025602	2.956947
7	6	0	-1.919827	-1.454177	-0.175178
8	8	0	-0.911054	1.856301	0.708533
9	6	0	-2.182298	2.038433	0.403183
10	8	0	-2.945086	1.092929	0.349700
11	6	0	-3.434356	-1.677721	-0.262850
12	8	0	-3.962695	-2.326962	0.586433
13	6	0	-4.110947	-1.130960	-1.480858
14	1	0	-3.574405	-1.425799	-2.379046
15	1	0	-5.129571	-1.496930	-1.516075
16	1	0	-4.102209	-0.046931	-1.434731
17	6	0	-2.540525	3.452751	0.124430
18	1	0	-2.027884	3.752585	-0.785824
19	1	0	-3.609915	3.546417	-0.001488
20	1	0	-2.188319	4.089993	0.928018
21	6	0	-1.089197	-2.588725	-0.721889
22	1	0	-1.356448	-3.493239	-0.183336
23	1	0	-1.317492	-2.729804	-1.774605
24	1	0	-0.028229	-2.410064	-0.613884
25	79	0	1.242010	0.053839	-0.034867
26	17	0	0.311798	1.036857	-1.944289
27	17	0	3.236117	-0.284257	-1.186035
28	17	0	2.142849	-1.045728	1.800840

Sum of electronic and zero-point Energies= -2091.424139

Zero-point correction= 0.203896 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

TSc1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.370125	-0.825945	-0.746046
2	6	0	-1.375589	-0.041816	-0.517692
3	6	0	-0.458479	-2.150325	-1.422276
4	1	0	-1.468492	-2.383998	-1.750695
5	1	0	0.194288	-2.155807	-2.290618
6	1	0	-0.110092	-2.922294	-0.744172
7	6	0	-2.026555	1.147338	-0.120888
8	8	0	-2.852734	-0.163859	-0.908219
9	6	0	-3.649321	-1.060721	-0.157648
10	8	0	-3.492774	-1.191539	1.004303
11	6	0	-2.380174	1.399291	1.343681
12	8	0	-1.426576	1.485126	2.056654
13	6	0	-3.789683	1.685263	1.761911
14	1	0	-4.468827	1.774261	0.920712
15	1	0	-4.125854	0.875794	2.401377
16	1	0	-3.800197	2.602583	2.341275
17	6	0	-4.638972	-1.720824	-1.052702
18	1	0	-5.254035	-2.390875	-0.467617
19	1	0	-5.252136	-0.967689	-1.538495
20	1	0	-4.119301	-2.270008	-1.831776
21	6	0	-2.075143	2.339361	-1.004227
22	1	0	-2.937978	2.963763	-0.799679
23	1	0	-1.162060	2.893589	-0.784280
24	1	0	-2.028390	2.053711	-2.046754
25	79	0	1.446886	-0.136705	-0.083792
26	17	0	1.448252	-1.912583	1.419438
27	17	0	3.535452	0.603894	0.664511
28	17	0	1.309827	1.606285	-1.643733

Sum of electronic and zero-point Energies= -2091.380013
Zero-point correction= 0.201431 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.726656	-0.774006	0.428640
2	6	0	1.806621	0.116323	0.352533
3	6	0	0.957730	-2.170964	0.839106
4	1	0	1.924726	-2.339193	1.294110
5	1	0	0.160924	-2.515422	1.490809
6	1	0	0.876309	-2.761210	-0.078149
7	6	0	1.747709	1.424393	-0.042434
8	8	0	3.029705	-0.372225	0.797233
9	6	0	3.994362	-0.640907	-0.132350
10	8	0	3.865012	-0.372523	-1.284135

11	6	0	0.552146	2.106650	-0.674769
12	8	0	0.436544	1.960464	-1.857850
13	6	0	-0.270764	3.042693	0.156283
14	1	0	0.248846	3.997536	0.222327
15	1	0	-1.220640	3.200067	-0.341115
16	1	0	-0.435072	2.666324	1.159172
17	6	0	5.176716	-1.285277	0.513982
18	1	0	5.965540	-1.398014	-0.216696
19	1	0	5.517906	-0.687380	1.352911
20	1	0	4.893413	-2.259349	0.902300
21	6	0	2.946581	2.299812	-0.005919
22	1	0	2.670836	3.339126	0.133992
23	1	0	3.644811	1.993598	0.763372
24	1	0	3.439228	2.211536	-0.974766
25	79	0	-1.210963	-0.339292	0.064352
26	17	0	-0.934558	-1.274780	-2.046359
27	17	0	-3.462518	0.134589	-0.294289
28	17	0	-1.279243	0.370688	2.302738

Sum of electronic and zero-point Energies= -2091.445039
Zero-point correction= 0.203442 (Hartree/Particle)
No imaginary frequency

TSc2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.502530	0.553087	0.971793
2	6	0	-1.803012	0.395012	0.431169
3	6	0	-0.381255	0.526853	2.476885
4	1	0	-1.202746	1.059850	2.947406
5	1	0	-0.382216	-0.505769	2.811698
6	1	0	0.559868	0.982577	2.759511
7	6	0	-2.983901	0.333962	-0.072327
8	8	0	-0.785784	1.964120	0.564211
9	6	0	-0.353968	2.441911	-0.684551
10	8	0	-0.330063	1.741496	-1.636256
11	6	0	-3.752346	-1.003347	-0.093096
12	8	0	-4.518303	-1.159848	-0.993600
13	6	0	-3.578435	-1.945272	1.053999
14	1	0	-2.531215	-2.198639	1.182560
15	1	0	-3.933798	-1.467234	1.964572
16	1	0	-4.154602	-2.841747	0.864949
17	6	0	-0.017293	3.887920	-0.580122
18	1	0	0.107749	4.293828	-1.574866
19	1	0	-0.789241	4.422246	-0.036720
20	1	0	0.912057	3.974326	-0.025390
21	6	0	-3.695670	1.476871	-0.743029
22	1	0	-4.681710	1.591785	-0.305744
23	1	0	-3.149269	2.404111	-0.652473
24	1	0	-3.820408	1.216058	-1.788629
25	79	0	1.089663	-0.420417	0.040201
26	17	0	2.423698	1.416498	0.577246
27	17	0	2.894905	-1.559802	-0.899171
28	17	0	-0.350025	-2.214730	-0.346421

Sum of electronic and zero-point Energies= -2091.390569

Zero-point correction= 0.202194 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

2 and 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.934260	-0.141196	1.001374
2	6	0	1.748461	0.087887	-0.187232
3	6	0	1.003162	0.648000	2.287411
4	1	0	0.739188	1.680448	2.135110
5	1	0	0.313438	0.208496	2.999786
6	1	0	2.012034	0.591738	2.685385
7	6	0	2.327373	-1.091375	-0.597630
8	8	0	1.810427	1.202547	-0.917481
9	6	0	2.176902	2.412694	-0.349409
10	8	0	2.710062	2.457071	0.708775
11	6	0	1.971491	-2.014476	0.381356
12	8	0	1.234209	-1.486804	1.315118
13	6	0	2.321461	-3.441359	0.519060
14	1	0	2.719735	-3.626923	1.512414
15	1	0	1.421357	-4.037130	0.401372
16	1	0	3.047128	-3.738615	-0.226887
17	6	0	1.841359	3.531846	-1.268954
18	1	0	0.760116	3.627003	-1.310127
19	1	0	2.282068	4.445047	-0.893832
20	1	0	2.198644	3.316161	-2.270316
21	6	0	3.116852	-1.331704	-1.838375
22	1	0	4.014426	-1.907560	-1.634207
23	1	0	2.526591	-1.871926	-2.574095
24	1	0	3.414778	-0.387198	-2.278179
25	79	0	-1.074856	-0.077456	0.086055
26	17	0	-0.949297	-2.315246	-0.539038
27	17	0	-3.244804	0.007213	-0.769674
28	17	0	-1.171862	2.218330	0.492143

Sum of electronic and zero-point Energies= -2091.503270
Zero-point correction= 0.207587 (Hartree/Particle)
No imaginary frequency

1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.034599	-1.826170	0.687983
2	6	0	0.141324	-1.055089	0.383235
3	6	0	1.940342	-2.889890	1.093013
4	1	0	1.333353	-3.705224	1.477692
5	1	0	2.518794	-3.233355	0.242130
6	1	0	2.610964	-2.550544	1.875577
7	6	0	-1.226871	-0.487041	0.262740
8	8	0	-1.709147	-0.098540	1.537173
9	6	0	-1.585519	-0.897626	2.624445
10	8	0	-1.255185	-2.042893	2.568501
11	6	0	-1.208010	0.811802	-0.592311

12	8	0	-0.266613	0.980081	-1.326333
13	6	0	-1.908643	-0.127322	3.863274
14	1	0	-2.003532	-0.809300	4.697226
15	1	0	-1.099610	0.573945	4.050050
16	1	0	-2.818030	0.448759	3.731095
17	79	0	2.083371	0.143621	-0.063522
18	17	0	1.582427	1.313078	1.894734
19	17	0	3.729136	1.660532	-0.583479
20	17	0	2.620556	-1.114237	-1.948814
21	6	0	-2.106296	-1.513967	-0.459432
22	6	0	-3.263413	-2.023610	0.108976
23	6	0	-1.732455	-1.914370	-1.738535
24	6	0	-4.041935	-2.927813	-0.596149
25	1	0	-3.560416	-1.732824	1.100435
26	6	0	-2.513774	-2.817120	-2.438030
27	1	0	-0.832353	-1.524225	-2.186038
28	6	0	-3.671001	-3.325907	-1.869243
29	1	0	-4.936681	-3.322630	-0.143860
30	1	0	-2.215682	-3.121180	-3.427622
31	1	0	-4.278040	-4.029798	-2.414274
32	6	0	-2.320247	1.788746	-0.540069
33	6	0	-3.568122	1.543950	0.030218
34	6	0	-2.074120	3.024583	-1.140503
35	6	0	-4.549247	2.518318	-0.005053
36	1	0	-3.783557	0.598015	0.487698
37	6	0	-3.052159	3.999550	-1.160877
38	1	0	-1.108994	3.201576	-1.581901
39	6	0	-4.292561	3.746546	-0.594324
40	1	0	-5.515094	2.318543	0.428562
41	1	0	-2.848818	4.953434	-1.618199
42	1	0	-5.058437	4.504815	-0.612665

TSd1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.821518	1.550622	1.477237
2	6	0	-0.351278	0.761123	0.623984
3	6	0	-1.710033	2.363402	2.274021
4	1	0	-1.349431	3.386873	2.283012
5	1	0	-2.679391	2.351469	1.779044
6	1	0	-1.802913	1.993060	3.288850
7	6	0	1.090029	0.530739	0.255169
8	8	0	1.864044	0.346955	1.444522
9	6	0	1.789450	1.220864	2.437508
10	8	0	1.014674	2.150706	2.455078
11	6	0	1.261941	-0.714851	-0.658860
12	8	0	0.488662	-0.798500	-1.574461
13	6	0	2.743929	0.904322	3.540161
14	1	0	2.741220	1.708881	4.262463
15	1	0	2.433563	-0.019913	4.020556
16	1	0	3.740653	0.751368	3.140966
17	79	0	-2.004277	-0.369053	-0.069533
18	17	0	-1.148076	-2.101383	1.244954
19	17	0	-3.749052	-1.699023	-0.804528
20	17	0	-2.858215	1.469343	-1.221300
21	6	0	1.668871	1.691688	-0.553596

22	6	0	3.042061	1.909306	-0.531731
23	6	0	0.861308	2.461923	-1.380461
24	6	0	3.598004	2.915498	-1.304247
25	1	0	3.678662	1.293945	0.081266
26	6	0	1.425276	3.462658	-2.154185
27	1	0	-0.199686	2.284868	-1.428498
28	6	0	2.790631	3.696067	-2.115065
29	1	0	4.662119	3.082962	-1.275134
30	1	0	0.791228	4.058992	-2.789098
31	1	0	3.223494	4.477898	-2.717247
32	6	0	2.417194	-1.640403	-0.538425
33	6	0	3.020129	-2.026461	-1.734991
34	6	0	2.854268	-2.195845	0.661687
35	6	0	4.072059	-2.922801	-1.728516
36	1	0	2.652783	-1.616118	-2.660001
37	6	0	3.890726	-3.113629	0.658962
38	1	0	2.364579	-1.944273	1.583247
39	6	0	4.508341	-3.467720	-0.530160
40	1	0	4.542286	-3.205019	-2.655847
41	1	0	4.211219	-3.558190	1.586716
42	1	0	5.320984	-4.175811	-0.524394

2d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.469052	1.167934	1.907334
2	6	0	-0.322793	0.582578	0.737149
3	6	0	-1.640950	1.412189	2.779848
4	1	0	-1.661890	2.452141	3.094703
5	1	0	-2.550485	1.201073	2.233850
6	1	0	-1.605878	0.785448	3.667846
7	6	0	1.053849	0.569504	0.133500
8	8	0	2.044382	0.457131	1.269246
9	6	0	1.846278	1.137610	2.313420
10	8	0	0.721215	1.646476	2.594205
11	6	0	1.330439	-0.613362	-0.831012
12	8	0	0.687985	-0.591345	-1.842954
13	6	0	2.979580	1.358762	3.235921
14	1	0	2.622881	1.611060	4.225037
15	1	0	3.606410	0.474782	3.253077
16	1	0	3.572745	2.182343	2.843105
17	79	0	-1.914547	-0.410020	-0.092452
18	17	0	-0.948681	-2.339532	0.817030
19	17	0	-3.724534	-1.617316	-0.948490
20	17	0	-2.863429	1.600409	-0.801600
21	6	0	1.459937	1.849823	-0.583304
22	6	0	2.808415	2.054389	-0.876678
23	6	0	0.518115	2.785933	-0.981792
24	6	0	3.208431	3.197165	-1.543573
25	1	0	3.543582	1.319445	-0.590225
26	6	0	0.927080	3.926013	-1.659322
27	1	0	-0.528224	2.624148	-0.790844
28	6	0	2.265928	4.137412	-1.935851
29	1	0	4.252019	3.349736	-1.764758
30	1	0	0.188203	4.645001	-1.971774
31	1	0	2.576650	5.025786	-2.460823

32	6	0	2.416477	-1.602306	-0.610760
33	6	0	3.173783	-1.941927	-1.729765
34	6	0	2.658743	-2.238965	0.603757
35	6	0	4.187067	-2.877837	-1.627038
36	1	0	2.954177	-1.468456	-2.671571
37	6	0	3.657055	-3.192204	0.695253
38	1	0	2.034797	-2.034620	1.454870
39	6	0	4.429668	-3.503005	-0.413917
40	1	0	4.775846	-3.128484	-2.493753
41	1	0	3.823946	-3.702834	1.629300
42	1	0	5.210427	-4.241896	-0.335291

TSd2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.222169	-2.165476	-0.132856
2	6	0	0.678643	-0.954865	-0.106500
3	6	0	0.567836	-3.462813	0.191029
4	1	0	1.265490	-4.099187	0.727307
5	1	0	-0.313830	-3.314537	0.799960
6	1	0	0.275384	-3.973741	-0.723509
7	6	0	1.347462	0.281762	-0.401332
8	8	0	2.898787	-0.447824	-1.546292
9	6	0	3.196782	-1.605860	-1.365689
10	8	0	2.515859	-2.430511	-0.585723
11	6	0	0.728912	1.166979	-1.508842
12	8	0	1.096929	1.032800	-2.641118
13	6	0	4.375492	-2.261456	-1.999491
14	1	0	4.929807	-2.821046	-1.253457
15	1	0	4.024785	-2.964562	-2.749957
16	1	0	5.002564	-1.513875	-2.464810
17	79	0	-1.356101	-0.812436	0.314166
18	17	0	-1.773987	-1.216813	-1.938628
19	17	0	-3.645523	-0.728547	0.791840
20	17	0	-0.826424	-0.492647	2.574293
21	6	0	2.228970	0.930242	0.554028
22	6	0	2.882875	2.117652	0.192089
23	6	0	2.455365	0.376115	1.818565
24	6	0	3.745731	2.729039	1.074487
25	1	0	2.728299	2.539098	-0.786760
26	6	0	3.312873	1.003453	2.702511
27	1	0	1.924616	-0.510635	2.113061
28	6	0	3.957336	2.173589	2.331860
29	1	0	4.251656	3.636437	0.791252
30	1	0	3.469729	0.585038	3.682220
31	1	0	4.623887	2.660406	3.025058
32	6	0	-0.304222	2.155988	-1.115984
33	6	0	-0.979831	2.787192	-2.161477
34	6	0	-0.634119	2.465274	0.203115
35	6	0	-1.967644	3.711575	-1.891347
36	1	0	-0.721915	2.527266	-3.172962
37	6	0	-1.628521	3.391657	0.467664
38	1	0	-0.138292	1.991706	1.031790
39	6	0	-2.294232	4.013162	-0.575559
40	1	0	-2.491916	4.189376	-2.702051
41	1	0	-1.887903	3.614443	1.488616

42	1	0	-3.073368	4.727377	-0.365084

3d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.337609	-1.880000	0.133560
2	6	0	0.629895	-0.703719	-0.008912
3	6	0	0.754969	-3.158323	0.609992
4	1	0	1.544144	-3.805013	0.975015
5	1	0	0.006228	-2.993432	1.374392
6	1	0	0.276548	-3.651853	-0.237076
7	6	0	1.195141	0.535774	-0.200664
8	8	0	2.643411	-1.081404	-2.276121
9	6	0	3.243345	-1.521386	-1.361111
10	8	0	2.615764	-2.041417	-0.226850
11	6	0	0.515757	1.575540	-1.075037
12	8	0	1.014583	1.696983	-2.166168
13	6	0	4.717028	-1.679631	-1.208899
14	1	0	5.051852	-1.097289	-0.355296
15	1	0	4.960861	-2.719717	-1.018245
16	1	0	5.204856	-1.337983	-2.111151
17	79	0	-1.436624	-0.875972	0.126843
18	17	0	-1.552821	-1.084527	-2.179077
19	17	0	-3.756470	-1.090751	0.345879
20	17	0	-1.147137	-0.739974	2.461243
21	6	0	2.459894	0.934396	0.405679
22	6	0	3.328980	1.831825	-0.232521
23	6	0	2.790596	0.448492	1.678935
24	6	0	4.515571	2.190918	0.374764
25	1	0	3.083111	2.201014	-1.212054
26	6	0	3.971091	0.832162	2.285672
27	1	0	2.092026	-0.183725	2.200494
28	6	0	4.838015	1.696198	1.632501
29	1	0	5.189564	2.862590	-0.130073
30	1	0	4.207146	0.469570	3.272056
31	1	0	5.757894	1.995502	2.107587
32	6	0	-0.609825	2.383511	-0.588475
33	6	0	-1.318157	3.140557	-1.521857
34	6	0	-0.955603	2.432799	0.759616
35	6	0	-2.371789	3.928384	-1.106986
36	1	0	-1.034041	3.084553	-2.558473
37	6	0	-2.008669	3.231475	1.170852
38	1	0	-0.422501	1.846595	1.489006
39	6	0	-2.716693	3.972699	0.238805
40	1	0	-2.930902	4.502647	-1.826612
41	1	0	-2.282594	3.260467	2.211632
42	1	0	-3.544630	4.583858	0.559062

4d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.697448	2.036373	1.037442

2	6	0	-0.307515	1.310292	0.630800
3	6	0	1.118400	2.140183	2.465959
4	1	0	1.101401	3.183913	2.768602
5	1	0	0.466489	1.561580	3.106938
6	1	0	2.131245	1.763108	2.571646
7	6	0	-1.393987	0.623305	0.345098
8	8	0	0.061985	2.796719	-1.476607
9	6	0	1.154186	3.029574	-1.065114
10	8	0	1.531701	2.737715	0.213151
11	6	0	-1.274287	-0.802014	-0.011710
12	8	0	-0.189658	-1.375552	-0.205218
13	6	0	2.288003	3.641600	-1.815738
14	1	0	2.799996	4.379496	-1.208709
15	1	0	2.994863	2.852586	-2.058797
16	1	0	1.913429	4.084257	-2.728550
17	79	0	1.804192	-0.838647	0.012841
18	17	0	1.872587	-0.257104	-2.235177
19	17	0	4.026397	-0.407336	0.233783
20	17	0	1.658912	-1.461731	2.249614
21	6	0	-2.698081	1.347350	0.278691
22	6	0	-3.419888	1.398391	-0.909587
23	6	0	-3.174618	2.031333	1.391774
24	6	0	-4.603755	2.112250	-0.976781
25	1	0	-3.048953	0.888859	-1.783509
26	6	0	-4.361297	2.742936	1.324025
27	1	0	-2.614293	2.000912	2.312394
28	6	0	-5.079450	2.782836	0.139754
29	1	0	-5.151419	2.149978	-1.904073
30	1	0	-4.722632	3.265085	2.194857
31	1	0	-6.002127	3.336979	0.085165
32	6	0	-2.456329	-1.669331	-0.183609
33	6	0	-3.594856	-1.545383	0.611877
34	6	0	-2.377066	-2.700390	-1.121557
35	6	0	-4.636093	-2.444004	0.468015
36	1	0	-3.662307	-0.766767	1.349491
37	6	0	-3.434584	-3.573902	-1.282301
38	1	0	-1.488632	-2.797892	-1.720911
39	6	0	-4.562653	-3.448986	-0.484210
40	1	0	-5.506341	-2.355990	1.096494
41	1	0	-3.376384	-4.356028	-2.020574
42	1	0	-5.383366	-4.137583	-0.602183

TSd3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.802781	2.520971	0.994463
2	6	0	-2.016789	1.512731	0.178556
3	6	0	-1.523106	2.506611	2.449430
4	1	0	-2.252648	3.110567	2.981986
5	1	0	-1.551561	1.489244	2.815499
6	1	0	-0.530364	2.903286	2.638663
7	6	0	-2.040493	0.149027	-0.010459
8	8	0	-1.818743	3.777222	0.411292
9	6	0	-2.068611	3.661787	-0.871496
10	8	0	-2.248198	2.525033	-1.289403
11	6	0	-0.773526	-0.424847	-0.247870

12	8	0	0.181197	0.359153	-0.567691
13	6	0	-2.080982	4.899681	-1.683974
14	1	0	-2.642601	4.731299	-2.592871
15	1	0	-2.498805	5.720514	-1.113646
16	1	0	-1.055111	5.149226	-1.944306
17	79	0	2.146372	0.161917	0.005151
18	17	0	2.751117	0.101602	-2.237782
19	17	0	4.338580	0.086226	0.635792
20	17	0	1.453520	0.285503	2.229912
21	6	0	-3.337450	-0.571187	-0.061760
22	6	0	-3.613976	-1.491565	-1.071221
23	6	0	-4.329412	-0.305916	0.880597
24	6	0	-4.835949	-2.139844	-1.122893
25	1	0	-2.868277	-1.698364	-1.820633
26	6	0	-5.555559	-0.946436	0.823508
27	1	0	-4.135127	0.404798	1.668177
28	6	0	-5.812468	-1.870285	-0.176947
29	1	0	-5.028102	-2.849888	-1.910790
30	1	0	-6.306979	-0.728905	1.565295
31	1	0	-6.764779	-2.372846	-0.220769
32	6	0	-0.522371	-1.876447	-0.151785
33	6	0	0.336152	-2.480339	-1.069497
34	6	0	-1.097079	-2.639250	0.862466
35	6	0	0.606439	-3.834800	-0.975882
36	1	0	0.782226	-1.891859	-1.853482
37	6	0	-0.806094	-3.986724	0.963319
38	1	0	-1.752915	-2.172618	1.576575
39	6	0	0.041318	-4.586281	0.042406
40	1	0	1.264045	-4.297883	-1.692477
41	1	0	-1.237574	-4.569057	1.760363
42	1	0	0.262822	-5.638132	0.121448

5d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.501917	2.164028	0.856734
2	6	0	-0.360197	1.717217	-0.056765
3	6	0	0.734327	1.910241	2.290148
4	1	0	0.552453	2.804987	2.879441
5	1	0	0.073436	1.117025	2.617678
6	1	0	1.757405	1.582137	2.449924
7	6	0	-1.460522	0.771104	-0.092576
8	8	0	1.373177	3.044067	0.211087
9	6	0	1.039865	3.075517	-1.027282
10	8	0	0.017379	2.360429	-1.267605
11	6	0	-1.137426	-0.486981	-0.519425
12	8	0	0.053168	-0.753681	-1.012168
13	6	0	1.760094	3.857062	-2.039264
14	1	0	1.066793	4.209160	-2.793077
15	1	0	2.278149	4.682665	-1.568431
16	1	0	2.486260	3.195069	-2.505223
17	79	0	1.784217	-0.754539	0.050422
18	17	0	2.763800	0.432392	-1.725549
19	17	0	3.775564	-0.705157	1.205933
20	17	0	0.754746	-1.837317	1.823191

21	6	0	-2.815830	1.305326	0.189005
22	6	0	-3.869306	1.089559	-0.700636
23	6	0	-3.058744	2.089259	1.316185
24	6	0	-5.123783	1.619118	-0.457118
25	1	0	-3.698431	0.500974	-1.585971
26	6	0	-4.312843	2.626349	1.556995
27	1	0	-2.262609	2.271967	2.020280
28	6	0	-5.352311	2.390397	0.672546
29	1	0	-5.922769	1.436544	-1.157319
30	1	0	-4.477709	3.223138	2.439527
31	1	0	-6.329242	2.805518	0.858804
32	6	0	-2.083417	-1.627927	-0.559292
33	6	0	-1.976226	-2.542727	-1.603904
34	6	0	-3.028543	-1.844416	0.439985
35	6	0	-2.822555	-3.635919	-1.665912
36	1	0	-1.223042	-2.388774	-2.357166
37	6	0	-3.861950	-2.947115	0.384095
38	1	0	-3.098081	-1.162264	1.269106
39	6	0	-3.767217	-3.840268	-0.672468
40	1	0	-2.737194	-4.333061	-2.483423
41	1	0	-4.580570	-3.113186	1.169877
42	1	0	-4.419627	-4.697389	-0.714963

TSd4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.704905	-2.160261	-0.789973
2	6	0	1.808330	-1.483623	-0.442282
3	6	0	-0.415931	-2.799882	-1.506495
4	1	0	-1.063254	-3.330663	-0.815437
5	1	0	-0.991308	-2.048888	-2.028840
6	1	0	-0.027199	-3.506420	-2.231078
7	6	0	1.936443	-0.055274	-0.318275
8	8	0	1.592847	-3.861546	-0.426613
9	6	0	2.700744	-3.498763	-0.088700
10	8	0	2.934404	-2.204435	-0.101049
11	6	0	0.731670	0.553017	-0.472311
12	8	0	-0.231509	-0.280853	-0.821708
13	6	0	3.821017	-4.361043	0.358594
14	1	0	3.584575	-5.397023	0.160412
15	1	0	4.734199	-4.069761	-0.148741
16	1	0	3.970935	-4.217498	1.425178
17	79	0	-2.060829	-0.244104	0.169195
18	17	0	-3.093204	-0.124768	-1.915988
19	17	0	-4.089030	-0.290443	1.217361
20	17	0	-0.950748	-0.439880	2.203060
21	6	0	3.251294	0.594131	-0.117788
22	6	0	3.756816	1.461038	-1.083429
23	6	0	4.003417	0.361247	1.032170
24	6	0	4.978859	2.086678	-0.900962
25	1	0	3.183812	1.645985	-1.977100
26	6	0	5.228044	0.982038	1.211645
27	1	0	3.617475	-0.296624	1.793488
28	6	0	5.718800	1.847200	0.245867
29	1	0	5.353255	2.758160	-1.656312
30	1	0	5.794588	0.797417	2.109933

31	1	0	6.670299	2.333137	0.387832
32	6	0	0.414686	1.981469	-0.326644
33	6	0	-0.541656	2.549315	-1.168229
34	6	0	1.026182	2.769438	0.646862
35	6	0	-0.869774	3.888608	-1.044329
36	1	0	-1.024886	1.940854	-1.913716
37	6	0	0.688802	4.104587	0.769798
38	1	0	1.746803	2.332509	1.315026
39	6	0	-0.256040	4.667154	-0.076211
40	1	0	-1.607971	4.319085	-1.700385
41	1	0	1.156686	4.704730	1.532590
42	1	0	-0.517395	5.707960	0.024482

TSe1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.808042	-0.919959	1.456111
2	6	0	-0.372619	-0.809206	1.049244
3	6	0	1.476226	-1.542222	2.628682
4	1	0	0.735000	-1.979602	3.287245
5	1	0	2.162064	-2.307939	2.281397
6	1	0	2.047793	-0.789908	3.162619
7	6	0	-1.573073	-0.495289	0.259316
8	8	0	-2.582837	-0.041502	1.169415
9	6	0	-2.588205	-0.712988	2.314256
10	8	0	-1.689139	-1.478395	2.572707
11	6	0	-1.247639	0.643009	-0.778008
12	8	0	-0.504240	0.336492	-1.665784
13	6	0	-3.764618	-0.427372	3.178488
14	1	0	-3.574774	-0.781943	4.182029
15	1	0	-3.981254	0.634928	3.175698
16	1	0	-4.627482	-0.945809	2.768520
17	79	0	2.100883	0.037423	0.075524
18	17	0	1.612062	2.069364	1.108001
19	17	0	3.693503	1.029331	-1.284494
20	17	0	2.560987	-2.070378	-0.803774
21	6	0	-2.114953	-1.691955	-0.517512
22	6	0	-3.478984	-1.773825	-0.769995
23	6	0	-1.253032	-2.648044	-1.035920
24	6	0	-3.981323	-2.825671	-1.518554
25	1	0	-4.147301	-1.019054	-0.391623
26	6	0	-1.763137	-3.695085	-1.785471
27	1	0	-0.191575	-2.578827	-0.869032
28	6	0	-3.124725	-3.789459	-2.024771
29	1	0	-5.040285	-2.886767	-1.708543
30	1	0	-1.089641	-4.436025	-2.182749
31	1	0	-3.515734	-4.607478	-2.607178
32	6	0	-1.912432	1.964291	-0.719945
33	6	0	-2.235359	2.539294	-1.948343
34	6	0	-2.141026	2.673878	0.456293
35	6	0	-2.816921	3.791944	-1.997237
36	1	0	-2.023594	1.993907	-2.851999
37	6	0	-2.697833	3.938650	0.399074
38	1	0	-1.848767	2.263465	1.404918
39	6	0	-3.047970	4.492333	-0.822950
40	1	0	-3.076932	4.226131	-2.948155

41	1	0	-2.851183	4.495945	1.308169
42	1	0	-3.490295	5.474469	-0.860397

2e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.553173	-0.071888	1.539614
2	6	0	0.581858	0.539480	1.274949
3	6	0	-0.991516	-0.394927	2.932084
4	1	0	-0.289408	-0.063175	3.690263
5	1	0	-1.956392	0.067781	3.117754
6	1	0	-1.124996	-1.469863	3.021217
7	6	0	1.337749	1.005412	0.048314
8	8	0	2.693561	1.262081	0.667019
9	6	0	2.589932	1.231972	1.928946
10	8	0	1.464547	0.889106	2.386801
11	6	0	1.568542	-0.085234	-1.038870
12	8	0	0.966856	0.032727	-2.066629
13	6	0	3.728799	1.560375	2.803185
14	1	0	3.425016	1.538504	3.840453
15	1	0	4.516377	0.832892	2.625271
16	1	0	4.112426	2.539341	2.534480
17	79	0	-1.871335	-0.678701	0.101760
18	17	0	-0.624983	-2.643748	-0.064316
19	17	0	-3.432829	-1.418280	-1.484543
20	17	0	-3.113094	1.252709	0.545615
21	6	0	0.928454	2.332868	-0.540694
22	6	0	1.711511	2.882992	-1.555912
23	6	0	-0.164135	3.035452	-0.060334
24	6	0	1.401382	4.121750	-2.077231
25	1	0	2.559559	2.341314	-1.940896
26	6	0	-0.481591	4.275283	-0.598728
27	1	0	-0.797774	2.612153	0.697105
28	6	0	0.298964	4.820401	-1.599975
29	1	0	2.008867	4.538926	-2.863118
30	1	0	-1.348194	4.801003	-0.234840
31	1	0	0.049427	5.782110	-2.017366
32	6	0	2.571704	-1.160522	-0.826895
33	6	0	3.221447	-1.629219	-1.965167
34	6	0	2.866809	-1.727440	0.410568
35	6	0	4.174144	-2.626951	-1.864770
36	1	0	2.964073	-1.206088	-2.920976
37	6	0	3.807678	-2.736250	0.506216
38	1	0	2.316719	-1.440236	1.290224
39	6	0	4.470481	-3.179432	-0.628925
40	1	0	4.676106	-2.979683	-2.750264
41	1	0	4.010220	-3.190955	1.461839
42	1	0	5.204906	-3.964232	-0.550788

TSe2

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

1	6	0	0.263644	-0.492990	1.525016
2	6	0	-0.972515	-0.135573	1.194063
3	6	0	0.646886	-0.815063	2.930468
4	1	0	-0.160033	-0.651455	3.636746
5	1	0	0.960206	-1.854808	2.988048
6	1	0	1.502479	-0.206420	3.209743
7	6	0	-1.561143	0.128485	-0.118486
8	8	0	-2.855413	1.408210	0.798464
9	6	0	-2.856631	0.902246	1.909447
10	8	0	-1.966628	-0.016366	2.204302
11	6	0	-0.825515	0.994848	-1.150634
12	8	0	-0.624265	0.435155	-2.198613
13	6	0	-3.816083	1.232087	2.994519
14	1	0	-4.313003	0.322436	3.317677
15	1	0	-3.273041	1.631821	3.845558
16	1	0	-4.539858	1.951637	2.638984
17	79	0	1.743336	-0.812139	0.159866
18	17	0	2.661037	1.228074	0.824234
19	17	0	3.494375	-1.223297	-1.349388
20	17	0	0.745731	-2.880541	-0.274339
21	6	0	-2.576764	-0.764286	-0.640589
22	6	0	-3.359881	-0.398526	-1.745418
23	6	0	-2.768763	-2.016729	-0.045894
24	6	0	-4.321240	-1.259277	-2.225087
25	1	0	-3.220411	0.560758	-2.210584
26	6	0	-3.721193	-2.882423	-0.546126
27	1	0	-2.131068	-2.326105	0.762720
28	6	0	-4.499424	-2.502634	-1.628696
29	1	0	-4.925449	-0.972707	-3.068945
30	1	0	-3.843905	-3.856344	-0.103957
31	1	0	-5.240985	-3.180443	-2.018944
32	6	0	-0.427429	2.396690	-0.917065
33	6	0	-0.060746	3.115327	-2.056997
34	6	0	-0.374287	3.019467	0.327383
35	6	0	0.331793	4.434348	-1.955099
36	1	0	-0.084692	2.619461	-3.011517
37	6	0	0.027816	4.338111	0.426637
38	1	0	-0.606131	2.476243	1.222285
39	6	0	0.374805	5.047981	-0.711549
40	1	0	0.611615	4.980991	-2.839940
41	1	0	0.084031	4.807357	1.394450
42	1	0	0.687700	6.076034	-0.628926

3e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.204892	-1.412200	0.721104
2	6	0	-1.113943	-1.057874	0.455116
3	6	0	0.498930	-2.529246	1.646064
4	1	0	-0.379116	-3.023788	2.038361
5	1	0	1.130167	-3.253287	1.134525
6	1	0	1.100172	-2.125215	2.460599
7	6	0	-1.553270	-0.043327	-0.379665
8	8	0	-2.678697	-0.189224	2.423239
9	6	0	-2.815314	-1.316634	2.060820

10	8	0	-2.088001	-1.861272	1.048691
11	6	0	-0.613597	1.004876	-0.959260
12	8	0	-0.274092	0.817771	-2.099105
13	6	0	-3.786078	-2.312417	2.604804
14	1	0	-4.516185	-2.553743	1.837143
15	1	0	-3.275418	-3.231464	2.872697
16	1	0	-4.285598	-1.892219	3.466619
17	79	0	1.884403	-0.651730	-0.116404
18	17	0	2.207508	0.576870	1.846602
19	17	0	3.862062	0.139674	-1.070926
20	17	0	1.486397	-2.159800	-1.857116
21	6	0	-2.923886	0.078881	-0.843188
22	6	0	-3.450828	1.346636	-1.130555
23	6	0	-3.709268	-1.055144	-1.107195
24	6	0	-4.735044	1.477965	-1.617655
25	1	0	-2.862175	2.228143	-0.945612
26	6	0	-4.977408	-0.916015	-1.630678
27	1	0	-3.305334	-2.036054	-0.937875
28	6	0	-5.498266	0.348396	-1.872544
29	1	0	-5.135183	2.458504	-1.811889
30	1	0	-5.560194	-1.792971	-1.857142
31	1	0	-6.494527	0.451496	-2.270170
32	6	0	-0.269405	2.193535	-0.167342
33	6	0	-0.795808	2.411426	1.104800
34	6	0	0.596373	3.125391	-0.741520
35	6	0	-0.461070	3.564043	1.792805
36	1	0	-1.449870	1.687944	1.564078
37	6	0	0.934901	4.265228	-0.042498
38	1	0	0.999958	2.928129	-1.719742
39	6	0	0.403979	4.484617	1.222643
40	1	0	-0.862601	3.735271	2.777362
41	1	0	1.615239	4.979253	-0.475127
42	1	0	0.672374	5.375028	1.767634

TSe3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.539007	-0.663228	0.715456
2	6	0	-0.378633	0.434314	0.503506
3	6	0	0.287877	-1.754776	1.670964
4	1	0	-0.741187	-1.841113	1.996894
5	1	0	0.658707	-2.700344	1.290399
6	1	0	0.911840	-1.493187	2.529909
7	6	0	-1.681556	0.293543	0.152180
8	8	0	0.052952	2.047488	-1.598115
9	6	0	0.427614	2.405811	-0.532607
10	8	0	0.205581	1.661992	0.614601
11	6	0	-2.093341	-1.112757	-0.152812
12	8	0	-1.224240	-1.867851	-0.541301
13	6	0	1.191751	3.637064	-0.186947
14	1	0	1.295613	4.251697	-1.070258
15	1	0	0.682197	4.181653	0.601310
16	1	0	2.169962	3.350837	0.189160
17	79	0	2.436961	-0.460930	0.036840
18	17	0	1.857979	-1.477663	-1.966554

19	17	0	4.641871	-0.177963	-0.667118
20	17	0	2.887797	0.486962	2.137972
21	6	0	-2.578782	1.433859	-0.058725
22	6	0	-2.631272	2.482900	0.861842
23	6	0	-3.396883	1.478472	-1.188747
24	6	0	-3.490287	3.547505	0.657012
25	1	0	-2.007614	2.454364	1.739205
26	6	0	-4.239323	2.553424	-1.398411
27	1	0	-3.355637	0.681384	-1.912027
28	6	0	-4.291310	3.586793	-0.474442
29	1	0	-3.533298	4.346181	1.378822
30	1	0	-4.854647	2.585696	-2.281838
31	1	0	-4.954335	4.420725	-0.636025
32	6	0	-3.477639	-1.593236	0.047469
33	6	0	-4.380015	-0.971193	0.908901
34	6	0	-3.847635	-2.768543	-0.607225
35	6	0	-5.634871	-1.518799	1.108646
36	1	0	-4.106794	-0.070021	1.428956
37	6	0	-5.108145	-3.300634	-0.419510
38	1	0	-3.134430	-3.246536	-1.256604
39	6	0	-6.001744	-2.676604	0.440175
40	1	0	-6.325894	-1.041120	1.782884
41	1	0	-5.393911	-4.201384	-0.936547
42	1	0	-6.983764	-3.094558	0.590440

2e and 3d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.490285	-0.060312	-1.320669
2	6	0	-0.146356	1.078596	-0.670984
3	6	0	1.158631	-0.017394	-2.675774
4	1	0	1.994549	0.661563	-2.681823
5	1	0	1.511745	-1.012118	-2.924796
6	1	0	0.432124	0.300709	-3.417761
7	6	0	-1.423049	0.756920	-0.284007
8	8	0	0.458647	2.211118	-0.302141
9	6	0	0.987430	3.061767	-1.250359
10	8	0	0.720576	2.942638	-2.401682
11	6	0	-1.632237	-0.540697	-0.785815
12	8	0	-0.573229	-0.986469	-1.406139
13	6	0	1.844641	4.087693	-0.599155
14	1	0	2.727276	3.594768	-0.202142
15	1	0	2.127938	4.832218	-1.330124
16	1	0	1.314668	4.544712	0.229928
17	79	0	1.870739	-0.705514	0.267628
18	17	0	0.210635	-1.979468	1.287388
19	17	0	3.396379	-1.455888	1.874337
20	17	0	3.510890	0.714390	-0.595449
21	6	0	-2.311336	1.587026	0.550903
22	6	0	-2.770399	2.814598	0.083845
23	6	0	-2.667495	1.160242	1.827775
24	6	0	-3.583679	3.603144	0.881463
25	1	0	-2.495963	3.145474	-0.905089
26	6	0	-3.480660	1.951571	2.620993
27	1	0	-2.296935	0.217288	2.195798

28	6	0	-3.940654	3.171850	2.149258
29	1	0	-3.937720	4.551587	0.512299
30	1	0	-3.749048	1.617536	3.609567
31	1	0	-4.572688	3.786032	2.769476
32	6	0	-2.795376	-1.402787	-0.771858
33	6	0	-2.626271	-2.773948	-0.985354
34	6	0	-4.077782	-0.880063	-0.590695
35	6	0	-3.725907	-3.606992	-1.007238
36	1	0	-1.633755	-3.171149	-1.103565
37	6	0	-5.173331	-1.721355	-0.626140
38	1	0	-4.217013	0.175148	-0.439815
39	6	0	-4.998989	-3.082139	-0.829661
40	1	0	-3.592529	-4.665011	-1.157376
41	1	0	-6.162338	-1.315791	-0.494866
42	1	0	-5.855812	-3.735572	-0.848454