Supporting Information

Theoretical insights into the reaction of Cp*(Cl)Hf(diene) with isonitriles

Ming-Ran Du,[a,c] Xiang-Biao Zhang,*[a] Sheng-Meng Si[a,c]

and Lei Wang*[b]

[a]*School of Chemical Engineering, Anhui University of Science and Technology, Huainan, Anhui 232001, People's Republic of China.*

[b]*Department of Chemistry, Huaibei Normal University, Huaibei, Anhui 235000, People's Republic of China.*

[c]*These authors contributed equally.*

**Corresponding Authors*

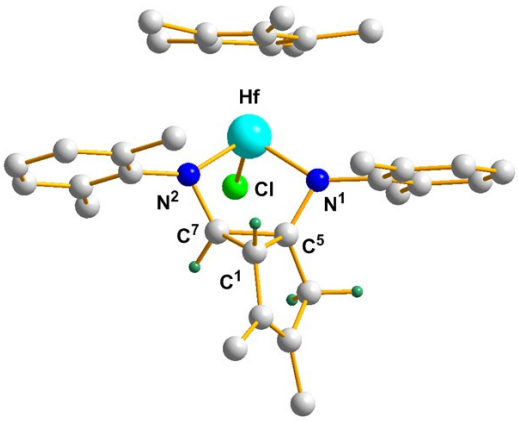
E-mail: xbzhang_theochem@yahoo.com (X.-B. Zhang)

leiwang@chnu.edu.cn (L. Wang)

CONTENTS

1. Choice of calculated method

In order to obtain more accurate geometry structures for studied molecules, eight theoretical models, the B3LYP/BS1, BP86/BS1, B3LYP/def2-SVP, BP86/def2-SVP, BP86/BS2, BP86/LANL2DZ, B3LYP/BS3, and BP86/BS3, were examined by calculating the geometry structure for the enantiomer of diazahafnacyclopentane, **18ArIS**, and by comparing the calculated bond parameters to the X-ray crystal structure of **18ArIS**.[1] These calculated methods have been applied to studies of the hafnium, and the same group metal (Ti and Zr) complexes.[2-10] As shown in **Table 1**, the calculated results at the level of the B3LYP/BS1 are closer to the experimental ones. In the BS1, Hf and Cl atoms are described with the LANL2DZ basis sets improved with a set of f- or d-polarization functions (α = 0.784 for Hf; α = 0.640 for Cl) with effective core potentials (ECP),[11-15] while other atoms are represented by the 6-311+G(d,p) basis sets, except for the atoms on the methyls and 2,6-dimethylphenyl (Ar) substituent groups which are described with the 6-31G basis sets.[16-18] In the BS2, Hf atom is represented by the LANL2DZ basis sets with ECP, Cl atom by the 6-311+G(d,p) basis set and other atoms by the same basis sets as in the BS1. In the BS3, Hf atom is described with the LANL2DZ basis sets with ECP, which are modified by Couty and Hall.[19] While the atoms on the methyls and Ar substituent groups are described with the 6-31G basis sets, other H atoms are represented by the 6-311G(d,p) basis sets, and C, N, Cl atoms by the D95 basis sets.[20] All calculations were performed in n-pentane with the G09 program and the polarizable continuum model (PCM) using the integral equation formalism variant (IEFPCM) was adopted for the SCRF calculations.[21,22]



18ArIS

Atomic numbering for **18ArIS**

(The H atoms on the methyl and Ar groups were omitted for clarity.)

Table 1. Calculated main bond parameters and corresponding experimental values (bond length in angstrom and angle in degree) for **18ArIS**

	Bond Parameters									
Methods	Hf-N^1	Hf-N^2	Hf-C^5	Hf- C^7	C^5-N^1	C^7-N^2	C^7-C^5	C^5-C^1	C^7-C^1	N^1-Hf-N^2
B3LYP/BS1	2.037	2.028	2.628	2.588	1.451	1.449	1.576	1.525	1.524	93.5
BP86/BS1	2.044	2.035	2.609	2.567	1.454	1.452	1.593	1.536	1.535	94.1
B3LYP/def2-SVP	2.065	2.058	2.645	2.606	1.448	1.445	1.576	1.525	1.524	92.5
BP86/def2-SVP	2.069	2.060	2.626	2.584	1.450	1.447	1.592	1.535	1.534	93.3
BP86/BS2	2.052	2.045	2.622	2.583	1.454	1.451	1.594	1.535	1.535	93.7
BP86/LANL2DZ	2.040	2.030	2.644	2.596	1.477	1.477	1.606	1.553	1.558	94.6
B3LYP/BS3	2.039	2.030	2.657	2.618	1.473	1.471	1.596	1.542	1.546	93.9
BP86/BS3	2.045	2.036	2.643	2.600	1.477	1.474	1.608	1.556	1.558	94.9
Exp.[1]	2.010	1.991	2.527	2.490	1.423	1.444	1.552	1.493	1.507	95.0

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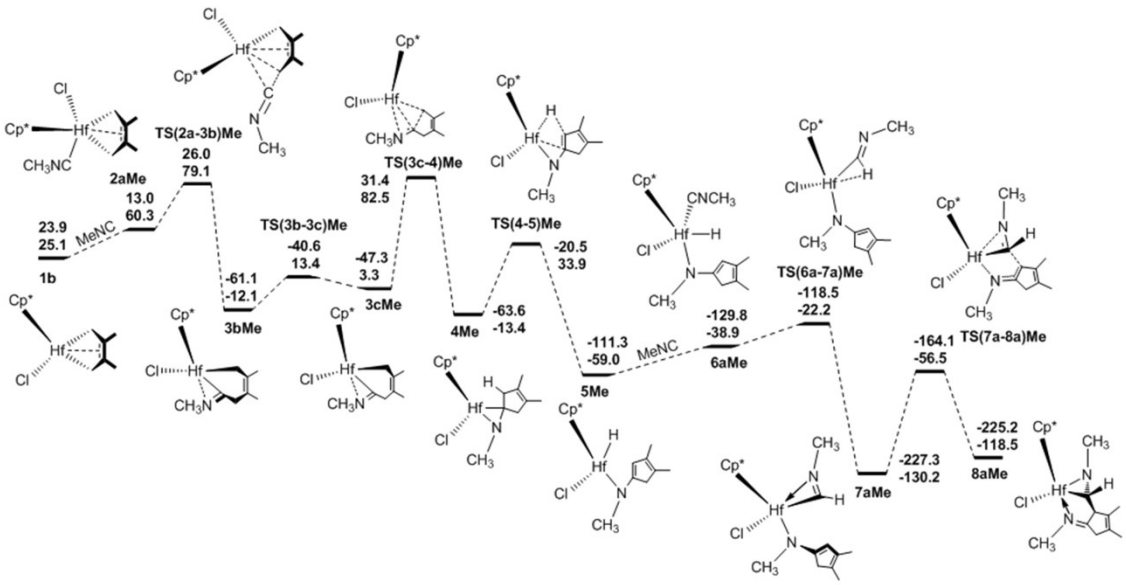
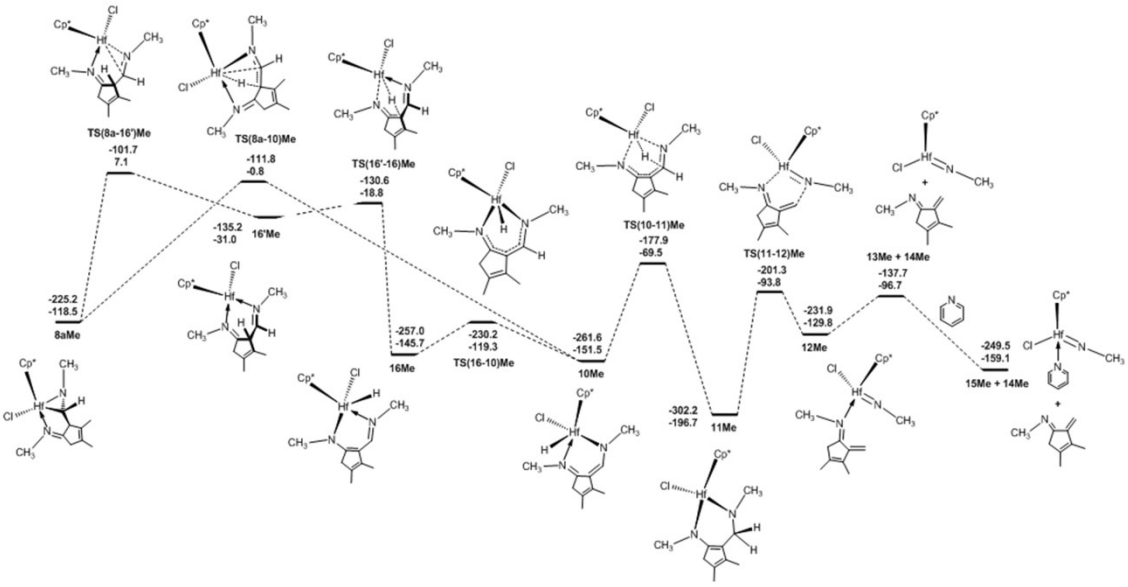
2. Figure S1. Energy profiles for (a) the bis-insertion of a methyl-substituted isonitrile (MeNC) and (b) the fragmentation of hafnaaziridine **8aMe**. The Born-Oppenheimer energies (above) and Gibbs free energies (below) are given in kJ mol^{-1}.

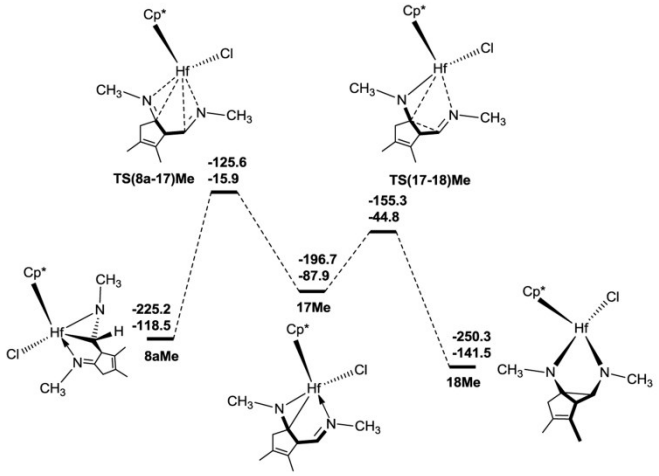


(a)



(b)

3. Figure S2. Energy profiles for the formation of diazahafnacyclopentane **18Me** via (a) the insertion reaction pathway and (b) the isomerization reaction pathway and energy profile for β-H elimination from Hf complex **8bMe**. The Born-Oppenheimer energies (above) and Gibbs free energies (below) are given in kJ mol^{-1}.



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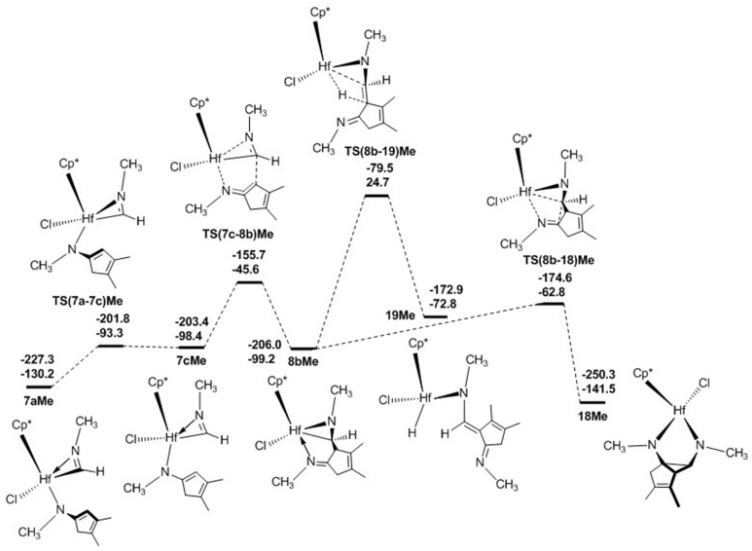
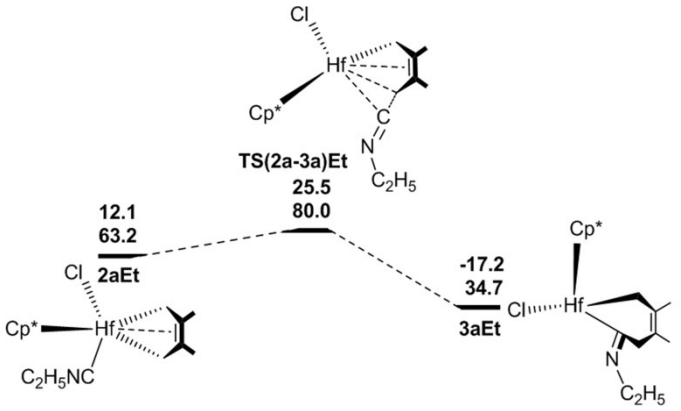


(b)

4. Figure S3. Energy profiles for (a) migratory insertion of an ethyl-substituted isonitrile (EtNC) into the Hf–C bond in Hf complex **2aEt**, (b) C–C reductive elimination in Hf complex **3cEt**, (c) the fragmentation of the hafnaaziridine **8aEt**, and the formation of the diazahafnacyclopentane **18Et** via (d) the insertion reaction pathway and (e) the isomerization reaction pathway and energy profile for β-H elimination from Hf complex **8bEt**. The Born-Oppenheimer energies (above) and Gibbs free energies (below) are given in kJ mol^{-1}.



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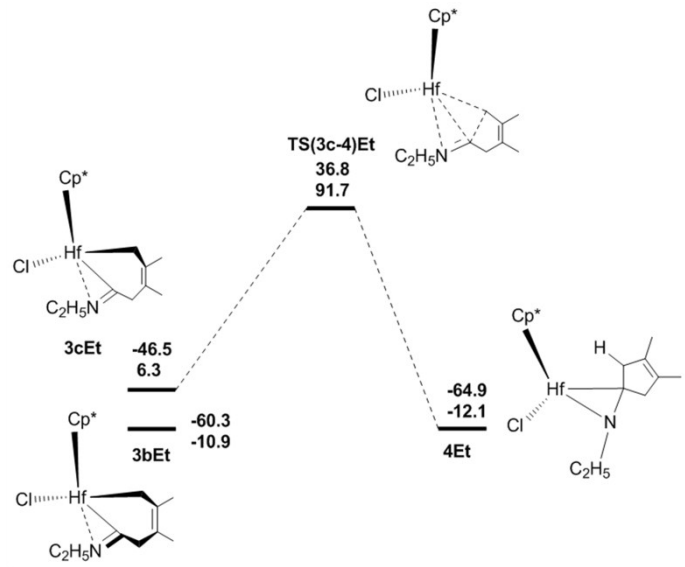

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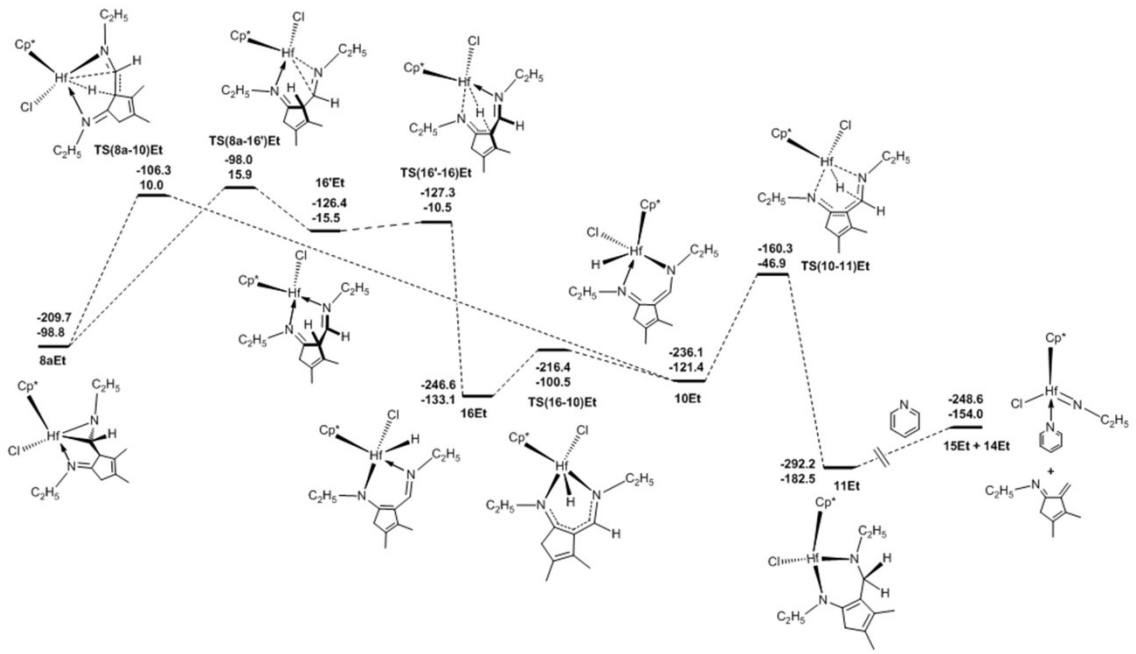
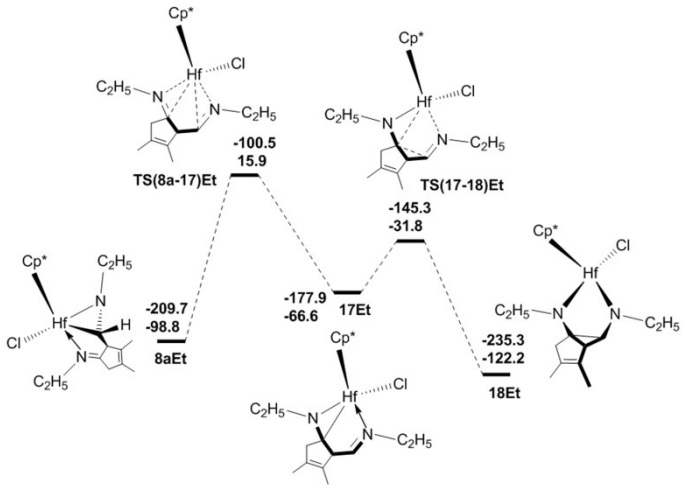
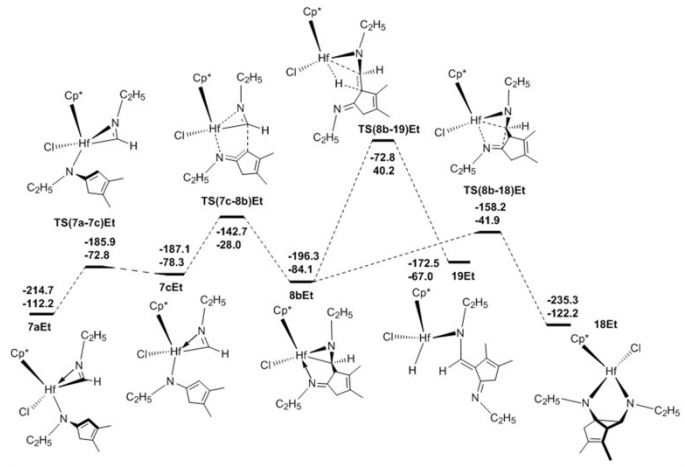

TS(8a-10)Et
-106.3
10.0
TS(8a-16')Et
-98.0
15.9
16'Et
-126.4
-15.5
TS(16'-16)Et
-127.3
-10.5
-209.7
-98.8
8aEt
-246.6
-133.1
16Et
-216.4
-100.5
TS(16-10)Et
-236.1
-121.4
10Et
-160.3
-46.9
TS(10-11)Et
-292.2
-182.5
11Et
-248.6
-154.0
15Et + 14Et

(c)

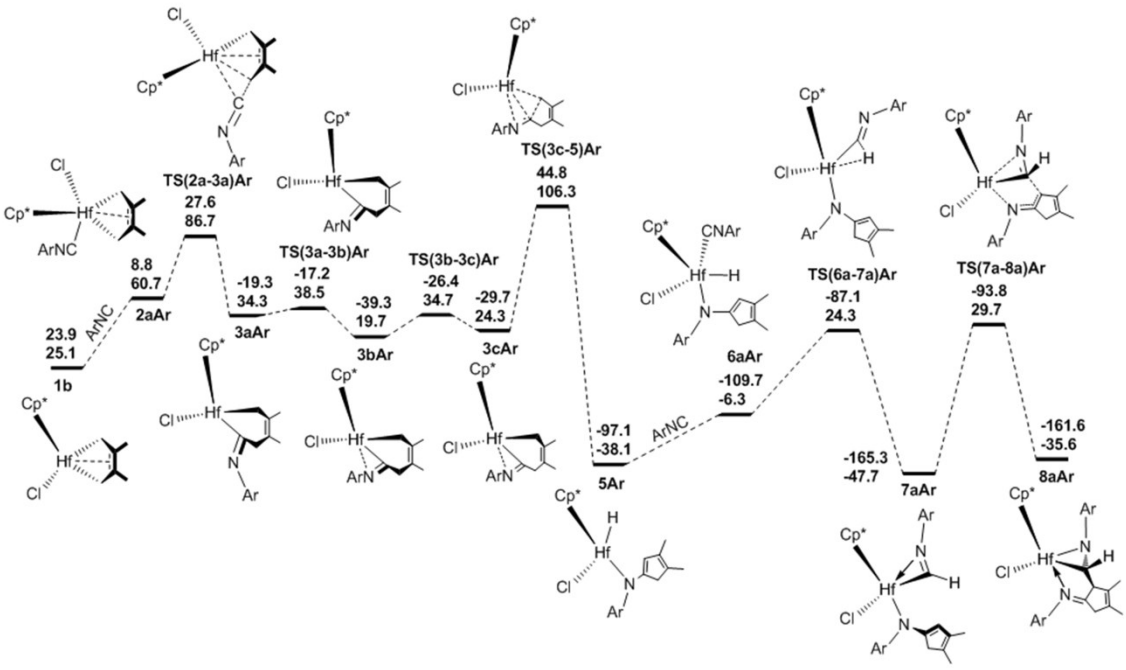

TS(8a-17)Et
-100.5
15.9
TS(17-18)Et
-145.3
-31.8
-209.7
-98.8
8aEt
-177.9
-66.6
17Et
-235.3
-122.2
18Et

(d)

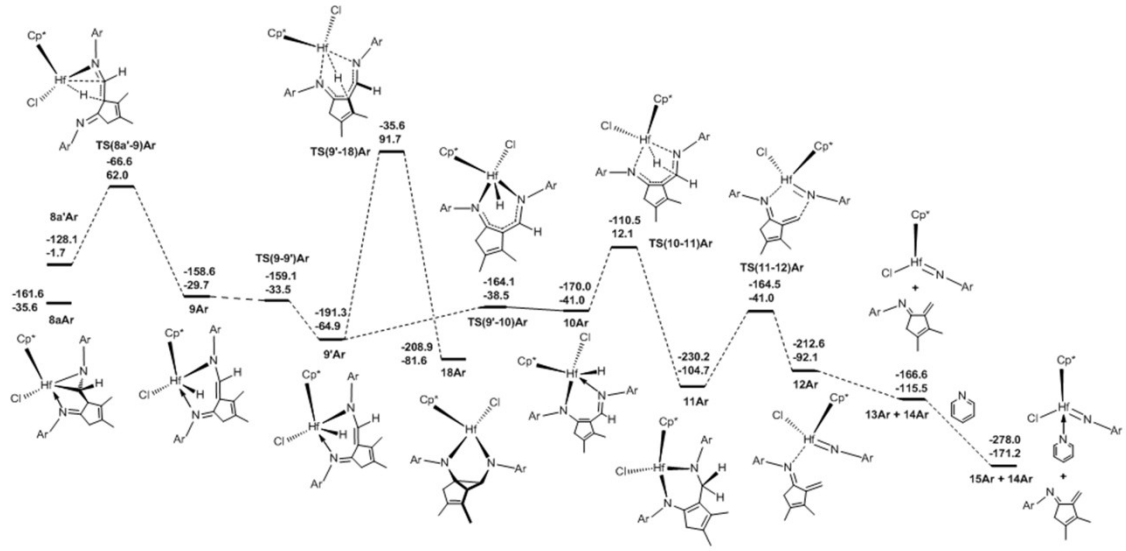

TS(7a-7c)Et
-185.9
-72.8
TS(7c-8b)Et
-142.7
-28.0
TS(8b-19)Et
-72.8
40.2
TS(8b-18)Et
-158.2
-41.9
-214.7
-112.2
7aEt
-187.1
-78.3
7cEt
-196.3
-84.1
8bEt
-172.5
-67.0
19Et
-235.3
-122.2
18Et

(e)

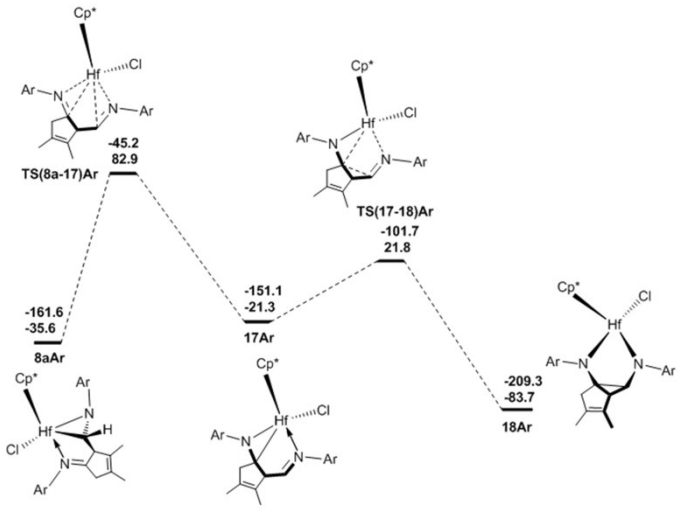
5. Figure S4. Energy profiles for (a) the bis-insertion of N-2,6-dimethylphenyl-substituted isonitriles (ArNC), (b) the fragmentation of the hafnaaziridine **8aAr**; the formation of the diazahafnacyclopentane **18Ar** via (c) the insertion reaction pathway and (d) the isomerization reaction pathway and the energy profile for β-H elimination from Hf complex **8bAr** (d). The Born-Oppenheimer energies (above) and Gibbs free energies (below) are given in kJ mol^{-1}.



(a)



(b)



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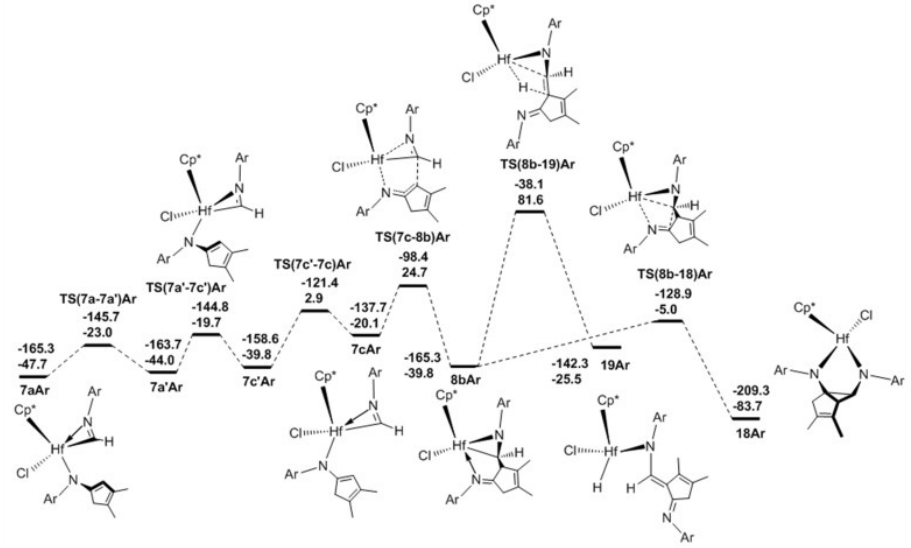
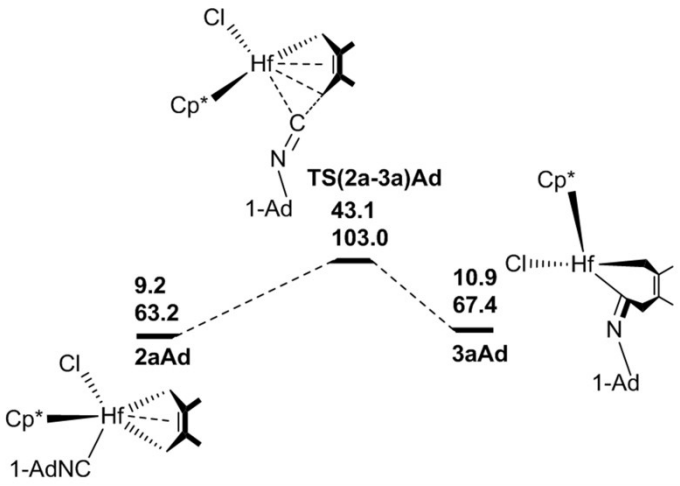
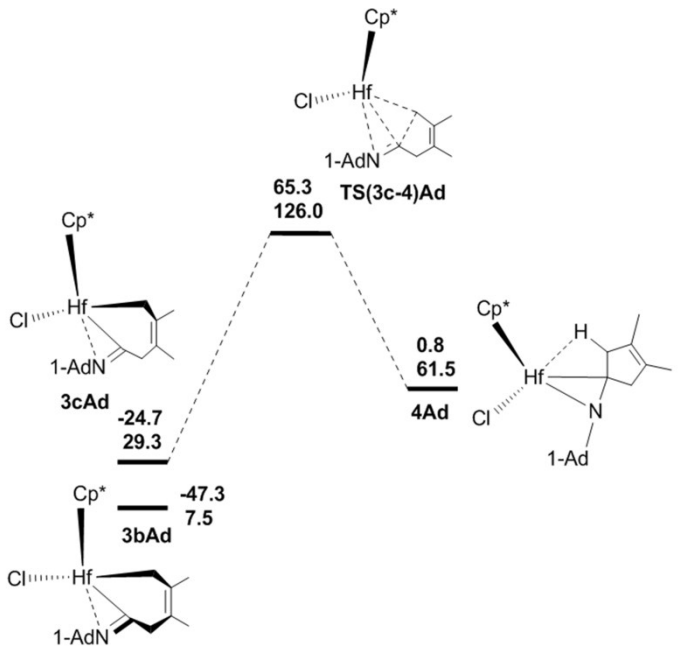


(d)

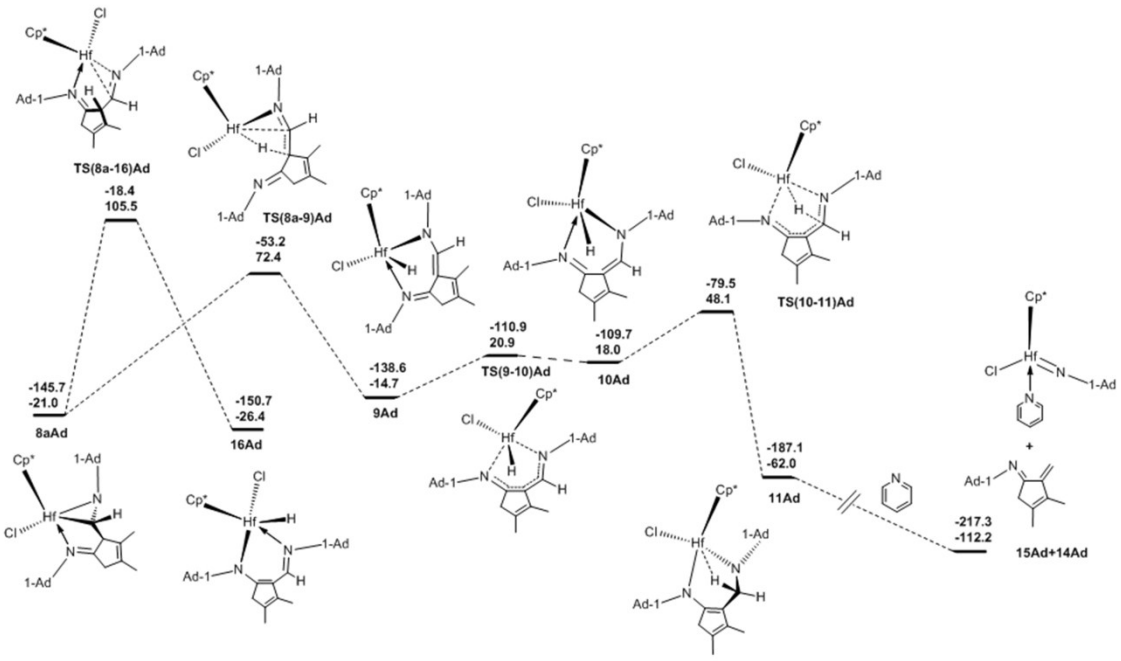
6. Figure S5. Energy profiles for (a) migratory insertion of N-1-adamantyl-substituted isonitrile (1-AdNC) into the Hf–C bond in Hf complex **2aAd**, (b) C–C reductive elimination in Hf complex **3cAd**, (c) the fragmentation of the hafnaaziridine **8aAd**; the formation of the diazahafnacyclopentane **18Ad** via (d) the insertion reaction pathway and (e) the isomerization reaction pathway and energy profile for β-H elimination from Hf complex **8bAd** (e). The Born-Oppenheimer energies (above) and Gibbs free energies (below) are given in kJ mol^{-1}.


Cl
Hf
Cp*
C
N
1-Ad
TS(2a-3a)Ad
43.1
103.0
9.2
63.2
2aAd
10.9
67.4
3aAd
Cp*
Cl
Hf
N
1-Ad
Cl
Cp*
Hf
1-AdNC

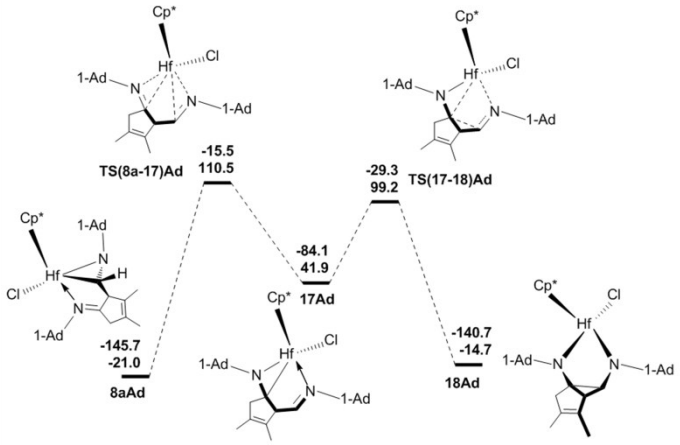
(a)


Cp*
Cl
Hf
1-AdN
65.3
126.0
TS(3c-4)Ad
Cp*
Cl
Hf
1-AdN
3cAd
-24.7
29.3
0.8
61.5
4Ad
Cp*
H
Hf
Cl
N
1-Ad
Cp*
-47.3
7.5
3bAd
Cl
Hf
1-AdN

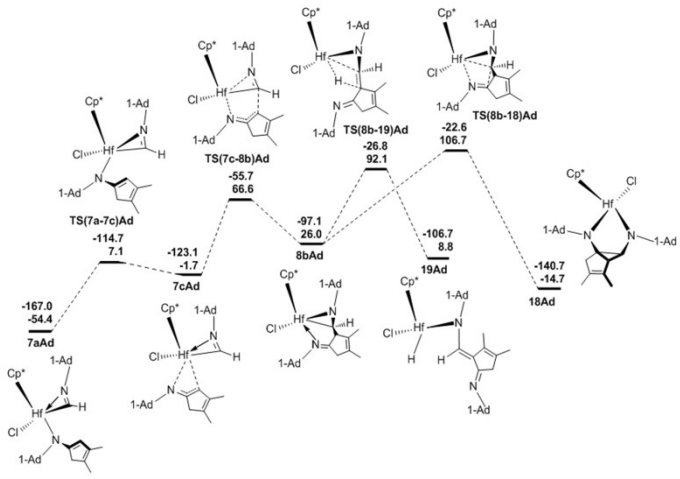
(b)


TS(8a-16)Ad
-18.4
105.5
TS(8a-9)Ad
-53.2
72.4
-145.7
-21.0
8aAd
-150.7
-26.4
16Ad
-138.6
-14.7
9Ad
-110.9
20.9
TS(9-10)Ad
-109.7
18.0
10Ad
-79.5
48.1
TS(10-11)Ad
-187.1
-62.0
11Ad
-217.3
-112.2
15Ad+14Ad

(c)


TS(8a-17)Ad
-15.5
110.5
-29.3
99.2
TS(17-18)Ad
-84.1
41.9
17Ad
-145.7
-21.0
8aAd
-140.7
-14.7
18Ad

(d)


TS(7a-7c)Ad
-114.7
7.1
TS(7c-8b)Ad
-55.7
66.6
TS(8b-19)Ad
-26.8
92.1
TS(8b-18)Ad
-22.6
106.7
-167.0
-54.4
7aAd
-123.1
-1.7
7cAd
-97.1
26.0
8bAd
-106.7
8.8
19Ad
-140.7
-14.7
18Ad

(e)

7. Calculated Cartesian coordinates and electronic energies (**E**) for the involved species in the paper.

In n-pentane

By B3LYP/BS1

18ArIS (E = -1494.9933299 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.119371	-0.814532	-0.388549
2	7	1.496547	0.626186	-0.012346
3	7	-1.453930	0.394356	0.072461
4	17	0.089480	-0.938992	-2.837136
5	6	-0.863785	-2.866640	0.769827
6	6	2.856020	0.948633	0.318205
7	6	0.694108	1.702950	-0.555640
8	6	-2.821851	0.408601	0.507031
9	6	-0.876094	1.616176	-0.455470
10	6	3.212640	1.316428	1.639820
11	6	3.853542	0.883966	-0.692513
12	6	4.558465	1.600996	1.931061
13	6	2.196039	1.415459	2.756429
14	6	5.540768	1.539534	0.943284
15	1	4.828876	1.872547	2.947947
16	6	5.183749	1.182836	-0.359839
17	1	6.575128	1.763144	1.185030
18	1	5.943081	1.130937	-1.134793
19	6	3.513566	0.497726	-2.114877
20	1	4.422352	0.439573	-2.721806
21	1	2.842773	1.223292	-2.589996
22	1	3.002065	-0.468431	-2.170885
23	1	2.616639	1.050271	3.700466
24	1	1.296828	0.841244	2.527982
25	1	1.888048	2.456330	2.924364
26	6	-3.173124	0.892390	1.794085
27	6	-3.831452	-0.105948	-0.352119
28	6	-5.164406	-0.120478	0.089703
29	6	-3.510447	-0.646550	-1.728477
30	6	-5.512985	0.353641	1.356101
31	1	-5.932048	-0.510002	-0.572674
32	6	-4.518609	0.850921	2.198698
33	1	-6.547753	0.331574	1.683210
34	1	-4.779031	1.213370	3.189266
35	6	-2.145415	1.450219	2.752689
36	1	-2.487736	1.346403	3.787673
37	1	-1.968032	2.517850	2.571553
38	1	-1.184332	0.940634	2.649808
39	1	-4.431512	-0.923405	-2.251084
40	1	-2.872548	-1.536718	-1.687063
41	1	-2.973469	0.078899	-2.346120
42	6	-0.091777	2.656521	0.336953
43	6	-1.609029	2.395091	-1.557018
44	6	-1.209338	3.842046	-1.346047
45	1	-1.348978	2.027008	-2.555368
46	1	-2.693393	2.274542	-1.444435
47	6	-0.406825	3.982495	-0.276232
48	6	-1.719105	4.903121	-2.283655
49	6	0.201492	5.240339	0.286528
50	1	0.059048	2.558549	1.401367
51	1	1.046166	2.134479	-1.492412
52	1	-1.388641	5.905814	-1.995575
53	1	-2.818362	4.903490	-2.309957

54	1	-1.377730	4.719057	-3.312097
55	1	-0.123591	6.134880	-0.253290
56	1	1.298813	5.197382	0.244183
57	1	-0.072142	5.367078	1.343388
58	6	-0.232686	-3.344656	-0.414480
59	6	0.152060	-2.344820	1.628554
60	6	-2.313703	-3.056509	1.148166
61	6	1.172493	-3.123802	-0.287607
62	6	-0.897508	-4.093026	-1.544633
63	6	1.413810	-2.517332	0.979000
64	6	2.223099	-3.575879	-1.274327
65	6	2.769785	-2.289640	1.602755
66	6	-0.057612	-1.924098	3.064100
67	1	-2.958656	-3.140159	0.268961
68	1	-2.693830	-2.230415	1.755430
69	1	-2.431277	-3.981028	1.731249
70	1	-0.444239	-3.851977	-2.510511
71	1	-1.965186	-3.863065	-1.614688
72	1	-0.803582	-5.176918	-1.387994
73	1	2.461049	-4.637998	-1.120369
74	1	3.154984	-3.012695	-1.161333
75	1	1.884418	-3.457340	-2.308282
76	1	2.744329	-1.503713	2.361415
77	1	3.523080	-2.003121	0.863193
78	1	3.116636	-3.211978	2.090013
79	1	-0.018431	-2.802989	3.723622
80	1	-1.031896	-1.448741	3.211120
81	1	0.712540	-1.226527	3.405170

By BP86/BS1

18ArIS (E = -1495.1130607 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.108146	-0.813257	-0.392206
2	7	1.521373	0.594962	0.010349
3	7	-1.456418	0.404899	0.104227
4	17	0.077494	-0.897870	-2.839974
5	6	-0.922473	-2.853447	0.731129
6	6	2.885536	0.903103	0.350767
7	6	0.729751	1.671364	-0.557643
8	6	-2.825797	0.447381	0.542892
9	6	-0.858033	1.610186	-0.445458
10	6	3.242709	1.230897	1.693556
11	6	3.893013	0.861604	-0.664877
12	6	4.597778	1.494065	2.002639
13	6	2.210609	1.310723	2.804825
14	6	5.589953	1.450082	1.010432
15	1	4.867299	1.735905	3.038113
16	6	5.233377	1.136250	-0.313192
17	1	6.635581	1.655469	1.265606
18	1	6.002009	1.098336	-1.094339
19	6	3.549739	0.535919	-2.106734
20	1	4.465508	0.334594	-2.689040
21	1	3.018845	1.372874	-2.601042
22	1	2.879621	-0.337795	-2.185564
23	1	2.600474	0.872550	3.742226
24	1	1.285717	0.782954	2.521639
25	1	1.940431	2.361773	3.027938
26	6	-3.166190	0.949530	1.836580
27	6	-3.853811	-0.062180	-0.313186
28	6	-5.193519	-0.050437	0.136908
29	6	-3.539396	-0.626483	-1.686660
30	6	-5.530072	0.443588	1.409066
31	1	-5.976312	-0.436601	-0.526657

32	6	-4.518400	0.933829	2.250698
33	1	-6.573562	0.441881	1.743037
34	1	-4.769581	1.312320	3.248944
35	6	-2.114992	1.498597	2.783112
36	1	-2.442008	1.397903	3.833078
37	1	-1.926469	2.572905	2.594740
38	1	-1.153779	0.971856	2.656199
39	1	-4.469548	-0.909162	-2.209024
40	1	-2.897935	-1.525315	-1.627242
41	1	-2.989794	0.091938	-2.318924
42	6	-0.044367	2.659172	0.326124
43	6	-1.578981	2.380849	-1.566753
44	6	-1.152693	3.828347	-1.390503
45	1	-1.324047	1.975714	-2.562444
46	1	-2.674976	2.277346	-1.448511
47	6	-0.341301	3.979741	-0.313448
48	6	-1.645416	4.882757	-2.352896
49	6	0.286706	5.245971	0.223121
50	1	0.122645	2.572463	1.399588
51	1	1.075407	2.082966	-1.517835
52	1	-1.305973	5.894633	-2.071595
53	1	-2.753882	4.891163	-2.391479
54	1	-1.292662	4.679703	-3.384255
55	1	-0.034514	6.138745	-0.340453
56	1	1.392866	5.189641	0.176829
57	1	0.017839	5.399149	1.287586
58	6	-0.294321	-3.326236	-0.468359
59	6	0.108542	-2.359100	1.603693
60	6	-2.378074	-3.026099	1.114481
61	6	1.123053	-3.125716	-0.337554
62	6	-0.968669	-4.043556	-1.619262
63	6	1.375609	-2.540665	0.947546
64	6	2.169185	-3.567220	-1.341157
65	6	2.738323	-2.340872	1.576875
66	6	-0.097002	-1.958009	3.050266
67	1	-3.023646	-3.149658	0.228565
68	1	-2.762288	-2.163722	1.686094
69	1	-2.499602	-3.930437	1.744482
70	1	-0.556160	-3.724712	-2.592488
71	1	-2.056146	-3.854588	-1.638334
72	1	-0.821304	-5.138332	-1.525873
73	1	2.405433	-4.642228	-1.205764
74	1	3.111109	-3.003563	-1.222700
75	1	1.819123	-3.427358	-2.378872
76	1	2.722293	-1.554078	2.348918
77	1	3.501612	-2.054649	0.833280
78	1	3.073366	-3.281142	2.059691
79	1	-0.084309	-2.857698	3.698824
80	1	-1.067756	-1.455663	3.202345
81	1	0.698193	-1.282440	3.408864

By B3LYP/def2-SVP

18ArIS (E = -1938.2727841 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.115157	-0.821816	-0.401553
2	7	1.501121	0.646584	-0.003943
3	7	-1.467760	0.418755	0.068811
4	17	0.088523	-0.991986	-2.851758
5	6	-0.859889	-2.856751	0.840279
6	6	2.855493	0.958885	0.317772
7	6	0.694481	1.714177	-0.550248
8	6	-2.825663	0.424367	0.501151
9	6	-0.876393	1.629267	-0.462897

10	6	3.217923	1.371118	1.624238
11	6	3.855041	0.841481	-0.685299
12	6	4.565232	1.653912	1.903044
13	6	2.207853	1.520247	2.736455
14	6	5.546578	1.546381	0.921254
15	1	4.841078	1.963551	2.915544
16	6	5.185969	1.141227	-0.364542
17	1	6.589895	1.772834	1.155973
18	1	5.950716	1.051167	-1.141206
19	6	3.514442	0.386553	-2.083395
20	1	4.404164	0.418446	-2.728748
21	1	2.736242	1.008494	-2.550548
22	1	3.127204	-0.644396	-2.098201
23	1	2.634105	1.199407	3.699819
24	1	1.300871	0.935828	2.541627
25	1	1.901354	2.573067	2.859387
26	6	-3.183810	0.915094	1.783522
27	6	-3.831360	-0.112209	-0.348786
28	6	-5.161365	-0.140118	0.095375
29	6	-3.507029	-0.658076	-1.718640
30	6	-5.515635	0.343108	1.354521
31	1	-5.930457	-0.550500	-0.565023
32	6	-4.527256	0.862205	2.187659
33	1	-6.556836	0.310904	1.685633
34	1	-4.794234	1.234689	3.180999
35	6	-2.165350	1.491012	2.735677
36	1	-2.509626	1.399394	3.776721
37	1	-1.995843	2.562939	2.541362
38	1	-1.193509	0.988613	2.642451
39	1	-4.426265	-0.961583	-2.240290
40	1	-2.847447	-1.539109	-1.675784
41	1	-2.984394	0.075233	-2.348669
42	6	-0.098207	2.675979	0.327111
43	6	-1.598337	2.401142	-1.579057
44	6	-1.198414	3.850456	-1.382231
45	1	-1.331786	2.018227	-2.579505
46	1	-2.692134	2.281010	-1.475263
47	6	-0.404151	4.000922	-0.298403
48	6	-1.691877	4.899937	-2.330514
49	6	0.197721	5.256582	0.256437
50	1	0.045193	2.587223	1.402561
51	1	1.057003	2.151807	-1.492820
52	1	-1.359565	5.910661	-2.053525
53	1	-2.796182	4.905748	-2.372511
54	1	-1.344959	4.702572	-3.360657
55	1	-0.120570	6.155114	-0.291154
56	1	1.301099	5.213171	0.226949
57	1	-0.080040	5.392502	1.316796
58	6	-0.258379	-3.372619	-0.349817
59	6	0.183874	-2.330044	1.667869
60	6	-2.300923	-3.008468	1.244371
61	6	1.154358	-3.167007	-0.258192
62	6	-0.956086	-4.125232	-1.448936
63	6	1.431342	-2.526994	0.989917
64	6	2.171563	-3.643620	-1.258725
65	6	2.798703	-2.280202	1.565159
66	6	0.012273	-1.852127	3.083771
67	1	-2.974582	-3.049447	0.377049
68	1	-2.645046	-2.183929	1.884106
69	1	-2.443955	-3.946229	1.811087
70	1	-0.527116	-3.901838	-2.436226
71	1	-2.029225	-3.889218	-1.493586
72	1	-0.870491	-5.214671	-1.287024

73	1	2.386309	-4.717941	-1.116369
74	1	3.127200	-3.108404	-1.158760
75	1	1.822138	-3.512602	-2.293389
76	1	2.791429	-1.487078	2.324529
77	1	3.530044	-1.986127	0.798816
78	1	3.182211	-3.195906	2.050049
79	1	0.068105	-2.702754	3.787067
80	1	-0.961996	-1.368301	3.242239
81	1	0.793843	-1.138928	3.380742

By BP86/def2-SVP

18ArIS (E = -1938.3534139 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.112947	-0.816801	-0.396251
2	7	1.516827	0.634291	0.014720
3	7	-1.475926	0.413433	0.097443
4	17	0.108174	-0.973034	-2.846055
5	6	-0.882942	-2.847597	0.827819
6	6	2.874801	0.939616	0.336046
7	6	0.709228	1.692149	-0.553488
8	6	-2.839698	0.429133	0.517061
9	6	-0.877362	1.614226	-0.453502
10	6	3.240701	1.324151	1.659346
11	6	3.877226	0.837980	-0.677951
12	6	4.598186	1.588060	1.946347
13	6	2.220981	1.463021	2.767472
14	6	5.584640	1.488924	0.956937
15	1	4.878259	1.876160	2.973576
16	6	5.218805	1.116217	-0.345764
17	1	6.638843	1.697676	1.199712
18	1	5.988838	1.034128	-1.130789
19	6	3.523252	0.441496	-2.092684
20	1	4.436368	0.316212	-2.707422
21	1	2.888183	1.204435	-2.591471
22	1	2.942292	-0.502635	-2.135502
23	1	2.623560	1.090522	3.732173
24	1	1.290974	0.912184	2.532060
25	1	1.943979	2.527768	2.929256
26	6	-3.215730	0.979341	1.779531
27	6	-3.837491	-0.154089	-0.325179
28	6	-5.180520	-0.165109	0.105431
29	6	-3.483708	-0.767236	-1.660790
30	6	-5.553851	0.377563	1.343679
31	1	-5.945567	-0.610175	-0.552185
32	6	-4.571750	0.939322	2.170520
33	1	-6.607537	0.358315	1.664744
34	1	-4.853511	1.358024	3.151179
35	6	-2.201759	1.595512	2.714384
36	1	-2.556253	1.557086	3.764052
37	1	-2.019406	2.663435	2.467856
38	1	-1.224259	1.078166	2.649240
39	1	-4.398681	-1.059029	-2.213427
40	1	-2.860705	-1.681069	-1.548975
41	1	-2.895608	-0.080352	-2.300703
42	6	-0.081525	2.676788	0.317055
43	6	-1.598681	2.370296	-1.586372
44	6	-1.190390	3.824757	-1.420492
45	1	-1.334116	1.957822	-2.585531
46	1	-2.702114	2.250353	-1.476420
47	6	-0.386541	3.993610	-0.330695
48	6	-1.677633	4.864919	-2.386296
49	6	0.219847	5.262320	0.196790
50	1	0.078110	2.598186	1.400913

51	1	1.061665	2.117151	-1.517541
52	1	-1.334805	5.884782	-2.121439
53	1	-2.790166	4.880366	-2.430479
54	1	-1.331120	4.651342	-3.422375
55	1	-0.104117	6.155933	-0.372453
56	1	1.331510	5.220535	0.163950
57	1	-0.053678	5.423623	1.263360
58	6	-0.272729	-3.364029	-0.368412
59	6	0.163866	-2.316782	1.664695
60	6	-2.324906	-2.999676	1.236807
61	6	1.148130	-3.152761	-0.271317
62	6	-0.960787	-4.109372	-1.481952
63	6	1.422105	-2.512974	0.987838
64	6	2.169428	-3.617771	-1.276735
65	6	2.789853	-2.265392	1.567222
66	6	-0.020089	-1.834480	3.079963
67	1	-2.997970	-3.119898	0.365529
68	1	-2.694371	-2.131773	1.818174
69	1	-2.453959	-3.902805	1.874887
70	1	-0.594599	-3.793403	-2.479777
71	1	-2.058489	-3.958486	-1.466109
72	1	-0.781132	-5.203816	-1.390831
73	1	2.397452	-4.698547	-1.138003
74	1	3.127659	-3.069640	-1.177373
75	1	1.812843	-3.486431	-2.318193
76	1	2.779056	-1.472527	2.339344
77	1	3.527310	-1.959146	0.798809
78	1	3.180301	-3.189909	2.048889
79	1	0.001057	-2.691670	3.790502
80	1	-0.992118	-1.321958	3.223523
81	1	0.780886	-1.136565	3.393240

By BP86/BS2

18ArIS (E = -1940.3799704 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.119071	-0.816654	-0.385808
2	7	1.512590	0.628960	0.001145
3	7	-1.464847	0.392829	0.103735
4	17	0.086602	-0.912688	-2.838778
5	6	-0.868937	-2.859320	0.772125
6	6	2.874421	0.948931	0.338541
7	6	0.702934	1.693091	-0.562164
8	6	-2.836487	0.412675	0.536444
9	6	-0.884563	1.604544	-0.451391
10	6	3.227210	1.307986	1.673994
11	6	3.884235	0.884011	-0.673043
12	6	4.580963	1.584777	1.978327
13	6	2.193977	1.402445	2.783535
14	6	5.574795	1.522301	0.988870
15	1	4.848076	1.851169	3.008380
16	6	5.222824	1.173581	-0.327575
17	1	6.618800	1.739420	1.240869
18	1	5.992872	1.119663	-1.106369
19	6	3.542219	0.508990	-2.103474
20	1	4.460524	0.391283	-2.704274
21	1	2.915940	1.278718	-2.593544
22	1	2.963149	-0.430252	-2.157827
23	1	2.586318	0.982894	3.728343
24	1	1.272010	0.864626	2.508429
25	1	1.918095	2.455893	2.987946
26	6	-3.196086	0.932509	1.817580
27	6	-3.846945	-0.134195	-0.316913
28	6	-5.190732	-0.137649	0.120531

29	6	-3.504650	-0.727537	-1.671580
30	6	-5.547430	0.377203	1.378967
31	1	-5.960307	-0.551859	-0.541553
32	6	-4.551823	0.901051	2.219579
33	1	-6.593789	0.364842	1.703606
34	1	-4.818404	1.293905	3.208261
35	6	-2.162005	1.512965	2.764181
36	1	-2.498950	1.427647	3.812402
37	1	-1.984861	2.585876	2.558007
38	1	-1.192804	0.996360	2.657237
39	1	-4.424281	-1.008481	-2.213765
40	1	-2.877428	-1.634978	-1.576665
41	1	-2.927949	-0.028781	-2.301661
42	6	-0.089659	2.669049	0.318446
43	6	-1.616862	2.358566	-1.576504
44	6	-1.217979	3.814204	-1.402147
45	1	-1.350474	1.956882	-2.570768
46	1	-2.711009	2.232468	-1.462430
47	6	-0.409002	3.982420	-0.325724
48	6	-1.725697	4.857472	-2.368985
49	6	0.198171	5.260417	0.206857
50	1	0.073480	2.588157	1.392803
51	1	1.040335	2.111928	-1.522585
52	1	-1.406085	5.876068	-2.088238
53	1	-2.833910	4.845429	-2.412655
54	1	-1.364163	4.658765	-3.398180
55	1	-0.134179	6.145480	-0.362332
56	1	1.305244	5.220340	0.164746
57	1	-0.076745	5.414829	1.269503
58	6	-0.252142	-3.336879	-0.431386
59	6	0.167994	-2.342556	1.624517
60	6	-2.318231	-3.039770	1.175205
61	6	1.165099	-3.120936	-0.321771
62	6	-0.931062	-4.076300	-1.565367
63	6	1.428344	-2.518830	0.953144
64	6	2.199866	-3.571628	-1.332499
65	6	2.797682	-2.290725	1.558015
66	6	-0.022938	-1.918261	3.066393
67	1	-2.975073	-3.168257	0.298460
68	1	-2.700033	-2.179371	1.751244
69	1	-2.425269	-3.944444	1.807496
70	1	-0.530186	-3.769417	-2.547542
71	1	-2.020280	-3.897637	-1.577306
72	1	-0.772955	-5.168434	-1.457878
73	1	2.417833	-4.651650	-1.206265
74	1	3.151437	-3.024791	-1.212590
75	1	1.848367	-3.417795	-2.368240
76	1	2.780051	-1.500197	2.326063
77	1	3.543214	-1.994052	0.800370
78	1	3.158154	-3.222338	2.039374
79	1	0.005891	-2.805591	3.731454
80	1	-0.996044	-1.420784	3.221395
81	1	0.770836	-1.228883	3.401187

By BP86/LANL2DZ

18ArIS (E = -1494.9861192 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.097038	-0.813112	-0.392338
2	7	1.533057	0.569055	-0.006965
3	7	-1.451827	0.422388	0.094844
4	17	0.060233	-0.878851	-2.889064
5	6	-0.966786	-2.863599	0.723938
6	6	2.905602	0.853203	0.352220

7	6	0.756082	1.691420	-0.570394
8	6	-2.825928	0.457494	0.544911
9	6	-0.844967	1.656769	-0.442987
10	6	3.255685	1.166959	1.704532
11	6	3.922199	0.821672	-0.661867
12	6	4.616143	1.420961	2.027214
13	6	2.215449	1.248684	2.814770
14	6	5.621551	1.382219	1.037203
15	1	4.880441	1.651737	3.068389
16	6	5.268925	1.083943	-0.299387
17	1	6.668013	1.579047	1.302426
18	1	6.043635	1.052585	-1.077130
19	6	3.584280	0.530390	-2.117517
20	1	4.493011	0.258949	-2.685177
21	1	3.137995	1.416887	-2.611792
22	1	2.844422	-0.283535	-2.217590
23	1	2.586430	0.772040	3.742356
24	1	1.273596	0.761391	2.513478
25	1	1.986455	2.304602	3.063137
26	6	-3.164527	0.963327	1.842015
27	6	-3.856106	-0.054632	-0.314234
28	6	-5.201045	-0.050753	0.138898
29	6	-3.536249	-0.610103	-1.694895
30	6	-5.540175	0.442964	1.419500
31	1	-5.985849	-0.439358	-0.523435
32	6	-4.521803	0.941448	2.261655
33	1	-6.584359	0.436139	1.756611
34	1	-4.774069	1.321202	3.260945
35	6	-2.110552	1.525052	2.785145
36	1	-2.436900	1.438165	3.837954
37	1	-1.928395	2.597785	2.578921
38	1	-1.146735	0.999955	2.663224
39	1	-4.463607	-0.870695	-2.237421
40	1	-2.910873	-1.521800	-1.634791
41	1	-2.960586	0.105255	-2.308192
42	6	-0.003333	2.696957	0.345548
43	6	-1.578605	2.448219	-1.552787
44	6	-1.118955	3.900909	-1.370944
45	1	-1.343486	2.048217	-2.559571
46	1	-2.677107	2.363913	-1.412927
47	6	-0.284826	4.036073	-0.289109
48	6	-1.606985	4.971932	-2.320645
49	6	0.367206	5.293007	0.247529
50	1	0.173605	2.603920	1.419563
51	1	1.120437	2.102433	-1.525090
52	1	-1.233242	5.976354	-2.051675
53	1	-2.716133	5.013644	-2.333232
54	1	-1.287821	4.759516	-3.361958
55	1	0.067920	6.194467	-0.316691
56	1	1.472997	5.215237	0.206848
57	1	0.099108	5.454994	1.311875
58	6	-0.333933	-3.337472	-0.489568
59	6	0.076542	-2.378551	1.612454
60	6	-2.426061	-3.024265	1.099875
61	6	1.099999	-3.150149	-0.351864
62	6	-1.011695	-4.037552	-1.649760
63	6	1.357075	-2.571901	0.951796
64	6	2.143994	-3.597466	-1.355891
65	6	2.722986	-2.389230	1.581105
66	6	-0.134522	-1.967129	3.056148
67	1	-3.075712	-3.120105	0.211991
68	1	-2.803089	-2.173512	1.694876
69	1	-2.561416	-3.942586	1.707904

70	1	-0.598944	-3.709782	-2.621183
71	1	-2.100610	-3.848558	-1.666934
72	1	-0.867975	-5.134724	-1.572366
73	1	2.348206	-4.682576	-1.246676
74	1	3.103356	-3.066703	-1.214546
75	1	1.810107	-3.423625	-2.395374
76	1	2.712696	-1.632358	2.384018
77	1	3.486715	-2.077583	0.846068
78	1	3.062428	-3.346126	2.028784
79	1	-0.149128	-2.863527	3.710327
80	1	-1.097069	-1.443042	3.199377
81	1	0.672263	-1.308567	3.424302

By B3LYP/BS3

18ArIS (E = -1940.0209502 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.133134	-0.802973	-0.399700
2	7	1.494111	0.660689	-0.042233
3	7	-1.463840	0.378063	0.061817
4	17	0.088382	-0.937730	-2.896199
5	6	-0.818230	-2.870404	0.800666
6	6	2.852108	0.981368	0.319364
7	6	0.671824	1.751708	-0.587341
8	6	-2.829504	0.347117	0.519119
9	6	-0.915734	1.637517	-0.469981
10	6	3.183548	1.367320	1.641936
11	6	3.869039	0.897351	-0.669300
12	6	4.525147	1.648916	1.955362
13	6	2.147481	1.489238	2.737770
14	6	5.526683	1.567919	0.989085
15	1	4.776276	1.934425	2.973402
16	6	5.193744	1.194444	-0.315316
17	1	6.557148	1.790241	1.248357
18	1	5.967499	1.129264	-1.074865
19	6	3.553756	0.487608	-2.090376
20	1	4.458814	0.512050	-2.705210
21	1	2.813214	1.145621	-2.557585
22	1	3.136628	-0.523857	-2.142895
23	1	2.549917	1.139075	3.695285
24	1	1.249969	0.914205	2.505737
25	1	1.842804	2.534191	2.883991
26	6	-3.187533	0.852073	1.795652
27	6	-3.825440	-0.230078	-0.315104
28	6	-5.152827	-0.283727	0.138905
29	6	-3.489897	-0.799904	-1.675382
30	6	-5.508823	0.212562	1.394255
31	1	-5.910095	-0.720634	-0.505654
32	6	-4.527169	0.770397	2.213087
33	1	-6.539413	0.161334	1.731366
34	1	-4.793019	1.151177	3.195339
35	6	-2.175058	1.473953	2.729880
36	1	-2.510418	1.394096	3.769203
37	1	-2.032434	2.539963	2.513657
38	1	-1.198350	0.991968	2.641579
39	1	-4.403293	-1.095290	-2.201269
40	1	-2.848976	-1.686990	-1.601395
41	1	-2.948620	-0.086883	-2.303127
42	6	-0.135232	2.704829	0.323738
43	6	-1.686985	2.399126	-1.566532
44	6	-1.311435	3.866690	-1.365202
45	1	-1.429802	2.034974	-2.568035
46	1	-2.767311	2.251057	-1.438222
47	6	-0.484326	4.029557	-0.295842

48	6	-1.857406	4.913719	-2.296417
49	6	0.104912	5.301877	0.251609
50	1	0.028202	2.615330	1.385953
51	1	1.017028	2.185734	-1.523187
52	1	-1.541254	5.922801	-2.016870
53	1	-2.956132	4.892168	-2.303753
54	1	-1.529188	4.731604	-3.328978
55	1	-0.242796	6.185592	-0.290731
56	1	1.201763	5.278944	0.197450
57	1	-0.160203	5.429802	1.310057
58	6	-0.193003	-3.352196	-0.402830
59	6	0.214283	-2.321883	1.648458
60	6	-2.253475	-3.084988	1.209940
61	6	1.225802	-3.110533	-0.297643
62	6	-0.859045	-4.121943	-1.514552
63	6	1.481628	-2.486355	0.974446
64	6	2.263163	-3.567451	-1.292424
65	6	2.841927	-2.242454	1.575965
66	6	0.019326	-1.889140	3.080007
67	1	-2.919627	-3.166974	0.347019
68	1	-2.627794	-2.272811	1.838741
69	1	-2.342370	-4.018355	1.783248
70	1	-0.451902	-3.851006	-2.492903
71	1	-1.938341	-3.945102	-1.542272
72	1	-0.706283	-5.200510	-1.371654
73	1	2.496838	-4.630006	-1.138391
74	1	3.198442	-3.008820	-1.187664
75	1	1.913836	-3.449419	-2.322685
76	1	2.818785	-1.456779	2.334734
77	1	3.580020	-1.948481	0.824378
78	1	3.206243	-3.160124	2.058329
79	1	0.054728	-2.763232	3.745428
80	1	-0.949573	-1.403949	3.231048
81	1	0.799495	-1.197596	3.409696

By BP86/BS3

18ArIS (E = -1940.1792467 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.123069	-0.808568	-0.379661
2	7	1.521236	0.626031	-0.013421
3	7	-1.473197	0.381783	0.087408
4	17	0.094498	-0.934578	-2.871236
5	6	-0.871271	-2.857151	0.798635
6	6	2.894232	0.935983	0.324061
7	6	0.704567	1.718628	-0.572283
8	6	-2.854033	0.376225	0.517290
9	6	-0.896505	1.628982	-0.455032
10	6	3.256644	1.322890	1.648505
11	6	3.898804	0.845732	-0.689963
12	6	4.614966	1.590640	1.941562
13	6	2.231497	1.465332	2.760629
14	6	5.603633	1.495869	0.950041
15	1	4.888709	1.877086	2.964710
16	6	5.242541	1.127026	-0.357853
17	1	6.651140	1.706549	1.193783
18	1	6.007265	1.053475	-1.140646
19	6	3.544969	0.461814	-2.115180
20	1	4.458110	0.342697	-2.724131
21	1	2.914103	1.228152	-2.604246
22	1	2.967368	-0.478323	-2.161835
23	1	2.637107	1.101203	3.722541
24	1	1.311366	0.905950	2.528466
25	1	1.948988	2.526032	2.911683

26	6	-3.236795	0.913330	1.783994
27	6	-3.846073	-0.203504	-0.335205
28	6	-5.192434	-0.235005	0.093106
29	6	-3.482655	-0.792755	-1.686339
30	6	-5.569535	0.288698	1.341327
31	1	-5.947157	-0.675331	-0.569710
32	6	-4.593959	0.853954	2.178176
33	1	-6.617506	0.254610	1.659971
34	1	-4.877245	1.259854	3.157148
35	6	-2.228044	1.547397	2.723807
36	1	-2.588591	1.511430	3.767180
37	1	-2.053942	2.610208	2.469030
38	1	-1.252338	1.035022	2.667630
39	1	-4.392771	-1.083015	-2.240292
40	1	-2.847421	-1.693631	-1.585911
41	1	-2.906504	-0.086410	-2.308118
42	6	-0.093650	2.701864	0.335792
43	6	-1.650270	2.395198	-1.567715
44	6	-1.253514	3.863907	-1.380217
45	1	-1.389219	2.008787	-2.570403
46	1	-2.743235	2.261459	-1.441401
47	6	-0.425139	4.029006	-0.296826
48	6	-1.779796	4.915606	-2.326741
49	6	0.174898	5.307698	0.240645
50	1	0.069618	2.602006	1.409135
51	1	1.045596	2.143016	-1.526110
52	1	-1.457296	5.932003	-2.042002
53	1	-2.887854	4.900653	-2.351081
54	1	-1.433960	4.726329	-3.362462
55	1	-0.177392	6.196264	-0.310299
56	1	1.280355	5.279021	0.179781
57	1	-0.086202	5.443140	1.309063
58	6	-0.239157	-3.345548	-0.409806
59	6	0.168100	-2.317939	1.660198
60	6	-2.317662	-3.053044	1.197974
61	6	1.190337	-3.116725	-0.294032
62	6	-0.908332	-4.097959	-1.539078
63	6	1.446087	-2.494950	0.989927
64	6	2.232441	-3.571479	-1.293199
65	6	2.810684	-2.258008	1.598375
66	6	-0.034706	-1.870646	3.092012
67	1	-2.984100	-3.121221	0.321824
68	1	-2.685252	-2.228967	1.832463
69	1	-2.423447	-3.995221	1.772035
70	1	-0.513426	-3.785673	-2.521713
71	1	-2.000446	-3.937504	-1.545962
72	1	-0.731921	-5.186190	-1.427887
73	1	2.466079	-4.644457	-1.142122
74	1	3.175498	-3.008242	-1.182460
75	1	1.877904	-3.445858	-2.331209
76	1	2.784823	-1.470295	2.369147
77	1	3.556036	-1.956455	0.842623
78	1	3.173019	-3.188910	2.078260
79	1	-0.013461	-2.747311	3.770150
80	1	-1.009144	-1.370211	3.229120
81	1	0.757768	-1.178112	3.423457

In Benzene
By B3LYP/BS1
1a (E = -688.7914314 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.960414	0.913657	-0.688473
2	6	1.842265	-0.425906	-1.170414

3	6	1.951814	0.872921	0.737353
4	17	-1.143136	2.419406	-0.006881
5	6	1.766612	-1.291153	-0.038610
6	6	1.829641	-0.491814	1.141506
7	6	-1.391023	-1.243526	-1.447495
8	6	-2.572954	-0.742579	-0.713385
9	1	-1.052810	-2.249475	-1.184058
10	6	-1.400636	-1.256847	1.410735
11	6	-2.577614	-0.749246	0.673157
12	1	-1.059196	-2.259754	1.139530
13	1	-1.464123	-1.155441	2.491282
14	6	-3.668266	-0.113584	1.515712
15	6	-3.657447	-0.098507	-1.557483
16	1	-4.328498	0.553820	-0.996305
17	1	-4.263547	-0.880752	-2.035325
18	1	-3.207889	0.496312	-2.362196
19	1	-4.334447	0.545208	0.956272
20	1	-3.224827	0.472107	2.330443
21	1	-4.278693	-0.900541	1.980135
22	6	1.945839	-0.859959	-2.613384
23	6	2.183261	2.145928	-1.533122
24	6	2.160773	2.055655	1.653579
25	6	1.921515	-1.008713	2.557618
26	6	1.760963	-2.800334	-0.080632
27	1	2.996622	-1.024418	-2.891091
28	1	1.540515	-0.105557	-3.295298
29	1	1.405263	-1.793756	-2.795434
30	1	3.258622	2.343068	-1.645450
31	1	1.725791	3.032338	-1.083854
32	1	1.764520	2.031319	-2.538228
33	1	3.233998	2.238550	1.804055
34	1	1.715663	1.889790	2.640151
35	1	1.721167	2.968737	1.241339
36	1	2.969371	-1.198018	2.830601
37	1	1.372247	-1.946882	2.683108
38	1	1.518586	-0.291168	3.279485
39	1	2.790261	-3.185552	-0.068841
40	1	1.280641	-3.182157	-0.987044
41	1	1.242270	-3.232267	0.781306
42	1	-1.446746	-1.130873	-2.527382
43	72	-0.328885	0.113899	-0.008383

TS1a-1b (E = -688.7687437 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.445191	-0.855031	-0.001722
2	6	-2.649939	-1.954601	-0.535523
3	6	-2.255276	-2.432153	0.747593
4	6	-1.714002	-2.450592	-1.495518
5	17	-1.381289	1.340516	0.379856
6	6	-1.079679	-3.229063	0.582998
7	6	-0.749420	-3.240791	-0.805648
8	6	1.240774	-1.107265	1.421773
9	6	2.520649	-1.048637	0.589374
10	1	1.264456	-1.975372	2.088815
11	6	1.179933	-0.652615	-1.502595
12	6	2.492831	-0.841398	-0.746539
13	1	1.163156	-1.293282	-2.391919
14	1	1.136468	0.379435	-1.895575
15	6	3.723012	-0.742464	-1.632421
16	6	3.787239	-1.211895	1.412380
17	1	4.709767	-1.168101	0.827874
18	1	3.770523	-2.173127	1.945969

19	1	3.837575	-0.428346	2.182374
20	1	3.748773	0.237549	-2.130752
21	1	3.675166	-1.497304	-2.430542
22	1	4.669357	-0.874515	-1.101782
23	6	-3.002772	-2.224140	2.044360
24	6	-3.901592	-1.167522	-0.847355
25	6	-1.807283	-2.254383	-2.990301
26	6	0.357915	-4.053553	-1.430403
27	6	-0.434618	-4.084388	1.645700
28	1	-3.706731	-3.050196	2.216703
29	1	-3.581604	-1.295435	2.036549
30	1	-2.326407	-2.189224	2.905228
31	1	-4.737703	-1.850601	-1.052385
32	1	-3.775537	-0.530192	-1.728355
33	1	-4.196081	-0.522111	-0.014701
34	1	-2.460655	-3.017205	-3.436189
35	1	-0.829057	-2.335611	-3.472960
36	1	-2.226215	-1.276158	-3.249656
37	1	0.046515	-5.101554	-1.541355
38	1	1.267343	-4.041101	-0.820878
39	1	0.621284	-3.681164	-2.424271
40	1	-0.917101	-5.071360	1.681725
41	1	-0.523823	-3.638058	2.641090
42	1	0.629576	-4.244376	1.447314
43	1	1.212687	-0.231061	2.095600

1b (E = -688.7820158 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.936613	-0.805882	0.710200
2	6	1.936773	-0.805887	-0.709229
3	6	0.688841	-1.348727	1.156486
4	17	1.738064	2.606207	0.000858
5	6	0.689115	-1.348753	-1.155791
6	6	-0.066573	-1.714669	0.000264
7	6	-1.336242	1.677667	-1.471537
8	6	-2.327735	0.910438	-0.696465
9	1	-1.425032	1.594223	-2.549617
10	6	-1.337140	1.677715	1.471178
11	6	-2.328157	0.910464	0.695537
12	1	-1.426587	1.594336	2.549209
13	1	-1.207262	2.726076	1.176215
14	6	-3.277661	0.061593	1.526448
15	6	-3.276759	0.061556	-1.527915
16	1	-3.767000	-0.741543	-0.975268
17	1	-2.749000	-0.382943	-2.379966
18	1	-4.061831	0.708246	-1.943984
19	1	-4.062949	0.708294	1.942090
20	1	-2.750380	-0.382927	2.378786
21	1	-3.767606	-0.741491	0.973520
22	6	3.070869	-0.378863	-1.608997
23	6	3.070532	-0.378911	1.610215
24	6	0.340597	-1.679455	2.589949
25	6	-1.313315	-2.565031	0.000130
26	6	0.341236	-1.679550	-2.589326
27	1	3.673979	-1.249578	-1.901972
28	1	3.732338	0.336746	-1.113657
29	1	2.706493	0.091762	-2.528634
30	1	3.673571	-1.249650	1.903268
31	1	2.705980	0.091678	2.529800
32	1	3.732109	0.336713	1.115040
33	1	0.748470	-2.661923	2.867630
34	1	-0.741421	-1.716097	2.747954
35	1	0.752087	-0.943924	3.288510

36	1	-1.033634	-3.628128	0.000178
37	1	-1.931549	-2.389489	-0.883867
38	1	-1.931753	-2.389466	0.883981
39	1	0.749269	-2.661985	-2.866885
40	1	0.752813	-0.943997	-3.287813
41	1	-0.740740	-1.716307	-2.747576
42	1	-1.206587	2.726051	-1.176559
43	72	0.107861	0.810553	0.000270

2a (E = -939.449465 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	2.992721	0.131698	0.155112
2	6	-1.823689	-1.789706	-0.783650
3	6	-2.363751	-1.294554	0.447175
4	6	-0.513663	-2.279636	-0.531652
5	17	-0.163131	0.323073	-2.695056
6	6	-1.384062	-1.503889	1.463031
7	6	-0.234217	-2.087481	0.857549
8	6	1.833373	0.135223	0.059086
9	6	4.449798	0.207848	0.244139
10	6	0.224398	2.587463	-0.530795
11	6	-1.130796	2.642589	-0.085012
12	1	1.014499	2.809535	0.178924
13	6	-0.280068	1.437388	1.855033
14	6	-1.415257	2.045994	1.158009
15	1	0.622355	2.041923	1.949185
16	1	-0.537475	0.967688	2.799857
17	6	-2.767330	2.187942	1.832326
18	6	-2.201088	3.251588	-0.973879
19	1	-2.329579	4.314856	-0.723396
20	1	-3.178259	2.767822	-0.872271
21	1	-1.896930	3.196948	-2.024013
22	1	-2.817824	3.162108	2.342469
23	1	-2.907556	1.420959	2.599104
24	1	-3.611990	2.136986	1.138037
25	6	4.887536	1.534319	-0.414304
26	6	4.831184	0.175805	1.739817
27	1	4.579824	1.566852	-1.463528
28	1	4.449255	2.389970	0.107916
29	1	4.387699	1.022535	2.272239
30	1	4.492634	-0.752948	2.209178
31	6	-3.817456	-0.937368	0.660166
32	6	-2.598197	-1.941404	-2.070410
33	6	0.368415	-2.991849	-1.528002
34	6	0.965963	-2.616083	1.608444
35	6	-1.611630	-1.404428	2.950655
36	1	-4.429034	-1.850379	0.702593
37	1	-4.215635	-0.319332	-0.152043
38	1	-3.971986	-0.395320	1.595917
39	1	-3.174849	-2.877870	-2.054364
40	1	-1.935217	-1.963104	-2.938215
41	1	-3.307991	-1.121048	-2.220942
42	1	0.100338	-4.056379	-1.586972
43	1	1.425544	-2.933931	-1.248448
44	1	0.267548	-2.561370	-2.528371
45	1	0.737157	-3.593939	2.055789
46	1	1.267274	-1.945277	2.420167
47	1	1.828677	-2.751289	0.949268
48	1	-2.012130	-2.356468	3.328977
49	1	-2.329761	-0.622485	3.212099
50	1	-0.684110	-1.199096	3.493557
51	1	5.919799	0.236362	1.833064
52	1	5.977825	1.615418	-0.365770

53	1	0.427091	2.906823	-1.546525
54	6	5.035695	-1.006659	-0.507379
55	1	6.128286	-0.967223	-0.459145
56	1	4.701434	-1.944221	-0.052284
57	1	4.732139	-0.995685	-1.558482
58	72	-0.425359	0.251637	-0.185632

TS2a-3a (E = -939.4372334 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-1.050069	-0.680384	-0.611704
2	7	-3.165569	1.180384	-2.380759
3	6	1.461721	-0.994239	-0.937759
4	6	1.294426	-0.244610	0.260691
5	6	0.992299	-0.200284	-2.026352
6	17	-1.277725	-2.722237	-2.020488
7	6	0.736396	1.027196	-0.088148
8	6	0.551891	1.052654	-1.502032
9	6	-2.640531	0.366141	-1.633027
10	6	-4.536273	1.678290	-2.686967
11	6	-1.824019	0.062629	1.454661
12	6	-2.227292	-1.332028	1.489482
13	1	-2.604494	0.804260	1.276820
14	6	-3.647614	-0.761333	-0.456147
15	6	-3.052653	-1.773114	0.460927
16	1	-4.282594	-1.235505	-1.195675
17	1	-4.158641	0.047668	0.067335
18	6	-3.563901	-3.194819	0.343654
19	6	-1.693752	-2.250283	2.574458
20	1	-1.512564	-3.271748	2.227482
21	1	-2.419160	-2.303100	3.398907
22	1	-0.760237	-1.857361	2.989518
23	1	-4.538006	-3.286862	0.846502
24	1	-2.885219	-3.926407	0.790188
25	1	-3.698006	-3.468871	-0.706624
26	6	-5.554667	0.532372	-2.875785
27	6	-4.966662	2.620155	-1.539245
28	1	-5.168842	-0.220220	-3.571708
29	1	-5.804337	0.044625	-1.930665
30	1	-5.057880	2.076827	-0.593359
31	1	-4.238500	3.427556	-1.409679
32	6	1.782912	-0.647332	1.632693
33	6	2.125043	-2.345218	-1.059501
34	6	1.088394	-0.562494	-3.487968
35	6	0.149172	2.259500	-2.314937
36	6	0.589566	2.219036	0.826789
37	1	2.813483	-0.299606	1.791508
38	1	1.782741	-1.734496	1.764056
39	1	1.168516	-0.214923	2.429043
40	1	3.191920	-2.225181	-1.295671
41	1	1.670304	-2.945741	-1.852311
42	1	2.057963	-2.918817	-0.129094
43	1	2.076067	-0.289866	-3.886695
44	1	0.334636	-0.038183	-4.084104
45	1	0.944957	-1.635077	-3.645055
46	1	1.038311	2.846442	-2.586975
47	1	-0.525932	2.916306	-1.758468
48	1	-0.362574	1.976622	-3.238684
49	1	1.458193	2.885375	0.724461
50	1	0.527076	1.920005	1.876692
51	1	-0.305036	2.807313	0.596179
52	1	-5.938877	3.066735	-1.775111
53	1	-6.479923	0.941513	-3.296504

54	1	-1.145461	0.374417	2.242037
55	6	-4.411998	2.477272	-4.002630
56	1	-5.376591	2.921270	-4.271392
57	1	-3.674032	3.278328	-3.894287
58	1	-4.090599	1.822303	-4.819535

3a (E = -939.4515093 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.593575	0.281198	-0.131490
2	7	2.235967	-0.922499	-0.188354
3	6	-2.306993	-1.443466	-0.803586
4	6	-2.805190	-0.806095	0.374302
5	6	-1.126979	-2.157466	-0.448073
6	17	-0.902763	1.301834	-2.324756
7	6	-1.946841	-1.144843	1.460485
8	6	-0.900402	-1.972879	0.951957
9	6	1.589375	0.022716	0.379390
10	6	3.728976	-1.130923	-0.171925
11	6	-0.786162	1.789431	1.513858
12	6	0.085668	2.737182	0.775158
13	1	-0.316637	1.316196	2.381730
14	6	2.094336	1.251530	1.158736
15	6	1.410162	2.480517	0.560735
16	1	3.175395	1.388001	1.137852
17	1	1.807951	1.125853	2.210906
18	6	2.332165	3.355197	-0.261169
19	6	-0.627154	3.961225	0.219524
20	1	-0.118379	4.422106	-0.628497
21	1	-0.725961	4.716582	1.011902
22	1	-1.639984	3.700693	-0.107860
23	1	3.120856	3.779210	0.377940
24	1	1.822835	4.183605	-0.755190
25	1	2.836814	2.762595	-1.035803
26	6	4.457582	-0.022998	-0.967611
27	6	4.270721	-1.242483	1.273420
28	1	4.015763	0.077846	-1.965307
29	1	4.404887	0.948081	-0.468859
30	1	4.191120	-0.300893	1.823032
31	1	3.718503	-2.010691	1.827107
32	6	-4.080430	-0.001597	0.465829
33	6	-2.994646	-1.469663	-2.147325
34	6	-0.316871	-3.053761	-1.353937
35	6	0.129086	-2.711191	1.771062
36	6	-2.198214	-0.834294	2.915588
37	1	-4.940632	-0.662763	0.641591
38	1	-4.280422	0.553146	-0.457060
39	1	-4.047548	0.718788	1.289277
40	1	-3.715025	-2.298871	-2.185487
41	1	-2.283264	-1.606585	-2.966439
42	1	-3.541244	-0.542747	-2.343778
43	1	-0.619816	-4.102428	-1.223050
44	1	0.750790	-2.972190	-1.133130
45	1	-0.461971	-2.797973	-2.408334
46	1	-0.239747	-3.714057	2.029739
47	1	0.353575	-2.190396	2.707616
48	1	1.065365	-2.822591	1.218633
49	1	-2.818035	-1.620379	3.369151
50	1	-2.723706	0.116426	3.046633
51	1	-1.267244	-0.780871	3.489024
52	1	5.327801	-1.534037	1.253466
53	1	5.516055	-0.283643	-1.087684
54	1	-1.750141	2.208609	1.799686
55	6	3.956481	-2.480679	-0.889395

56	1	5.024486	-2.724654	-0.933018
57	1	3.437176	-3.287385	-0.359976
58	1	3.564956	-2.437290	-1.911386

TS3a-3b (E = -939.4515018 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-0.044622	-0.057121	-0.041520
2	6	0.012849	0.081484	4.596516
3	6	1.427323	0.044335	4.794976
4	6	-0.297163	-0.771189	3.498568
5	17	-0.409529	3.047928	2.903943
6	6	1.987535	-0.845566	3.833787
7	6	0.923634	-1.348212	3.025242
8	6	1.022124	0.510441	0.374849
9	6	3.200155	1.674920	2.327209
10	6	2.852711	2.795492	1.418219
11	1	3.654995	0.809919	1.835351
12	6	2.178437	1.170677	-0.395528
13	6	2.339632	2.581755	0.170224
14	1	2.037717	1.220014	-1.475249
15	1	3.085545	0.579048	-0.216791
16	6	1.886800	3.677540	-0.770387
17	6	3.042337	4.183399	2.013688
18	1	2.417420	4.950632	1.553845
19	1	4.093197	4.487592	1.906883
20	1	2.815935	4.175684	3.086029
21	1	2.503241	3.672138	-1.681476
22	1	1.944630	4.676488	-0.336114
23	1	0.849256	3.510096	-1.088729
24	6	2.176960	0.754326	5.897593
25	6	-0.983418	0.785487	5.486005
26	6	-1.680071	-1.115807	2.998436
27	6	1.021854	-2.460961	2.011825
28	6	3.423623	-1.306315	3.785882
29	1	1.738774	1.731916	6.126745
30	1	3.227864	0.911897	5.636389
31	1	2.152323	0.162315	6.823211
32	1	-1.297757	0.118358	6.300967
33	1	-1.878482	1.087678	4.935513
34	1	-0.560067	1.687132	5.938605
35	1	-2.034270	-2.046083	3.465150
36	1	-1.683469	-1.253105	1.913805
37	1	-2.403271	-0.330146	3.239397
38	1	0.787612	-3.425547	2.484414
39	1	2.028231	-2.535924	1.587497
40	1	0.323115	-2.303978	1.186233
41	1	3.559151	-2.193054	4.420782
42	1	4.112475	-0.535697	4.144649
43	1	3.731265	-1.580712	2.771678
44	1	3.804705	1.973202	3.183032
45	72	1.036460	1.120258	2.538461
46	6	-0.425062	-0.325038	-1.475602
47	6	0.644684	-1.188086	-2.186412
48	6	-1.742690	-1.128747	-1.402873
49	6	-0.693669	0.990371	-2.242914
50	1	1.592849	-0.657544	-2.308321
51	1	0.834906	-2.103535	-1.614316
52	1	-1.592806	-2.059083	-0.843790
53	1	-2.515207	-0.544678	-0.891144
54	1	-1.398232	1.616773	-1.684288
55	1	0.220052	1.565861	-2.410860
56	1	0.288537	-1.478583	-3.182184
57	1	-1.136218	0.767960	-3.221382

58	1	-2.101951	-1.380708	-2.407607

3b (E = -939.4744958 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-1.259455	1.245779	0.185472
2	6	2.553963	1.085930	-0.084187
3	6	2.888257	-0.274785	-0.365727
4	6	1.967948	1.135840	1.215947
5	17	0.096086	-0.163741	-2.703254
6	6	2.504270	-1.063970	0.758054
7	6	1.927915	-0.190967	1.734360
8	6	-1.380095	0.208547	0.924978
9	6	-2.199184	2.375677	-0.139186
10	6	-0.437204	-2.255252	0.226980
11	6	-1.920827	-2.397843	0.007436
12	1	-0.200878	-2.351677	1.293422
13	6	-2.493556	-0.510969	1.604355
14	6	-2.864447	-1.670543	0.656696
15	1	-2.130998	-0.894430	2.567114
16	1	-3.382616	0.094445	1.808621
17	6	-4.363642	-1.880317	0.556680
18	6	-2.275849	-3.450721	-1.031503
19	1	-3.322390	-3.438746	-1.343856
20	1	-2.039650	-4.457075	-0.657216
21	1	-1.660291	-3.293011	-1.927098
22	1	-4.636328	-2.728664	-0.073889
23	1	-4.871965	-0.989703	0.157450
24	1	-4.790389	-2.064027	1.554172
25	6	-3.385809	1.813780	-0.951990
26	6	-2.679091	3.039058	1.168530
27	1	-3.026505	1.294430	-1.846202
28	1	-3.978086	1.111503	-0.358447
29	1	-3.248475	2.339994	1.788637
30	1	-1.826516	3.404713	1.751393
31	6	3.632172	-0.764019	-1.586737
32	6	2.876476	2.270996	-0.965200
33	6	1.570788	2.385733	1.965076
34	6	1.517817	-0.587004	3.133047
35	6	2.818240	-2.526514	0.960562
36	1	4.717603	-0.680008	-1.434716
37	1	3.374937	-0.184144	-2.478347
38	1	3.411196	-1.813951	-1.804149
39	1	3.901980	2.620209	-0.778939
40	1	2.204514	3.114398	-0.776443
41	1	2.802566	2.019654	-2.028050
42	1	2.408785	2.749755	2.575857
43	1	0.726968	2.205349	2.638850
44	1	1.284390	3.193841	1.285028
45	1	2.389725	-0.596417	3.802553
46	1	1.075008	-1.587986	3.160744
47	1	0.787101	0.110648	3.554374
48	1	3.794927	-2.642573	1.451291
49	1	2.861428	-3.069273	0.010895
50	1	2.072458	-3.022020	1.589460
51	1	-3.326234	3.892326	0.936779
52	1	-4.040243	2.634668	-1.266441
53	1	0.099287	-3.055777	-0.294950
54	6	-1.408081	3.385507	-0.990510
55	1	-2.048564	4.228850	-1.270660
56	1	-0.551218	3.776636	-0.430485
57	1	-1.037767	2.910765	-1.904876
58	72	0.365119	-0.160258	-0.269178

TS3b-3c (E = -939.4640629 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.251109	-0.387672	-0.347924
2	7	-0.955980	1.437302	-0.784444
3	6	2.558750	-1.490676	0.215385
4	6	2.050944	-0.896428	1.406235
5	6	2.846532	-0.448762	-0.712492
6	17	0.097015	-1.680760	-2.393318
7	6	1.990077	0.516336	1.201651
8	6	2.499273	0.792881	-0.108520
9	6	-1.688537	0.509505	-0.298326
10	6	-1.271631	2.831809	-1.267106
11	6	-0.973875	-1.659351	1.128250
12	6	-2.333624	-2.093812	0.633518
13	1	-1.075953	-0.970541	1.982001
14	6	-3.095883	0.251369	0.111589
15	6	-3.318177	-1.255306	0.232269
16	1	-3.257467	0.767116	1.073273
17	1	-3.832947	0.681674	-0.574714
18	6	-4.727550	-1.665585	-0.150748
19	6	-2.498473	-3.606683	0.624404
20	1	-3.395517	-3.955420	0.108000
21	1	-2.517543	-4.001958	1.650361
22	1	-1.632020	-4.061437	0.125300
23	1	-4.920716	-2.732646	-0.026310
24	1	-4.945551	-1.403511	-1.197824
25	1	-5.464304	-1.127756	0.465815
26	6	-0.869215	3.813708	-0.146687
27	6	-0.423399	3.065024	-2.532604
28	1	-1.452160	3.627575	0.762467
29	1	0.192881	3.718119	0.096466
30	1	0.640849	2.938549	-2.317075
31	1	-0.703159	2.356005	-3.319531
32	6	1.835367	-1.594974	2.725838
33	6	2.835000	-2.959156	-0.002586
34	6	3.505521	-0.632132	-2.057875
35	6	2.859593	2.156070	-0.651788
36	6	1.667277	1.537582	2.270706
37	1	2.743138	-1.519588	3.341339
38	1	1.615558	-2.658363	2.594540
39	1	1.011895	-1.156891	3.298727
40	1	3.875772	-3.204273	0.252868
41	1	2.674734	-3.246460	-1.046910
42	1	2.188082	-3.589501	0.616397
43	1	4.594320	-0.732600	-1.943629
44	1	3.320992	0.219759	-2.720266
45	1	3.139777	-1.529199	-2.567259
46	1	3.900426	2.399908	-0.394547
47	1	2.229089	2.946067	-0.234881
48	1	2.776518	2.201013	-1.742485
49	1	2.555299	1.750362	2.883220
50	1	0.883096	1.183994	2.949550
51	1	1.331282	2.486776	1.842185
52	1	-0.582106	4.081094	-2.910221
53	1	-1.054548	4.844323	-0.469176
54	1	-0.432576	-2.530903	1.507519
55	6	-2.766800	2.994677	-1.602692
56	1	-2.934782	3.989009	-2.031062
57	1	-3.089006	2.250687	-2.338921
58	1	-3.394290	2.905052	-0.710891

3c (E = -939.4654124 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-1.178422	1.539430	-0.136678
2	6	2.493104	-1.258069	0.457736
3	6	2.053940	-0.451280	1.549426
4	6	2.812618	-0.395109	-0.627534
5	17	0.109403	-1.088202	-2.466583
6	6	2.085983	0.913272	1.129952
7	6	2.548112	0.945873	-0.223642
8	6	-1.809804	0.425549	-0.202871
9	6	-1.698923	2.945323	0.050119
10	6	-0.879037	-1.620198	1.168831
11	6	-2.156585	-2.251142	0.652040
12	1	-1.098486	-0.975664	2.036208
13	6	-3.201994	-0.059933	-0.035361
14	6	-3.221805	-1.572029	0.170948
15	1	-3.725502	0.471461	0.774926
16	1	-3.769685	0.178094	-0.946626
17	6	-4.554126	-2.181232	-0.223506
18	6	-2.131449	-3.770691	0.732866
19	1	-2.975640	-4.258091	0.240383
20	1	-2.104994	-4.104308	1.780357
21	1	-1.212959	-4.143675	0.258935
22	1	-4.640125	-3.242275	0.017501
23	1	-4.737878	-2.063450	-1.302892
24	1	-5.377091	-1.662969	0.292267
25	6	-1.953920	3.167723	1.556349
26	6	-0.618777	3.910852	-0.467209
27	1	-2.713109	2.474123	1.933698
28	1	-1.034657	3.023000	2.133010
29	1	0.310805	3.794946	0.095693
30	1	-0.407989	3.723395	-1.525849
31	6	1.819870	-0.920127	2.965452
32	6	2.696706	-2.754330	0.482713
33	6	3.443442	-0.812445	-1.932202
34	6	2.890331	2.176973	-1.032380
35	6	1.928390	2.097547	2.057243
36	1	2.755264	-0.866795	3.540865
37	1	1.471017	-1.955964	3.002107
38	1	1.079603	-0.304164	3.487188
39	1	3.718281	-3.003751	0.803098
40	1	2.545581	-3.199381	-0.506437
41	1	2.007410	-3.246431	1.176511
42	1	4.538166	-0.841869	-1.833628
43	1	3.200177	-0.117352	-2.741422
44	1	3.108391	-1.805307	-2.246049
45	1	3.967912	2.386802	-0.976557
46	1	2.364454	3.063682	-0.668361
47	1	2.638005	2.053906	-2.091601
48	1	2.844227	2.237025	2.649438
49	1	1.103567	1.964484	2.765937
50	1	1.751652	3.026866	1.509468
51	1	-0.956926	4.947279	-0.360849
52	1	-2.308748	4.190094	1.728822
53	1	-0.225518	-2.407651	1.555679
54	6	-2.996206	3.144139	-0.762074
55	1	-3.302856	4.194629	-0.709878
56	1	-2.837390	2.887590	-1.815377
57	1	-3.817819	2.536069	-0.374539
58	72	0.235177	-0.157152	-0.216593

TS3c-4 (E = -939.4298399 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)

		X	Y	Z
1	72	0.662008	-0.015132	-0.808069
2	7	-0.720886	1.488875	-0.561060
3	6	2.971282	-1.090188	-0.570743
4	6	2.562014	-0.624539	0.714728
5	6	3.191178	0.045622	-1.402551
6	17	0.413440	-1.182771	-2.954997
7	6	2.529280	0.805638	0.674244
8	6	2.921438	1.218794	-0.638770
9	6	-1.354210	0.280811	-0.572147
10	6	-1.268842	2.825485	-0.187936
11	6	-0.929627	-0.877433	0.942876
12	6	-2.281772	-1.539387	1.009709
13	1	-0.690173	-0.315761	1.853782
14	6	-2.796903	-0.056689	-0.815362
15	6	-3.206406	-1.169631	0.111795
16	1	-3.469027	0.796609	-0.662269
17	1	-2.923079	-0.355031	-1.866258
18	6	-4.602495	-1.718580	-0.051351
19	6	-2.454679	-2.590900	2.085225
20	1	-3.463613	-3.012462	2.110815
21	1	-2.242518	-2.164492	3.075685
22	1	-1.746113	-3.418560	1.938507
23	1	-4.842900	-2.493664	0.680627
24	1	-4.732196	-2.150208	-1.053817
25	1	-5.349024	-0.917694	0.048101
26	6	-1.986188	2.743030	1.179371
27	6	-0.100331	3.823379	-0.102911
28	1	-2.816423	2.030217	1.153745
29	1	-1.287273	2.424369	1.961142
30	1	0.594100	3.543050	0.693073
31	1	0.446256	3.851951	-1.051322
32	6	2.422177	-1.457312	1.968999
33	6	3.239577	-2.524376	-0.962297
34	6	3.740895	0.011790	-2.807238
35	6	3.226078	2.628279	-1.094228
36	6	2.375549	1.680359	1.899088
37	1	3.373859	-1.478739	2.518995
38	1	2.152453	-2.494812	1.745634
39	1	1.663261	-1.055322	2.649012
40	1	4.312196	-2.751116	-0.882852
41	1	2.933360	-2.723642	-1.994179
42	1	2.708506	-3.230274	-0.315025
43	1	4.835445	-0.090884	-2.789266
44	1	3.504534	0.929469	-3.355459
45	1	3.334179	-0.828123	-3.378621
46	1	4.312827	2.788255	-1.129396
47	1	2.804273	3.374267	-0.417042
48	1	2.834804	2.834110	-2.096812
49	1	3.221861	1.521544	2.582025
50	1	1.460343	1.465846	2.463157
51	1	2.362791	2.741194	1.637868
52	1	-0.476285	4.830825	0.108373
53	1	-2.386899	3.724820	1.457539
54	1	-0.178991	-1.686641	0.887646
55	6	-2.242334	3.316277	-1.289959
56	1	-2.588906	4.331429	-1.062069
57	1	-1.732332	3.333481	-2.259420
58	1	-3.120303	2.671098	-1.377960

4 (E = -939.4540671 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	7	-0.825881	1.498187	0.034003
2	6	2.410429	-1.581821	0.089572
3	6	2.107313	-1.010426	1.362372
4	6	2.756474	-0.523342	-0.797579
5	17	-0.237289	-1.392972	-2.218674
6	6	2.275236	0.406548	1.259020
7	6	2.679317	0.709460	-0.081087
8	6	-1.815119	0.492442	0.110389
9	6	-1.146580	2.949113	-0.005568
10	6	-1.820833	-0.453404	1.235898
11	6	-2.956541	-1.407173	0.963543
12	1	-1.747022	-0.064176	2.257226
13	6	-3.000572	0.183152	-0.791653
14	6	-3.601598	-1.054702	-0.161856
15	1	-3.754024	0.985033	-0.798204
16	1	-2.721164	0.013223	-1.839129
17	6	-4.791178	-1.723984	-0.795533
18	6	-3.229515	-2.556744	1.896620
19	1	-4.100720	-3.140664	1.585812
20	1	-3.411778	-2.199006	2.919782
21	1	-2.368957	-3.239323	1.944197
22	1	-5.155978	-2.572367	-0.208658
23	1	-4.539126	-2.090813	-1.799851
24	1	-5.620215	-1.012541	-0.914245
25	6	-2.040821	3.307874	1.203879
26	6	0.164701	3.748944	0.062571
27	1	-2.964787	2.719147	1.190746
28	1	-1.515081	3.099624	2.143126
29	1	0.705386	3.528871	0.987766
30	1	0.807561	3.503330	-0.787951
31	6	1.864747	-1.773508	2.646024
32	6	2.445771	-3.054957	-0.240474
33	6	3.256596	-0.687340	-2.212143
34	6	3.226637	2.026240	-0.582427
35	6	2.253048	1.360027	2.432357
36	1	2.817509	-1.978489	3.155112
37	1	1.376901	-2.736045	2.461786
38	1	1.237216	-1.210541	3.345182
39	1	3.459497	-3.457406	-0.103030
40	1	2.151697	-3.241477	-1.277908
41	1	1.774123	-3.632596	0.403411
42	1	4.337720	-0.887340	-2.215593
43	1	3.086023	0.214869	-2.808301
44	1	2.759853	-1.518037	-2.721957
45	1	4.325791	1.998544	-0.583521
46	1	2.919768	2.861933	0.049840
47	1	2.905764	2.247987	-1.605930
48	1	3.181636	1.268304	3.013758
49	1	1.420282	1.158409	3.115276
50	1	2.168744	2.400128	2.108678
51	1	-0.045149	4.824152	0.034833
52	1	-2.307924	4.370968	1.185097
53	1	-0.780449	-1.155813	1.263585
54	6	-1.872371	3.313064	-1.327080
55	1	-2.030558	4.396842	-1.385164
56	1	-1.267973	3.002930	-2.186839
57	1	-2.848212	2.825670	-1.398401
58	72	0.285665	-0.195929	-0.147947

TS4-5 (E = -939.4540248 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	0.284781	-0.195778	-0.131417
2	7	-0.835456	1.498659	0.062585
3	6	2.411020	-1.580049	0.087429
4	6	2.113863	-1.021006	1.367008
5	6	2.749414	-0.513412	-0.792284
6	17	-0.251330	-1.369830	-2.209864
7	6	2.276989	0.396921	1.274991
8	6	2.673216	0.712817	-0.064507
9	6	-1.837806	0.510984	0.153878
10	6	-1.147902	2.950283	-0.024185
11	6	-1.817543	-0.458994	1.238949
12	6	-2.951086	-1.413059	0.974876
13	1	-1.681524	-0.115205	2.268155
14	6	-3.011702	0.192133	-0.762074
15	6	-3.607287	-1.052952	-0.142140
16	1	-3.768614	0.990050	-0.770990
17	1	-2.721158	0.028949	-1.807225
18	6	-4.800688	-1.718138	-0.772545
19	6	-3.210168	-2.571747	1.900025
20	1	-4.080781	-3.157379	1.590868
21	1	-3.386121	-2.224032	2.927659
22	1	-2.345230	-3.249389	1.933956
23	1	-5.155515	-2.575629	-0.192813
24	1	-4.558305	-2.071141	-1.784178
25	1	-5.634134	-1.008994	-0.872906
26	6	-2.056886	3.347600	1.161904
27	6	0.167368	3.743363	0.043525
28	1	-2.986309	2.767583	1.150158
29	1	-1.547138	3.157740	2.113742
30	1	0.695067	3.539118	0.979926
31	1	0.819335	3.477161	-0.793501
32	6	1.878001	-1.797366	2.643512
33	6	2.443644	-3.050206	-0.255581
34	6	3.243651	-0.663140	-2.210563
35	6	3.224285	2.032795	-0.552798
36	6	2.255161	1.343320	2.454035
37	1	2.833082	-2.004903	3.147191
38	1	1.391404	-2.758621	2.450402
39	1	1.251099	-1.243463	3.350344
40	1	3.455251	-3.457305	-0.116163
41	1	2.154645	-3.226504	-1.296179
42	1	1.766074	-3.630994	0.379134
43	1	4.326384	-0.854011	-2.220467
44	1	3.062758	0.241718	-2.799639
45	1	2.751602	-1.494426	-2.723870
46	1	4.323410	2.001573	-0.551447
47	1	2.918834	2.863424	0.086790
48	1	2.906868	2.264753	-1.575071
49	1	3.203770	1.284179	3.006734
50	1	1.452000	1.105463	3.160223
51	1	2.120812	2.381319	2.140184
52	1	-0.035899	4.818887	-0.008761
53	1	-2.312853	4.412395	1.112318
54	1	-0.736092	-1.205089	1.212671
55	6	-1.850682	3.283460	-1.365989
56	1	-1.996755	4.366686	-1.456394
57	1	-1.237157	2.943756	-2.207925
58	1	-2.830563	2.804446	-1.438531

5 (E = -939.4830697 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	0.466285	0.034447	-0.402952
2	7	-1.037999	1.220688	0.385958
3	6	2.252651	-1.839734	-0.225336
4	6	1.505367	-1.844750	0.991639
5	6	2.944742	-0.604265	-0.312671
6	17	1.109368	1.413707	-2.281044
7	6	1.738750	-0.607613	1.663483
8	6	2.618439	0.169134	0.846177
9	6	-2.067140	0.291764	0.250961
10	6	-1.326583	2.665268	0.665788
11	6	-2.040246	-0.954698	0.813646
12	6	-3.124039	-1.790311	0.280840
13	1	-1.372811	-1.255222	1.610123
14	6	-3.243510	0.320045	-0.719586
15	6	-3.849011	-1.058746	-0.597020
16	1	-3.976890	1.098753	-0.478647
17	1	-2.892895	0.528088	-1.737006
18	6	-5.089202	-1.441794	-1.355672
19	6	-3.338180	-3.214275	0.722953
20	1	-4.245817	-3.644754	0.289743
21	1	-3.422381	-3.279600	1.816211
22	1	-2.492389	-3.848200	0.425141
23	1	-5.410690	-2.462119	-1.124341
24	1	-4.927036	-1.381048	-2.440976
25	1	-5.923761	-0.766020	-1.119868
26	6	-2.310730	2.775424	1.851935
27	6	0.009153	3.332240	1.051580
28	1	-3.273764	2.308691	1.616918
29	1	-1.899404	2.278395	2.737708
30	1	0.427532	2.862291	1.947997
31	1	0.737090	3.252298	0.236966
32	6	0.774489	-3.046115	1.542875
33	6	2.383780	-2.999560	-1.180904
34	6	3.961002	-0.228883	-1.362868
35	6	3.269829	1.479145	1.225822
36	6	1.295207	-0.256153	3.065487
37	1	1.496779	-3.797117	1.892379
38	1	0.142366	-3.524238	0.787374
39	1	0.141786	-2.785462	2.396616
40	1	3.236865	-3.634469	-0.901050
41	1	2.547291	-2.660303	-2.208492
42	1	1.485300	-3.623198	-1.179870
43	1	4.966158	-0.544132	-1.048842
44	1	3.986223	0.850581	-1.536591
45	1	3.746267	-0.708132	-2.322871
46	1	4.258678	1.294117	1.668771
47	1	2.679421	2.032379	1.961280
48	1	3.416751	2.129345	0.357248
49	1	2.033393	-0.612805	3.797666
50	1	0.333800	-0.712281	3.322124
51	1	1.191551	0.824277	3.202087
52	1	-0.146473	4.395699	1.263335
53	1	-2.494089	3.827656	2.097434
54	1	-0.170968	-1.366588	-1.395573
55	6	-1.901121	3.381350	-0.581608
56	1	-2.007524	4.454107	-0.381086
57	1	-1.230334	3.252033	-1.436768
58	1	-2.887697	2.994135	-0.851687

6a (E = -1190.1438901 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.186508	-0.547528	-0.087817
2	7	1.674783	-0.185378	-0.956339
3	6	-1.601627	-1.300625	1.987742
4	6	-0.213335	-1.445282	2.292648
5	6	-1.923199	-2.203808	0.940344
6	17	-1.410825	-1.028763	-2.271846
7	6	0.324642	-2.446410	1.432247
8	6	-0.732126	-2.901429	0.576009
9	6	2.363747	0.819215	-0.229189
10	6	2.365736	-0.671657	-2.222863
11	6	3.074006	0.683345	0.915283
12	6	3.585596	1.983908	1.369143
13	1	3.249436	-0.251904	1.432300
14	6	2.381226	2.294645	-0.598561
15	6	3.194778	2.942752	0.494749
16	1	2.817524	2.472056	-1.589286
17	1	1.356950	2.685365	-0.639294
18	6	3.481564	4.419661	0.509842
19	6	4.415365	2.132922	2.618822
20	1	4.719870	3.170326	2.788794
21	1	5.325698	1.520260	2.561997
22	1	3.857129	1.797522	3.503627
23	1	4.087467	4.709279	1.374828
24	1	2.553060	5.007809	0.542079
25	1	4.023248	4.731635	-0.394981
26	6	3.903888	-0.599809	-2.082284
27	6	1.982090	-2.148777	-2.457549
28	1	4.261694	0.428522	-1.969705
29	1	4.244682	-1.172054	-1.212591
30	1	2.331999	-2.768349	-1.623969
31	1	0.901695	-2.268203	-2.565047
32	6	0.494440	-0.791914	3.454297
33	6	-2.562544	-0.425266	2.754312
34	6	-3.292793	-2.471330	0.367724
35	6	-0.667773	-4.068163	-0.380911
36	6	1.690566	-3.081296	1.561291
37	1	0.342843	-1.375536	4.374199
38	1	0.120574	0.220936	3.630341
39	1	1.572053	-0.716356	3.283363
40	1	-2.840319	-0.899342	3.706397
41	1	-3.485623	-0.249113	2.193697
42	1	-2.119576	0.548910	2.987187
43	1	-3.726782	-3.375742	0.817391
44	1	-3.250302	-2.619612	-0.715486
45	1	-3.981954	-1.643117	0.561205
46	1	-1.032358	-4.982650	0.108842
47	1	0.354628	-4.261236	-0.718822
48	1	-1.283871	-3.893928	-1.268211
49	1	1.648918	-3.925715	2.264414
50	1	2.434552	-2.374750	1.940613
51	1	2.057490	-3.466487	0.605677
52	1	2.455181	-2.515715	-3.376663
53	1	4.368102	-1.024314	-2.980118
54	1	-0.033535	0.902929	1.040118
55	6	1.916044	0.179713	-3.435145
56	1	2.382958	-0.189617	-4.357257
57	1	0.829597	0.131242	-3.548140
58	1	2.207175	1.227858	-3.306296
59	6	-3.527466	3.889198	0.835720
60	6	-3.703509	2.961380	-0.384686
61	1	-3.712186	3.345906	1.767502
62	1	-2.515536	4.304189	0.865601
63	1	-4.241979	4.715306	0.766926

64	6	-3.403092	3.707828	-1.702871
65	6	-5.113371	2.333348	-0.411952
66	1	-3.496138	3.034239	-2.559707
67	1	-4.118252	4.527798	-1.821348
68	1	-2.391758	4.125329	-1.690671
69	1	-5.858855	3.128199	-0.512479
70	1	-5.216090	1.648081	-1.258483
71	1	-5.312926	1.784808	0.513759
72	7	-2.733215	1.873996	-0.268133
73	6	-1.943660	1.023830	-0.205294

TS6a-7a (E = -1190.1378188 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.978289	-0.221059	-0.219912
2	7	0.423010	-1.721976	-0.592520
3	6	-2.283851	1.334957	1.440798
4	6	-1.567809	0.339714	2.182559
5	6	-3.273238	0.681133	0.661758
6	17	-2.163785	-0.283859	-2.412357
7	6	-2.119725	-0.933239	1.857127
8	6	-3.166402	-0.720782	0.895921
9	6	1.693152	-1.406380	-0.056191
10	6	0.351501	-2.993929	-1.425071
11	6	2.069566	-1.424824	1.244810
12	6	3.447646	-0.938005	1.397234
13	1	1.446228	-1.753259	2.067145
14	6	2.877690	-0.887760	-0.860571
15	6	3.941854	-0.618375	0.176498
16	1	3.225948	-1.608673	-1.609587
17	1	2.594809	0.013213	-1.418896
18	6	5.311716	-0.119518	-0.195536
19	6	4.130711	-0.859184	2.738575
20	1	5.154904	-0.482365	2.657198
21	1	4.173211	-1.847608	3.216404
22	1	3.581643	-0.196265	3.421281
23	1	5.948148	0.019017	0.684672
24	1	5.260419	0.843254	-0.724049
25	1	5.823921	-0.822257	-0.868648
26	6	1.303113	-4.072647	-0.858451
27	6	-1.089366	-3.543864	-1.348668
28	1	2.354127	-3.775148	-0.927326
29	1	1.078112	-4.274483	0.194653
30	1	-1.354885	-3.776204	-0.310810
31	1	-1.810064	-2.830417	-1.756377
32	6	-0.574575	0.619692	3.285103
33	6	-2.124569	2.826021	1.608129
34	6	-4.316406	1.348324	-0.198220
35	6	-4.121680	-1.767674	0.372722
36	6	-1.819334	-2.237531	2.561353
37	1	-1.099946	0.796675	4.234766
38	1	0.031542	1.504202	3.068479
39	1	0.111339	-0.218045	3.438948
40	1	-2.735651	3.183779	2.448911
41	1	-2.439563	3.371351	0.713617
42	1	-1.086100	3.101438	1.817352
43	1	-5.250056	1.482759	0.366418
44	1	-4.541306	0.753582	-1.087923
45	1	-3.988194	2.335126	-0.539073
46	1	-5.038383	-1.783583	0.979236
47	1	-3.687358	-2.771310	0.408111
48	1	-4.409849	-1.565638	-0.663365
49	1	-2.477563	-2.356776	3.433910

50	1	-0.786732	-2.280094	2.920347
51	1	-1.977773	-3.102195	1.910099
52	1	-1.167546	-4.467759	-1.934111
53	1	1.176961	-5.002783	-1.424511
54	1	0.386282	0.936510	0.430397
55	6	0.705803	-2.697461	-2.902345
56	1	0.606965	-3.607486	-3.507519
57	1	0.034077	-1.934462	-3.306037
58	1	1.735943	-2.340029	-2.999191
59	6	2.136093	3.303564	0.368263
60	6	1.385131	3.718952	-0.909575
61	1	1.478492	3.343554	1.242849
62	1	2.533354	2.286725	0.287800
63	1	2.972246	3.990787	0.535848
64	6	2.316424	3.668094	-2.140405
65	6	0.770600	5.126156	-0.758830
66	1	1.767766	3.929731	-3.050247
67	1	3.137661	4.380275	-2.008442
68	1	2.740660	2.666546	-2.265856
69	1	1.566687	5.859781	-0.594418
70	1	0.218467	5.403909	-1.661903
71	1	0.084858	5.161939	0.093911
72	7	0.266641	2.786994	-1.188600
73	6	-0.235490	1.760569	-0.836970

7a (E = -1190.1828657 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	0.743379	-1.465784	-0.704729
2	6	-2.268627	0.775794	1.771304
3	6	-1.574512	-0.377493	2.255475
4	6	-3.049514	0.384833	0.659780
5	17	-1.564187	0.460815	-2.338358
6	6	-1.966276	-1.496090	1.457608
7	6	-2.857743	-1.023094	0.454360
8	6	1.905238	-1.158690	0.006194
9	6	0.835760	-2.480529	-1.819622
10	6	1.997247	-1.078934	1.364887
11	6	3.295010	-0.525107	1.771701
12	1	1.242078	-1.424151	2.056346
13	6	3.225562	-0.636830	-0.559247
14	6	4.034340	-0.274663	0.665146
15	1	3.752478	-1.372146	-1.177248
16	1	3.041319	0.228505	-1.204973
17	6	5.452570	0.215212	0.559415
18	6	3.675411	-0.345771	3.218961
19	1	4.692840	0.040794	3.331528
20	1	3.615497	-1.299333	3.761263
21	1	2.992735	0.351914	3.722830
22	1	5.889555	0.415715	1.543016
23	1	5.516461	1.141547	-0.029121
24	1	6.092091	-0.524022	0.055475
25	6	1.717235	-3.673806	-1.379256
26	6	-0.580988	-3.016004	-2.109456
27	1	2.755211	-3.378300	-1.197264
28	1	1.324348	-4.118647	-0.457996
29	1	-0.990336	-3.513047	-1.224512
30	1	-1.253583	-2.209770	-2.410213
31	6	-0.801778	-0.431541	3.553070
32	6	-2.261724	2.134665	2.428879
33	6	-4.047489	1.239125	-0.081829
34	6	-3.662205	-1.851553	-0.517818
35	6	-1.623287	-2.938886	1.748816
36	1	-1.486178	-0.322586	4.406505

37	1	-0.055181	0.367020	3.626161
38	1	-0.283520	-1.387381	3.676972
39	1	-3.056658	2.198968	3.185790
40	1	-2.432902	2.940884	1.707706
41	1	-1.311887	2.333946	2.935775
42	1	-5.061243	1.066654	0.307927
43	1	-4.052309	1.011214	-1.151390
44	1	-3.828612	2.306291	0.028772
45	1	-4.705872	-1.924875	-0.180121
46	1	-3.272633	-2.869130	-0.607407
47	1	-3.666257	-1.404820	-1.517564
48	1	-2.232618	-3.313614	2.583462
49	1	-0.571355	-3.071877	2.022576
50	1	-1.818075	-3.580745	0.885773
51	1	-0.538707	-3.749757	-2.923021
52	1	1.718735	-4.442053	-2.160963
53	1	1.093959	2.283140	1.601422
54	6	1.399708	-1.839489	-3.112087
55	1	1.397967	-2.573354	-3.927492
56	1	0.779790	-0.988230	-3.408618
57	1	2.428593	-1.492876	-2.976911
58	6	-0.451911	4.011054	-1.404783
59	6	0.846301	3.242199	-1.069263
60	1	-1.123908	3.383123	-1.995833
61	1	-0.969587	4.314443	-0.487336
62	1	-0.211668	4.912851	-1.979091
63	6	1.777343	4.102976	-0.198429
64	6	1.555321	2.809722	-2.368877
65	1	2.678589	3.549030	0.089396
66	1	2.088541	4.989155	-0.761304
67	1	1.274752	4.445685	0.713522
68	1	1.794532	3.690038	-2.975876
69	1	2.490872	2.284105	-2.146189
70	1	0.909451	2.144745	-2.948709
71	7	0.429128	1.990397	-0.355992
72	6	0.571245	1.659883	0.868115
73	72	-0.571071	0.034624	-0.058253

TS7a-8a (E = -1190.1560335 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.552006	-0.396686	0.054556
2	7	-1.984382	1.025824	-0.390435
3	6	-2.116753	0.786032	0.921154
4	7	0.836098	1.135922	0.931351
5	6	-2.021356	-2.426544	0.481778
6	6	-1.289185	-2.159457	1.681580
7	6	-1.098022	-2.845640	-0.509889
8	17	0.212286	-0.293851	-2.345232
9	6	0.087968	-2.440929	1.431994
10	6	0.211522	-2.843974	0.068549
11	6	-2.796199	1.896836	-1.289204
12	6	0.173232	2.093794	1.577544
13	6	2.301331	1.310005	0.557084
14	6	-1.074254	1.855466	2.234860
15	1	-3.067051	0.836291	1.450337
16	6	-1.614269	3.169949	2.666485
17	1	-1.131915	1.026594	2.931861
18	6	0.397570	3.602786	1.542995
19	6	-0.811073	4.170562	2.254853
20	1	1.325695	3.917782	2.030131
21	1	0.464041	3.946772	0.505644
22	6	-0.960206	5.656558	2.438078

23	6	-2.890188	3.265434	3.460520
24	1	-3.130990	4.297304	3.733516
25	1	-2.813567	2.679818	4.387546
26	1	-3.740621	2.859343	2.896605
27	1	-1.863912	5.909174	3.001662
28	1	-1.014836	6.178438	1.471549
29	1	-0.099957	6.078942	2.977958
30	6	-3.307222	1.025678	-2.458139
31	6	-3.987760	2.517568	-0.534559
32	6	-1.875658	3.014573	-1.832605
33	1	-1.010982	2.575089	-2.338386
34	1	-1.519295	3.648022	-1.012087
35	1	-3.644428	3.126435	0.309048
36	1	-4.662821	1.742597	-0.152298
37	1	-3.968924	0.234994	-2.084854
38	1	-2.466779	0.559651	-2.979617
39	6	3.126132	1.727417	1.798798
40	6	2.823952	-0.072361	0.110161
41	6	2.493886	2.310750	-0.606351
42	1	1.852106	2.042632	-1.450746
43	1	2.278575	3.339834	-0.309998
44	1	2.884217	2.731394	2.152822
45	1	2.958887	1.022084	2.620560
46	1	2.718391	-0.802318	0.917546
47	1	2.303396	-0.431667	-0.781932
48	6	-1.889909	-1.875376	3.036761
49	6	-3.524701	-2.378437	0.350592
50	6	-1.427326	-3.346838	-1.894445
51	6	1.444512	-3.369339	-0.627641
52	6	1.160373	-2.483950	2.498982
53	1	-2.176436	-2.813613	3.534297
54	1	-2.787759	-1.254261	2.960664
55	1	-1.181193	-1.361984	3.695669
56	1	-3.974793	-3.312023	0.717080
57	1	-3.837745	-2.248169	-0.689984
58	1	-3.954065	-1.556372	0.933111
59	1	-1.455414	-4.446083	-1.903286
60	1	-0.683044	-3.021307	-2.626623
61	1	-2.403979	-2.988555	-2.234698
62	1	1.362007	-4.453840	-0.784916
63	1	2.351359	-3.190554	-0.042451
64	1	1.581515	-2.903231	-1.609883
65	1	0.957245	-3.300713	3.205311
66	1	1.215070	-1.556404	3.080716
67	1	2.149479	-2.666224	2.069435
68	1	-4.561024	3.161294	-1.210989
69	1	-3.870802	1.638849	-3.171552
70	1	-2.418844	3.647362	-2.545349
71	1	3.888003	0.001024	-0.139880
72	1	4.192427	1.713806	1.547274
73	1	3.536244	2.275997	-0.943929

8a (E = -1190.1789291 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-0.554144	-1.481280	-0.512797
2	6	-0.894449	-1.123586	0.838291
3	7	-1.006262	1.621435	0.018068
4	6	2.469714	-1.378176	1.098175
5	6	1.990344	-0.418423	2.042453
6	6	3.200784	-0.676464	0.094313
7	17	1.217878	0.540062	-2.545678
8	6	2.443845	0.871226	1.628006
9	6	3.190806	0.711962	0.425114

10	6	-1.039394	-2.648427	-1.292893
11	6	-2.100097	1.085107	0.443286
12	6	-0.990294	3.015734	-0.616170
13	6	-2.096023	-0.236903	1.186028
14	1	-0.728248	-1.888688	1.602100
15	6	-3.554427	-0.683663	1.123804
16	1	-1.906992	0.036591	2.241781
17	6	-3.546807	1.522264	0.282843
18	6	-4.340336	0.277488	0.620106
19	1	-3.789709	2.323826	0.991587
20	1	-3.760990	1.915477	-0.713513
21	6	-5.833659	0.288343	0.431500
22	6	-3.973281	-2.001306	1.713696
23	1	-5.057171	-2.145282	1.675680
24	1	-3.659265	-2.064891	2.765822
25	1	-3.501372	-2.842584	1.194421
26	1	-6.294685	-0.657427	0.730330
27	1	-6.093390	0.470486	-0.621070
28	1	-6.300790	1.092552	1.018456
29	6	-0.050973	-2.892902	-2.453005
30	6	-1.104858	-3.919726	-0.415578
31	6	-2.437873	-2.337151	-1.881313
32	1	-2.379373	-1.465199	-2.542242
33	1	-3.159201	-2.115991	-1.089052
34	1	-1.779101	-3.786167	0.435912
35	1	-0.111541	-4.169099	-0.026461
36	1	0.942573	-3.147998	-2.064840
37	1	0.047031	-1.997443	-3.072190
38	6	-1.811458	4.037635	0.210134
39	6	0.471720	3.510497	-0.615386
40	6	-1.495456	2.942809	-2.075349
41	1	-0.886289	2.246510	-2.656357
42	1	-2.540342	2.626677	-2.135772
43	1	-2.887800	3.948723	0.058442
44	1	-1.594432	3.940698	1.280349
45	1	0.864576	3.555910	0.405356
46	1	1.115209	2.874635	-1.227849
47	6	1.354672	-0.722466	3.377574
48	6	2.378941	-2.878146	1.252259
49	6	3.979405	-1.295677	-1.042414
50	6	3.946477	1.782996	-0.324407
51	6	2.307126	2.133255	2.450428
52	1	2.123139	-0.787280	4.162412
53	1	0.816157	-1.674049	3.361655
54	1	0.643705	0.054950	3.678725
55	1	3.184562	-3.246845	1.903772
56	1	2.472972	-3.391484	0.290506
57	1	1.427821	-3.183745	1.699173
58	1	5.023872	-1.466423	-0.743735
59	1	3.983555	-0.650076	-1.925508
60	1	3.561395	-2.261726	-1.343567
61	1	5.021617	1.724411	-0.103106
62	1	3.609716	2.787350	-0.048720
63	1	3.824728	1.677367	-1.407888
64	1	2.987068	2.101697	3.313749
65	1	1.292721	2.266896	2.844523
66	1	2.561185	3.025671	1.871012
67	1	-1.465572	-4.769680	-1.006990
68	1	-0.397783	-3.722831	-3.080520
69	1	-2.811262	-3.189494	-2.463185
70	1	0.510843	4.519925	-1.038169
71	1	-1.525435	5.048331	-0.098912
72	1	-1.419101	3.936436	-2.531808

73	72	0.742606	-0.020981	-0.136856

2b (E = -939.46813 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.689074	-0.513928	-0.360712
2	7	-2.760463	0.159838	-3.135545
3	6	1.820517	-0.751259	-0.625650
4	6	1.607329	0.065964	0.526097
5	6	1.366894	-0.031583	-1.768790
6	17	-0.849193	-2.778354	-1.457793
7	6	1.026747	1.295730	0.089589
8	6	0.875462	1.234459	-1.326311
9	6	-2.112267	-0.052507	-2.195915
10	6	-3.590080	0.360106	-4.325186
11	6	-1.110211	-1.316288	1.734316
12	6	-2.473625	-1.384450	1.195801
13	1	-0.908840	-0.524972	2.458543
14	6	-2.157578	0.975555	0.611839
15	6	-3.005827	-0.229300	0.636912
16	1	-1.741322	1.290557	1.570911
17	1	-2.598755	1.822335	0.087589
18	6	-4.411359	-0.162791	0.065778
19	6	-3.202815	-2.712217	1.228312
20	1	-3.969911	-2.806684	0.454870
21	1	-3.688429	-2.845719	2.206261
22	1	-2.492709	-3.535368	1.096959
23	1	-4.731494	-1.093346	-0.413192
24	1	-4.490161	0.645462	-0.668998
25	1	-5.127266	0.061834	0.870198
26	6	-4.654658	-0.757864	-4.345205
27	6	-4.243181	1.754048	-4.215048
28	1	-4.181752	-1.743351	-4.384786
29	1	-5.288817	-0.706819	-3.455272
30	1	-4.872790	1.820366	-3.322586
31	1	-3.482356	2.539295	-4.169710
32	6	2.098443	-0.230186	1.922824
33	6	2.530027	-2.083316	-0.651159
34	6	1.508696	-0.488185	-3.201480
35	6	0.421270	2.375598	-2.206789
36	6	0.797016	2.516350	0.946800
37	1	3.129839	0.128583	2.051694
38	1	2.091590	-1.303374	2.136176
39	1	1.481926	0.259789	2.682978
40	1	3.601554	-1.943039	-0.854013
41	1	2.121909	-2.740222	-1.424283
42	1	2.440553	-2.607518	0.305551
43	1	2.519946	-0.273809	-3.575489
44	1	0.799776	0.020819	-3.862766
45	1	1.337355	-1.564657	-3.297158
46	1	1.255290	3.063342	-2.406571
47	1	-0.378764	2.957424	-1.736732
48	1	0.052113	2.019920	-3.173915
49	1	1.704165	3.137111	0.980216
50	1	0.545017	2.249220	1.978043
51	1	-0.016670	3.136853	0.559194
52	1	-4.869363	1.926827	-5.095549
53	1	-5.285390	-0.635221	-5.231073
54	1	-0.697753	-2.270824	2.056638
55	6	-2.665479	0.271344	-5.558226
56	1	-3.262672	0.411058	-6.464461
57	1	-1.896372	1.049279	-5.525787
58	1	-2.178573	-0.707006	-5.608430

TS2b-3d (E = -939.432908 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.701367	-0.696807	-0.659131
2	7	-3.150078	0.996561	-2.325311
3	6	1.813868	-0.612120	-0.701341
4	6	1.414831	0.240524	0.374241
5	6	1.379966	-0.018884	-1.923540
6	17	-0.617547	-2.848419	-1.803949
7	6	0.718134	1.350816	-0.185245
8	6	0.705556	1.198111	-1.606119
9	6	-2.299188	0.379715	-1.695250
10	6	-3.450319	0.839761	-3.789267
11	6	-1.024876	-1.386481	1.476659
12	6	-2.385095	-1.781257	1.051262
13	1	-0.994843	-0.556451	2.187187
14	6	-2.650039	0.556441	0.275491
15	6	-3.184201	-0.824805	0.471684
16	1	-1.994348	0.935030	1.060945
17	1	-3.398942	1.302900	0.050545
18	6	-4.615691	-1.057206	0.037599
19	6	-2.796447	-3.226357	1.234200
20	1	-3.633289	-3.529588	0.600915
21	1	-3.081545	-3.396227	2.282606
22	1	-1.951444	-3.888873	1.016315
23	1	-4.844931	-2.109522	-0.145522
24	1	-4.839816	-0.492556	-0.872154
25	1	-5.300006	-0.695005	0.819657
26	6	-4.904150	0.326528	-3.875838
27	6	-3.352560	2.248869	-4.409171
28	1	-4.988910	-0.673506	-3.437436
29	1	-5.582729	1.000641	-3.343228
30	1	-4.022721	2.942643	-3.891459
31	1	-2.331324	2.637206	-4.338709
32	6	1.838398	0.094647	1.814738
33	6	2.667099	-1.851695	-0.575155
34	6	1.710562	-0.520531	-3.308720
35	6	0.273550	2.257313	-2.590576
36	6	0.255197	2.577199	0.565996
37	1	2.818041	0.568443	1.969921
38	1	1.928089	-0.954809	2.110412
39	1	1.130592	0.571224	2.499672
40	1	3.732496	-1.589986	-0.644397
41	1	2.447536	-2.574275	-1.366055
42	1	2.513798	-2.354521	0.385105
43	1	2.703128	-0.163226	-3.617197
44	1	0.988258	-0.169601	-4.052097
45	1	1.719683	-1.613477	-3.349734
46	1	1.084166	2.985499	-2.735832
47	1	-0.607829	2.804769	-2.244935
48	1	0.036925	1.830571	-3.568979
49	1	1.057699	3.327434	0.603297
50	1	-0.019763	2.345007	1.600171
51	1	-0.610911	3.045810	0.088228
52	1	-3.635748	2.211888	-5.466934
53	1	-5.217790	0.271139	-4.924315
54	1	-0.418960	-2.215580	1.842323
55	6	-2.498349	-0.139516	-4.502101
56	1	-2.784371	-0.232930	-5.555794
57	1	-1.463401	0.214822	-4.460924
58	1	-2.536576	-1.132391	-4.043243

3d (E = -939.4489857 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.706931	-0.707506	-0.799033
2	7	-3.394362	0.951472	-2.201016
3	6	1.803284	-0.645218	-0.901257
4	6	1.453890	0.123761	0.248379
5	6	1.340642	0.049366	-2.060104
6	17	-0.692537	-2.923174	-1.758286
7	6	0.754741	1.281604	-0.199684
8	6	0.697707	1.248807	-1.625570
9	6	-2.548358	0.541167	-1.337768
10	6	-3.308935	0.725202	-3.670183
11	6	-1.133646	-1.124413	1.352898
12	6	-2.533330	-1.577910	1.079319
13	1	-1.079137	-0.221706	1.967560
14	6	-3.043440	0.696386	0.131868
15	6	-3.442118	-0.723438	0.530918
16	1	-2.286772	1.110657	0.804889
17	1	-3.902139	1.372040	0.147314
18	6	-4.876016	-1.060167	0.197129
19	6	-2.831735	-3.027566	1.414202
20	1	-3.779283	-3.387542	1.008584
21	1	-2.856255	-3.155285	2.505541
22	1	-2.034913	-3.675944	1.030432
23	1	-5.100905	-2.126946	0.252059
24	1	-5.116856	-0.704091	-0.812027
25	1	-5.552805	-0.534992	0.887626
26	6	-4.645857	0.046590	-4.058013
27	6	-3.241988	2.123084	-4.328908
28	1	-4.722404	-0.943693	-3.594032
29	1	-5.491891	0.652849	-3.718727
30	1	-4.072577	2.745126	-3.978945
31	1	-2.304817	2.630057	-4.076014
32	6	1.911559	-0.147154	1.659464
33	6	2.652510	-1.893830	-0.908050
34	6	1.661576	-0.345957	-3.483178
35	6	0.259636	2.403994	-2.492370
36	6	0.312144	2.438792	0.664565
37	1	2.893811	0.315001	1.830730
38	1	2.013183	-1.218484	1.858071
39	1	1.221119	0.264125	2.401579
40	1	3.716467	-1.627660	-0.981650
41	1	2.410597	-2.542212	-1.754696
42	1	2.522789	-2.481619	0.006178
43	1	2.716048	-0.130536	-3.704460
44	1	1.055704	0.204878	-4.207168
45	1	1.499788	-1.414559	-3.658851
46	1	1.038501	3.179658	-2.496878
47	1	-0.665530	2.862420	-2.131747
48	1	0.096384	2.099533	-3.528914
49	1	1.125516	3.171704	0.762237
50	1	0.043302	2.116915	1.675832
51	1	-0.548659	2.962437	0.236999
52	1	-3.305588	2.035935	-5.419942
53	1	-4.712376	-0.075224	-5.145738
54	1	-0.528178	-1.902814	1.819267
55	6	-2.142109	-0.152998	-4.157335
56	1	-2.188417	-0.265595	-5.247090
57	1	-1.176368	0.294289	-3.910404
58	1	-2.186199	-1.154705	-3.716090

6b (E = -1190.1354416 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.319960	-0.161233	0.179956
2	7	2.358136	0.462847	-0.534706

3	6	-0.806236	-2.447596	0.237915
4	6	-0.608739	-2.084697	1.606160
5	6	0.476191	-2.629492	-0.359655
6	17	-0.383864	0.421503	-2.233860
7	6	0.796024	-2.059278	1.852707
8	6	1.463554	-2.401549	0.643444
9	6	2.205053	0.786101	0.687796
10	6	3.388402	0.874826	-1.556306
11	6	-0.049266	1.242357	2.094414
12	6	0.466780	2.637505	1.916897
13	1	0.561530	0.699475	2.822630
14	6	2.806493	1.793704	1.617701
15	6	1.779797	2.926934	1.740958
16	1	2.966180	1.308667	2.591517
17	1	3.770572	2.198304	1.296539
18	6	2.389057	4.312647	1.660601
19	6	-0.611408	3.709915	1.951686
20	1	-0.270267	4.696338	1.628080
21	1	-1.025716	3.807077	2.965772
22	1	-1.441958	3.414243	1.296995
23	1	1.650009	5.111527	1.755312
24	1	2.924318	4.465203	0.711116
25	1	3.129342	4.456110	2.462707
26	6	3.119135	2.343392	-1.951903
27	6	4.813269	0.705288	-0.984792
28	1	2.102309	2.449998	-2.341820
29	1	3.235002	3.011545	-1.092818
30	1	5.007275	1.388062	-0.153292
31	1	4.969277	-0.320895	-0.634330
32	6	-1.681122	-1.926409	2.657665
33	6	-2.118168	-2.764211	-0.440291
34	6	0.716060	-3.142319	-1.760298
35	6	2.946391	-2.635700	0.501807
36	6	1.453432	-1.886854	3.200708
37	1	-1.814764	-2.862483	3.218310
38	1	-2.647729	-1.668055	2.214558
39	1	-1.429683	-1.142284	3.379639
40	1	-2.252389	-3.852511	-0.519430
41	1	-2.163057	-2.351189	-1.453785
42	1	-2.970116	-2.367904	0.119532
43	1	0.576379	-4.232413	-1.799051
44	1	1.733196	-2.927204	-2.100535
45	1	0.027331	-2.689592	-2.480047
46	1	3.198243	-3.669877	0.776819
47	1	3.526113	-1.971203	1.150386
48	1	3.286326	-2.474067	-0.525048
49	1	1.615537	-2.865415	3.675429
50	1	0.836337	-1.292091	3.880809
51	1	2.428572	-1.394799	3.121148
52	1	5.549402	0.912682	-1.770054
53	1	3.826637	2.655697	-2.729103
54	1	-1.071974	1.269750	2.479426
55	6	3.214573	-0.040424	-2.783065
56	1	3.915943	0.254621	-3.572098
57	1	3.418942	-1.084259	-2.518887
58	1	2.194134	0.026205	-3.167542
59	7	-3.099164	0.756793	0.209857
60	6	-1.992867	0.398317	0.209890
61	6	-4.468796	1.262800	0.125506
62	6	-5.287293	0.273355	-0.731242
63	1	-6.315095	0.638938	-0.819490
64	1	-4.859683	0.184541	-1.734152
65	1	-5.310135	-0.717940	-0.268066

66	6	-4.407859	2.653567	-0.542940
67	1	-5.422426	3.055120	-0.628486
68	1	-3.807578	3.346195	0.054683
69	1	-3.971640	2.583313	-1.543517
70	6	-5.031440	1.357355	1.559257
71	1	-4.428803	2.036771	2.169564
72	1	-6.056248	1.739416	1.520718
73	1	-5.045313	0.373091	2.037815

TS6b-7b (E = -1190.1031877 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.341076	-0.482186	-0.099537
2	7	2.304729	0.421702	-0.631760
3	6	-0.854651	-2.680226	0.359194
4	6	-0.668836	-2.066617	1.632119
5	6	0.433310	-3.009634	-0.162383
6	17	-0.137708	-0.597992	-2.545933
7	6	0.735063	-1.999894	1.893948
8	6	1.413965	-2.586588	0.784972
9	6	1.991122	0.752144	0.564953
10	6	3.374467	0.858706	-1.592512
11	6	-0.564261	1.549695	1.740958
12	6	0.106984	2.829493	1.395500
13	1	0.073577	0.856398	2.287899
14	6	2.414488	1.813934	1.531046
15	6	1.454095	2.991287	1.315655
16	1	2.307951	1.415576	2.547689
17	1	3.446350	2.148627	1.417113
18	6	2.177074	4.292072	1.021205
19	6	-0.857421	3.978294	1.144692
20	1	-0.372665	4.891260	0.796743
21	1	-1.411947	4.224349	2.060902
22	1	-1.595163	3.690267	0.387171
23	1	1.508308	5.136930	0.849550
24	1	2.822493	4.197415	0.135794
25	1	2.836564	4.559591	1.860493
26	6	2.775033	1.987091	-2.462367
27	6	4.655362	1.336509	-0.878598
28	1	1.877616	1.633734	-2.977833
29	1	2.506894	2.853275	-1.847940
30	1	4.514140	2.298016	-0.377490
31	1	4.991670	0.600693	-0.139003
32	6	-1.763795	-1.734750	2.616757
33	6	-2.181415	-3.010784	-0.279052
34	6	0.699194	-3.803097	-1.419427
35	6	2.898479	-2.853068	0.710241
36	6	1.371218	-1.598300	3.203729
37	1	-1.956142	-2.597840	3.269778
38	1	-2.699679	-1.489150	2.107905
39	1	-1.499474	-0.889444	3.259887
40	1	-2.583956	-3.950819	0.124549
41	1	-2.083259	-3.126611	-1.362206
42	1	-2.920808	-2.223539	-0.101830
43	1	0.633164	-4.879853	-1.208021
44	1	1.697148	-3.604978	-1.822261
45	1	-0.021659	-3.566620	-2.206105
46	1	3.146711	-3.783246	1.240667
47	1	3.481385	-2.047617	1.168826
48	1	3.239381	-2.963034	-0.323300
49	1	1.403757	-2.455855	3.891009
50	1	0.813302	-0.801727	3.707060
51	1	2.399452	-1.249296	3.066086
52	1	5.454810	1.462652	-1.617441

53	1	3.508864	2.307024	-3.211209
54	1	-1.473493	1.699732	2.312620
55	6	3.695077	-0.368653	-2.471204
56	1	4.411175	-0.092481	-3.253196
57	1	4.137600	-1.170653	-1.869090
58	1	2.783382	-0.744877	-2.942878
59	7	-2.762919	0.732081	0.026024
60	6	-1.569965	0.578068	0.241585
61	6	-4.001877	1.413299	0.456487
62	6	-4.288328	2.521794	-0.583235
63	1	-5.254288	2.990977	-0.366642
64	1	-3.514414	3.294951	-0.558681
65	1	-4.321095	2.097705	-1.591431
66	6	-3.966325	1.999762	1.884567
67	1	-4.962730	2.380285	2.137405
68	1	-3.703467	1.230431	2.618471
69	1	-3.260795	2.827736	1.970274
70	6	-5.115418	0.339906	0.378296
71	1	-4.929775	-0.464347	1.099020
72	1	-6.087431	0.790088	0.607716
73	1	-5.154054	-0.095222	-0.624570

7b (E = -1190.1623931 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.042608	-0.558372	0.081051
2	7	1.805435	0.419630	-0.704035
3	6	-0.925862	-2.891918	0.528119
4	6	-0.791087	-2.282412	1.806588
5	6	0.387418	-3.066541	-0.018367
6	17	-0.877571	-0.697970	-2.343275
7	6	0.598591	-2.057060	2.045499
8	6	1.324382	-2.558183	0.922232
9	6	1.653218	0.716332	0.532225
10	6	2.718795	0.879103	-1.805626
11	6	-0.673993	1.966725	2.447791
12	6	0.143149	3.143117	1.880189
13	1	-0.096785	1.482040	3.242665
14	6	2.231966	1.731663	1.484257
15	6	1.420249	3.040454	1.458513
16	1	2.178980	1.297168	2.488008
17	1	3.281436	1.964213	1.291119
18	6	2.238613	4.209776	0.938022
19	6	-0.644603	4.442156	1.887538
20	1	-0.101744	5.292603	1.474453
21	1	-0.937458	4.699108	2.915450
22	1	-1.573469	4.334529	1.313061
23	1	1.686237	5.147897	0.880271
24	1	2.626406	3.994036	-0.065578
25	1	3.112313	4.374498	1.584589
26	6	1.984708	2.000321	-2.574673
27	6	4.083729	1.367070	-1.279849
28	1	1.024252	1.633210	-2.947672
29	1	1.801281	2.865682	-1.928374
30	1	4.002160	2.304772	-0.723835
31	1	4.545075	0.613534	-0.631127
32	6	-1.908486	-2.031939	2.791098
33	6	-2.198984	-3.418600	-0.091476
34	6	0.700054	-3.797381	-1.302062
35	6	2.828616	-2.637413	0.815182
36	6	1.204629	-1.569512	3.339829
37	1	-2.119865	-2.938114	3.376345
38	1	-2.836929	-1.740938	2.288703
39	1	-1.652737	-1.236209	3.498557

40	1	-2.282279	-4.504349	0.062017
41	1	-2.230116	-3.229825	-1.169418
42	1	-3.085221	-2.954615	0.352609
43	1	0.618923	-4.884159	-1.155171
44	1	1.716199	-3.586479	-1.650064
45	1	0.011346	-3.512156	-2.103191
46	1	3.202731	-3.558599	1.284075
47	1	3.317092	-1.793620	1.314310
48	1	3.161086	-2.641004	-0.227518
49	1	1.348905	-2.405135	4.040020
50	1	0.565523	-0.833256	3.838394
51	1	2.183226	-1.105499	3.179831
52	1	4.757290	1.541750	-2.126606
53	1	2.591995	2.328044	-3.426473
54	1	-1.583026	2.359949	2.907677
55	6	2.924579	-0.339159	-2.730308
56	1	3.521116	-0.051380	-3.603440
57	1	3.454852	-1.139998	-2.201932
58	1	1.958713	-0.722803	-3.069312
59	7	-1.841845	0.697909	0.517971
60	6	-0.933992	0.921122	1.392659
61	6	-3.156824	1.334459	0.164776
62	6	-2.883003	2.354097	-0.963558
63	1	-3.824560	2.808875	-1.292831
64	1	-2.216277	3.152138	-0.618371
65	1	-2.415704	1.853116	-1.816263
66	6	-3.834323	2.011791	1.373001
67	1	-4.847835	2.321536	1.093618
68	1	-3.914035	1.317501	2.217519
69	1	-3.295946	2.904013	1.703289
70	6	-4.057276	0.198800	-0.364689
71	1	-4.270135	-0.527571	0.428487
72	1	-5.010266	0.608677	-0.718018
73	1	-3.564209	-0.319695	-1.191076

TS8a-9 (E = -1190.1348497 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.630231	-0.264385	-0.165254
2	7	-0.140954	-0.545031	1.691250
3	6	-0.629341	0.750158	1.548691
4	7	-1.882238	-0.840343	-0.789595
5	6	2.953524	0.470202	0.534289
6	6	2.225258	1.662816	0.224460
7	6	3.172004	-0.233791	-0.683031
8	17	1.092241	-2.612384	-0.789066
9	6	1.973499	1.672120	-1.186025
10	6	2.544849	0.488969	-1.737147
11	6	-0.206780	-1.258943	2.994337
12	6	-2.351670	0.198730	-0.213672
13	6	-2.776097	-1.833607	-1.499320
14	6	-1.353341	1.163945	0.351825
15	1	-0.348741	1.532475	2.249935
16	6	-2.101038	2.480129	0.417199
17	1	-0.554364	1.210320	-0.742374
18	6	-3.726766	0.829738	-0.094456
19	6	-3.410695	2.282006	0.186566
20	1	-4.333291	0.701360	-0.993247
21	1	-4.296816	0.387466	0.733104
22	6	-4.537495	3.278039	0.237417
23	6	-1.440277	3.779032	0.785938
24	1	-2.172724	4.583886	0.890457
25	1	-0.715319	4.087486	0.023320

26	1	-0.897997	3.697360	1.735277
27	1	-4.193459	4.293101	0.452744
28	1	-5.268955	2.999280	1.009478
29	1	-5.078926	3.302220	-0.718695
30	6	0.682391	-2.511501	2.900385
31	6	0.272256	-0.362585	4.160765
32	6	-1.676748	-1.677564	3.240929
33	1	-2.017791	-2.352205	2.448581
34	1	-2.328085	-0.795654	3.251031
35	1	-0.372029	0.515113	4.284887
36	1	1.299358	-0.021810	3.992467
37	1	1.730821	-2.232567	2.750901
38	1	0.377523	-3.137772	2.057495
39	6	-3.213927	-1.208314	-2.847053
40	6	-1.970537	-3.109952	-1.801399
41	6	-3.998276	-2.240429	-0.640138
42	1	-3.673049	-2.557839	0.356921
43	1	-4.733526	-1.441151	-0.529273
44	1	-3.818751	-0.306899	-2.711614
45	1	-2.333506	-0.944496	-3.443099
46	1	-1.093824	-2.890134	-2.412680
47	1	-1.621126	-3.584267	-0.881336
48	6	2.103079	2.845274	1.157721
49	6	3.625728	0.168771	1.853246
50	6	4.072070	-1.430687	-0.847411
51	6	2.559448	0.111182	-3.200195
52	6	1.438513	2.829611	-1.996866
53	1	3.061134	3.384602	1.201125
54	1	1.853227	2.544250	2.180037
55	1	1.344992	3.556226	0.823895
56	1	4.633639	0.609359	1.882580
57	1	3.733781	-0.907962	2.018535
58	1	3.063873	0.579528	2.697093
59	1	5.108804	-1.094399	-0.996522
60	1	3.785534	-2.040364	-1.707616
61	1	4.052255	-2.080524	0.032125
62	1	3.453343	0.509105	-3.701904
63	1	1.685758	0.508379	-3.729451
64	1	2.562853	-0.975680	-3.333764
65	1	2.267349	3.456259	-2.357934
66	1	0.774584	3.469841	-1.410326
67	1	0.877502	2.489122	-2.873461
68	1	0.249489	-0.928903	5.098838
69	1	0.608559	-3.097511	3.823716
70	1	-1.774144	-2.192129	4.204248
71	1	-2.609830	-3.817156	-2.342376
72	1	-3.807506	-1.933297	-3.415115
73	1	-4.503739	-3.087884	-1.115908

9 (E = -1190.1733043 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.377497	-0.244598	-0.371081
2	7	-0.290506	-0.306390	1.725793
3	6	-0.979244	0.829402	1.772406
4	7	-1.948507	-0.837190	-0.477163
5	6	2.828899	0.304534	0.336809
6	6	2.095077	1.532428	0.366916
7	6	2.933404	-0.103938	-1.022205
8	17	0.887544	-2.487645	-1.215472
9	6	1.725376	1.856443	-0.966459
10	6	2.230905	0.832322	-1.824436
11	6	-0.056461	-1.080424	2.991629
12	6	-2.388422	0.362385	-0.241137

13	6	-2.750987	-1.910763	-1.168677
14	6	-1.710054	1.282320	0.666072
15	1	-0.987772	1.434648	2.682531
16	6	-2.366681	2.603272	0.567536
17	1	-0.376559	0.705791	-1.734180
18	6	-3.546279	1.150803	-0.852730
19	6	-3.384736	2.550608	-0.313001
20	1	-3.498796	1.103930	-1.946292
21	1	-4.519928	0.750846	-0.560367
22	6	-4.334994	3.634464	-0.740014
23	6	-1.948295	3.782645	1.407091
24	1	-2.528436	4.676753	1.162548
25	1	-0.887132	4.021927	1.267039
26	1	-2.092249	3.580404	2.477568
27	1	-4.101479	4.597602	-0.276423
28	1	-5.372445	3.379608	-0.478094
29	1	-4.308966	3.772793	-1.830465
30	6	0.800387	-2.312614	2.649743
31	6	0.634463	-0.239506	4.089993
32	6	-1.437907	-1.556452	3.509178
33	1	-1.947066	-2.148151	2.742281
34	1	-2.075805	-0.702452	3.766063
35	1	0.046579	0.643674	4.363367
36	1	1.627162	0.089725	3.773003
37	1	1.787800	-2.023093	2.282314
38	1	0.312391	-2.919051	1.880783
39	6	-2.367351	-1.959095	-2.665694
40	6	-2.395382	-3.243616	-0.465318
41	6	-4.287963	-1.749340	-1.045332
42	1	-4.584386	-1.520069	-0.015287
43	1	-4.692783	-0.987189	-1.714712
44	1	-2.592160	-1.003872	-3.153775
45	1	-1.304151	-2.170369	-2.793361
46	1	-1.321159	-3.421259	-0.472845
47	1	-2.743675	-3.223614	0.574418
48	6	1.987223	2.454533	1.557375
49	6	3.662534	-0.258531	1.463324
50	6	3.803493	-1.224871	-1.528423
51	6	2.137137	0.811386	-3.330698
52	6	1.070484	3.136362	-1.422279
53	1	2.908831	3.046078	1.658916
54	1	1.843604	1.910254	2.494301
55	1	1.158712	3.160088	1.451123
56	1	4.674956	0.171146	1.433577
57	1	3.771954	-1.345669	1.391251
58	1	3.243011	-0.027078	2.445643
59	1	4.835868	-0.865895	-1.652220
60	1	3.460348	-1.600191	-2.496143
61	1	3.822590	-2.073574	-0.838824
62	1	2.989073	1.338041	-3.784727
63	1	1.218956	1.294395	-3.678495
64	1	2.137632	-0.212456	-3.719736
65	1	1.825924	3.922033	-1.570223
66	1	0.341756	3.506886	-0.695547
67	1	0.540523	2.994174	-2.368076
68	1	0.752717	-0.847221	4.993935
69	1	0.937492	-2.931924	3.543035
70	1	-1.314379	-2.174853	4.405578
71	1	-2.892702	-4.075556	-0.977688
72	1	-2.942017	-2.746028	-3.168641
73	1	-4.754832	-2.701198	-1.320847

TS9-10 (E = -1190.1649824 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		

		X	Y	Z
1	72	0.412916	-0.086370	-0.266122
2	7	-0.129159	-0.253089	1.763995
3	6	-1.056682	0.719355	2.021231
4	7	-1.942624	-0.199506	-0.788744
5	6	2.819685	0.702416	0.296601
6	6	2.234178	1.680933	-0.558224
7	6	2.967971	-0.500565	-0.448971
8	17	0.354962	-2.600904	-0.688257
9	6	2.070231	1.100337	-1.853027
10	6	2.502429	-0.246458	-1.782408
11	6	0.247446	-1.070834	2.989074
12	6	-2.636907	0.555153	0.009084
13	6	-2.528465	-0.867426	-2.030054
14	6	-2.112157	1.134782	1.245734
15	1	-0.990695	1.202191	2.993444
16	6	-3.071795	2.149724	1.727239
17	1	-0.269304	1.487020	-0.895752
18	6	-4.058470	1.110075	-0.130260
19	6	-4.190005	2.120608	0.979084
20	1	-4.212089	1.589074	-1.095625
21	1	-4.809298	0.314535	-0.046164
22	6	-5.454444	2.920486	1.120037
23	6	-2.799099	3.020442	2.925822
24	1	-3.582042	3.771654	3.061334
25	1	-1.840772	3.545759	2.820816
26	1	-2.745917	2.429781	3.850865
27	1	-5.396460	3.648168	1.934841
28	1	-6.315930	2.265945	1.317641
29	1	-5.679626	3.468584	0.193778
30	6	1.386705	-2.043471	2.646033
31	6	0.694839	-0.183476	4.178877
32	6	-1.003252	-1.892698	3.389573
33	1	-1.311626	-2.538510	2.560973
34	1	-1.842554	-1.235833	3.645669
35	1	-0.121527	0.413108	4.598347
36	1	1.504666	0.490068	3.882769
37	1	2.309155	-1.507164	2.417959
38	1	1.126600	-2.669423	1.790910
39	6	-1.396479	-1.005915	-3.077673
40	6	-3.055578	-2.255738	-1.599547
41	6	-3.665441	-0.099545	-2.757565
42	1	-4.616522	-0.126566	-2.225051
43	1	-3.387425	0.939568	-2.963003
44	1	-1.006445	-0.016344	-3.345385
45	1	-0.584133	-1.639341	-2.725045
46	1	-2.259926	-2.845271	-1.140863
47	1	-3.875457	-2.146772	-0.879341
48	6	2.015807	3.132890	-0.210361
49	6	3.394708	1.009878	1.659417
50	6	3.723342	-1.745056	-0.051609
51	6	2.646394	-1.210066	-2.935414
52	6	1.622392	1.838490	-3.089928
53	1	2.923179	3.721537	-0.411254
54	1	1.767901	3.264296	0.848554
55	1	1.197022	3.561825	-0.795489
56	1	4.327975	1.580188	1.547962
57	1	3.632405	0.105087	2.223922
58	1	2.715876	1.616038	2.268397
59	1	4.638399	-1.837642	-0.653399
60	1	3.125990	-2.648905	-0.212568
61	1	4.024863	-1.721617	0.999173
62	1	3.683271	-1.210557	-3.301964

63	1	2.001518	-0.938512	-3.777518
64	1	2.394785	-2.231810	-2.636218
65	1	2.464534	2.388070	-3.534759
66	1	0.832971	2.560823	-2.859976
67	1	1.238100	1.156278	-3.855219
68	1	1.064588	-0.829228	4.982981
69	1	1.579381	-2.691646	3.508374
70	1	-0.780901	-2.520927	4.259974
71	1	-3.437418	-2.795798	-2.474370
72	1	-1.798107	-1.465162	-3.987555
73	1	-3.827416	-0.592247	-3.722178

10 (E = -1190.1641448 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.637739	-0.094101	0.024318
2	7	0.281052	1.766573	-0.347715
3	6	1.523515	1.800631	0.231286
4	7	1.380294	-1.251040	-0.403534
5	6	-2.747489	0.815776	1.196088
6	6	-2.171048	-0.139840	2.082351
7	6	-3.205515	0.119926	0.037838
8	17	-0.950089	-0.532280	-2.488145
9	6	-2.311017	-1.432319	1.494541
10	6	-2.938282	-1.273659	0.231089
11	6	2.455727	-0.561492	-0.152234
12	6	2.473038	0.815478	0.332734
13	1	1.845756	2.771769	0.600249
14	6	3.823318	1.084790	0.873594
15	1	0.264707	-0.426142	1.585738
16	6	3.922538	-0.993987	-0.201467
17	6	4.656291	0.069732	0.575140
18	1	4.109591	-1.993755	0.184513
19	1	4.259425	-0.996652	-1.246590
20	6	6.126202	-0.076215	0.851314
21	6	4.165748	2.360051	1.597887
22	1	5.184561	2.333883	1.994109
23	1	3.480677	2.532539	2.438285
24	1	4.091961	3.232419	0.933861
25	1	6.523994	0.761780	1.431267
26	1	6.700508	-0.136550	-0.084967
27	1	6.333612	-1.000398	1.409712
28	6	-1.713841	0.137727	3.492732
29	6	-3.056286	2.242099	1.590836
30	6	-4.069853	0.650560	-1.080752
31	6	-3.439885	-2.358951	-0.690138
32	6	-1.950918	-2.724569	2.187725
33	1	-2.569337	0.120100	4.184598
34	1	-1.237901	1.119780	3.579518
35	1	-0.988576	-0.608239	3.829268
36	1	-3.900234	2.255011	2.295409
37	1	-3.338997	2.861451	0.736162
38	1	-2.210321	2.725085	2.090901
39	1	-5.068720	0.194814	-1.030242
40	1	-3.647179	0.417347	-2.064023
41	1	-4.202606	1.733845	-1.016456
42	1	-4.536075	-2.420717	-0.633405
43	1	-3.042675	-3.342175	-0.421458
44	1	-3.169656	-2.157310	-1.731578
45	1	-2.626108	-2.901887	3.036405
46	1	-0.928560	-2.702560	2.583117

47	1	-2.037075	-3.586059	1.518960
48	6	-0.079493	3.074879	-1.036607
49	6	-0.153736	4.246830	-0.027109
50	6	0.992049	3.367093	-2.116505
51	6	-1.439544	2.930128	-1.736919
52	1	-0.886716	4.036569	0.756999
53	1	0.809651	4.457284	0.448852
54	1	1.982060	3.521259	-1.673661
55	1	1.056401	2.530256	-2.819781
56	1	-1.426925	2.102686	-2.449318
57	1	-2.237556	2.756383	-1.014414
58	6	1.471608	-2.742789	-0.720141
59	6	0.064450	-3.288515	-1.041185
60	6	2.361843	-3.030273	-1.952597
61	6	1.948053	-3.504051	0.547544
62	1	-0.649292	-3.038098	-0.249338
63	1	-0.315639	-2.907049	-1.987094
64	1	2.074901	-2.373859	-2.780694
65	1	3.427675	-2.906614	-1.757303
66	1	2.944031	-3.217210	0.885347
67	1	1.250806	-3.326168	1.372363
68	1	1.963806	-4.578949	0.335016
69	1	2.205553	-4.066942	-2.271292
70	1	0.113983	-4.381806	-1.093298
71	1	-0.462071	5.158555	-0.551365
72	1	-1.671598	3.855254	-2.276562
73	1	0.724594	4.272123	-2.673774

TS10-11 (E = -1190.1494677 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.724331	0.302693	0.114016
2	7	-0.040939	0.133624	-1.750679
3	6	-1.119581	-0.735246	-1.469369
4	7	-1.321781	0.833832	1.011904
5	6	2.769075	-1.153807	-0.328194
6	6	2.077085	-1.767366	0.759065
7	6	3.278891	0.095933	0.127512
8	17	1.125529	2.809750	-0.056962
9	6	2.195720	-0.912210	1.899086
10	6	2.930232	0.239117	1.508406
11	6	-2.385240	0.500815	0.286335
12	6	-2.310167	-0.345897	-0.856969
13	1	-1.160569	-1.650125	-2.062808
14	6	-3.643006	-0.910535	-1.118993
15	1	-0.330289	-1.258743	0.174975
16	6	-3.873766	0.705122	0.561816
17	6	-4.558887	-0.292468	-0.341942
18	1	-4.160190	0.576354	1.604082
19	1	-4.162259	1.727481	0.284609
20	6	-6.056366	-0.421727	-0.341969
21	6	-3.884775	-1.958959	-2.172991
22	1	-4.945442	-2.213227	-2.253331
23	1	-3.337478	-2.883685	-1.945796
24	1	-3.543269	-1.615693	-3.158941
25	1	-6.405465	-1.158508	-1.071894
26	1	-6.537914	0.538247	-0.579947
27	1	-6.430884	-0.727250	0.645748
28	6	1.572510	-3.190009	0.788417
29	6	3.084487	-1.840981	-1.636177
30	6	4.204318	1.029485	-0.615093
31	6	3.421215	1.361409	2.390312
32	6	1.765457	-1.301053	3.295214

33	1	2.382337	-3.875526	1.080214
34	1	1.203612	-3.509016	-0.191104
35	1	0.754233	-3.313306	1.504102
36	1	3.906883	-2.557365	-1.496719
37	1	3.397042	-1.132232	-2.407439
38	1	2.226248	-2.399231	-2.023869
39	1	5.234560	0.915332	-0.248369
40	1	3.913324	2.075986	-0.478483
41	1	4.213257	0.824225	-1.689352
42	1	4.506554	1.276189	2.541285
43	1	2.950483	1.343183	3.377711
44	1	3.224218	2.340752	1.941090
45	1	2.389770	-2.125992	3.666102
46	1	0.724517	-1.644042	3.330461
47	1	1.870416	-0.472698	4.001847
48	6	0.125851	0.536166	-3.192866
49	6	0.116847	-0.691030	-4.137192
50	6	-1.025327	1.498960	-3.572544
51	6	1.468111	1.275320	-3.342868
52	1	0.872461	-1.423062	-3.832110
53	1	-0.859361	-1.186907	-4.165148
54	1	-2.000669	1.014090	-3.457987
55	1	-1.002965	2.383289	-2.927778
56	1	1.517984	2.131457	-2.665867
57	1	2.307823	0.608042	-3.127715
58	6	-1.515364	1.490176	2.374782
59	6	-0.135727	1.891421	2.936241
60	6	-2.361919	2.784059	2.292648
61	6	-2.117019	0.458068	3.365187
62	1	0.554538	1.042383	2.932568
63	1	0.308501	2.710093	2.370405
64	1	-1.993623	3.421317	1.482047
65	1	-3.425243	2.597393	2.138949
66	1	-3.091326	0.077003	3.056131
67	1	-1.440965	-0.397044	3.469558
68	1	-2.235145	0.924670	4.349958
69	1	-2.259685	3.337884	3.232669
70	1	-0.249991	2.207577	3.978891
71	1	0.347715	-0.365703	-5.157613
72	1	1.576588	1.635761	-4.372174
73	1	-0.920641	1.821065	-4.615601

11 (E = -1190.1946865 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.704899	-0.007078	-0.206806
2	7	0.462020	1.611383	-0.192266
3	6	1.272653	1.183182	0.987423
4	7	0.925501	-1.416267	-0.227145
5	6	-2.389058	1.215853	1.294591
6	6	-1.900945	0.106367	2.052170
7	6	-3.165784	0.700155	0.222294
8	17	-1.360267	-0.155359	-2.561091
9	6	-2.432400	-1.093039	1.476493
10	6	-3.198987	-0.727341	0.340140
11	6	2.198003	-0.924995	0.089211
12	6	2.423348	0.293409	0.669536
13	1	1.524370	2.032144	1.626067
14	6	3.860694	0.528944	0.857829
15	1	0.592411	0.579104	1.635365
16	6	3.571736	-1.521419	-0.207979
17	6	4.551854	-0.523628	0.363919
18	1	3.730741	-2.521215	0.204069
19	1	3.715751	-1.603263	-1.290758

20	6	6.034867	-0.775683	0.334652
21	6	4.411225	1.758105	1.535874
22	1	5.500098	1.710673	1.633016
23	1	3.991460	1.876653	2.544587
24	1	4.168126	2.672000	0.977346
25	1	6.596154	0.051584	0.782040
26	1	6.403445	-0.905281	-0.693689
27	1	6.301369	-1.691190	0.883902
28	6	-1.238895	0.179013	3.411105
29	6	-2.250280	2.667913	1.682645
30	6	-3.968442	1.499900	-0.775198
31	6	-4.036005	-1.634099	-0.528976
32	6	-2.389082	-2.441140	2.158595
33	1	-1.996468	0.095664	4.203994
34	1	-0.715257	1.128175	3.561965
35	1	-0.517390	-0.631135	3.565416
36	1	-3.026350	2.942256	2.411508
37	1	-2.359219	3.330933	0.819954
38	1	-1.278483	2.879105	2.138847
39	1	-5.017978	1.569143	-0.454883
40	1	-3.952122	1.038464	-1.767435
41	1	-3.588137	2.520864	-0.878810
42	1	-5.103698	-1.498584	-0.306745
43	1	-3.798202	-2.689673	-0.366642
44	1	-3.890522	-1.419212	-1.593443
45	1	-3.033888	-2.425623	3.048958
46	1	-1.381777	-2.710132	2.494389
47	1	-2.752406	-3.244177	1.511296
48	6	0.864864	2.844205	-0.930866
49	6	1.195591	4.011178	0.032277
50	6	2.090800	2.547831	-1.832113
51	6	-0.319876	3.273684	-1.823410
52	1	0.363010	4.196712	0.719975
53	1	2.099404	3.821298	0.620471
54	1	2.950820	2.219842	-1.240743
55	1	1.847519	1.754839	-2.546871
56	1	-0.595356	2.477908	-2.519760
57	1	-1.195442	3.522420	-1.213619
58	6	0.798133	-2.890433	-0.562754
59	6	-0.673753	-3.191281	-0.920302
60	6	1.633087	-3.296391	-1.808373
61	6	1.178104	-3.758377	0.662954
62	1	-1.352136	-2.856595	-0.133066
63	1	-0.960509	-2.721271	-1.863918
64	1	1.516550	-2.549613	-2.601067
65	1	2.694552	-3.420059	-1.592452
66	1	2.199371	-3.570076	1.002245
67	1	0.502492	-3.549901	1.499322
68	1	1.095064	-4.822744	0.411827
69	1	1.265520	-4.256429	-2.189433
70	1	-0.810024	-4.273121	-1.026238
71	1	1.369825	4.924369	-0.547403
72	1	-0.044620	4.161440	-2.404233
73	1	2.377816	3.447107	-2.391308

TS11-12 (E = -1190.1617747 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.357061	-0.305678	-0.107617
2	7	0.401850	-0.424372	1.762001
3	6	-0.478507	1.655278	1.539360
4	7	-1.864662	0.299409	-0.571996
5	6	2.803221	0.413489	-0.214102
6	6	2.065314	1.481440	-0.808764

7	6	2.715334	-0.707513	-1.080849
8	17	0.034943	-2.721004	-0.575190
9	6	1.582845	1.033941	-2.083572
10	6	1.977150	-0.315326	-2.247659
11	6	0.521538	-0.906474	3.134331
12	6	-2.511819	0.988681	0.358161
13	6	-2.627318	-0.232745	-1.783683
14	6	-1.852814	1.574314	1.480266
15	1	0.038741	2.052307	2.399396
16	6	-2.849698	1.940228	2.494237
17	1	0.047714	1.865375	0.605456
18	6	-4.006336	1.200497	0.587094
19	6	-4.089766	1.731214	2.001812
20	1	-4.409732	1.945720	-0.106253
21	1	-4.589434	0.288797	0.443110
22	6	-5.425567	2.022861	2.625158
23	6	-2.466809	2.541258	3.820268
24	1	-3.344907	2.784405	4.424946
25	1	-1.889696	3.465295	3.676037
26	1	-1.837858	1.857227	4.403881
27	1	-5.327008	2.424724	3.638103
28	1	-6.041501	1.114112	2.685369
29	1	-5.993979	2.751927	2.028945
30	6	1.379623	-2.201545	3.100943
31	6	1.210012	0.118992	4.071043
32	6	-0.883822	-1.257527	3.690155
33	1	-1.350866	-2.026107	3.065254
34	1	-1.534386	-0.377656	3.688430
35	1	0.599293	1.020271	4.193703
36	1	2.185453	0.411853	3.669778
37	1	2.395467	-1.979611	2.756262
38	1	0.935151	-2.931603	2.418417
39	6	-3.604258	0.805975	-2.394777
40	6	-1.602448	-0.565586	-2.886061
41	6	-3.373365	-1.531209	-1.391892
42	1	-2.666203	-2.280482	-1.027020
43	1	-4.123035	-1.355900	-0.615628
44	1	-4.548968	0.879795	-1.854957
45	1	-3.141744	1.798880	-2.438833
46	1	-1.101693	0.340218	-3.233689
47	1	-0.860844	-1.291518	-2.549341
48	6	2.090493	2.927695	-0.362763
49	6	3.678462	0.525716	1.009640
50	6	3.449236	-2.018018	-0.925330
51	6	1.810889	-1.183960	-3.470240
52	6	0.966852	1.949353	-3.116942
53	1	2.939649	3.452330	-0.824466
54	1	2.203281	3.022458	0.722324
55	1	1.182222	3.468057	-0.654497
56	1	4.685218	0.866069	0.726114
57	1	3.785886	-0.434185	1.522464
58	1	3.277582	1.242459	1.732102
59	1	4.401491	-1.992552	-1.475309
60	1	2.860158	-2.855703	-1.309816
61	1	3.678281	-2.231826	0.123401
62	1	2.781532	-1.342363	-3.960765
63	1	1.140238	-0.730621	-4.206070
64	1	1.410363	-2.171640	-3.212957
65	1	1.690161	2.721684	-3.414238
66	1	0.074757	2.469980	-2.747113
67	1	0.684676	1.405100	-4.022543
68	1	1.362575	-0.317551	5.065488
69	1	1.441060	-2.643168	4.103691

70	1	-0.812194	-1.636297	4.717684
71	1	-2.124715	-1.012240	-3.739223
72	1	-3.844211	0.502606	-3.419479
73	1	-3.887895	-1.936539	-2.271128

12 (E = -1190.1677161 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.741356	-0.552543	-0.309577
2	7	0.666764	-0.668856	1.510089
3	6	-0.456658	2.373520	0.802894
4	7	-1.657989	0.171337	-0.833221
5	6	3.224351	-0.064022	-0.407640
6	6	2.578998	1.170806	-0.728971
7	6	3.041220	-0.949996	-1.503788
8	17	0.439633	-2.953929	-0.891275
9	6	2.019890	1.043951	-2.042913
10	6	2.301570	-0.265726	-2.515075
11	6	0.726444	-0.912997	2.941567
12	6	-2.299555	0.883128	0.029560
13	6	-2.417939	-0.555283	-1.949983
14	6	-1.650668	1.800034	0.997086
15	1	-0.014157	3.046194	1.525676
16	6	-2.602671	2.044736	2.088389
17	1	0.096461	2.212710	-0.112000
18	6	-3.786064	0.918458	0.378832
19	6	-3.807777	1.534555	1.760795
20	1	-4.340630	1.559931	-0.314166
21	1	-4.249902	-0.068270	0.344220
22	6	-5.090850	1.569509	2.537579
23	6	-2.223052	2.823668	3.317086
24	1	-3.046945	2.884325	4.032748
25	1	-1.930061	3.849018	3.052976
26	1	-1.366447	2.362913	3.823651
27	1	-4.975044	2.056008	3.509602
28	1	-5.466056	0.551194	2.710757
29	1	-5.872346	2.104710	1.979737
30	6	1.608566	-2.157756	3.223214
31	6	1.318351	0.311663	3.686480
32	6	-0.706457	-1.188268	3.472292
33	1	-1.129036	-2.063905	2.966646
34	1	-1.358140	-0.330153	3.273428
35	1	0.713998	1.203760	3.488077
36	1	2.340016	0.509430	3.343929
37	1	2.633103	-1.983387	2.877216
38	1	1.209886	-3.026495	2.688476
39	6	-3.558579	0.305763	-2.553782
40	6	-1.404054	-0.797116	-3.086429
41	6	-2.967175	-1.906081	-1.437547
42	1	-2.161430	-2.536874	-1.056961
43	1	-3.709367	-1.770485	-0.645591
44	1	-4.472680	0.292230	-1.958967
45	1	-3.237978	1.344574	-2.694037
46	1	-1.015113	0.155202	-3.461638
47	1	-0.573414	-1.427722	-2.765047
48	6	2.791031	2.462006	0.031979
49	6	4.148680	-0.285285	0.765037
50	6	3.682018	-2.306982	-1.663119
51	6	2.026074	-0.817983	-3.893225
52	6	1.399197	2.164921	-2.846993
53	1	3.820794	2.819671	-0.113327
54	1	2.635431	2.338264	1.108782
55	1	2.124313	3.257985	-0.314636
56	1	5.167427	0.049297	0.517149

57	1	4.206757	-1.341999	1.042857
58	1	3.820764	0.270300	1.647653
59	1	4.648502	-2.213437	-2.180259
60	1	3.051732	-2.985643	-2.244454
61	1	3.866892	-2.783654	-0.695597
62	1	2.945383	-0.824277	-4.496538
63	1	1.286765	-0.219540	-4.434322
64	1	1.658872	-1.850317	-3.854031
65	1	2.177356	2.751613	-3.356298
66	1	0.828862	2.863139	-2.223674
67	1	0.721981	1.786360	-3.619508
68	1	1.345357	0.141236	4.770763
69	1	1.637744	-2.386682	4.296702
70	1	-0.697720	-1.379156	4.553621
71	1	-1.901327	-1.313499	-3.914206
72	1	-3.813454	-0.100011	-3.538042
73	1	-3.453630	-2.432054	-2.267066

13 (E = -666.6958806 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.011471	0.701890	-0.202820
2	7	1.802987	0.463099	-0.145061
3	6	-0.840155	-1.362796	0.937479
4	6	-0.860651	-1.638254	-0.465075
5	6	-1.848814	-0.380665	1.204649
6	17	-0.673003	3.030086	-0.652366
7	6	-1.880971	-0.823602	-1.053972
8	6	-2.499124	-0.057986	-0.022671
9	6	3.236644	0.226430	-0.078052
10	6	3.754263	0.621506	1.328905
11	6	3.550302	-1.268162	-0.339341
12	6	3.947331	1.094404	-1.147983
13	1	3.726808	2.154196	-0.980242
14	1	3.594531	0.824746	-2.150337
15	1	3.181330	-1.566936	-1.327259
16	1	3.065352	-1.897569	0.415660
17	1	3.259005	0.018387	2.098907
18	1	3.542674	1.678352	1.526657
19	6	-0.098399	-2.743261	-1.160076
20	6	-0.047666	-2.123745	1.975673
21	6	-2.235112	0.143354	2.570461
22	6	-3.682525	0.864491	-0.185454
23	6	-2.314438	-0.859486	-2.503086
24	1	-0.669105	-3.682171	-1.123117
25	1	0.871394	-2.922930	-0.688626
26	1	0.085213	-2.514265	-2.214970
27	1	-0.606162	-3.009752	2.309865
28	1	0.158886	-1.514217	2.861463
29	1	0.912667	-2.464814	1.579104
30	1	-3.033827	-0.472818	3.006407
31	1	-2.608159	1.172096	2.523260
32	1	-1.393057	0.122633	3.270671
33	1	-4.624029	0.317899	-0.034261
34	1	-3.715827	1.309411	-1.184772
35	1	-3.659101	1.687912	0.535364
36	1	-3.129596	-1.583252	-2.641860
37	1	-1.498157	-1.161763	-3.167726
38	1	-2.683005	0.113847	-2.844581
39	1	4.630711	-1.456479	-0.302134
40	1	4.837110	0.462756	1.408131
41	1	5.034829	0.951635	-1.113012

14 (E = -523.4597698 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)

		X	Y	Z
1	7	1.249707	0.739158	-0.017290
2	6	0.070391	0.274623	-0.069988
3	6	2.501634	-0.066433	0.020623
4	6	-1.128359	1.180695	-0.048542
5	6	-2.323279	0.327750	0.010851
6	6	-0.477848	-1.155829	-0.118382
7	6	-1.974777	-0.976992	-0.014275
8	1	-0.209591	-1.654303	-1.056219
9	1	-0.079134	-1.778873	0.689869
10	6	-2.865339	-2.185878	0.026875
11	6	-3.707720	0.913533	0.084126
12	1	-4.480697	0.141988	0.132865
13	1	-3.911214	1.541556	-0.793586
14	1	-3.812420	1.555207	0.969110
15	1	-3.925127	-1.925210	0.094282
16	1	-2.616758	-2.821811	0.888497
17	1	-2.724121	-2.803333	-0.871807
18	6	2.547415	-1.235295	-0.993423
19	6	3.635408	0.927172	-0.323078
20	6	2.701327	-0.587836	1.464518
21	1	2.685176	0.244636	2.175934
22	1	1.914961	-1.296730	1.745789
23	1	1.911644	-2.073713	-0.697781
24	1	2.241046	-0.895811	-1.989810
25	1	3.508631	1.312736	-1.341158
26	1	3.614527	1.776663	0.366805
27	1	4.614452	0.439027	-0.254503
28	1	3.574064	-1.611646	-1.067295
29	1	3.668004	-1.097405	1.550255
30	6	-1.081206	2.520644	-0.078880
31	1	-1.980310	3.124975	-0.057922
32	1	-0.126969	3.031016	-0.124841

15 (E = -914.996662 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.282866	-0.051077	-0.499308
2	7	-0.833090	1.689986	-0.296072
3	6	-1.938922	-1.142504	1.029790
4	6	-0.708398	-1.092813	1.753699
5	6	-1.777217	-2.078640	-0.036573
6	17	-0.157285	-0.601253	-2.912341
7	6	0.193535	-2.028912	1.152627
8	6	-0.466314	-2.636430	0.050156
9	6	-1.384793	3.029089	-0.182291
10	6	-2.807923	3.062831	-0.798277
11	6	-1.461848	3.462372	1.304773
12	6	-0.478408	4.023456	-0.955724
13	1	-0.414971	3.729115	-2.009009
14	1	0.535348	4.018457	-0.537543
15	1	-0.463128	3.445635	1.758255
16	1	-2.104831	2.776428	1.868045
17	1	-3.467772	2.367991	-0.266228
18	1	-2.766501	2.761034	-1.850769
19	6	-0.476534	-0.351081	3.051438
20	6	-3.232212	-0.475308	1.435528
21	6	-2.848470	-2.518812	-1.007979
22	6	0.070577	-3.733825	-0.836890
23	6	1.547511	-2.411432	1.703039
24	1	-0.778602	-0.965111	3.912458
25	1	-1.050258	0.579997	3.090357
26	1	0.579638	-0.094319	3.191793
27	1	-3.799047	-1.122351	2.121084

28	1	-3.873083	-0.268558	0.572580
29	1	-3.052161	0.475090	1.945557
30	1	-3.357552	-3.421133	-0.639216
31	1	-2.428590	-2.752251	-1.991623
32	1	-3.611971	-1.746708	-1.149143
33	1	-0.361677	-4.706685	-0.562627
34	1	1.158804	-3.826763	-0.752388
35	1	-0.166121	-3.552261	-1.891272
36	1	1.444338	-3.192489	2.469551
37	1	2.055077	-1.561746	2.172708
38	1	2.210466	-2.806108	0.925780
39	1	-1.868186	4.477427	1.404185
40	1	-3.242930	4.069287	-0.739647
41	1	-0.871835	5.046940	-0.899039
42	7	1.990168	0.326454	-0.202653
43	6	2.908914	-0.397651	-0.888272
44	6	2.430352	1.309506	0.621384
45	6	4.279621	-0.169977	-0.773479
46	1	2.519413	-1.161908	-1.550508
47	6	3.785679	1.585062	0.797442
48	1	1.660921	1.883318	1.121667
49	6	4.729897	0.835786	0.087607
50	1	4.973281	-0.769455	-1.350049
51	1	4.088438	2.379667	1.468341
52	1	5.789911	1.034813	0.198130

TS8a-16 (E = -1190.1287637 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.848368	0.029754	-0.158329
2	7	-0.550666	-1.394105	-0.761354
3	6	-1.536627	-1.264320	0.168249
4	7	-0.846316	1.496807	-0.582179
5	6	2.411594	-1.560769	1.133932
6	6	1.593155	-0.863878	2.074149
7	6	3.290434	-0.615664	0.543799
8	17	2.082120	0.474344	-2.229455
9	6	1.972432	0.521293	2.066259
10	6	3.012716	0.668392	1.107430
11	6	-0.750124	-2.454642	-1.817338
12	6	-1.914708	1.083007	0.076832
13	6	-0.878962	2.645787	-1.575941
14	6	-1.653342	-0.038767	1.021323
15	1	-2.226317	-2.073095	0.375780
16	6	-2.879767	-0.089035	1.920016
17	1	-0.725315	0.230033	1.633481
18	6	-3.324360	1.595148	0.310952
19	6	-3.807006	0.777850	1.490010
20	1	-3.335631	2.656849	0.576036
21	1	-3.992615	1.493218	-0.554280
22	6	-5.194456	1.008926	2.026934
23	6	-2.975784	-1.057423	3.068747
24	1	-3.987090	-1.094528	3.484043
25	1	-2.292484	-0.780206	3.882336
26	1	-2.702009	-2.072874	2.755598
27	1	-5.427835	0.360143	2.875993
28	1	-5.947665	0.828994	1.246972
29	1	-5.319384	2.050589	2.354664
30	6	0.525852	-2.587677	-2.666607
31	6	-1.049820	-3.829746	-1.168519
32	6	-1.928857	-2.033431	-2.724752
33	1	-1.708603	-1.080405	-3.216176
34	1	-2.847034	-1.913821	-2.139936

35	1	-2.000885	-3.836782	-0.627036
36	1	-0.251004	-4.109737	-0.473458
37	1	1.386834	-2.851212	-2.042817
38	1	0.755998	-1.656427	-3.187253
39	6	-2.015649	3.672894	-1.349068
40	6	0.445546	3.431546	-1.430530
41	6	-1.032891	2.061106	-2.998910
42	1	-0.205654	1.392995	-3.243682
43	1	-1.972132	1.500775	-3.074703
44	1	-3.005023	3.263625	-1.562941
45	1	-2.000394	4.075183	-0.330898
46	1	0.517815	3.864472	-0.425581
47	1	1.315834	2.800564	-1.607592
48	6	0.709829	-1.536237	3.099791
49	6	2.471751	-3.060722	0.972329
50	6	4.433211	-0.931148	-0.386911
51	6	3.780618	1.934469	0.810042
52	6	1.526418	1.577775	3.052336
53	1	1.327553	-1.978702	3.894631
54	1	0.106070	-2.339673	2.665935
55	1	0.029000	-0.826302	3.576765
56	1	3.144248	-3.503400	1.722294
57	1	2.846811	-3.348795	-0.014843
58	1	1.487547	-3.521565	1.102238
59	1	5.353031	-1.104845	0.190190
60	1	4.623430	-0.112581	-1.086357
61	1	4.238044	-1.829819	-0.980367
62	1	4.720398	1.961433	1.380314
63	1	3.207997	2.827733	1.080329
64	1	4.037898	2.010570	-0.251788
65	1	2.195510	1.595747	3.925835
66	1	0.511435	1.393773	3.418173
67	1	1.536886	2.578363	2.607758
68	1	-1.109908	-4.596415	-1.949183
69	1	0.387263	-3.378608	-3.412435
70	1	-2.102180	-2.792293	-3.496513
71	1	0.468855	4.250392	-2.159063
72	1	-1.853937	4.509760	-2.037449
73	1	-1.056008	2.872238	-3.736675

16 (E = -1190.1773008 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.713569	-0.575300	-0.009873
2	7	-1.084559	-1.724453	-1.071868
3	6	-2.055768	-1.428548	-0.271508
4	7	-0.535207	1.085543	-0.709010
5	6	2.982741	-0.865392	1.204405
6	6	1.985272	-0.933843	2.206205
7	6	3.000966	0.468690	0.679094
8	17	2.102213	-1.373531	-1.896033
9	6	1.348674	0.344210	2.279260
10	6	2.014850	1.219551	1.368715
11	6	-1.263726	-2.835779	-2.075489
12	6	-1.541620	0.971054	0.165465
13	6	-0.463230	2.184863	-1.736575
14	6	-2.038705	-0.282860	0.590351
15	1	-2.957844	-2.036069	-0.226690
16	6	-3.006490	-0.065046	1.690494
17	1	0.116910	-1.900589	1.079553
18	6	-2.305396	2.040888	0.940662
19	6	-3.158410	1.256530	1.910936
20	1	-1.626830	2.744461	1.431993
21	1	-2.940752	2.638397	0.275272

22	6	-4.035264	1.964112	2.906962
23	6	-3.681568	-1.208509	2.402389
24	1	-4.285328	-0.861106	3.245771
25	1	-2.938206	-1.921053	2.782864
26	1	-4.347084	-1.767400	1.730122
27	1	-4.597162	1.261740	3.530200
28	1	-4.762572	2.616407	2.401999
29	1	-3.444615	2.606395	3.575848
30	6	-0.290698	-3.981594	-1.712685
31	6	-2.700392	-3.408225	-2.111877
32	6	-0.938612	-2.259043	-3.472177
33	1	0.064944	-1.832048	-3.491415
34	1	-1.661210	-1.478779	-3.739212
35	1	-3.446144	-2.633935	-2.328178
36	1	-2.973097	-3.912549	-1.177604
37	1	-0.514136	-4.367945	-0.711554
38	1	0.744883	-3.638901	-1.731178
39	6	-0.588182	3.625077	-1.178122
40	6	0.883984	2.055466	-2.472130
41	6	-1.613953	1.934845	-2.744618
42	1	-1.512222	0.945140	-3.199086
43	1	-2.590125	1.987495	-2.248172
44	1	-1.590271	3.840031	-0.800879
45	1	0.134497	3.813565	-0.382816
46	1	1.723994	2.249282	-1.798089
47	1	1.008704	1.054486	-2.892776
48	6	1.766408	-2.078962	3.163232
49	6	3.979696	-1.949334	0.873756
50	6	4.047718	1.005723	-0.265228
51	6	1.872619	2.720100	1.348221
52	6	0.343263	0.742535	3.334441
53	1	2.434174	-1.979562	4.032033
54	1	1.971859	-3.045433	2.692916
55	1	0.736301	-2.104494	3.529745
56	1	4.874100	-1.853093	1.506666
57	1	4.298151	-1.895678	-0.170752
58	1	3.563551	-2.948524	1.041727
59	1	5.011340	1.113059	0.253194
60	1	3.775835	1.990444	-0.658177
61	1	4.199590	0.336265	-1.117913
62	1	2.524210	3.163471	2.115362
63	1	0.850665	3.040801	1.568468
64	1	2.163467	3.152110	0.386827
65	1	0.842783	0.912236	4.299516
66	1	-0.415143	-0.032259	3.486479
67	1	-0.180949	1.666035	3.071890
68	1	-2.753015	-4.153142	-2.912599
69	1	-0.399386	-4.800743	-2.433092
70	1	-0.997624	-3.053506	-4.225420
71	1	0.930714	2.783100	-3.289601
72	1	-0.387579	4.333386	-1.990239
73	1	-1.592714	2.690636	-3.538422

TS8a-17 (E = -1190.1272702 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.329606	-0.363045	0.413680
2	7	1.597553	0.419570	0.081922
3	6	1.443439	0.726842	-1.231227
4	7	-1.630239	1.052959	-0.416686
5	6	-0.427519	-2.364499	-1.137954
6	6	-1.727283	-2.381088	-0.538698
7	6	0.523898	-2.725831	-0.133109
8	17	-0.678978	0.175265	2.793985

9	6	-1.567030	-2.644571	0.844537
10	6	-0.172433	-2.855132	1.098828
11	6	-0.573010	1.911975	-0.543806
12	6	0.461807	1.775457	-1.662098
13	1	2.150623	0.329987	-1.961433
14	6	1.081388	3.157611	-1.796148
15	1	-0.045159	1.467262	-2.587734
16	6	-0.280397	3.239085	0.164859
17	6	0.661893	3.947099	-0.795302
18	1	-1.158330	3.845640	0.381111
19	1	0.212041	3.081683	1.135877
20	6	1.019761	5.385242	-0.532889
21	6	2.023504	3.481112	-2.924598
22	1	2.431414	4.494252	-2.851385
23	1	1.515412	3.391464	-3.895669
24	1	2.870986	2.781849	-2.943238
25	1	1.724007	5.785381	-1.268614
26	1	1.470974	5.492607	0.464460
27	1	0.122006	6.019543	-0.541718
28	6	-3.004535	-2.438502	-1.342277
29	6	-0.173048	-2.333389	-2.629016
30	6	1.931906	-3.177502	-0.433609
31	6	0.384736	-3.329291	2.420181
32	6	-2.653176	-2.847163	1.873546
33	1	-3.021993	-3.371312	-1.924439
34	1	-3.096436	-1.613556	-2.054780
35	1	-3.894780	-2.440002	-0.707906
36	1	-0.350181	-3.325528	-3.072202
37	1	0.857744	-2.048503	-2.860222
38	1	-0.833683	-1.624173	-3.138660
39	1	1.910875	-4.207297	-0.819445
40	1	2.573306	-3.177942	0.451017
41	1	2.408914	-2.557817	-1.198434
42	1	0.072562	-4.364938	2.617099
43	1	0.030048	-2.712802	3.253327
44	1	1.478318	-3.308303	2.432929
45	1	-2.749668	-3.912987	2.125366
46	1	-3.626949	-2.503581	1.512815
47	1	-2.433704	-2.307736	2.801527
48	6	2.985163	0.373138	0.686461
49	6	4.075417	-0.105424	-0.296246
50	6	3.289918	1.836017	1.102249
51	6	2.969495	-0.508637	1.944961
52	1	3.881529	-1.118229	-0.658482
53	1	4.170309	0.563640	-1.157995
54	1	3.257664	2.500247	0.232525
55	1	2.554293	2.188014	1.832804
56	1	2.179197	-0.190842	2.631415
57	1	2.810285	-1.559751	1.696692
58	6	-3.088470	1.462641	-0.413728
59	6	-3.883848	0.476701	0.458817
60	6	-3.369209	2.885302	0.124397
61	6	-3.563576	1.409359	-1.887910
62	1	-3.725105	-0.550596	0.138299
63	1	-3.579579	0.562608	1.507125
64	1	-2.996815	3.010911	1.145440
65	1	-2.940719	3.659233	-0.518339
66	1	-2.971090	2.100338	-2.499147
67	1	-3.449578	0.403967	-2.300740
68	1	5.040203	-0.111042	0.222630
69	1	3.929982	-0.427039	2.466045
70	1	4.286697	1.895025	1.554882
71	1	-4.454878	3.036939	0.141899

72	1	-4.955556	0.696030	0.389222
73	1	-4.618644	1.700576	-1.963424

17 (E = -1190.1579384 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.364196	-0.095517	0.235496
2	7	-0.642465	1.782358	-0.869023
3	6	-1.902928	1.606171	-1.031162
4	7	-0.742400	-1.393216	-0.842660
5	6	2.791500	-0.703579	-0.706982
6	6	2.427037	-1.633549	0.310937
7	6	3.032695	0.560078	-0.080448
8	17	-0.328994	0.778798	2.479051
9	6	2.394409	-0.928861	1.552718
10	6	2.783513	0.421803	1.309137
11	6	-1.723618	-0.713589	-0.045800
12	6	-2.628187	0.357972	-0.667786
13	1	-2.500224	2.391013	-1.493069
14	6	-3.730700	0.550064	0.377767
15	1	-3.133030	0.066385	-1.612097
16	6	-2.574544	-1.415237	1.021616
17	6	-3.692962	-0.434948	1.285703
18	1	-3.008988	-2.373476	0.690041
19	1	-2.015938	-1.640036	1.941098
20	6	-4.616003	-0.648584	2.456250
21	6	-4.712991	1.688280	0.270978
22	1	-5.519706	1.599677	1.004825
23	1	-5.172209	1.722520	-0.728198
24	1	-4.226444	2.660524	0.435396
25	1	-5.424232	0.088066	2.501399
26	1	-4.053935	-0.591195	3.398664
27	1	-5.069491	-1.649248	2.415452
28	6	2.408280	-3.139896	0.195371
29	6	3.208103	-1.029365	-2.125909
30	6	3.795522	1.696304	-0.725696
31	6	3.066195	1.450537	2.375019
32	6	2.223535	-1.557754	2.917042
33	1	3.398335	-3.542870	0.455620
34	1	2.171350	-3.479422	-0.815084
35	1	1.684391	-3.596718	0.877334
36	1	4.277524	-0.815726	-2.262506
37	1	2.662772	-0.450209	-2.880841
38	1	3.059013	-2.086918	-2.355256
39	1	4.870460	1.569923	-0.528135
40	1	3.513743	2.680240	-0.339837
41	1	3.670874	1.714473	-1.812032
42	1	4.020964	1.232443	2.875249
43	1	2.280919	1.462148	3.137264
44	1	3.139364	2.460004	1.956822
45	1	3.192830	-1.910627	3.299563
46	1	1.549804	-2.421461	2.891376
47	1	1.814799	-0.843101	3.636050
48	6	-0.030763	3.099194	-1.308251
49	6	0.908719	2.770138	-2.486406
50	6	-1.057335	4.156507	-1.771398
51	6	0.733570	3.672249	-0.096594
52	1	1.595429	1.964600	-2.222424
53	1	0.327372	2.452225	-3.359436
54	1	-1.606012	3.847477	-2.667818
55	1	-1.774954	4.405561	-0.981690
56	1	0.039326	3.901272	0.718206

57	1	1.476963	2.970460	0.285030
58	6	-1.032821	-2.524077	-1.774695
59	6	-1.045964	-3.874209	-1.009135
60	6	-2.405969	-2.342449	-2.466716
61	6	0.051430	-2.567724	-2.869571
62	1	-0.089953	-4.042834	-0.508194
63	1	-1.835985	-3.885720	-0.252488
64	1	-3.218540	-2.286007	-1.736193
65	1	-2.420959	-1.432466	-3.076905
66	1	0.075343	-1.621377	-3.422471
67	1	1.038090	-2.735409	-2.436241
68	1	1.249241	4.594412	-0.385948
69	1	-0.511867	5.071588	-2.023679
70	1	1.497126	3.651347	-2.763536
71	1	-1.224642	-4.706060	-1.702552
72	1	-0.151697	-3.378765	-3.579423
73	1	-2.600709	-3.195895	-3.127087

TS17-18 (E = -1190.1336249 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.012089	-0.627488	-0.265443
2	7	-1.550640	0.992517	0.152392
3	6	-0.842246	2.040911	-0.238275
4	7	1.675099	0.248983	0.480277
5	6	-0.161810	-2.629685	1.376377
6	6	0.811356	-3.002019	0.401152
7	6	-1.442843	-2.618410	0.734588
8	17	-0.098412	-0.500608	-2.746699
9	6	0.139034	-3.159480	-0.843808
10	6	-1.254789	-2.951465	-0.633158
11	6	1.238068	1.325892	-0.337455
12	6	0.473225	2.488860	0.303980
13	1	-1.232570	2.660162	-1.048691
14	6	0.982695	3.735749	-0.382630
15	1	0.486628	2.516318	1.398582
16	6	2.043712	1.926175	-1.499300
17	6	1.823647	3.420235	-1.381998
18	1	3.112430	1.681472	-1.429054
19	1	1.720650	1.555535	-2.479813
20	6	2.515808	4.354068	-2.339486
21	6	0.501434	5.095877	0.052284
22	1	0.921843	5.902240	-0.556769
23	1	0.771756	5.288489	1.100431
24	1	-0.594722	5.167429	-0.008818
25	1	2.265100	5.404348	-2.160685
26	1	2.246693	4.112577	-3.377275
27	1	3.607539	4.248366	-2.264230
28	6	2.212849	-3.509272	0.647462
29	6	0.009813	-2.605454	2.880740
30	6	-2.744804	-2.633660	1.502074
31	6	-2.312156	-3.251772	-1.668651
32	6	0.753351	-3.704674	-2.110251
33	1	2.191667	-4.606855	0.717529
34	1	2.647837	-3.133406	1.574668
35	1	2.893950	-3.253093	-0.169611
36	1	-0.598058	-3.397987	3.339107
37	1	-0.299801	-1.656187	3.333860
38	1	1.047236	-2.784410	3.170668
39	1	-2.942926	-3.654219	1.862802
40	1	-3.604494	-2.332842	0.898160
41	1	-2.708182	-1.985811	2.383194
42	1	-2.227718	-4.297349	-1.994796

43	1	-2.204934	-2.621492	-2.558944
44	1	-3.322473	-3.115855	-1.272567
45	1	0.722135	-4.804601	-2.104884
46	1	1.800697	-3.405218	-2.219899
47	1	0.218124	-3.353315	-2.995815
48	6	-3.058820	1.079363	-0.090253
49	6	-3.695825	0.896302	1.306104
50	6	-3.520485	2.451486	-0.642149
51	6	-3.534272	-0.006835	-1.068581
52	1	-3.374637	-0.040163	1.763426
53	1	-3.400530	1.718451	1.967780
54	1	-3.181941	3.284193	-0.014772
55	1	-3.189070	2.624969	-1.671359
56	1	-3.065313	0.122395	-2.048996
57	1	-3.285921	-1.001008	-0.702325
58	6	2.946497	0.336365	1.285802
59	6	4.113703	-0.323779	0.510320
60	6	3.324303	1.806107	1.597786
61	6	2.743445	-0.378255	2.636547
62	1	3.877302	-1.361458	0.265395
63	1	4.310860	0.209250	-0.425075
64	1	3.462852	2.400473	0.692292
65	1	2.557939	2.289709	2.211868
66	1	1.922066	0.086617	3.192946
67	1	2.508034	-1.431407	2.496666
68	1	5.031336	-0.309330	1.112440
69	1	4.264396	1.820340	2.161724
70	1	3.655516	-0.310514	3.242040
71	1	-4.621891	0.049209	-1.192116
72	1	-4.789575	0.890838	1.226573
73	1	-4.615643	2.462508	-0.646331

18 (E = -1190.1771398 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.640262	-0.018357	0.251572
2	7	-0.448302	1.641987	-0.216878
3	6	-1.678459	1.029315	0.199449
4	7	-0.794494	-1.321962	-0.416423
5	6	2.658386	-0.665414	-1.258704
6	6	2.790154	-1.445031	-0.071529
7	6	2.850532	0.708056	-0.906939
8	17	0.286956	-0.055284	2.690606
9	6	3.048456	-0.554101	1.008855
10	6	3.093252	0.774522	0.495857
11	6	-1.878322	-0.526848	0.101666
12	6	-2.712025	0.428790	-0.749101
13	1	-2.107228	1.419236	1.120852
14	6	-4.105176	0.370548	-0.216309
15	1	-2.516507	0.514558	-1.811343
16	6	-2.828052	-1.028244	1.211586
17	6	-4.168064	-0.396062	0.888573
18	1	-2.903011	-2.119273	1.221849
19	1	-2.455302	-0.741868	2.199742
20	6	-5.354876	-0.668693	1.773926
21	6	-5.211692	1.145719	-0.884094
22	1	-6.182681	0.972361	-0.410230
23	1	-5.298520	0.864184	-1.942868
24	1	-5.011166	2.226003	-0.857943
25	1	-6.266587	-0.185024	1.409533
26	1	-5.172859	-0.313743	2.798164
27	1	-5.549580	-1.748829	1.844173
28	6	2.903717	-2.948721	0.038924
29	6	2.690908	-1.149537	-2.691256

30	6	3.108706	1.783824	-1.938223
31	6	3.500079	1.983002	1.307245
32	6	3.443111	-0.968617	2.404668
33	1	3.953097	-3.230105	0.205534
34	1	2.569830	-3.459064	-0.867514
35	1	2.326171	-3.349409	0.879290
36	1	3.634787	-0.836159	-3.159699
37	1	1.876891	-0.741267	-3.299872
38	1	2.643177	-2.238172	-2.757971
39	1	3.950775	1.480211	-2.576243
40	1	3.385678	2.733741	-1.474877
41	1	2.254538	1.965666	-2.599002
42	1	4.554411	1.899554	1.605037
43	1	2.909025	2.078828	2.225233
44	1	3.388135	2.911121	0.742158
45	1	4.524775	-1.165374	2.444254
46	1	2.926456	-1.878942	2.723100
47	1	3.212979	-0.191208	3.137406
48	6	-1.142078	-2.637074	-1.058674
49	6	-0.984694	-3.790009	-0.033883
50	6	-2.575747	-2.651868	-1.647038
51	6	-0.173318	-2.884571	-2.230222
52	1	0.030442	-3.796471	0.375423
53	1	-1.682718	-3.685124	0.801426
54	1	-3.350212	-2.492576	-0.893995
55	1	-2.689464	-1.883521	-2.418449
56	1	-0.243947	-2.076356	-2.965401
57	1	0.854228	-2.943999	-1.876115
58	6	-0.553028	3.084831	-0.615034
59	6	-0.746181	3.176415	-2.149233
60	6	-1.739886	3.792300	0.086759
61	6	0.734076	3.818582	-0.198286
62	1	0.088008	2.694033	-2.669382
63	1	-1.672782	2.677372	-2.452136
64	1	-2.703375	3.360584	-0.200047
65	1	-1.642219	3.738309	1.176905
66	1	0.864602	3.769832	0.887956
67	1	1.607481	3.376867	-0.674498
68	1	0.682028	4.872900	-0.494731
69	1	-0.799009	4.223249	-2.473201
70	1	-1.745340	4.849515	-0.201019
71	1	-0.416365	-3.830715	-2.727995
72	1	-1.170562	-4.758363	-0.515314
73	1	-2.754271	-3.627896	-2.112473

TS7a-7c (E = -1190.1633484 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.264231	0.009905	-0.119083
2	7	-0.219149	1.805763	-1.476314
3	6	0.945746	1.277674	-1.445338
4	7	1.082606	-1.717296	-0.024979
5	6	-0.926226	0.655942	2.274485
6	6	-1.223679	-0.744058	2.212582
7	6	-1.844349	1.340704	1.423225
8	17	-1.491268	-1.079982	-1.994603
9	6	-2.306303	-0.916229	1.314923
10	6	-2.683821	0.369113	0.813556
11	6	2.171178	-0.947465	0.231985
12	6	2.155096	0.051577	1.193474
13	1	1.782001	1.668268	-2.035543
14	6	3.340124	0.913714	1.041768
15	1	1.561730	0.009655	2.089915
16	6	3.439714	-0.750547	-0.602229

17	6	4.101483	0.458471	0.021841
18	1	4.106258	-1.620002	-0.590217
19	1	3.168197	-0.581032	-1.648331
20	6	5.437137	0.951141	-0.465053
21	6	3.612875	2.075061	1.962095
22	1	4.579783	2.544038	1.755989
23	1	3.611681	1.751890	3.012082
24	1	2.837858	2.847824	1.864614
25	1	5.794424	1.807466	0.116252
26	1	5.395175	1.259721	-1.519835
27	1	6.199771	0.161187	-0.397870
28	6	-0.587251	-1.805863	3.077330
29	6	-0.091883	1.336915	3.337319
30	6	-2.031399	2.838472	1.421674
31	6	-3.906854	0.616818	-0.034214
32	6	-3.062442	-2.186219	1.016528
33	1	-0.855862	-1.657632	4.132482
34	1	0.506410	-1.802317	3.008210
35	1	-0.924274	-2.805070	2.788793
36	1	-0.749569	1.738710	4.121823
37	1	0.495869	2.173599	2.944570
38	1	0.598737	0.641805	3.824826
39	1	-2.580871	3.146823	2.323234
40	1	-2.604626	3.181228	0.557491
41	1	-1.076321	3.374251	1.426460
42	1	-4.815879	0.365983	0.530696
43	1	-3.898643	0.004005	-0.941890
44	1	-3.986122	1.664054	-0.337139
45	1	-4.048431	-2.160360	1.502414
46	1	-2.536941	-3.072181	1.381672
47	1	-3.226583	-2.311931	-0.058810
48	6	-0.636153	2.963405	-2.359280
49	6	0.040838	2.839351	-3.741447
50	6	-2.163135	2.903638	-2.528872
51	6	-0.203444	4.274794	-1.669267
52	1	-0.212765	1.883523	-4.212097
53	1	1.130721	2.916314	-3.670743
54	1	-0.307455	3.648459	-4.392211
55	1	-2.669907	3.031798	-1.569519
56	1	-2.465292	1.940341	-2.950930
57	1	-2.497039	3.701958	-3.200931
58	1	0.885082	4.304627	-1.543244
59	1	-0.669932	4.374507	-0.685002
60	1	-0.502054	5.134214	-2.280067
61	6	1.242837	-3.104817	-0.588029
62	6	2.328931	-3.867188	0.212977
63	6	-0.088643	-3.858081	-0.383953
64	6	1.597162	-3.096263	-2.095459
65	1	2.084537	-3.863555	1.281244
66	1	3.324129	-3.431519	0.088208
67	1	2.375479	-4.908123	-0.126800
68	1	-0.903844	-3.372752	-0.921668
69	1	-0.340134	-3.898453	0.680937
70	1	0.009267	-4.886108	-0.752277
71	1	2.584829	-2.662466	-2.278309
72	1	0.852316	-2.524744	-2.656043
73	1	1.608420	-4.123404	-2.480320

7c (E =-1190.1672187 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.000198	-0.380442	-0.149304
2	7	-1.967187	0.430644	-0.874094
3	6	-1.018170	1.141460	-1.350779
4	7	1.998158	0.704972	-0.106305
5	6	-0.167728	-1.519092	2.185458
6	6	1.101834	-1.950612	1.694317
7	6	-1.180464	-2.088802	1.359745
8	17	0.534659	-1.277727	-2.438482
9	6	0.874458	-2.773237	0.560745
10	6	-0.537057	-2.846100	0.340091
11	6	1.362328	1.772157	0.366649
12	6	0.367995	1.584424	1.358023
13	1	-1.191880	1.953016	-2.062664
14	6	-0.367358	2.860355	1.518681
15	1	0.586268	0.967283	2.217545
16	6	1.270362	3.214946	-0.130390
17	6	0.129101	3.795004	0.680888
18	1	2.200084	3.774073	0.030741
19	1	1.076047	3.238162	-1.205812
20	6	-0.268696	5.237255	0.515073
21	6	-1.466429	3.016624	2.536034
22	1	-1.883738	4.028241	2.544062
23	1	-1.093932	2.798197	3.546745
24	1	-2.286189	2.312744	2.339671
25	1	-1.085100	5.516822	1.188852
26	1	-0.597349	5.451576	-0.512428
27	1	0.578434	5.908215	0.721617
28	6	2.423560	-1.660970	2.363594
29	6	-0.412863	-0.866064	3.526205
30	6	-2.642570	-2.150235	1.729473
31	6	-1.203978	-3.770589	-0.649738
32	6	1.887617	-3.593119	-0.197846
33	1	2.409768	-1.994225	3.409712
34	1	2.665641	-0.591122	2.353383
35	1	3.243107	-2.183825	1.862954
36	1	-0.656214	-1.631332	4.277600
37	1	-1.246131	-0.155777	3.500923
38	1	0.471419	-0.331325	3.888183
39	1	-2.814847	-2.995963	2.411547
40	1	-3.288141	-2.298320	0.860747
41	1	-2.973029	-1.244929	2.247722
42	1	-1.196812	-4.803656	-0.272282
43	1	-0.688260	-3.761137	-1.614493
44	1	-2.247079	-3.492474	-0.828425
45	1	1.759572	-4.659161	0.037762
46	1	2.913158	-3.317003	0.060117
47	1	1.769955	-3.475284	-1.280049
48	6	-3.435147	0.547976	-1.210335
49	6	-3.691227	1.670830	-2.233124
50	6	-3.874921	-0.805186	-1.806117
51	6	-4.196562	0.852874	0.095269
52	1	-3.166542	1.483844	-3.176629
53	1	-3.378998	2.647607	-1.846821
54	1	-4.763485	1.722030	-2.448997
55	1	-3.703526	-1.620763	-1.099133
56	1	-3.315108	-1.022798	-2.721761
57	1	-4.943220	-0.778435	-2.048292
58	1	-3.885607	1.819944	0.505565
59	1	-4.014000	0.081890	0.846711
60	1	-5.273786	0.893885	-0.101498
61	6	3.257616	0.809002	-0.922740
62	6	4.308853	1.616411	-0.120524
63	6	3.805928	-0.619696	-1.115315

64	6	3.034700	1.452926	-2.313031
65	1	4.471712	1.158385	0.861540
66	1	4.004232	2.656189	0.030867
67	1	5.262238	1.622479	-0.660948
68	1	3.105243	-1.234017	-1.683416
69	1	3.984870	-1.091264	-0.144183
70	1	4.756679	-0.580955	-1.659326
71	1	2.775177	2.512754	-2.239482
72	1	2.241932	0.929105	-2.853545
73	1	3.958576	1.379888	-2.899337

TS7c-8b (E = -1190.1417998 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.620837	-0.077280	-0.282217
2	7	-0.132122	1.940454	-0.627373
3	6	0.955714	1.211485	-0.905180
4	7	1.246284	-1.449382	-0.221838
5	6	-1.345029	-0.089434	2.120344
6	6	-1.478467	-1.466474	1.745097
7	6	-2.398648	0.642048	1.484463
8	17	-1.655801	-0.643950	-2.426217
9	6	-2.552320	-1.562632	0.822298
10	6	-3.113531	-0.255247	0.654895
11	6	2.277246	-0.755408	0.222718
12	6	2.108251	0.605686	0.671990
13	1	1.730511	1.523484	-1.601689
14	6	3.460236	1.187636	0.849778
15	1	1.369651	0.847894	1.431094
16	6	3.774995	-1.028610	0.141090
17	6	4.410907	0.294949	0.505829
18	1	4.073115	-1.796957	0.864537
19	1	4.087932	-1.392002	-0.841567
20	6	5.907880	0.447439	0.492461
21	6	3.654463	2.599868	1.335195
22	1	4.709571	2.835454	1.504206
23	1	3.115633	2.765494	2.278335
24	1	3.260306	3.324658	0.610775
25	1	6.221198	1.437915	0.837458
26	1	6.318781	0.303378	-0.517737
27	1	6.389991	-0.300294	1.139642
28	6	-0.744887	-2.593650	2.434473
29	6	-0.510903	0.412721	3.279699
30	6	-2.833190	2.029158	1.885434
31	6	-4.351878	0.042658	-0.153966
32	6	-3.162728	-2.809811	0.229995
33	1	-0.966044	-2.577022	3.510591
34	1	0.342353	-2.521337	2.321448
35	1	-1.057657	-3.570183	2.055266
36	1	-1.066028	0.305501	4.223781
37	1	-0.253678	1.472253	3.173756
38	1	0.422854	-0.149374	3.386169
39	1	-3.358596	1.981636	2.850566
40	1	-3.524549	2.469332	1.162335
41	1	-1.990138	2.713248	2.008587
42	1	-5.249922	-0.330574	0.359273
43	1	-4.309789	-0.434247	-1.138983
44	1	-4.483853	1.117390	-0.312830
45	1	-4.186145	-2.943978	0.606741
46	1	-2.596221	-3.707595	0.490399
47	1	-3.223168	-2.755251	-0.863469
48	6	-0.345153	3.391839	-0.924333
49	6	0.010074	4.237418	0.320184
50	6	0.545439	3.832804	-2.108174

51	6	-1.823555	3.587886	-1.313906
52	1	-0.629255	3.979111	1.168888
53	1	1.052316	4.070252	0.612186
54	1	-0.119278	5.305390	0.106967
55	1	1.610260	3.763788	-1.860934
56	1	0.352786	3.213752	-2.991553
57	1	0.326857	4.875439	-2.364213
58	1	-2.060636	3.006529	-2.211443
59	1	-2.486687	3.263265	-0.509586
60	1	-2.025728	4.645322	-1.520654
61	6	1.425164	-2.806598	-0.877199
62	6	0.054791	-3.510526	-0.942414
63	6	1.922951	-2.586308	-2.328400
64	6	2.380907	-3.748829	-0.101724
65	1	-0.299155	-3.769552	0.056515
66	1	-0.694809	-2.894374	-1.442747
67	1	0.153843	-4.438577	-1.516368
68	1	1.197286	-1.989845	-2.889550
69	1	2.885732	-2.068510	-2.356195
70	1	2.042408	-3.553373	-2.830965
71	1	3.434019	-3.499473	-0.237849
72	1	2.152333	-3.738823	0.969916
73	1	2.240827	-4.772622	-0.465790

8b (E = -1190.159509 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.657926	-0.050262	-0.297275
2	7	-0.118188	1.899945	-0.325478
3	6	1.086895	1.204312	-0.604711
4	7	1.356637	-1.433893	-0.203878
5	6	-1.434358	-0.340850	2.077075
6	6	-1.660767	-1.645792	1.532030
7	6	-2.420869	0.538411	1.530690
8	17	-1.514449	-0.439920	-2.561263
9	6	-2.710375	-1.546279	0.582862
10	6	-3.175426	-0.190922	0.577851
11	6	2.317034	-0.724381	0.278835
12	6	2.090400	0.775495	0.489445
13	1	1.549390	1.314589	-1.590074
14	6	3.516358	1.317051	0.551618
15	1	1.607270	0.959984	1.461216
16	6	3.774320	-1.037105	0.553416
17	6	4.425331	0.331264	0.583007
18	1	3.870591	-1.542039	1.525847
19	1	4.232397	-1.702305	-0.180004
20	6	5.925539	0.422536	0.669623
21	6	3.765242	2.797918	0.608106
22	1	4.832051	3.039321	0.629396
23	1	3.300884	3.236277	1.502638
24	1	3.318808	3.299819	-0.258734
25	1	6.277421	1.457881	0.685235
26	1	6.400243	-0.081860	-0.184161
27	1	6.297149	-0.073086	1.578236
28	6	-1.072839	-2.904447	2.126099
29	6	-0.566430	-0.035583	3.278815
30	6	-2.740772	1.894264	2.107561
31	6	-4.361722	0.298482	-0.217996
32	6	-3.355184	-2.663854	-0.201137
33	1	-1.458873	-3.041314	3.146447
34	1	0.019013	-2.869262	2.198720
35	1	-1.346323	-3.797412	1.557613
36	1	-1.108672	-0.242037	4.214258
37	1	-0.264916	1.017049	3.302504

38	1	0.344613	-0.644707	3.292805
39	1	-3.121839	1.775624	3.132271
40	1	-3.514288	2.409978	1.532629
41	1	-1.862685	2.544170	2.156545
42	1	-5.301104	-0.081057	0.209517
43	1	-4.313164	-0.040220	-1.258890
44	1	-4.419807	1.391110	-0.228944
45	1	-4.383603	-2.836757	0.145974
46	1	-2.809459	-3.606022	-0.092161
47	1	-3.405198	-2.430400	-1.271441
48	6	-0.363354	3.332709	-0.657883
49	6	0.076357	4.239283	0.517542
50	6	0.425790	3.734580	-1.928181
51	6	-1.864823	3.531396	-0.950078
52	1	-0.515585	4.029436	1.414385
53	1	1.130943	4.067033	0.756398
54	1	-0.049168	5.299569	0.263299
55	1	1.506375	3.664329	-1.768132
56	1	0.159410	3.084336	-2.769217
57	1	0.187574	4.769140	-2.202026
58	1	-2.169414	2.913621	-1.802083
59	1	-2.474324	3.256530	-0.088362
60	1	-2.070654	4.581178	-1.191772
61	6	1.590947	-2.830779	-0.769383
62	6	0.227985	-3.432593	-1.162383
63	6	2.419099	-2.679832	-2.071529
64	6	2.277214	-3.787596	0.233479
65	1	-0.400374	-3.602508	-0.288261
66	1	-0.306053	-2.782913	-1.861216
67	1	0.388035	-4.397399	-1.655600
68	1	1.893899	-2.028179	-2.776995
69	1	3.413084	-2.262235	-1.895318
70	1	2.543569	-3.663119	-2.538158
71	1	3.319523	-3.530201	0.427517
72	1	1.740588	-3.803794	1.187362
73	1	2.260284	-4.803139	-0.177123

TS8b-18 (E = -1190.1353338 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.441362	-0.047591	0.000336
2	7	-0.415196	1.739513	-0.433328
3	6	-1.571064	1.004911	-0.060282
4	7	-0.942420	-1.574140	-1.090334
5	6	2.774113	0.640366	-0.904234
6	6	2.785987	-0.782664	-1.048443
7	6	2.774542	0.939394	0.492414
8	17	-0.231274	-0.775084	2.277985
9	6	2.778877	-1.360968	0.253581
10	6	2.756862	-0.296370	1.198062
11	6	-2.116138	-1.054225	-0.770797
12	6	-2.500639	0.364982	-1.095170
13	1	-2.065198	1.234278	0.885611
14	6	-3.985522	0.424570	-0.806323
15	1	-2.227645	0.649309	-2.116613
16	6	-3.273317	-1.681745	-0.000771
17	6	-4.400567	-0.690680	-0.185145
18	1	-3.542019	-2.684342	-0.335448
19	1	-2.979699	-1.782661	1.053341
20	6	-5.768414	-1.030111	0.341572
21	6	-4.816796	1.630968	-1.155511
22	1	-5.887065	1.432452	-1.043072
23	1	-4.637136	1.943822	-2.192283
24	1	-4.571179	2.487111	-0.513885

25	1	-6.505158	-0.251792	0.123310
26	1	-5.740856	-1.169575	1.431899
27	1	-6.132008	-1.973930	-0.089413
28	6	3.125843	-1.453385	-2.361326
29	6	3.101843	1.569380	-2.051823
30	6	3.053988	2.268149	1.163239
31	6	2.963805	-0.449721	2.684215
32	6	3.016120	-2.804700	0.638933
33	1	4.111748	-1.105912	-2.701886
34	1	2.411244	-1.219203	-3.158476
35	1	3.179463	-2.540159	-2.270515
36	1	4.062756	1.276457	-2.498641
37	1	3.196559	2.604901	-1.722885
38	1	2.353640	1.543857	-2.852275
39	1	3.871743	2.148687	1.885434
40	1	2.195437	2.672264	1.710994
41	1	3.372158	3.022322	0.438350
42	1	4.040419	-0.452165	2.913971
43	1	2.535240	-1.382959	3.057875
44	1	2.502133	0.366830	3.246487
45	1	3.921852	-2.879334	1.255451
46	1	3.169155	-3.443407	-0.235476
47	1	2.193199	-3.228704	1.227169
48	6	-0.516143	3.231648	-0.556694
49	6	-1.682794	3.600827	-1.503395
50	6	-0.773528	3.847509	0.840438
51	6	0.770040	3.820930	-1.151852
52	1	-1.530062	3.156863	-2.493915
53	1	-2.636888	3.248936	-1.107549
54	1	-1.741294	4.689557	-1.619354
55	1	-1.686517	3.438552	1.286333
56	1	0.062290	3.632002	1.514903
57	1	-0.888068	4.935819	0.766817
58	1	1.630193	3.615424	-0.517013
59	1	0.956657	3.408419	-2.147529
60	1	0.669784	4.908980	-1.244738
61	6	-0.840170	-3.085795	-1.274034
62	6	-0.943781	-3.874630	0.052691
63	6	-1.898535	-3.556641	-2.307062
64	6	0.528286	-3.366012	-1.908930
65	1	-0.238868	-3.481820	0.791569
66	1	-1.942166	-3.836817	0.492274
67	1	-0.700844	-4.927471	-0.132877
68	1	-2.928661	-3.437977	-1.967415
69	1	-1.780435	-2.996695	-3.241471
70	1	-1.742845	-4.619411	-2.523631
71	1	0.644510	-2.796160	-2.834824
72	1	1.329746	-3.097027	-1.227257
73	1	0.618686	-4.432375	-2.143274

TS8b-19 (E = -1190.1263068 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.804957	0.016141	0.198686
2	7	-0.064696	1.774240	-0.554249
3	6	0.968155	0.868766	-0.883147
4	7	2.099003	-1.826061	-1.023086
5	6	-1.488896	-0.216090	2.611352
6	6	-2.116734	-1.311792	1.942761
7	6	-2.097485	0.989726	2.144682
8	17	-1.570752	-1.208504	-1.779259
9	6	-3.105130	-0.787246	1.069266
10	6	-3.086808	0.637954	1.174122
11	6	2.630861	-0.909852	-0.334125

12	6	1.740950	0.226388	0.162921
13	1	1.096148	0.494293	-1.895330
14	6	2.585990	0.977312	1.167822
15	1	0.897677	-0.486083	0.991435
16	6	4.035382	-0.644871	0.205527
17	6	3.844870	0.504940	1.165115
18	1	4.463940	-1.519424	0.701544
19	1	4.725845	-0.377719	-0.604649
20	6	5.029661	0.996651	1.953093
21	6	2.048029	2.108704	1.995859
22	1	2.833556	2.586357	2.588049
23	1	1.279298	1.749297	2.690458
24	1	1.576480	2.866078	1.364839
25	1	4.778073	1.822868	2.623475
26	1	5.829305	1.339653	1.280911
27	1	5.453798	0.185244	2.561592
28	6	-1.838294	-2.774978	2.196667
29	6	-0.543727	-0.343884	3.784871
30	6	-1.893522	2.360615	2.746441
31	6	-4.134169	1.547812	0.574531
32	6	-4.119690	-1.588440	0.294048
33	1	-2.492162	-3.163454	2.990687
34	1	-0.803503	-2.940240	2.514927
35	1	-2.012980	-3.382282	1.302325
36	1	-1.104661	-0.598371	4.695743
37	1	-0.010876	0.590314	3.983650
38	1	0.205363	-1.127571	3.629406
39	1	-2.472097	2.452935	3.676784
40	1	-2.227624	3.152189	2.071397
41	1	-0.845645	2.558138	2.991560
42	1	-5.091034	1.421823	1.101486
43	1	-4.314325	1.327800	-0.483535
44	1	-3.852245	2.600441	0.653071
45	1	-5.026047	-1.732487	0.900066
46	1	-3.736414	-2.576035	0.022710
47	1	-4.410794	-1.086925	-0.633120
48	6	-0.255053	3.006495	-1.370395
49	6	0.931710	3.973511	-1.148277
50	6	-0.345333	2.646874	-2.875277
51	6	-1.563401	3.687023	-0.936973
52	1	0.948713	4.341428	-0.116493
53	1	1.881635	3.467164	-1.353608
54	1	0.848829	4.838882	-1.816315
55	1	0.594487	2.221871	-3.243673
56	1	-1.144696	1.918866	-3.049419
57	1	-0.557604	3.548005	-3.462392
58	1	-2.419469	3.033822	-1.129374
59	1	-1.536869	3.928710	0.130272
60	1	-1.709252	4.618117	-1.496153
61	6	2.732848	-2.998613	-1.670398
62	6	1.886432	-4.217979	-1.233333
63	6	2.555887	-2.767218	-3.191612
64	6	4.222314	-3.274126	-1.360485
65	1	1.986508	-4.390170	-0.154948
66	1	0.830502	-4.040714	-1.458876
67	1	2.216266	-5.121050	-1.759434
68	1	1.504408	-2.571010	-3.422512
69	1	3.149276	-1.906820	-3.523102
70	1	2.884473	-3.650944	-3.750507
71	1	4.864543	-2.442123	-1.665114
72	1	4.383221	-3.477398	-0.296682
73	1	4.542876	-4.161512	-1.918318

19 (E = -1190.158953 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.856747	0.027023	-0.403267
2	7	-0.307757	1.483633	1.027264
3	6	1.028781	1.286510	0.729980
4	7	3.526629	0.600820	-0.543361
5	6	-2.167526	-2.006853	0.423431
6	6	-2.079683	-2.155427	-0.991180
7	6	-2.976751	-0.863734	0.704842
8	17	-0.705763	1.387871	-2.383025
9	6	-2.812516	-1.095934	-1.589341
10	6	-3.365405	-0.289312	-0.544284
11	6	2.963640	-0.230306	0.233137
12	6	1.693940	0.105876	0.958615
13	1	1.565047	2.029784	0.140769
14	6	1.507848	-0.917731	2.004807
15	1	0.361036	-1.235123	-0.892376
16	6	3.340118	-1.642828	0.685735
17	6	2.441173	-1.888501	1.872465
18	1	3.143855	-2.362728	-0.118754
19	1	4.397602	-1.740719	0.947381
20	6	2.683081	-3.085854	2.747328
21	6	0.545022	-0.763490	3.155449
22	1	0.700044	-1.540671	3.908855
23	1	-0.499891	-0.800951	2.838154
24	1	0.689759	0.211833	3.634543
25	1	1.962883	-3.165514	3.566187
26	1	3.691627	-3.053772	3.184686
27	1	2.626716	-4.012232	2.157522
28	6	-1.455301	-3.324176	-1.712336
29	6	-1.643016	-3.007237	1.427733
30	6	-3.508141	-0.492776	2.071433
31	6	-4.367287	0.819988	-0.766693
32	6	-3.106703	-0.947160	-3.062051
33	1	-2.202237	-4.114786	-1.875881
34	1	-0.629819	-3.753448	-1.137352
35	1	-1.059922	-3.033535	-2.690360
36	1	-2.127099	-3.981835	1.278145
37	1	-1.851144	-2.691155	2.453717
38	1	-0.561094	-3.161674	1.336633
39	1	-4.154898	-1.295706	2.450517
40	1	-4.110897	0.418001	2.031617
41	1	-2.716363	-0.332990	2.811100
42	1	-5.338917	0.395783	-1.056377
43	1	-4.055634	1.497876	-1.568626
44	1	-4.524347	1.419065	0.133577
45	1	-4.017070	-1.504421	-3.325625
46	1	-2.289671	-1.333587	-3.679346
47	1	-3.260188	0.098957	-3.340816
48	6	-0.729938	2.862605	1.445599
49	6	-0.327129	3.064223	2.925645
50	6	-0.069740	3.961317	0.575184
51	6	-2.256406	2.968623	1.305700
52	1	-0.829412	2.330648	3.565642
53	1	0.755825	2.946903	3.048713
54	1	-0.604963	4.069090	3.265373
55	1	1.010664	4.025710	0.740211
56	1	-0.249497	3.776848	-0.489027
57	1	-0.500610	4.934364	0.836273
58	1	-2.555931	2.870779	0.257321
59	1	-2.752560	2.190819	1.892200
60	1	-2.602613	3.942900	1.667590
61	6	4.810513	0.375791	-1.263522

62	6	4.890593	1.506214	-2.315218
63	6	5.984301	0.529924	-0.266065
64	6	4.885273	-0.985292	-1.997542
65	1	4.060759	1.423375	-3.025709
66	1	4.820585	2.482746	-1.824979
67	1	5.834575	1.456089	-2.870531
68	1	5.927480	1.500224	0.239337
69	1	5.971625	-0.256035	0.496525
70	1	6.941158	0.474057	-0.798066
71	1	5.010958	-1.826443	-1.310906
72	1	3.979042	-1.150858	-2.591189
73	1	5.742738	-0.985082	-2.680408

2aMe (E = -821.5267384 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.068018	0.398870	0.161196
2	7	-3.269308	1.056229	-0.890843
3	6	1.447959	-1.656657	0.140104
4	6	0.642412	-1.787518	-1.030272
5	6	0.585076	-1.790612	1.276695
6	17	-0.783512	0.943607	2.521172
7	6	-0.710875	-1.962399	-0.620749
8	6	-0.742961	-1.982326	0.808579
9	6	-2.188941	0.793820	-0.550290
10	6	0.446245	1.227784	-1.995140
11	6	1.576290	1.641686	-1.161256
12	1	-0.227252	2.013149	-2.338717
13	6	-0.099587	2.848726	0.093270
14	6	1.270297	2.490970	-0.079986
15	1	-0.366714	3.373831	1.002833
16	1	-0.678064	3.132902	-0.779497
17	6	2.310761	2.953555	0.925212
18	6	3.006077	1.329731	-1.563469
19	1	3.680561	1.187227	-0.713294
20	1	3.403836	2.161994	-2.164179
21	1	3.052642	0.435462	-2.191036
22	1	2.771332	3.889526	0.576732
23	1	3.115891	2.228203	1.082562
24	1	1.839399	3.160705	1.891296
25	6	1.144618	-1.999801	-2.436496
26	6	2.957943	-1.706854	0.200359
27	6	1.047908	-1.907935	2.708801
28	6	-1.945671	-2.283399	1.668936
29	6	-1.858684	-2.300383	-1.543905
30	1	1.324421	-3.071353	-2.607597
31	1	2.085811	-1.477529	-2.627678
32	1	0.420013	-1.664955	-3.184865
33	1	3.295356	-2.737914	0.380455
34	1	3.361100	-1.089176	1.010326
35	1	3.415298	-1.370351	-0.732918
36	1	1.321395	-2.949646	2.931734
37	1	0.267639	-1.602010	3.409417
38	1	1.928747	-1.288075	2.907306
39	1	-1.983495	-3.354231	1.914672
40	1	-2.882022	-2.029385	1.161234
41	1	-1.915377	-1.721244	2.606530
42	1	-1.832727	-3.366164	-1.812092
43	1	-1.816257	-1.725968	-2.475432
44	1	-2.827594	-2.104844	-1.074668
45	1	0.712724	0.556893	-2.806605
46	6	-4.589058	1.440994	-1.289312
47	1	-4.792158	2.454427	-0.935406
48	1	-4.663342	1.416723	-2.378921

49	1	-5.321043	0.753502	-0.859258

TS(2a-3b)Me (E = -821.5222523 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-1.114178	-0.589800	-0.664500
2	7	-3.305246	1.304397	-2.363383
3	6	1.402287	-1.036713	-0.905040
4	6	1.250125	-0.237324	0.260734
5	6	0.986019	-0.261326	-2.030675
6	17	-1.414676	-2.574181	-2.146337
7	6	0.744474	1.041415	-0.140566
8	6	0.589483	1.026803	-1.558328
9	6	-2.645479	0.548924	-1.681557
10	6	-1.824080	0.117316	1.442154
11	6	-2.185216	-1.290592	1.472938
12	1	-2.634471	0.837607	1.320164
13	6	-3.659415	-0.729603	-0.407041
14	6	-3.046998	-1.739315	0.474521
15	1	-4.303189	-1.168009	-1.164115
16	1	-4.131336	0.102597	0.115190
17	6	-3.520304	-3.173973	0.353780
18	6	-1.606095	-2.208955	2.533326
19	1	-1.421299	-3.225078	2.172243
20	1	-2.307428	-2.279695	3.377210
21	1	-0.667737	-1.806564	2.926162
22	1	-4.437410	-3.316000	0.944282
23	1	-2.778659	-3.896519	0.705488
24	1	-3.747845	-3.415688	-0.687990
25	6	1.722400	-0.598276	1.649023
26	6	2.004719	-2.419483	-0.973640
27	6	1.117519	-0.666758	-3.478124
28	6	0.249735	2.219559	-2.421392
29	6	0.625776	2.266870	0.733258
30	1	2.759276	-0.264778	1.797145
31	1	1.700501	-1.679175	1.821355
32	1	1.115639	-0.122889	2.426198
33	1	3.067896	-2.359911	-1.246390
34	1	1.501535	-3.039428	-1.721648
35	1	1.941885	-2.939872	-0.012374
36	1	2.118691	-0.413280	-3.855440
37	1	0.385707	-0.154478	-4.111079
38	1	0.967947	-1.741638	-3.608639
39	1	1.165716	2.760333	-2.699337
40	1	-0.406336	2.923796	-1.901093
41	1	-0.255557	1.923690	-3.345303
42	1	1.534326	2.881029	0.652701
43	1	0.498788	2.004111	1.786981
44	1	-0.222646	2.896571	0.444833
45	1	-1.121306	0.432508	2.206718
46	6	-4.739405	1.549055	-2.495902
47	1	-4.938575	2.596520	-2.252590
48	1	-5.023262	1.388770	-3.539536
49	1	-5.338994	0.901777	-1.849466

3bMe (E = -821.5517528 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.155859	0.103373	-0.424985
2	7	-0.506926	2.162425	-0.225083
3	6	2.152516	-1.538060	-0.032998
4	6	1.717490	-1.071929	1.240263
5	6	2.675871	-0.426337	-0.756486
6	17	-0.145993	-0.854877	-2.650691

7	6	1.950607	0.338720	1.295664
8	6	2.553328	0.734284	0.060672
9	6	-1.523444	1.410877	-0.457228
10	6	-0.481838	3.566768	0.219882
11	6	-1.447996	-0.801797	0.958301
12	6	-2.900055	-0.843418	0.512194
13	1	-1.350656	-0.152843	1.845100
14	6	-2.980028	1.563822	-0.260714
15	6	-3.611670	0.204155	0.037450
16	1	-3.228992	2.314207	0.507815
17	1	-3.413378	1.949125	-1.196112
18	6	-5.098041	0.196775	-0.269316
19	6	-3.514177	-2.227257	0.672557
20	1	-4.516405	-2.324002	0.249763
21	1	-3.558804	-2.512641	1.733485
22	1	-2.873084	-2.966959	0.173289
23	1	-5.610464	-0.708627	0.060326
24	1	-5.278653	0.314438	-1.349142
25	1	-5.590646	1.047739	0.225122
26	6	1.297759	-1.930886	2.407346
27	6	2.161030	-2.970640	-0.509756
28	6	3.346593	-0.499458	-2.106381
29	6	3.104017	2.103623	-0.267506
30	6	1.782933	1.198853	2.528561
31	1	2.170881	-2.175060	3.029038
32	1	0.854029	-2.876307	2.080302
33	1	0.567488	-1.428083	3.049380
34	1	3.145981	-3.430599	-0.346447
35	1	1.937181	-3.038381	-1.579532
36	1	1.422477	-3.579040	0.022294
37	1	4.390405	-0.827023	-1.998234
38	1	3.357694	0.473426	-2.608487
39	1	2.840543	-1.207493	-2.769714
40	1	4.174755	2.155776	-0.025273
41	1	2.600937	2.891177	0.301341
42	1	2.998839	2.344288	-1.331066
43	1	2.643688	1.078889	3.201695
44	1	0.886049	0.930972	3.098224
45	1	1.713808	2.262163	2.278309
46	1	-1.159390	-1.797734	1.306258
47	1	0.125861	3.657134	1.124709
48	1	-1.491408	3.940445	0.420795
49	1	-0.022906	4.179547	-0.562128

TS(3b-3c)Me (E = -821.5490193 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.291955	-0.484937	-0.416266
2	7	-0.875391	1.380299	-0.697526
3	6	2.591978	-1.468251	0.313206
4	6	2.023384	-0.794334	1.434929
5	6	2.884006	-0.497050	-0.686577
6	17	0.194720	-1.646088	-2.539982
7	6	1.935551	0.594664	1.114727
8	6	2.467925	0.776828	-0.201954
9	6	-1.615370	0.445703	-0.240978
10	6	-1.220241	2.777309	-1.019066
11	6	-0.947932	-1.840871	0.978873
12	6	-2.337042	-2.171755	0.477094
13	1	-1.007923	-1.235550	1.895365
14	6	-3.017174	0.241544	0.193157
15	6	-3.300267	-1.262981	0.182553
16	1	-3.127072	0.675264	1.201053

17	1	-3.742662	0.775105	-0.436926
18	6	-4.733594	-1.583321	-0.195907
19	6	-2.565704	-3.669426	0.330669
20	1	-3.486015	-3.931965	-0.195601
21	1	-2.581912	-4.158608	1.315252
22	1	-1.728657	-4.109376	-0.228276
23	1	-4.965436	-2.649458	-0.166739
24	1	-4.968335	-1.214780	-1.206652
25	1	-5.431916	-1.079671	0.490206
26	6	1.761088	-1.406384	2.788911
27	6	2.924109	-2.939762	0.240344
28	6	3.595813	-0.760896	-1.990873
29	6	2.702239	2.101475	-0.892291
30	6	1.523855	1.696215	2.066894
31	1	2.679802	-1.394475	3.392307
32	1	1.430712	-2.446466	2.712342
33	1	0.995088	-0.858238	3.346439
34	1	3.937900	-3.131701	0.619770
35	1	2.882126	-3.312236	-0.788395
36	1	2.231861	-3.541112	0.839174
37	1	4.684922	-0.755522	-1.841597
38	1	3.361998	-0.000149	-2.742425
39	1	3.322020	-1.732647	-2.412950
40	1	3.722677	2.461968	-0.700253
41	1	2.010807	2.871379	-0.536411
42	1	2.582469	2.024392	-1.978477
43	1	2.387218	2.047193	2.649754
44	1	0.765879	1.356972	2.781332
45	1	1.115103	2.562844	1.536736
46	1	-0.430511	-2.764974	1.260543
47	1	-0.625998	3.449782	-0.392474
48	1	-2.284729	2.975931	-0.856103
49	1	-0.967156	2.975082	-2.064855

3cMe (E = -821.5517535 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.020992	0.098015	-0.134626
2	7	-1.208273	1.916656	-0.113958
3	6	2.384942	-0.876511	0.176971
4	6	1.969727	-0.336908	1.427611
5	6	2.498690	0.198180	-0.753246
6	17	-0.269888	-1.260382	-2.148504
7	6	1.802892	1.074788	1.264198
8	6	2.140596	1.404744	-0.085640
9	6	-1.992752	0.898639	-0.096523
10	6	-1.530637	3.332753	0.134180
11	6	-1.157161	-0.951677	1.572007
12	6	-2.577644	-1.443314	1.349034
13	1	-1.154358	-0.162156	2.342510
14	6	-3.405848	0.697403	0.285855
15	6	-3.598412	-0.710932	0.848194
16	1	-3.774307	1.473753	0.976652
17	1	-4.023229	0.795724	-0.619907
18	6	-5.046892	-1.155951	0.762437
19	6	-2.761004	-2.892963	1.776584
20	1	-3.734153	-3.316096	1.518684
21	1	-2.615133	-3.000277	2.861117
22	1	-1.993509	-3.512240	1.291943
23	1	-5.249420	-2.095620	1.279162
24	1	-5.363034	-1.270692	-0.286079
25	1	-5.704084	-0.392607	1.205908
26	6	1.929447	-1.071305	2.744858
27	6	2.745066	-2.315486	-0.104667

28	6	3.020932	0.081517	-2.164296
29	6	2.249535	2.796706	-0.665825
30	6	1.528557	2.052383	2.385376
31	1	2.895728	-0.974801	3.260073
32	1	1.734960	-2.139957	2.611248
33	1	1.158913	-0.676780	3.414879
34	1	3.830484	-2.469390	-0.023692
35	1	2.442601	-2.614198	-1.113816
36	1	2.263123	-2.999377	0.601543
37	1	4.120072	0.060915	-2.165456
38	1	2.707309	0.926868	-2.785403
39	1	2.668453	-0.833569	-2.649891
40	1	3.283084	3.163427	-0.594038
41	1	1.611646	3.509440	-0.134796
42	1	1.967342	2.823866	-1.724040
43	1	2.453347	2.276463	2.935783
44	1	0.808140	1.655962	3.109593
45	1	1.136342	3.003344	2.011374
46	1	-0.567705	-1.766182	2.002581
47	1	-1.345615	3.905163	-0.780030
48	1	-0.881494	3.727383	0.920959
49	1	-2.577726	3.458484	0.429173

TS(3c-4)Me (E = 821.520227 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.709627	-0.224671	-0.918636
2	7	-0.579238	1.329155	-0.692286
3	6	3.096355	-1.094459	-0.590851
4	6	2.586606	-0.683210	0.678628
5	6	3.222453	0.062735	-1.413834
6	17	0.580045	-1.607201	-2.947568
7	6	2.394516	0.734772	0.634645
8	6	2.786283	1.193025	-0.662160
9	6	-1.295426	0.162267	-0.666964
10	6	-0.978668	2.603409	-0.096561
11	6	-0.896189	-0.972824	0.869079
12	6	-2.301188	-1.504834	1.015978
13	1	-0.573878	-0.428377	1.765539
14	6	-2.784256	0.036787	-0.765622
15	6	-3.248096	-1.023858	0.196859
16	1	-3.295444	0.987369	-0.545441
17	1	-3.061416	-0.223186	-1.796768
18	6	-4.705252	-1.411028	0.144118
19	6	-2.503173	-2.552744	2.089764
20	1	-3.543666	-2.878426	2.176082
21	1	-2.188122	-2.167093	3.069508
22	1	-1.887744	-3.440437	1.885501
23	1	-4.977073	-2.153672	0.898354
24	1	-4.958831	-1.823712	-0.842568
25	1	-5.345210	-0.529573	0.292911
26	6	2.471121	-1.546727	1.914425
27	6	3.543002	-2.486168	-0.969866
28	6	3.816995	0.087346	-2.800958
29	6	2.875480	2.635022	-1.106941
30	6	2.033421	1.605545	1.816223
31	1	3.407416	-1.517412	2.489045
32	1	2.274512	-2.594835	1.665331
33	1	1.670439	-1.208498	2.580518
34	1	4.632648	-2.583048	-0.863240
35	1	3.286957	-2.721726	-2.007706
36	1	3.082837	-3.249015	-0.333462
37	1	4.914954	0.078752	-2.748271

38	1	3.521522	0.985597	-3.352507
39	1	3.504032	-0.781348	-3.388689
40	1	3.889418	3.026665	-0.943901
41	1	2.183786	3.273242	-0.549538
42	1	2.647192	2.750680	-2.171764
43	1	2.929491	1.836410	2.409433
44	1	1.318495	1.115941	2.486541
45	1	1.593786	2.556287	1.501600
46	1	-0.219292	-1.845527	0.793039
47	1	-0.268398	3.381809	-0.389430
48	1	-0.996670	2.544910	1.002889
49	1	-1.977485	2.908090	-0.435837

4Me (E = -821.5584879 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.547688	-1.031972	0.009039
2	7	1.038250	-1.086981	1.142605
3	6	-1.892590	1.089232	-0.298543
4	6	-1.966189	0.736888	1.086345
5	6	-2.609675	0.097383	-1.042140
6	17	-0.450949	-2.829584	-1.635252
7	6	-2.692647	-0.486039	1.187978
8	6	-3.101767	-0.872116	-0.129948
9	6	1.431353	-0.106988	0.067339
10	6	1.967462	-1.430981	2.208618
11	6	1.911623	1.258558	0.599794
12	6	3.411752	1.268202	0.375400
13	1	1.645173	1.395667	1.655907
14	6	2.606306	-0.604145	-0.815561
15	6	3.792097	0.246170	-0.405536
16	1	2.784085	-1.677769	-0.674079
17	1	2.406003	-0.475973	-1.889395
18	6	5.171615	-0.087190	-0.909743
19	6	4.258799	2.365909	0.963709
20	1	5.317037	2.264989	0.701617
21	1	4.182770	2.375409	2.060730
22	1	3.918292	3.352137	0.615414
23	1	5.930332	0.619033	-0.556891
24	1	5.195285	-0.087039	-2.009186
25	1	5.472336	-1.094879	-0.588863
26	6	-1.506431	1.590470	2.244634
27	6	-1.377918	2.394035	-0.860503
28	6	-2.864879	0.126872	-2.530735
29	6	-3.980239	-2.051025	-0.476127
30	6	-3.097467	-1.173202	2.473854
31	1	-2.308664	2.275775	2.553142
32	1	-0.636178	2.198396	1.982500
33	1	-1.237061	0.985483	3.116062
34	1	-2.204655	3.108236	-0.982394
35	1	-0.909661	2.264091	-1.841799
36	1	-0.638617	2.855533	-0.200684
37	1	-3.794065	0.670621	-2.752522
38	1	-2.964283	-0.881253	-2.944952
39	1	-2.056704	0.629858	-3.072342
40	1	-5.038439	-1.754067	-0.475363
41	1	-3.871310	-2.868880	0.244045
42	1	-3.747829	-2.451707	-1.467428
43	1	-4.075704	-0.805319	2.813666
44	1	-2.380489	-0.985373	3.279808
45	1	-3.187048	-2.258450	2.351003
46	1	1.453942	2.100530	0.061614
47	1	1.494649	-2.139953	2.897325
48	1	2.275313	-0.546484	2.784990

49	1	2.877228	-1.900413	1.807297

TS(4-5)Me (E = -821.5409287 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.188886	-0.292742	-0.083366
2	7	0.766804	-0.996731	1.513669
3	6	-2.029870	1.402991	-0.093496
4	6	-2.017153	0.786618	1.199867
5	6	-2.459991	0.423978	-1.040404
6	17	0.167426	-1.595631	-2.133465
7	6	-2.436244	-0.572152	1.045219
8	6	-2.705617	-0.792080	-0.337702
9	6	1.810571	-0.508315	0.677750
10	6	0.972448	-1.439180	2.885364
11	6	2.095764	0.987034	0.682960
12	6	3.375474	1.103869	-0.114928
13	1	2.156179	1.462309	1.674929
14	6	3.075013	-1.226990	0.249754
15	6	3.915478	-0.108687	-0.333872
16	1	3.615321	-1.698157	1.090147
17	1	2.893183	-2.025225	-0.481959
18	6	5.199405	-0.432793	-1.050270
19	6	3.900401	2.456324	-0.521741
20	1	4.855991	2.388577	-1.050328
21	1	4.046384	3.101871	0.356128
22	1	3.189281	2.973336	-1.182331
23	1	5.732912	0.461207	-1.387026
24	1	5.002112	-1.061794	-1.929319
25	1	5.873537	-1.003872	-0.396434
26	6	-1.766867	1.494373	2.512534
27	6	-1.814053	2.874914	-0.376065
28	6	-2.721744	0.649651	-2.509965
29	6	-3.267549	-2.054440	-0.944831
30	6	-2.730411	-1.543283	2.164514
31	1	-2.706449	1.890723	2.922956
32	1	-1.081374	2.340667	2.395713
33	1	-1.336299	0.822359	3.261124
34	1	-2.763243	3.423450	-0.298007
35	1	-1.422404	3.045982	-1.384603
36	1	-1.116016	3.330935	0.333798
37	1	-3.793557	0.814372	-2.689558
38	1	-2.411997	-0.211999	-3.109945
39	1	-2.188260	1.527587	-2.888862
40	1	-4.358824	-1.976950	-1.052351
41	1	-3.059165	-2.929614	-0.321218
42	1	-2.846523	-2.245845	-1.936762
43	1	-3.802061	-1.531204	2.408900
44	1	-2.184407	-1.284276	3.075637
45	1	-2.465312	-2.571859	1.898725
46	1	1.256052	1.598411	0.190493
47	1	0.029265	-1.786644	3.317897
48	1	1.362974	-0.622088	3.513821
49	1	1.693656	-2.268091	2.933359

5Me (E = -821.5743328 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.218484	0.015926	-0.176452
2	7	0.808118	-1.051661	1.305354
3	6	-2.232397	1.538603	-0.212607
4	6	-2.026648	1.129275	1.139313
5	6	-2.578445	0.380611	-0.968234
6	17	0.221370	-1.393769	-2.086245

7	6	-2.297551	-0.270552	1.229472
8	6	-2.625553	-0.737103	-0.075725
9	6	2.023654	-0.515885	0.958869
10	6	0.771994	-2.437386	1.788542
11	6	2.241019	0.839462	0.865346
12	6	3.531554	1.089197	0.200441
13	1	1.654836	1.599282	1.367171
14	6	3.228655	-1.230637	0.366174
15	6	4.126154	-0.094486	-0.076120
16	1	3.725136	-1.871053	1.107383
17	1	2.935836	-1.880283	-0.466675
18	6	5.471462	-0.359759	-0.693424
19	6	4.036887	2.483065	-0.058977
20	1	5.031353	2.481555	-0.514878
21	1	4.093182	3.060960	0.873699
22	1	3.355763	3.021210	-0.731448
23	1	6.003858	0.568125	-0.924984
24	1	5.376315	-0.931529	-1.627405
25	1	6.108320	-0.951911	-0.020404
26	6	-1.720865	2.038750	2.307588
27	6	-2.246168	2.960795	-0.717206
28	6	-2.964703	0.363464	-2.428280
29	6	-3.075420	-2.130963	-0.445397
30	6	-2.378195	-1.050973	2.518584
31	1	-2.649557	2.425996	2.750466
32	1	-1.119909	2.902420	2.003750
33	1	-1.176138	1.512243	3.098261
34	1	-3.259080	3.380878	-0.635887
35	1	-1.941412	3.021875	-1.765730
36	1	-1.570875	3.600201	-0.141689
37	1	-4.042886	0.543997	-2.543007
38	1	-2.735569	-0.598672	-2.895583
39	1	-2.438205	1.138403	-2.994772
40	1	-4.172362	-2.195037	-0.429728
41	1	-2.691544	-2.883092	0.251053
42	1	-2.740840	-2.409587	-1.449117
43	1	-3.272570	-0.752848	3.082760
44	1	-1.508268	-0.876855	3.160577
45	1	-2.452672	-2.127111	2.337223
46	1	0.343131	1.648409	-0.795955
47	1	-0.264686	-2.761492	1.892499
48	1	1.260531	-2.526441	2.768399
49	1	1.272029	-3.125522	1.091451

6aMe (E = -954.3139493 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.946949	0.246516	-0.214565
2	7	0.646524	-1.097393	-0.334370
3	6	-2.617431	1.227569	1.518357
4	6	-1.800024	0.246256	2.166544
5	6	-3.392261	0.571675	0.521407
6	17	-1.661043	0.236763	-2.574125
7	6	-2.078665	-1.018665	1.577368
8	6	-3.056653	-0.814352	0.543375
9	6	1.977105	-1.097171	0.062725
10	6	0.212345	-2.333049	-1.032389
11	6	2.609429	-0.302097	0.969827
12	6	4.040274	-0.625834	1.012993
13	1	2.138022	0.462263	1.572136
14	6	3.023718	-2.029875	-0.533800
15	6	4.310586	-1.631791	0.146626
16	1	2.784402	-3.085852	-0.350812

17	1	3.079536	-1.913315	-1.624250
18	6	5.611724	-2.329458	-0.143891
19	6	4.994084	0.095975	1.930702
20	1	6.016705	-0.284463	1.843653
21	1	4.683733	-0.008235	2.979766
22	1	5.015251	1.171868	1.708009
23	1	6.435006	-1.912558	0.446238
24	1	5.890142	-2.244713	-1.204849
25	1	5.554342	-3.404816	0.083146
26	6	-0.939431	0.473018	3.386545
27	6	-2.765598	2.665405	1.952685
28	6	-4.446276	1.206322	-0.351730
29	6	-3.755349	-1.893143	-0.252454
30	6	-1.571842	-2.350248	2.081198
31	1	-1.522610	0.302688	4.302879
32	1	-0.552095	1.495371	3.423019
33	1	-0.081843	-0.206348	3.409456
34	1	-3.520829	2.743298	2.747145
35	1	-3.084282	3.310000	1.128416
36	1	-1.828988	3.069211	2.349884
37	1	-5.438789	1.109466	0.110634
38	1	-4.488576	0.734653	-1.337905
39	1	-4.255193	2.272879	-0.505936
40	1	-4.703273	-2.164867	0.232640
41	1	-3.154558	-2.805193	-0.324696
42	1	-3.984141	-1.562262	-1.269873
43	1	-2.176713	-2.687193	2.934700
44	1	-0.530994	-2.289342	2.413248
45	1	-1.629795	-3.127140	1.313437
46	1	0.263120	1.365402	0.731340
47	6	0.738603	4.490157	0.125583
48	7	-0.244728	3.566637	-0.403057
49	6	-0.590003	2.431742	-0.341283
50	1	0.227262	5.333305	0.595648
51	1	1.378635	3.984117	0.856799
52	1	1.347496	4.872244	-0.697081
53	1	-0.859460	-2.285193	-1.264350
54	1	0.378384	-3.228003	-0.417347
55	1	0.728271	-2.461181	-1.992857

TS(6a-7a)Me (E = -954.3139493 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.257627	-0.319069	-0.082990
2	7	-0.515700	1.611883	-0.333267
3	6	2.476881	-1.501279	-0.157534
4	6	2.169891	-1.324798	1.223200
5	6	2.693519	-0.209986	-0.735179
6	17	-0.345417	-1.289978	-2.209750
7	6	2.157497	0.077541	1.489330
8	6	2.509349	0.764513	0.287142
9	6	-1.792033	1.226935	-0.005208
10	6	-0.346086	2.667269	-1.339568
11	6	-2.091432	0.553729	1.156567
12	6	-3.466297	0.029889	1.085374
13	1	-1.488052	0.566795	2.055678
14	6	-3.022037	1.196902	-0.899988
15	6	-4.026911	0.409368	-0.086306
16	1	-3.387295	2.208632	-1.121313
17	1	-2.801496	0.723075	-1.863456
18	6	-5.422619	0.169978	-0.592233
19	6	-4.073273	-0.768003	2.208094
20	1	-5.115232	-1.033870	2.007009
21	1	-4.043672	-0.205344	3.151259

22	1	-3.510591	-1.697138	2.368845
23	1	-6.028289	-0.386034	0.130295
24	1	-5.414313	-0.402307	-1.530702
25	1	-5.938252	1.118390	-0.801515
26	6	2.047398	-2.424066	2.249832
27	6	2.676344	-2.826624	-0.853853
28	6	3.163333	0.047051	-2.147674
29	6	2.791941	2.243841	0.191664
30	6	1.954697	0.725207	2.840218
31	1	3.039739	-2.682938	2.646468
32	1	1.610452	-3.331039	1.822637
33	1	1.418163	-2.122096	3.091818
34	1	3.721041	-3.155883	-0.762078
35	1	2.438534	-2.762972	-1.919668
36	1	2.044452	-3.609290	-0.421676
37	1	4.255879	-0.052757	-2.211093
38	1	2.904273	1.054514	-2.488296
39	1	2.723436	-0.663193	-2.854092
40	1	3.732654	2.480513	0.707528
41	1	2.001087	2.844925	0.652619
42	1	2.900497	2.569727	-0.846849
43	1	2.910497	0.809650	3.376770
44	1	1.276392	0.142520	3.472485
45	1	1.541855	1.735113	2.746572
46	1	-0.462140	-1.533870	1.087796
47	1	0.711171	2.767786	-1.589757
48	1	-0.703748	3.634441	-0.960931
49	1	-0.891626	2.438212	-2.266623

7aMe (E = -821.5743292 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.622186	0.042345	-0.346875
2	7	1.177990	-1.006560	-0.224234
3	6	-2.552377	0.968038	1.092184
4	6	-1.500523	0.535765	1.961592
5	6	-3.073198	-0.172841	0.430352
6	17	-1.404386	-0.942470	-2.489382
7	6	-1.395292	-0.885542	1.855299
8	6	-2.351781	-1.322393	0.891758
9	6	2.474576	-0.564781	-0.001939
10	6	1.063487	-2.457396	-0.511735
11	6	2.909641	0.534884	0.675041
12	6	4.370615	0.643848	0.574969
13	1	2.286244	1.226221	1.223900
14	6	3.701481	-1.263270	-0.574640
15	6	4.858784	-0.392098	-0.148277
16	1	3.810283	-2.285752	-0.189663
17	1	3.626934	-1.352724	-1.666344
18	6	6.281625	-0.736806	-0.495186
19	6	5.133465	1.767425	1.229397
20	1	6.212732	1.680215	1.069731
21	1	4.953433	1.784776	2.313358
22	1	4.813057	2.742121	0.835689
23	1	6.986135	-0.000232	-0.094147
24	1	6.434349	-0.781493	-1.583663
25	1	6.568370	-1.720856	-0.094725
26	6	-0.770363	1.392162	2.969051
27	6	-3.069058	2.382393	0.977256
28	6	-4.261121	-0.213869	-0.498838
29	6	-2.699506	-2.750494	0.540861
30	6	-0.524502	-1.762630	2.724342
31	1	-1.291382	1.374887	3.936973
32	1	-0.709947	2.435779	2.645433

33	1	0.251371	1.037867	3.139867
34	1	-3.823181	2.583069	1.750870
35	1	-3.539770	2.565621	0.005922
36	1	-2.268720	3.119428	1.104171
37	1	-5.162789	-0.522951	0.048877
38	1	-4.106383	-0.921430	-1.318788
39	1	-4.464415	0.766248	-0.941795
40	1	-3.620660	-3.055698	1.056729
41	1	-1.911505	-3.447508	0.842515
42	1	-2.865460	-2.874531	-0.534487
43	1	-1.011053	-1.940746	3.693691
44	1	0.449486	-1.303789	2.920656
45	1	-0.341886	-2.738261	2.264731
46	1	0.786752	2.989444	-0.005165
47	6	-0.555228	2.919834	-2.441536
48	7	-0.382108	1.943407	-1.362504
49	6	0.258588	2.063301	-0.263312
50	1	-1.620329	3.141420	-2.559272
51	1	-0.005476	3.843608	-2.227381
52	1	-0.198370	2.481547	-3.377684
53	1	0.011916	-2.741148	-0.616142
54	1	1.500053	-3.061958	0.295276
55	1	1.555113	-2.721129	-1.457288

TS(7a-8a)Me (E = -954.3378816 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.825144	-0.020753	-0.034898
2	7	-2.132193	1.207537	-0.473864
3	6	-2.389496	1.306660	0.816337
4	7	0.532047	-1.481058	0.938998
5	6	-2.006908	1.535908	0.535323
6	6	-1.266541	0.864546	1.698679
7	6	-1.076063	0.573963	-0.482331
8	17	0.148505	-1.543183	-2.332151
9	6	0.123436	-0.507196	1.399543
10	6	0.243017	-0.685928	0.048629
11	6	-2.721505	2.025494	-1.281284
12	6	-0.033396	-0.945745	1.653276
13	6	1.923437	-2.953286	0.478169
14	6	-1.336922	0.543754	2.230875
15	1	-3.374412	2.302995	1.253199
16	6	-1.679433	0.750251	2.695080
17	1	-1.564216	0.733261	2.890251
18	6	0.481579	-1.602096	1.789751
19	6	-0.675114	-0.419268	2.435563
20	1	1.385338	-2.116037	2.416080
21	1	0.772749	-2.363386	0.816640
22	6	-0.585409	-0.672075	2.713231
23	6	-2.997436	2.140781	3.365536
24	1	-3.080852	2.144774	3.692368
25	1	-3.131176	2.670141	4.246931
26	1	-3.835978	2.728231	2.687832
27	1	-1.480125	0.255461	3.219292
28	1	-0.461171	-1.302209	1.785027
29	1	0.281320	-1.206155	3.349275
30	6	-1.857158	1.525750	3.058816
31	6	-3.512276	3.025315	0.457477
32	6	-1.400170	0.850196	-1.845436
33	6	1.516073	-1.947097	-0.670245
34	6	1.254612	-1.544243	2.387137
35	1	-2.022330	1.819502	3.611399
36	1	-2.820761	2.426189	2.980107
37	1	-1.194506	0.856082	3.668084
38	1	-3.853282	3.549743	0.891324
39	1	-3.869864	3.265959	-0.576624
40	1	-4.005427	3.443737	1.007773
41	1	-1.322769	1.049961	-1.833684
42	1	-0.713966	-0.000823	-2.610079
43	1	-2.417805	1.723598	-2.159667
44	1	1.651267	-1.913582	-0.670342
45	1	2.397727	-2.837839	-0.191327
46	1	1.502749	-2.084819	-1.712133
47	1	1.416890	-1.472430	2.951801
48	1	1.046293	-1.415419	3.112286
49	1	2.197311	-2.562936	1.888270
50	1	2.284036	-3.257337	0.007090
51	1	2.585511	-3.462080	1.317296
52	1	1.982302	-3.256973	-0.266667
53	1	-2.351637	1.801392	-0.946799
54	1	-2.442435	1.829153	-2.329413
55	1	-3.817386	3.100685	-1.195649

8aMe (E = -954.3630249 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.545750	-0.020753	-0.322417
2	7	0.788032	1.207537	-1.126827
3	6	1.132488	1.306660	0.266974
4	7	1.016857	-1.481058	0.512760
5	6	-2.311740	1.535908	0.521201
6	6	-1.812099	0.864546	1.680324
7	6	-3.001361	0.573963	-0.278324
8	17	-0.794926	-1.543183	-2.290004
9	6	-2.203368	-0.507196	1.597244
10	6	-2.941135	-0.685928	0.391104
11	6	1.378261	2.025494	-2.175532
12	6	2.177070	-0.945745	0.655899
13	6	0.908030	-2.953286	0.396967
14	6	2.341434	0.543754	0.817265
15	1	1.027106	2.302995	0.714203
16	6	3.790258	0.750251	0.371515
17	1	2.312009	0.733261	1.906533
18	6	3.528635	-1.602096	0.529705
19	6	4.436714	-0.419268	0.232273
20	1	3.815649	-2.116037	1.459760
21	1	3.537671	-2.363386	-0.258976
22	6	5.875060	-0.672075	-0.131064
23	6	4.345431	2.140781	0.241650
24	1	5.391077	2.144774	-0.079823
25	1	4.283915	2.670141	1.203724
26	1	3.762686	2.728231	-0.477821
27	1	6.420244	0.255461	-0.327793
28	1	5.946683	-1.302209	-1.028920
29	1	6.397505	-1.206155	0.675754
30	6	-1.179758	1.525750	2.881455
31	6	-2.239667	3.025315	0.272580
32	6	-3.764845	0.850196	-1.553417
33	6	-3.637699	-1.947097	-0.060365
34	6	-1.985250	-1.544243	2.675739
35	1	-1.950356	1.819502	3.609582
36	1	-0.626258	2.426189	2.600129
37	1	-0.481257	0.856082	3.394505
38	1	-3.028879	3.549743	0.830209
39	1	-2.370496	3.265959	-0.787077
40	1	-1.278770	3.443737	0.590651
41	1	-4.823358	1.049961	-1.333452
42	1	-3.723349	-0.000823	-2.240527
43	1	-3.370678	1.723598	-2.083575
44	1	-4.705071	-1.913582	0.200497
45	1	-3.212548	-2.837839	0.413978
46	1	-3.561225	-2.084819	-1.143588
47	1	-2.764651	-1.472430	3.447550
48	1	-1.018983	-1.415419	3.175871
49	1	-2.020514	-2.562936	2.275245
50	1	-0.089736	-3.257337	0.718743
51	1	1.649424	-3.462080	1.020461
52	1	1.031158	-3.256973	-0.647218
53	1	2.447002	1.801392	-2.310108
54	1	0.870341	1.829153	-3.126809
55	1	1.288430	3.100685	-1.948322

TS(8a-10)Me (E = -954.3175976 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	0.473828	-0.135718	-0.423418
2	7	-0.263689	-0.501257	1.419601
3	6	-0.616892	0.838069	1.439410
4	7	-1.792209	-0.381270	-0.996689
5	6	2.759714	0.533433	0.523289
6	6	2.154962	1.704327	-0.030264
7	6	3.038947	-0.358739	-0.543031
8	17	0.598241	-2.482006	-1.230483
9	6	2.073236	1.535706	-1.454568
10	6	2.609215	0.253694	-1.763914
11	6	-0.264124	-1.286035	2.644809
12	6	-2.332373	0.579918	-0.345158
13	6	-2.591928	-1.394597	-1.692954
14	6	-1.359457	1.497745	0.305823
15	1	-0.290459	1.484473	2.252626
16	6	-2.208722	2.709240	0.664677
17	1	-0.629631	1.780952	-0.607174
18	6	-3.738075	1.089298	-0.179136
19	6	-3.509935	2.465843	0.419717
20	1	-4.266876	1.136274	-1.139077
21	1	-4.343331	0.449301	0.476890
22	6	-4.695640	3.348383	0.703744
23	6	-1.604781	3.952210	1.256307
24	1	-2.370980	4.673533	1.552953
25	1	-0.940195	4.447750	0.536535
26	1	-1.002024	3.719521	2.142736
27	1	-4.406486	4.313685	1.127924
28	1	-5.382723	2.862352	1.411048
29	1	-5.267881	3.541870	-0.214279
30	6	1.961012	3.013163	0.697285
31	6	3.144729	0.348615	1.971050
32	6	3.791009	-1.662026	-0.438665
33	6	2.809706	-0.318014	-3.147751
34	6	1.718900	2.614268	-2.454484
35	1	2.872993	3.624125	0.623754
36	1	1.749406	2.863061	1.759877
37	1	1.143115	3.602404	0.272939
38	1	4.109142	0.831660	2.184912
39	1	3.241675	-0.710481	2.229420
40	1	2.401599	0.786816	2.646048
41	1	4.864884	-1.494093	-0.605142
42	1	3.442297	-2.387628	-1.178265
43	1	3.675361	-2.119957	0.548898
44	1	3.832515	-0.126929	-3.503160
45	1	2.122775	0.130438	-3.874077
46	1	2.647654	-1.400500	-3.162023
47	1	2.616420	3.181481	-2.743385
48	1	0.996254	3.327513	-2.045211
49	1	1.287500	2.197540	-3.370814
50	1	-3.665255	-1.183095	-1.634865
51	1	-2.287133	-1.435892	-2.742524
52	1	-1.292612	-1.441340	3.003592
53	1	0.191833	-2.260783	2.449268
54	1	0.299816	-0.789366	3.450470
55	1	-2.388149	-2.373711	-1.253099

10Me (E = -954.3761803 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	0.544071	0.091114	-0.770158
2	7	-0.079352	0.108271	1.327074
3	6	-1.050988	0.858777	1.880695
4	7	-1.696666	0.467464	-0.981306
5	6	2.825175	0.641557	0.362737
6	6	2.537842	1.627870	-0.628254
7	6	3.017321	-0.601703	-0.297976
8	17	0.149511	-2.189004	-1.564071
9	6	2.640530	1.009758	-1.912155
10	6	2.904876	-0.367760	-1.708258
11	6	0.505783	-0.864826	2.279716
12	6	-2.411847	1.181971	-0.156802
13	6	-2.303395	0.181006	-2.299430
14	6	-2.073253	1.483052	1.201782
15	1	-1.050378	0.924778	2.971429
16	6	-3.134032	2.337026	1.762404
17	1	0.203863	1.346792	-2.054307
18	6	-3.754975	1.827903	-0.446078
19	6	-4.093617	2.555309	0.835880
20	1	-3.690704	2.499593	-1.312707
21	1	-4.511665	1.074514	-0.702700
22	6	-5.358213	3.360487	0.945122
23	6	-3.088065	2.842389	3.180183
24	1	-3.927692	3.506578	3.403131
25	1	-2.158203	3.395151	3.370922
26	1	-3.122158	2.011182	3.898129
27	1	-5.457260	3.842415	1.922621
28	1	-6.246329	2.729624	0.792987
29	1	-5.394618	4.147993	0.178252
30	6	2.342833	3.102984	-0.365487
31	6	3.076595	0.964583	1.816350
32	6	3.486836	-1.908114	0.299671
33	6	3.224337	-1.381370	-2.779513
34	6	2.631018	1.719665	-3.243324
35	1	3.304487	3.636265	-0.384432
36	1	1.890289	3.282751	0.616085
37	1	1.695577	3.562697	-1.119896
38	1	3.956644	1.616476	1.900072
39	1	3.277993	0.067766	2.407612
40	1	2.234294	1.490532	2.278713
41	1	4.508129	-2.134404	-0.036643
42	1	2.850772	-2.748416	-0.002009
43	1	3.506933	-1.876090	1.393454
44	1	4.312263	-1.454925	-2.922681
45	1	2.782520	-1.105662	-3.742489
46	1	2.850470	-2.375448	-2.517968
47	1	3.658531	1.965609	-3.548579
48	1	2.059451	2.650559	-3.196299
49	1	2.189055	1.102916	-4.032427
50	1	-3.290438	-0.282836	-2.182195
51	1	-2.408857	1.099857	-2.889525
52	1	-0.199300	-1.686892	2.457032
53	1	1.419809	-1.296134	1.876795
54	1	0.734708	-0.392072	3.244530
55	1	-1.667857	-0.511269	-2.850467

TS(10-11)Me (E = -954.340542 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.622040	0.332815	0.232339
2	7	-0.117432	0.387793	-1.670221
3	6	-1.181163	-0.511426	-1.507506
4	7	-1.356697	0.730201	1.099723
5	6	2.550744	-1.204026	-0.386528

6	6	1.915030	-1.782917	0.757866
7	6	3.158697	0.018499	0.020086
8	17	0.966949	2.808519	0.577261
9	6	2.130910	-0.910104	1.868144
10	6	2.904235	0.196767	1.414108
11	6	0.352936	0.571131	-3.046612
12	6	-2.443607	0.439410	0.389458
13	6	-1.558756	1.383105	2.409288
14	6	-2.397183	-0.220405	-0.848541
15	1	-1.213154	-1.316535	-2.249392
16	6	-3.744784	-0.725929	-1.154826
17	1	-0.441903	-1.238272	-0.011432
18	6	-3.887035	0.515120	0.835818
19	6	-4.621889	-0.279077	-0.223371
20	1	-4.016619	0.087708	1.837440
21	1	-4.243207	1.552681	0.895152
22	6	-6.117445	-0.425319	-0.177757
23	6	-4.039057	-1.549838	-2.380834
24	1	-5.105088	-1.776415	-2.471896
25	1	-3.497538	-2.505351	-2.356165
26	1	-3.724902	-1.024189	-3.292902
27	1	-6.498029	-1.016024	-1.016792
28	1	-6.614504	0.555505	-0.207967
29	1	-6.442953	-0.917029	0.750384
30	6	1.350080	-3.180927	0.839236
31	6	2.691329	-1.875215	-1.732830
32	6	4.013611	0.928675	-0.830033
33	6	3.499771	1.282802	2.274908
34	6	1.716177	-1.187009	3.296363
35	1	2.141154	-3.892742	1.117579
36	1	0.930124	-3.504328	-0.117601
37	1	0.555727	-3.255365	1.588209
38	1	3.514198	-2.603838	-1.715736
39	1	2.910348	-1.153999	-2.525811
40	1	1.781755	-2.416011	-2.015738
41	1	5.080659	0.712051	-0.678344
42	1	3.850346	1.982090	-0.579818
43	1	3.804509	0.803379	-1.897614
44	1	4.533481	1.024007	2.545474
45	1	2.939669	1.419609	3.205300
46	1	3.513653	2.245527	1.757004
47	1	2.468574	-1.803606	3.808475
48	1	0.764502	-1.727624	3.345574
49	1	1.606279	-0.263806	3.875289
50	1	-0.588575	1.564989	2.875733
51	1	-2.156300	0.751360	3.078609
52	1	-2.061549	2.350910	2.295019
53	1	1.293773	1.126999	-3.038197
54	1	0.516147	-0.391876	-3.556248
55	1	-0.375233	1.147570	-3.632693

11Me (E = -954.3931395 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.673358	0.122362	-0.448880
2	7	0.397086	1.839344	-0.543217
3	6	1.847221	1.930892	-0.393715
4	7	0.912635	-1.093666	-0.911528
5	6	-1.724238	0.709494	1.785971
6	6	-0.933363	-0.470673	1.964801
7	6	-2.829129	0.370211	0.957449
8	17	-2.000898	0.124887	-2.497337
9	6	-1.584354	-1.547237	1.283966
10	6	-2.742175	-1.025908	0.648266

11	6	-0.202246	3.172448	-0.701684
12	6	2.179259	-0.651767	-0.527791
13	6	0.826136	-2.429799	-1.523045
14	6	2.588504	0.623732	-0.258763
15	1	2.263679	2.486320	-1.254873
16	6	4.007268	0.588891	0.161832
17	1	2.075827	2.559583	0.484563
18	6	3.345077	-1.591580	-0.281762
19	6	4.466997	-0.684286	0.148988
20	1	3.098795	-2.336486	0.486566
21	1	3.609622	-2.157849	-1.184470
22	6	5.841678	-1.214344	0.452892
23	6	4.776734	1.836227	0.520699
24	1	5.821174	1.610419	0.755114
25	1	4.340800	2.338726	1.395051
26	1	4.769031	2.562490	-0.303181
27	1	6.533052	-0.415020	0.739285
28	1	6.274402	-1.729367	-0.417646
29	1	5.821948	-1.944466	1.275239
30	6	0.269943	-0.597446	2.871025
31	6	-1.490328	2.032132	2.477405
32	6	-3.973917	1.273668	0.563359
33	6	-3.787364	-1.811771	-0.105035
34	6	-1.174684	-2.999706	1.345918
35	1	-0.042467	-0.852904	3.893770
36	1	0.839503	0.335790	2.924715
37	1	0.954451	-1.380546	2.530111
38	1	-1.931973	2.019948	3.483836
39	1	-1.944260	2.864815	1.931561
40	1	-0.423436	2.250478	2.588040
41	1	-4.841799	1.104785	1.216574
42	1	-4.296998	1.090976	-0.467058
43	1	-3.704989	2.331847	0.646206
44	1	-4.652057	-2.019149	0.541108
45	1	-3.399151	-2.774399	-0.453084
46	1	-4.148835	-1.265446	-0.982051
47	1	-1.618574	-3.485405	2.226310
48	1	-0.088821	-3.112747	1.422605
49	1	-1.507122	-3.558064	0.464895
50	1	-0.217308	-2.648856	-1.768929
51	1	1.190062	-3.221821	-0.854575
52	1	1.403185	-2.472926	-2.457362
53	1	-1.289924	3.097078	-0.807200
54	1	0.015382	3.820710	0.162649
55	1	0.183685	3.669512	-1.605079

TS(11-12)Me (E = -954.3516536 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.461320	-0.293648	0.039359
2	7	0.564797	-0.295252	1.910405
3	6	-0.452663	1.804770	1.767781
4	7	-1.617288	0.433594	-0.450579
5	6	2.874584	0.397390	-0.276141
6	6	2.086116	1.449506	-0.835702
7	6	2.708832	-0.751773	-1.098319
8	17	-0.152355	-2.630590	-0.481416
9	6	1.473884	0.957032	-2.035962
10	6	1.860099	-0.396907	-2.198342
11	6	-2.348217	1.093468	0.420826
12	6	-1.811712	1.653503	1.615362
13	1	-0.004538	2.133183	2.695907
14	6	-2.932277	1.921361	2.528926
15	1	0.138881	2.034418	0.886960

16	6	-3.853328	1.223269	0.469821
17	6	-4.104825	1.711779	1.884713
18	1	-4.222765	1.935672	-0.281157
19	1	-4.346782	0.267548	0.258350
20	6	-5.508098	1.927992	2.375806
21	6	-2.715147	2.417956	3.932244
22	1	-3.658592	2.594355	4.455892
23	1	-2.146889	3.358282	3.930821
24	1	-2.135428	1.692044	4.517843
25	1	-5.531231	2.288911	3.408327
26	1	-6.090365	0.996369	2.333829
27	1	-6.038507	2.662078	1.751844
28	6	2.137097	2.903719	-0.419439
29	6	3.818134	0.528310	0.895510
30	6	3.428274	-2.071903	-0.948579
31	6	1.533543	-1.304187	-3.359158
32	6	0.681453	1.797760	-3.010444
33	1	2.944981	3.423389	-0.954360
34	1	2.333382	3.018049	0.651976
35	1	1.206609	3.435435	-0.649948
36	1	4.801800	0.888197	0.560685
37	1	3.970480	-0.430842	1.399704
38	1	3.442308	1.234770	1.642288
39	1	4.337916	-2.088280	-1.566293
40	1	2.797187	-2.910054	-1.259507
41	1	3.730217	-2.253377	0.087995
42	1	2.412541	-1.436403	-4.005562
43	1	0.729744	-0.895472	-3.980445
44	1	1.218816	-2.296155	-3.017332
45	1	1.353698	2.402736	-3.635396
46	1	0.002464	2.490131	-2.499694
47	1	0.079753	1.180579	-3.685068
48	6	0.851470	-0.475079	3.309542
49	1	1.668158	0.173623	3.668398
50	1	-0.032738	-0.272837	3.936065
51	1	1.149902	-1.515929	3.509158
52	6	-2.301282	-0.058000	-1.668504
53	1	-1.560363	-0.415792	-2.384130
54	1	-2.959461	-0.900690	-1.425113
55	1	-2.892744	0.733146	-2.143822

12Me (E = -954.3635152 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.899473	0.138917	-0.552811
2	7	-0.660790	1.801503	-1.292756
3	6	2.334378	1.964901	-0.087353
4	7	1.197332	-0.895902	-0.515539
5	6	-2.335811	0.986826	1.315067
6	6	-1.101615	0.601867	1.918913
7	6	-2.990241	-0.201444	0.870683
8	17	-1.962091	-1.220128	-2.335046
9	6	-1.018270	-0.827840	1.884763
10	6	-2.182182	-1.322539	1.236901
11	6	2.429421	-0.555618	-0.329377
12	6	2.991765	0.794009	-0.065347
13	1	2.867120	2.890470	0.098989
14	6	4.438034	0.613136	0.172581
15	1	1.276231	2.021185	-0.324161
16	6	3.594648	-1.527455	-0.329523
17	6	4.790506	-0.679280	0.021997
18	1	3.437067	-2.342593	0.388018
19	1	3.701335	-2.008639	-1.311128
20	6	6.145298	-1.313165	0.145776

21	6	5.326220	1.779747	0.506611
22	1	6.361901	1.470462	0.667929
23	1	4.979091	2.289144	1.415172
24	1	5.317701	2.522061	-0.302520
25	1	6.921601	-0.589965	0.408625
26	1	6.436862	-1.795233	-0.798041
27	1	6.139209	-2.099411	0.913875
28	6	-0.157246	1.518226	2.664032
29	6	-2.909888	2.382949	1.286186
30	6	-4.371406	-0.284718	0.263663
31	6	-2.573872	-2.767509	1.040777
32	6	0.042495	-1.646895	2.582284
33	1	-0.433523	1.579112	3.727072
34	1	-0.180058	2.534981	2.259281
35	1	0.879547	1.168308	2.614904
36	1	-3.472769	2.589116	2.208155
37	1	-3.593517	2.521858	0.442824
38	1	-2.123938	3.139101	1.198248
39	1	-5.126445	-0.448888	1.046270
40	1	-4.446767	-1.107967	-0.453033
41	1	-4.639075	0.636370	-0.264018
42	1	-3.366299	-3.056388	1.745576
43	1	-1.728807	-3.444068	1.207152
44	1	-2.952204	-2.948530	0.028161
45	1	-0.163408	-1.702164	3.660638
46	1	1.041789	-1.211510	2.467347
47	1	0.077423	-2.674783	2.207232
48	6	-0.671287	3.159126	-1.776716
49	1	-1.433916	3.774927	-1.271920
50	1	0.300602	3.661315	-1.620401
51	1	-0.880857	3.203448	-2.857135
52	6	0.963915	-2.345390	-0.783517
53	1	-0.103369	-2.538510	-0.887480
54	1	1.445094	-2.643436	-1.721236
55	1	1.355018	-2.962480	0.031460

13Me (E = -548.7761331 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.018182	0.755607	-0.121944
2	7	1.811377	0.421807	-0.233003
3	6	-0.809560	-1.313498	1.008918
4	6	-0.776101	-1.585910	-0.392523
5	6	-1.848560	-0.354041	1.246265
6	17	-0.629725	2.942611	-1.038741
7	6	-1.781082	-0.778200	-1.015610
8	6	-2.456095	-0.033501	-0.000296
9	6	0.053188	-2.655507	-1.063463
10	6	-0.021839	-2.047926	2.070676
11	6	-2.281433	0.153721	2.604557
12	6	-3.648342	0.865884	-0.218673
13	6	-2.167881	-0.811730	-2.477620
14	1	-0.463225	-3.625020	-1.020838
15	1	1.026234	-2.774321	-0.577589
16	1	0.237197	-2.426848	-2.117900
17	1	-0.561691	-2.948240	2.396918
18	1	0.145224	-1.429849	2.959495
19	1	0.957512	-2.363982	1.699349
20	1	-3.035340	-0.514381	3.043431
21	1	-2.727830	1.152036	2.545502
22	1	-1.445149	0.200663	3.311296
23	1	-4.569766	0.273424	-0.306564
24	1	-3.547544	1.460895	-1.132235
25	1	-3.785489	1.565384	0.611868

26	1	-2.970230	-1.544123	-2.644223
27	1	-1.326971	-1.099856	-3.116981
28	1	-2.534633	0.160092	-2.824027
29	6	3.188769	-0.001148	-0.336341
30	1	3.278370	-1.088953	-0.485735
31	1	3.700298	0.489141	-1.178257
32	1	3.753903	0.249704	0.574268

14Me (E = -405.5480508 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.258431	0.784241	0.019151
2	6	0.069620	0.338226	0.002869
3	6	-1.136093	1.222341	0.033573
4	6	-2.315062	0.343778	0.001996
5	6	-0.435491	-1.103324	-0.048270
6	6	-1.939686	-0.953877	-0.043681
7	1	-0.081989	-1.627083	-0.945499
8	1	-0.082781	-1.689074	0.810101
9	6	-2.807961	-2.178529	-0.087329
10	6	-3.712699	0.901400	0.021041
11	1	-4.471781	0.115244	-0.006954
12	1	-3.878901	1.563713	-0.839061
13	1	-3.879646	1.501596	0.925446
14	1	-3.874593	-1.938333	-0.079362
15	1	-2.600441	-2.831911	0.772095
16	1	-2.599598	-2.769697	-0.990482
17	6	-1.111676	2.562681	0.080946
18	1	-2.021649	3.150501	0.101305
19	1	-0.166708	3.091707	0.100070
20	6	2.389206	-0.144617	-0.013153
21	1	3.010441	0.088571	-0.886008
22	1	3.009461	0.026156	0.874721
23	1	2.116288	-1.207786	-0.050994

15Me (E = -797.0775028 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.227446	-0.091118	-0.561970
2	7	-0.859507	1.619873	-0.371658
3	6	-1.855205	-1.077149	1.058334
4	6	-0.587863	-1.121384	1.711401
5	6	-1.813427	-2.001126	-0.029914
6	17	0.018249	-0.654696	-2.962330
7	6	0.214639	-2.111604	1.054930
8	6	-0.541381	-2.655188	-0.015823
9	6	-0.227043	-0.403326	2.992508
10	6	-3.061537	-0.295616	1.520876
11	6	-2.960108	-2.348117	-0.952750
12	6	-0.134775	-3.780708	-0.936283
13	6	1.563381	-2.593871	1.534406
14	1	-0.482154	-1.015029	3.870187
15	1	-0.764190	0.546091	3.085332
16	1	0.845498	-0.185226	3.051642
17	1	-3.619145	-0.859434	2.282869
18	1	-3.748914	-0.086312	0.695287
19	1	-2.774806	0.665393	1.958659
20	1	-3.521700	-3.210811	-0.565877
21	1	-2.606318	-2.606924	-1.956076
22	1	-3.665726	-1.517035	-1.054772
23	1	-0.636381	-4.717314	-0.654195
24	1	0.944307	-3.964193	-0.898185
25	1	-0.395020	-3.565362	-1.978457
26	1	1.443447	-3.349641	2.323586

27	1	2.165655	-1.780879	1.954708
28	1	2.143510	-3.057144	0.729165
29	7	1.994591	0.391815	-0.123761
30	6	2.992778	-0.348056	-0.665854
31	6	2.327272	1.486110	0.606187
32	6	4.339264	-0.027571	-0.498337
33	1	2.691377	-1.205438	-1.256150
34	6	3.651982	1.859436	0.828780
35	1	1.495825	2.062596	0.990962
36	6	4.678408	1.093410	0.266085
37	1	5.099738	-0.644991	-0.960278
38	1	3.868288	2.740337	1.420642
39	1	5.717057	1.366657	0.414519
40	6	-1.503207	2.891181	-0.148256
41	1	-2.337995	2.818611	0.569197
42	1	-0.799600	3.639751	0.255338
43	1	-1.913547	3.312739	-1.079718

TS(8a-16')Me (E = -954.3146031 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.673686	-0.195627	-0.392469
2	7	0.752217	1.181081	-0.859083
3	6	1.365285	1.361766	0.348018
4	7	1.140365	-1.490421	-0.183592
5	6	-2.306682	1.586110	0.377288
6	6	-1.862169	0.854510	1.525904
7	6	-3.092573	0.708073	-0.416599
8	17	-1.211205	-1.098660	-2.587329
9	6	-2.381078	-0.482897	1.436867
10	6	-3.135036	-0.565198	0.230282
11	6	1.098030	2.085078	-1.957718
12	6	2.065204	-0.965286	0.566607
13	6	1.486980	-2.681843	-0.987938
14	6	1.724066	0.252098	1.350656
15	1	1.706391	2.361194	0.611969
16	6	3.013183	0.536234	2.119957
17	1	0.919672	0.028451	2.095647
18	6	3.476750	-1.402335	0.841332
19	6	3.968193	-0.362004	1.828015
20	1	3.500081	-2.411198	1.282388
21	1	4.095411	-1.460001	-0.065020
22	6	5.383827	-0.425336	2.336995
23	6	3.083345	1.696439	3.074875
24	1	4.037103	1.733399	3.609368
25	1	2.279300	1.631503	3.821118
26	1	2.957260	2.653940	2.552112
27	1	5.592003	0.350288	3.079711
28	1	6.101964	-0.301825	1.513729
29	1	5.592563	-1.400452	2.798995
30	6	-1.251057	1.470254	2.763092
31	6	-2.086998	3.061910	0.151915
32	6	-3.839888	1.071570	-1.676529
33	6	-3.926984	-1.761700	-0.240723
34	6	-2.346146	-1.520918	2.537246
35	1	-2.044724	1.792058	3.453156
36	1	-0.641980	2.345687	2.520522
37	1	-0.617766	0.763223	3.310330
38	1	-2.773122	3.659679	0.769371
39	1	-2.256438	3.338770	-0.893227
40	1	-1.064743	3.359092	0.413063
41	1	-4.880828	1.335795	-1.441843
42	1	-3.858307	0.241161	-2.388801
43	1	-3.386873	1.929936	-2.182989

44	1	-4.971041	-1.693731	0.097079
45	1	-3.516594	-2.698858	0.151150
46	1	-3.935335	-1.835162	-1.332864
47	1	-3.201484	-1.392457	3.217660
48	1	-1.434222	-1.446521	3.138512
49	1	-2.396129	-2.539430	2.138104
50	1	1.851569	-3.491211	-0.344068
51	1	2.266196	-2.438046	-1.720341
52	1	2.142694	1.926366	-2.262563
53	1	0.442190	1.890000	-2.810684
54	1	0.604703	-3.025801	-1.526551
55	1	0.986451	3.138628	-1.660736

16'Me (E = -954.3273296 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.727157	-0.414037	-0.148619
2	7	0.627204	-0.678952	-1.746218
3	6	1.920448	-0.313318	-1.641218
4	7	0.977512	-1.162278	0.880501
5	6	-1.267085	2.038030	-0.297234
6	6	-0.953404	1.773678	1.074661
7	6	-2.494556	1.373862	-0.599744
8	17	-2.116148	-2.397625	-0.397644
9	6	-1.985977	0.947766	1.614916
10	6	-2.940537	0.710798	0.582672
11	6	0.293960	-1.506310	-2.927706
12	6	2.183783	-0.668231	0.578838
13	6	0.928798	-2.361705	1.742074
14	6	2.332228	0.438332	-0.418068
15	1	2.652750	-0.630006	-2.376814
16	6	3.805191	0.790267	-0.346577
17	1	1.693624	1.327961	-0.235317
18	6	3.521333	-0.985949	1.199799
19	6	4.453305	0.004787	0.528467
20	1	3.501451	-0.831728	2.292433
21	1	3.858491	-2.022678	1.057457
22	6	5.918330	0.001371	0.875238
23	6	4.360572	1.887901	-1.214878
24	1	5.439920	2.012220	-1.086509
25	1	3.880955	2.849798	-0.984890
26	1	4.166838	1.682900	-2.276259
27	1	6.478275	0.765390	0.327917
28	1	6.370074	-0.974795	0.649016
29	1	6.066686	0.178489	1.949912
30	6	0.153647	2.406657	1.887348
31	6	-0.555207	3.006055	-1.215397
32	6	-3.259564	1.473414	-1.899186
33	6	-4.265430	0.008588	0.750925
34	6	-2.122154	0.543024	3.064376
35	1	-0.244946	3.236360	2.488284
36	1	0.945575	2.814931	1.252787
37	1	0.617217	1.692550	2.576724
38	1	-1.039711	3.992359	-1.178946
39	1	-0.571688	2.667270	-2.256498
40	1	0.492558	3.145275	-0.932628
41	1	-3.965825	2.316222	-1.870782
42	1	-3.841243	0.567156	-2.098683
43	1	-2.590862	1.634954	-2.750893
44	1	-5.041819	0.728751	1.046341
45	1	-4.219583	-0.766527	1.521801
46	1	-4.591426	-0.473089	-0.175587
47	1	-2.681687	1.303684	3.628904
48	1	-1.145130	0.431253	3.545569

49	1	-2.659343	-0.404966	3.174625
50	1	-0.104500	-2.705928	1.833218
51	1	1.309504	-2.148484	2.749367
52	1	0.971487	-2.369204	-2.985113
53	1	-0.730754	-1.877262	-2.853990
54	1	1.526643	-3.173399	1.306793
55	1	0.387186	-0.924663	-3.853519

TS(16'-16)Me (E = -954.323311 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.517554	-0.200618	-0.599923
2	7	1.144714	0.350239	-2.090646
3	6	2.221350	0.382215	-1.367937
4	7	0.646508	-1.899163	-0.429600
5	6	-1.677657	1.360389	1.030158
6	6	-1.161103	0.270371	1.808432
7	6	-2.707955	0.842131	0.200269
8	17	-1.775497	-0.662105	-2.682169
9	6	-1.892164	-0.907522	1.467108
10	6	-2.837827	-0.559584	0.468259
11	6	1.252866	0.378974	-3.554643
12	6	1.567132	-1.236091	0.314153
13	6	0.672310	-3.354994	-0.544385
14	6	1.922525	0.185292	0.054545
15	1	3.231570	0.474294	-1.763379
16	6	2.919828	0.536129	1.126859
17	1	0.909407	1.028749	0.143606
18	6	2.310607	-1.706013	1.546597
19	6	3.131745	-0.503753	1.951368
20	1	1.638598	-2.028584	2.354804
21	1	2.953601	-2.571515	1.331896
22	6	4.048771	-0.578172	3.141635
23	6	3.522707	1.915294	1.172757
24	1	4.190520	2.042968	2.029345
25	1	2.736928	2.680484	1.237185
26	1	4.099776	2.128806	0.263099
27	1	4.586897	0.358778	3.311650
28	1	4.793597	-1.375339	3.010104
29	1	3.487519	-0.815686	4.056058
30	6	-0.225254	0.429338	2.983386
31	6	-1.353666	2.822221	1.237153
32	6	-3.607996	1.646242	-0.707602
33	6	-3.906443	-1.460863	-0.098697
34	6	-1.777492	-2.252220	2.144979
35	1	-0.769866	0.840631	3.845685
36	1	0.604951	1.108698	2.765590
37	1	0.203985	-0.526632	3.296183
38	1	-2.023540	3.262810	1.991149
39	1	-1.471899	3.401357	0.315313
40	1	-0.325518	2.962619	1.584686
41	1	-4.531548	1.929225	-0.182137
42	1	-3.889267	1.078144	-1.599251
43	1	-3.124877	2.570773	-1.042160
44	1	-4.846171	-1.337115	0.458796
45	1	-3.621481	-2.516239	-0.036342
46	1	-4.105095	-1.235166	-1.150233
47	1	-2.452318	-2.309059	3.011231
48	1	-0.762701	-2.440308	2.508828
49	1	-2.042050	-3.070665	1.467762
50	1	-0.174112	-3.676621	-1.156067
51	1	0.603107	-3.852143	0.433719
52	1	2.272562	0.635702	-3.868835
53	1	0.981280	-0.596324	-3.967669

54	1	1.601944	-3.685648	-1.030369
55	1	0.553274	1.114612	-3.958668

16Me (E = -954.3743706 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.665414	0.310061	-0.428501
2	7	1.314111	1.036002	-1.271860
3	6	2.480645	0.897970	-0.690450
4	7	0.686347	-1.303376	0.230270
5	6	-2.727941	1.417860	0.618718
6	6	-1.979209	0.810304	1.671785
7	6	-3.246399	0.381953	-0.197661
8	17	-1.274464	-0.206097	-2.743607
9	6	-2.095336	-0.605095	1.538598
10	6	-2.852536	-0.875364	0.364652
11	6	1.264850	1.961218	-2.420962
12	6	1.959252	-1.134923	0.608138
13	6	0.214936	-2.707334	0.250930
14	6	2.783000	-0.043238	0.310481
15	1	3.300202	1.528430	-1.042344
16	6	4.097523	-0.247377	0.952776
17	1	-0.441252	2.096263	-0.111597
18	6	2.786533	-2.131483	1.401533
19	6	4.113823	-1.434783	1.596928
20	1	2.295503	-2.393187	2.347887
21	1	2.907954	-3.074168	0.851014
22	6	5.219559	-2.081946	2.384545
23	6	5.211280	0.760683	0.842486
24	1	6.084666	0.465574	1.430930
25	1	4.884791	1.749166	1.192837
26	1	5.539274	0.880125	-0.199591
27	1	6.111153	-1.448821	2.433108
28	1	5.518656	-3.042134	1.938896
29	1	4.906395	-2.295232	3.416971
30	6	-1.328814	1.529436	2.830156
31	6	-3.032697	2.888632	0.477715
32	6	-4.222002	0.549911	-1.335598
33	6	-3.386500	-2.208113	-0.108416
34	6	-1.669509	-1.584867	2.606703
35	1	-2.049355	1.690335	3.645284
36	1	-0.944258	2.508803	2.527873
37	1	-0.491334	0.957222	3.244949
38	1	-3.995967	3.124846	0.952595
39	1	-3.098518	3.193604	-0.571945
40	1	-2.261794	3.503296	0.950258
41	1	-5.253549	0.451837	-0.966962
42	1	-4.068065	-0.202732	-2.113800
43	1	-4.130900	1.533688	-1.806705
44	1	-4.477949	-2.244040	0.013307
45	1	-2.971030	-3.043284	0.463681
46	1	-3.173172	-2.384625	-1.169479
47	1	-2.260532	-1.415120	3.516989
48	1	-0.613988	-1.475994	2.879768
49	1	-1.833097	-2.620923	2.300358
50	1	-0.818831	-2.754359	-0.085689
51	1	0.276367	-3.154256	1.249583
52	1	2.220526	2.486136	-2.543617
53	1	1.042133	1.404850	-3.336004
54	1	0.816169	-3.315768	-0.437042
55	1	0.472196	2.701677	-2.271337

TS(16-10)Me (E = -954.3623905 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)

		X	Y	Z
1	72	-0.920997	0.114749	0.063347
2	7	0.240254	1.207753	1.547303
3	6	1.251159	0.580977	2.141323
4	7	0.884162	-0.993918	-0.490177
5	6	-3.361335	0.360142	0.718791
6	6	-3.132832	-1.041509	0.572254
7	6	-3.236894	0.965114	-0.568367
8	17	-0.073552	1.896683	-1.580037
9	6	-2.844958	-1.298547	-0.802770
10	6	-2.918450	-0.060229	-1.508564
11	6	1.759957	-1.251161	0.466673
12	6	1.872983	-0.604131	1.732655
13	1	1.681976	1.073428	3.016319
14	6	2.978764	-1.251128	2.472433
15	1	-0.800911	-1.108652	1.432410
16	6	2.864367	-2.284670	0.376486
17	6	3.551100	-2.213897	1.718042
18	1	2.444741	-3.276512	0.162127
19	1	3.553264	-2.060857	-0.449557
20	6	4.711438	-3.115420	2.036120
21	6	3.368421	-0.828323	3.864878
22	1	4.151179	-1.470874	4.277386
23	1	2.506169	-0.867073	4.543903
24	1	3.746491	0.203418	3.879289
25	1	5.086734	-2.959724	3.052206
26	1	5.548792	-2.945752	1.343256
27	1	4.431134	-4.174526	1.941823
28	6	-3.375524	-2.088221	1.630209
29	6	-3.800442	1.043957	1.994536
30	6	-3.530762	2.404718	-0.914562
31	6	-2.822449	0.127965	-3.003371
32	6	-2.648067	-2.669858	-1.410395
33	1	-4.427037	-2.411050	1.608188
34	1	-3.160625	-1.705941	2.632064
35	1	-2.747912	-2.970403	1.476226
36	1	-4.885025	0.937999	2.138380
37	1	-3.579894	2.116573	1.978944
38	1	-3.309967	0.614124	2.874758
39	1	-4.564792	2.505587	-1.273929
40	1	-2.861485	2.772938	-1.697098
41	1	-3.420433	3.063719	-0.047018
42	1	-3.826448	0.137589	-3.450960
43	1	-2.260175	-0.681156	-3.481400
44	1	-2.328556	1.070073	-3.257652
45	1	-3.616972	-3.151905	-1.602894
46	1	-2.081144	-3.330521	-0.745229
47	1	-2.115586	-2.619790	-2.365878
48	6	1.125439	-1.573744	-1.825961
49	1	2.128848	-1.326789	-2.193075
50	1	1.015285	-2.666265	-1.814687
51	1	0.401934	-1.158407	-2.531384
52	6	0.015532	2.615700	1.929447
53	1	0.515263	2.847495	2.878698
54	1	0.405778	3.280236	1.150608
55	1	-1.053933	2.818055	2.045908

TS(8a-17)Me (E = -954.3242104 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.206208	-0.348561	0.458429
2	7	1.679418	0.453229	0.006893
3	6	1.443201	1.016097	-1.195190
4	7	-1.603508	0.935273	-0.375849

5	6	-0.289620	-2.309186	-1.097541
6	6	-1.629506	-2.218585	-0.602174
7	6	0.557854	-2.709811	-0.015904
8	17	-0.499297	0.192774	2.834831
9	6	-1.603580	-2.498858	0.787446
10	6	-0.250053	-2.794914	1.154194
11	6	-0.709468	1.967784	-0.370370
12	6	0.406475	2.083391	-1.384576
13	1	2.095328	0.751489	-2.033777
14	6	0.925637	3.507952	-1.207909
15	1	-0.025418	1.956959	-2.391853
16	6	-0.870142	3.295911	0.346928
17	6	0.216010	4.156701	-0.271338
18	1	-1.867852	3.735640	0.190353
19	1	-0.748012	3.218626	1.436778
20	6	0.371865	5.580817	0.191269
21	6	2.065808	4.019987	-2.047048
22	1	2.349463	5.042171	-1.779468
23	1	1.801394	4.012554	-3.114533
24	1	2.955435	3.386344	-1.933235
25	1	1.196039	6.098426	-0.308355
26	1	0.555631	5.614407	1.274545
27	1	-0.548680	6.153315	0.008226
28	6	-2.841984	-1.994036	-1.471539
29	6	0.095915	-2.255972	-2.559479
30	6	1.984468	-3.189464	-0.146285
31	6	0.193356	-3.287440	2.511579
32	6	-2.784913	-2.582921	1.724755
33	1	-2.980032	-2.841849	-2.156610
34	1	-2.746535	-1.087979	-2.080938
35	1	-3.755748	-1.905104	-0.876592
36	1	-0.072522	-3.232963	-3.036847
37	1	1.152030	-2.002524	-2.695104
38	1	-0.495467	-1.515427	-3.107734
39	1	2.001103	-4.261777	-0.389052
40	1	2.550860	-3.058738	0.781222
41	1	2.522568	-2.668051	-0.943957
42	1	-0.004798	-4.364104	2.614275
43	1	-0.334505	-2.770741	3.318845
44	1	1.266095	-3.134232	2.670146
45	1	-3.053750	-3.631392	1.916139
46	1	-3.668558	-2.086618	1.311433
47	1	-2.564820	-2.116735	2.691176
48	6	-3.014218	1.212399	-0.057152
49	1	-3.124914	1.692020	0.924917
50	1	-3.461534	1.869944	-0.815154
51	1	-3.567953	0.272471	-0.039400
52	6	3.062118	0.035949	0.287730
53	1	3.523384	-0.445135	-0.586258
54	1	3.661126	0.917964	0.546399
55	1	3.082164	-0.657338	1.130912

17Me (E = -954.3526973 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.359134	-0.104020	-0.172646
2	7	0.732214	1.945386	-0.067837
3	6	1.906262	1.914192	0.452936
4	7	0.708302	-1.113186	1.157437
5	6	-2.411138	1.100003	0.810196
6	6	-2.264653	-0.136448	1.507545
7	6	-2.777972	0.806828	-0.540120
8	17	-0.067725	-0.734693	-2.546270
9	6	-2.530882	-1.194095	0.589856

10	6	-2.856019	-0.607377	-0.671832
11	6	1.753173	-0.573155	0.332633
12	6	2.550546	0.631738	0.874043
13	1	2.454803	2.855202	0.568416
14	6	3.957650	0.461425	0.303703
15	1	2.613014	0.667369	1.981413
16	6	2.775418	-1.500088	-0.335421
17	6	4.062502	-0.708181	-0.347290
18	1	2.928560	-2.441164	0.221354
19	1	2.484171	-1.798726	-1.351229
20	6	5.282938	-1.277425	-1.022557
21	6	5.031078	1.491219	0.555767
22	1	6.006303	1.164042	0.182673
23	1	5.135033	1.691396	1.632296
24	1	4.804159	2.452223	0.072499
25	1	6.160016	-0.628368	-0.937990
26	1	5.085829	-1.443106	-2.090815
27	1	5.540752	-2.255947	-0.593335
28	6	-2.084481	-0.251496	3.002702
29	6	-2.455108	2.446085	1.500421
30	6	-3.158682	1.797196	-1.616850
31	6	-3.354359	-1.346809	-1.888938
32	6	-2.625873	-2.667924	0.914899
33	1	-3.006119	0.052633	3.520302
34	1	-1.274374	0.385418	3.375329
35	1	-1.863409	-1.277900	3.305661
36	1	-3.279642	2.463821	2.226767
37	1	-2.636786	3.260301	0.792598
38	1	-1.536918	2.674310	2.055770
39	1	-4.250943	1.852180	-1.726535
40	1	-2.747949	1.512849	-2.592451
41	1	-2.803413	2.807032	-1.388328
42	1	-4.452131	-1.411108	-1.872184
43	1	-2.962730	-2.367746	-1.933367
44	1	-3.059290	-0.845853	-2.815308
45	1	-3.666706	-2.951981	1.126273
46	1	-2.027373	-2.929708	1.792029
47	1	-2.280393	-3.292084	0.083609
48	6	0.238429	3.236389	-0.589293
49	1	0.996124	4.022118	-0.490719
50	1	-0.009034	3.115302	-1.648021
51	1	-0.662880	3.539940	-0.056816
52	6	0.975733	-1.972075	2.302458
53	1	1.580043	-2.845757	2.014420
54	1	1.528149	-1.433738	3.089679
55	1	0.041120	-2.339144	2.736784

TS(17-18)Me (E = -954.3354825 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.095135	-0.711169	-0.469405
2	7	-1.571830	0.743588	-0.187788
3	6	-0.957430	1.886194	-0.419843
4	7	1.611575	0.204441	0.432845
5	6	-0.154012	-2.317443	1.448091
6	6	0.802896	-2.905388	0.566623
7	6	-1.428408	-2.345007	0.798727
8	17	0.223773	-0.766881	-2.943807
9	6	0.125000	-3.262327	-0.634976
10	6	-1.255696	-2.927916	-0.487837
11	6	1.198626	1.313124	-0.357189
12	6	0.280721	2.366578	0.278483
13	1	-1.347815	2.524929	-1.223805
14	6	0.780829	3.694447	-0.247326

15	1	0.188582	2.312712	1.371697
16	6	2.145048	2.055634	-1.300759
17	6	1.791597	3.517507	-1.116034
18	1	3.198959	1.872856	-1.036544
19	1	2.045692	1.751518	-2.351070
20	6	2.549754	4.571905	-1.878333
21	6	0.135596	4.980866	0.199830
22	1	0.575496	5.858803	-0.283123
23	1	0.233817	5.109277	1.287298
24	1	-0.942043	4.983084	-0.021663
25	1	2.195430	5.585086	-1.665079
26	1	2.463858	4.402691	-2.960730
27	1	3.621113	4.529307	-1.636265
28	6	2.232803	-3.271756	0.892387
29	6	0.064044	-1.914878	2.888457
30	6	-2.731595	-1.975780	1.468537
31	6	-2.328740	-3.268466	-1.495374
32	6	0.719532	-4.033269	-1.788417
33	1	2.314112	-4.352962	1.072095
34	1	2.585121	-2.764195	1.794039
35	1	2.923124	-3.022457	0.079131
36	1	-0.231348	-2.729331	3.565660
37	1	-0.529473	-1.034540	3.159330
38	1	1.112260	-1.680118	3.092138
39	1	-2.984737	-2.717282	2.238822
40	1	-3.562109	-1.948929	0.757476
41	1	-2.680346	-0.997052	1.958321
42	1	-2.493167	-4.354386	-1.528715
43	1	-2.053150	-2.947515	-2.506537
44	1	-3.287923	-2.804560	-1.244354
45	1	0.572047	-5.113171	-1.641229
46	1	1.795913	-3.856701	-1.882219
47	1	0.256592	-3.755759	-2.739619
48	6	2.679581	0.358389	1.416577
49	1	3.615234	0.690547	0.943513
50	1	2.409364	1.102818	2.182277
51	1	2.875341	-0.592978	1.917870
52	6	-2.881302	0.562914	-0.857806
53	1	-3.689338	0.828270	-0.167520
54	1	-2.959184	1.199061	-1.749684
55	1	-3.019917	-0.474852	-1.162523

18Me (E = -954.3729549 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.538119	-0.140384	-0.230232
2	7	0.585017	1.431057	-0.818899
3	6	1.854453	0.770375	-0.714805
4	7	0.855349	-0.752011	1.098934
5	6	-2.179717	0.423224	1.617080
6	6	-2.605551	-0.827935	1.080434
7	6	-2.348902	1.418085	0.605036
8	17	-0.341332	-1.717834	-2.108794
9	6	-3.030095	-0.608404	-0.264197
10	6	-2.875716	0.780900	-0.556362
11	6	2.010963	-0.380552	0.326357
12	6	2.757756	0.939163	0.509832
13	1	2.380669	0.596763	-1.656248
14	6	4.203455	0.632502	0.289595
15	1	2.436662	1.655900	1.258856
16	6	3.071336	-1.423280	-0.055147
17	6	4.380984	-0.656196	-0.057991
18	1	3.094712	-2.244515	0.672447
19	1	2.849490	-1.879696	-1.025798

20	6	5.659193	-1.358980	-0.429769
21	6	5.237121	1.721272	0.415750
22	1	6.253454	1.349532	0.254223
23	1	5.200282	2.179061	1.414160
24	1	5.050433	2.525306	-0.310079
25	1	6.532289	-0.703490	-0.354088
26	1	5.614492	-1.741793	-1.459162
27	1	5.830314	-2.227134	0.223125
28	6	-2.712529	-2.140713	1.822467
29	6	-1.810808	0.722018	3.051125
30	6	-2.180841	2.901986	0.830505
31	6	-3.300976	1.457111	-1.839814
32	6	-3.689305	-1.631434	-1.157802
33	1	-3.736649	-2.290122	2.192230
34	1	-2.044170	-2.177533	2.687859
35	1	-2.470304	-2.994269	1.180241
36	1	-2.652181	1.209993	3.563209
37	1	-0.948766	1.393901	3.124575
38	1	-1.572820	-0.187121	3.609446
39	1	-3.001338	3.283989	1.454196
40	1	-2.199290	3.460600	-0.109227
41	1	-1.241471	3.138163	1.341656
42	1	-4.372526	1.699733	-1.810896
43	1	-3.134725	0.815769	-2.711682
44	1	-2.757791	2.392242	-2.008540
45	1	-4.775296	-1.639732	-0.987063
46	1	-3.313662	-2.641036	-0.966646
47	1	-3.517610	-1.417164	-2.216377
48	6	0.652055	2.776450	-1.377604
49	1	1.243311	3.451100	-0.738736
50	1	1.117376	2.768300	-2.376019
51	1	-0.353820	3.190436	-1.477662
52	6	1.131987	-1.234370	2.448601
53	1	1.782911	-2.120076	2.442387
54	1	1.624625	-0.460852	3.059026
55	1	0.196851	-1.516061	2.936807

TS(7a-7c)Me (E = -954.3522129 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.577076	0.132063	-0.470667
2	7	-0.518975	2.162007	-1.233984
3	6	0.658171	1.687930	-1.425903
4	7	1.163566	-1.047763	-0.208866
5	6	-1.269539	0.676771	1.850114
6	6	-1.157741	-0.752951	1.864115
7	6	-2.424671	1.018088	1.074472
8	17	-1.530920	-0.968489	-2.422618
9	6	-2.188805	-1.278057	1.044505
10	6	-2.968924	-0.180725	0.551482
11	6	2.439094	-0.597714	0.036023
12	6	2.831501	0.594180	0.579486
13	1	1.429314	2.274775	-1.938289
14	6	4.293648	0.700287	0.560055
15	1	2.171989	1.351845	0.983492
16	6	3.701727	-1.365389	-0.334528
17	6	4.828600	-0.429228	0.034828
18	1	3.778616	-2.317691	0.207567
19	1	3.703970	-1.619797	-1.402561
20	6	6.271571	-0.812992	-0.150464
21	6	5.014824	1.913668	1.089838
22	1	6.101982	1.813763	1.011944
23	1	4.767111	2.087201	2.146443
24	1	4.719939	2.817809	0.539027
25	1	6.948202	-0.016788	0.178509
26	1	6.502569	-1.027713	-1.204545
27	1	6.526257	-1.719419	0.419702
28	6	-0.190517	-1.528657	2.724600
29	6	-0.473105	1.619506	2.726406
30	6	-3.046997	2.389513	0.974646
31	6	-4.239396	-0.316257	-0.250084
32	6	-2.537564	-2.730882	0.823022
33	1	-0.490139	-1.467626	3.780130
34	1	0.830859	-1.143283	2.642991
35	1	-0.166260	-2.586838	2.450420
36	1	-0.952028	1.729652	3.709999
37	1	-0.393258	2.620958	2.289505
38	1	0.542663	1.249081	2.898533
39	1	-3.839611	2.498462	1.728184
40	1	-3.501851	2.569537	-0.004847
41	1	-2.314779	3.181286	1.158439
42	1	-5.073068	-0.621027	0.398710
43	1	-4.138681	-1.067777	-1.039662
44	1	-4.520166	0.628507	-0.726556
45	1	-3.459358	-2.988570	1.363057
46	1	-1.750017	-3.398988	1.183729
47	1	-2.708564	-2.951960	-0.236916
48	6	-1.035546	3.468529	-1.668726
49	6	1.033723	-2.511770	-0.366909
50	1	-1.933515	3.316268	-2.274833
51	1	-1.309244	4.069080	-0.797524
52	1	-0.280364	4.001473	-2.257328
53	1	1.571506	-2.864571	-1.258042
54	1	-0.016136	-2.783478	-0.502915
55	1	1.417356	-3.057935	0.506783

7cMe (E = -954.3531528 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.595075	0.088402	-0.497917
2	7	-0.284260	2.153432	-1.057243
3	6	0.576215	1.485202	-1.737732
4	7	1.116894	-1.102532	-0.166034
5	6	-1.340112	0.682744	1.799909
6	6	-1.204394	-0.742729	1.866663
7	6	-2.479747	0.976790	0.983717
8	17	-1.575615	-1.054143	-2.421606
9	6	-2.202954	-1.315522	1.039149
10	6	-2.990208	-0.250063	0.491959
11	6	2.383759	-0.605090	0.024948
12	6	2.753856	0.632122	0.477981
13	1	1.261325	1.992341	-2.426937
14	6	4.214022	0.765326	0.441560
15	1	2.085274	1.398782	0.849902
16	6	3.659564	-1.366191	-0.310799
17	6	4.768846	-0.385375	-0.010917
18	1	3.758930	-2.282099	0.287404
19	1	3.657154	-1.685036	-1.361338
20	6	6.218073	-0.749855	-0.186415
21	6	4.912707	2.026034	0.883481
22	1	6.001481	1.940154	0.812292
23	1	4.661425	2.269271	1.925415
24	1	4.602363	2.883625	0.270199
25	1	6.880338	0.077297	0.091466
26	1	6.446310	-1.019233	-1.228501
27	1	6.495410	-1.617016	0.432106
28	6	-0.239160	-1.470977	2.769192
29	6	-0.573549	1.667545	2.655651
30	6	-3.130756	2.328627	0.812426
31	6	-4.247777	-0.434533	-0.319201
32	6	-2.525631	-2.780163	0.860822
33	1	-0.556550	-1.378542	3.817210
34	1	0.777287	-1.071703	2.690715
35	1	-0.192718	-2.537310	2.532121
36	1	-1.059152	1.790016	3.634398
37	1	-0.518772	2.659301	2.194045
38	1	0.451295	1.329406	2.841459
39	1	-3.985276	2.423906	1.496917
40	1	-3.511298	2.482918	-0.203348
41	1	-2.439678	3.144239	1.041240
42	1	-5.086191	-0.715471	0.334372
43	1	-4.129560	-1.221336	-1.070502
44	1	-4.530435	0.483822	-0.843695
45	1	-3.466584	-3.029315	1.370845
46	1	-1.746548	-3.423654	1.279884
47	1	-2.649342	-3.043432	-0.196363
48	6	-0.491831	3.609666	-1.074517
49	6	1.014352	-2.570212	-0.281415
50	1	-1.522808	3.829513	-1.364757
51	1	-0.323067	4.017612	-0.073398
52	1	0.197521	4.083729	-1.782047
53	1	1.555223	-2.937797	-1.164674
54	1	-0.030783	-2.862834	-0.404279
55	1	1.412148	-3.084251	0.605677

TS(7c-8b)Me (E = -954.3347316 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.685688	0.156596	-0.519286
2	7	-0.028772	2.086031	-0.176773
3	6	1.025621	1.482777	-0.757727
4	7	0.986922	-1.294083	-0.389206
5	6	-1.785831	-0.093571	1.705157
6	6	-1.775255	-1.424491	1.177720
7	6	-2.720757	0.675085	0.941813
8	17	-1.325571	-0.056523	-2.871134
9	6	-2.659861	-1.460367	0.064111
10	6	-3.244053	-0.163440	-0.077836
11	6	2.139733	-0.790292	0.004721
12	6	2.281317	0.519695	0.565598
13	1	1.774987	2.064592	-1.297590
14	6	3.737833	0.794382	0.627526
15	1	1.670070	0.829318	1.407371
16	6	3.512948	-1.362327	-0.274831
17	6	4.448389	-0.240880	0.127898
18	1	3.692841	-2.276460	0.310286
19	1	3.616005	-1.652725	-1.328435
20	6	5.936480	-0.388581	-0.037527
21	6	4.258905	2.094651	1.180774
22	1	5.351998	2.141784	1.173595
23	1	3.921735	2.237685	2.217210
24	1	3.878714	2.946980	0.601581
25	1	6.476529	0.494815	0.317520
26	1	6.210499	-0.544318	-1.091275
27	1	6.314898	-1.258082	0.520221
28	6	-1.086102	-2.602475	1.824876
29	6	-1.102472	0.347745	2.980862
30	6	-3.204778	2.066877	1.272243
31	6	-4.334307	0.193012	-1.057569
32	6	-3.047961	-2.666760	-0.757541
33	1	-1.667554	-2.951402	2.689813
34	1	-0.083522	-2.347085	2.183475
35	1	-0.986791	-3.446497	1.136667
36	1	-1.745199	0.156952	3.852293
37	1	-0.873266	1.418376	2.970852
38	1	-0.163326	-0.191342	3.146745
39	1	-4.141757	2.015899	1.844775
40	1	-3.403691	2.661637	0.374219
41	1	-2.479403	2.612448	1.881813
42	1	-5.304577	-0.187496	-0.707208
43	1	-4.142886	-0.236496	-2.045945
44	1	-4.429112	1.276635	-1.180494
45	1	-4.059494	-3.005082	-0.492549
46	1	-2.369724	-3.509596	-0.590520
47	1	-3.047347	-2.441835	-1.830091
48	6	-0.064942	3.467142	0.300266
49	6	0.975061	-2.650024	-0.969535
50	1	-1.096431	3.815263	0.395177
51	1	0.422046	3.553221	1.283485
52	1	0.466482	4.125849	-0.400011
53	1	1.556144	-2.679467	-1.900214
54	1	-0.050586	-2.934610	-1.210272
55	1	1.388468	-3.394712	-0.277550

8bMe (E = -954.355415 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.504763	0.121893	-0.343155
2	7	0.346198	1.891484	-0.025967
3	6	1.431249	1.172781	-0.628267
4	7	1.109972	-1.403420	0.330577
5	6	-2.005402	0.506608	1.642923
6	6	-1.943750	-0.915578	1.507594
7	6	-2.729283	1.023358	0.526816
8	17	-0.760926	-0.571878	-2.700027
9	6	-2.626174	-1.274625	0.305411
10	6	-3.105044	-0.077727	-0.297567
11	6	2.284819	-0.894634	0.457110
12	6	2.499082	0.595884	0.325778
13	1	1.836617	1.580760	-1.560400
14	6	3.986814	0.670212	0.008617
15	1	2.337871	1.049210	1.320605
16	6	3.608452	-1.605178	0.558661
17	6	4.591835	-0.521988	0.147034
18	1	3.788088	-1.964322	1.583775
19	1	3.648623	-2.493043	-0.083898
20	6	6.043828	-0.875452	-0.028760
21	6	4.611604	1.990785	-0.346561
22	1	5.687682	1.908360	-0.524640
23	1	4.454639	2.720584	0.460469
24	1	4.146835	2.411618	-1.246620
25	1	6.645086	-0.013297	-0.330767
26	1	6.167419	-1.656198	-0.792705
27	1	6.468309	-1.272844	0.904510
28	6	-1.450214	-1.851437	2.589116
29	6	-1.557980	1.277938	2.863131
30	6	-3.195515	2.448837	0.335716
31	6	-3.989392	-0.009004	-1.518004
32	6	-2.924693	-2.665766	-0.203645
33	1	-2.155147	-1.858794	3.432214
34	1	-0.473445	-1.552578	2.986686
35	1	-1.363442	-2.881242	2.231657
36	1	-2.338879	1.263673	3.637589
37	1	-1.343583	2.323905	2.627399
38	1	-0.652153	0.849514	3.306420
39	1	-4.258009	2.541691	0.602091
40	1	-3.088267	2.786940	-0.700934
41	1	-2.637717	3.143285	0.969295
42	1	-5.036178	-0.205828	-1.243739
43	1	-3.693938	-0.744681	-2.272057
44	1	-3.951403	0.978188	-1.989654
45	1	-3.992924	-2.897137	-0.089796
46	1	-2.369470	-3.432169	0.346847
47	1	-2.679767	-2.770625	-1.267227
48	6	0.451456	3.292004	0.353469
49	6	0.968994	-2.876876	0.357455
50	1	-0.492289	3.656590	0.772367
51	1	1.240817	3.445602	1.107738
52	1	0.703848	3.916942	-0.518274
53	1	1.531535	-3.327941	-0.467718
54	1	-0.079805	-3.141207	0.235460
55	1	1.330449	-3.296620	1.302490

TS(8b-18)Me (E = -954.3429868 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.427639	0.037965	-0.203042
2	7	0.460746	1.819571	-0.303647
3	6	1.653830	1.090704	-0.525033
4	7	0.915805	-1.130941	1.054501
5	6	-2.223594	0.943612	1.299326
6	6	-2.204265	-0.458926	1.579309
7	6	-2.705474	1.121044	-0.032337
8	17	-0.248734	-1.181163	-2.340662
9	6	-2.648385	-1.147289	0.414611
10	6	-2.950421	-0.170156	-0.581706
11	6	2.090725	-0.685788	0.590653
12	6	2.564220	0.731548	0.652393
13	1	2.141432	1.135198	-1.501246
14	6	4.033566	0.656505	0.320216
15	1	2.312745	1.274837	1.568567
16	6	3.212913	-1.544443	0.032806
17	6	4.384204	-0.585137	-0.052363
18	1	3.414580	-2.387324	0.708597
19	1	2.952971	-1.989805	-0.935677
20	6	5.721236	-1.088543	-0.523250
21	6	4.876923	1.901531	0.356911
22	1	5.901654	1.721612	0.018678
23	1	4.923350	2.312328	1.375140
24	1	4.440786	2.680923	-0.282891
25	1	6.479340	-0.300139	-0.538763
26	1	5.646558	-1.506193	-1.537233
27	1	6.086492	-1.896417	0.126990
28	6	-1.915903	-1.046745	2.941748
29	6	-1.958406	2.025644	2.320552
30	6	-3.082382	2.426768	-0.694729
31	6	-3.599937	-0.454423	-1.913853
32	6	-2.902415	-2.628760	0.257388
33	1	-2.634498	-0.662992	3.678265
34	1	-0.910168	-0.797036	3.299042
35	1	-2.007081	-2.136913	2.938407
36	1	-2.852417	2.204420	2.935539
37	1	-1.686520	2.974066	1.848674
38	1	-1.143993	1.750033	2.999371
39	1	-4.175406	2.540153	-0.711829
40	1	-2.732067	2.486935	-1.731194
41	1	-2.674616	3.285531	-0.155010
42	1	-4.690375	-0.536013	-1.795603
43	1	-3.236344	-1.389870	-2.348620
44	1	-3.403860	0.342004	-2.638780
45	1	-3.980918	-2.827715	0.191525
46	1	-2.517428	-3.202126	1.106040
47	1	-2.441285	-3.028091	-0.653612
48	6	0.491375	3.278529	-0.367502
49	6	0.762392	-2.596912	1.203430
50	1	-0.508052	3.687922	-0.197622
51	1	0.841591	3.620745	-1.353533
52	1	1.170528	3.695216	0.392083
53	1	-0.245559	-2.807664	1.558647
54	1	1.469566	-2.987742	1.945549
55	1	0.913112	-3.137161	0.259432

18Me (E = -954.3729548 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.538079	-0.140311	-0.230269
2	7	0.585105	1.431185	-0.818821
3	6	1.854484	0.770491	-0.714682
4	7	0.855280	-0.752083	1.098869
5	6	-2.179671	0.423853	1.616992
6	6	-2.605180	-0.827686	1.081006
7	6	-2.349210	1.418145	0.604442
8	17	-0.341478	-1.717710	-2.108941
9	6	-3.029805	-0.608997	-0.263784
10	6	-2.875906	0.780240	-0.556603
11	6	2.010946	-0.380598	0.326397
12	6	2.757744	0.939061	0.510040
13	1	2.380913	0.596956	-1.656027
14	6	4.203437	0.632421	0.289741
15	1	2.436646	1.655686	1.259171
16	6	3.071292	-1.423321	-0.055203
17	6	4.380950	-0.656248	-0.057973
18	1	3.094632	-2.244630	0.672316
19	1	2.849462	-1.879644	-1.025898
20	6	5.659164	-1.359008	-0.429784
21	6	5.237072	1.721236	0.415833
22	1	6.253410	1.349563	0.254186
23	1	5.200316	2.179016	1.414248
24	1	5.050237	2.525254	-0.309974
25	1	6.532243	-0.703496	-0.354107
26	1	5.614452	-1.741824	-1.459173
27	1	5.830313	-2.227157	0.223110
28	6	-2.712044	-2.140084	1.823736
29	6	-1.810490	0.723673	3.050774
30	6	-2.181562	2.902220	0.829093
31	6	-3.301249	1.455762	-1.840389
32	6	-3.689029	-1.632748	-1.156570
33	1	-3.736582	-2.290171	2.192050
34	1	-2.044958	-2.175640	2.690155
35	1	-2.468084	-2.993889	1.182495
36	1	-2.651509	1.212682	3.562448
37	1	-0.947999	1.395051	3.123571
38	1	-1.573069	-0.185118	3.609903
39	1	-3.001729	3.284182	1.453243
40	1	-2.201018	3.460334	-0.110917
41	1	-1.241900	3.139059	1.339409
42	1	-4.372419	1.699990	-1.810859
43	1	-3.136633	0.813240	-2.711685
44	1	-2.756844	2.389925	-2.010587
45	1	-4.774817	-1.642040	-0.984619
46	1	-3.312208	-2.641973	-0.965729
47	1	-3.518704	-1.418444	-2.215357
48	6	0.652133	2.776572	-1.377506
49	6	1.131793	-1.234798	2.448455
50	1	-0.353742	3.190603	-1.477428
51	1	1.117336	2.768421	-2.375978
52	1	1.243498	3.451185	-0.738702
53	1	0.196555	-1.516249	2.936618
54	1	1.624703	-0.461536	3.058981
55	1	1.782415	-2.120716	2.442046

TS(8b-19)Me (E = -954.302582 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.848180	-0.127034	0.235287
2	7	-0.181209	1.657712	-0.418125
3	6	0.869801	0.833040	-0.868476
4	7	2.166572	-1.810425	-1.206269
5	6	-1.544747	-0.230639	2.656202
6	6	-2.217885	-1.324690	2.025320
7	6	-2.080460	0.980350	2.120173
8	17	-1.607946	-1.340201	-1.745600
9	6	-3.163132	-0.790862	1.107664
10	6	-3.062434	0.635257	1.141460
11	6	2.616078	-0.914182	-0.434322
12	6	1.704020	0.166386	0.120592
13	1	0.993384	0.586330	-1.921503
14	6	2.573661	0.928789	1.102123
15	1	0.939100	-0.566802	0.952234
16	6	4.007996	-0.704681	0.141772
17	6	3.831438	0.453045	1.094992
18	1	4.378630	-1.605938	0.646359
19	1	4.737391	-0.472508	-0.645985
20	6	5.025211	0.954821	1.862429
21	6	2.052767	2.098489	1.886394
22	1	2.840433	2.569544	2.480802
23	1	1.254213	1.791028	2.570996
24	1	1.623774	2.854249	1.219493
25	1	4.780063	1.785029	2.530206
26	1	5.814414	1.294772	1.176618
27	1	5.459491	0.149102	2.471107
28	6	-2.034633	-2.786890	2.360452
29	6	-0.606613	-0.353418	3.836081
30	6	-1.804814	2.379001	2.619037
31	6	-3.984799	1.595509	0.425618
32	6	-4.198680	-1.578787	0.345777
33	1	-2.728128	-3.093228	3.156683
34	1	-1.019367	-2.998218	2.712373
35	1	-2.227511	-3.428784	1.494426
36	1	-1.179311	-0.475164	4.766630
37	1	0.022216	0.533700	3.955321
38	1	0.057563	-1.218992	3.742738
39	1	-2.570323	2.676993	3.349536
40	1	-1.818772	3.113650	1.808414
41	1	-0.833145	2.454155	3.114711
42	1	-4.928290	1.712020	0.978259
43	1	-4.234938	1.244427	-0.580986
44	1	-3.536942	2.589226	0.328645
45	1	-5.111494	-1.681647	0.950036
46	1	-3.844588	-2.583449	0.098068
47	1	-4.470153	-1.089879	-0.593845
48	6	-0.417537	2.971460	-0.997592
49	6	3.065729	-2.833741	-1.744432
50	1	-1.382521	3.359861	-0.658451
51	1	0.368844	3.684736	-0.708786
52	1	-0.433966	2.920349	-2.097420
53	1	4.121340	-2.713928	-1.465775
54	1	2.720384	-3.818178	-1.407851
55	1	2.987370	-2.824536	-2.837175

19Me (E = -954.3395028 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	0.594420	-0.286564	-0.087751
2	7	-0.303869	-0.124244	1.769975
3	6	-1.547124	-0.635757	1.399763
4	7	-3.775987	-2.014964	0.160431
5	6	2.105623	1.630830	-0.765348
6	6	2.526840	0.501555	-1.529195
7	6	2.380470	1.362226	0.609835
8	17	0.461005	-2.640350	-0.610418
9	6	3.048055	-0.469863	-0.631533
10	6	2.953990	0.057913	0.695391
11	6	-3.609189	-0.764180	0.005358
12	6	-2.466291	-0.010079	0.603219
13	1	-1.782460	-1.657308	1.709923
14	6	-2.684613	1.414146	0.296391
15	1	-0.370089	0.540967	-1.415790
16	6	-4.456230	0.243681	-0.765256
17	6	-3.800148	1.565087	-0.454524
18	1	-4.454303	0.025770	-1.841566
19	1	-5.506277	0.228321	-0.448029
20	6	-4.417012	2.835525	-0.966397
21	6	-1.840808	2.529209	0.857094
22	1	-2.360173	3.489868	0.791740
23	1	-0.890638	2.627558	0.319703
24	1	-1.597426	2.337871	1.907385
25	1	-3.866165	3.728051	-0.657711
26	1	-5.454944	2.936885	-0.617878
27	1	-4.453187	2.827911	-2.065606
28	6	2.487877	0.389471	-3.033624
29	6	1.632705	2.946130	-1.335709
30	6	2.233773	2.354517	1.739582
31	6	3.564162	-0.592761	1.916464
32	6	3.747387	-1.753205	-1.008574
33	1	3.405011	0.804979	-3.474749
34	1	1.638198	0.934654	-3.455696
35	1	2.409525	-0.652440	-3.360023
36	1	2.493707	3.575069	-1.603699
37	1	1.028843	3.509892	-0.618125
38	1	1.029039	2.801723	-2.236308
39	1	3.111094	3.014891	1.780988
40	1	2.147240	1.860523	2.711160
41	1	1.350525	2.988652	1.614977
42	1	4.659464	-0.596538	1.831090
43	1	3.245502	-1.633988	2.041034
44	1	3.312994	-0.052335	2.833093
45	1	4.824580	-1.571980	-1.131864
46	1	3.366952	-2.163224	-1.948267
47	1	3.622728	-2.524166	-0.242653
48	6	0.081742	-0.393808	3.162209
49	6	-4.921642	-2.680878	-0.459616
50	1	1.146630	-0.208605	3.305790
51	1	-0.479048	0.249666	3.853673
52	1	-0.129258	-1.440882	3.431970
53	1	-5.634975	-2.010703	-0.958429
54	1	-4.550762	-3.404874	-1.195544
55	1	-5.456094	-3.251729	0.308528

2aEt (E = -860.834519 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.159394	-0.291183	0.153350
2	7	3.121937	-0.917067	-0.634486
3	6	-1.748463	1.677141	-0.215672
4	6	-0.866687	1.710045	-1.336540
5	6	-0.975174	1.980790	0.952461
6	17	0.431412	-0.529615	2.594617
7	6	0.445756	1.994225	-0.861066
8	6	0.374682	2.179247	0.554847
9	6	2.015113	-0.661500	-0.383653
10	6	-0.484129	-1.384466	-1.921169
11	6	-1.654410	-1.752482	-1.122301
12	1	0.242517	-2.171147	-2.124833
13	6	-0.028888	-2.730041	0.375594
14	6	-1.394165	-2.458282	0.068646
15	1	0.191349	-3.133781	1.356793
16	1	0.624721	-3.080843	-0.416025
17	6	-2.486009	-2.846953	1.050930
18	6	-3.062695	-1.556439	-1.653189
19	1	-3.801661	-1.349383	-0.872710
20	1	-3.383709	-2.469755	-2.177214
21	1	-3.098743	-0.743129	-2.383220
22	1	-2.887751	-3.835840	0.785665
23	1	-3.325513	-2.144054	1.068396
24	1	-2.076850	-2.921388	2.063648
25	6	-1.274252	1.734385	-2.788408
26	6	-3.259781	1.663303	-0.261789
27	6	-1.542734	2.235438	2.328034
28	6	1.500724	2.633764	1.450740
29	6	1.642221	2.280414	-1.738818
30	1	-1.480388	2.769490	-3.098087
31	1	-2.179600	1.151717	-2.978093
32	1	-0.486418	1.346940	-3.441432
33	1	-3.648912	2.691161	-0.223585
34	1	-3.695231	1.121599	0.585043
35	1	-3.636529	1.203835	-1.178464
36	1	-1.865972	3.283098	2.414840
37	1	-0.804269	2.039777	3.108908
38	1	-2.414280	1.605262	2.534916
39	1	1.490542	3.728125	1.555126
40	1	2.479104	2.350712	1.048673
41	1	1.415898	2.197063	2.449757
42	1	1.593796	3.307535	-2.127779
43	1	1.688806	1.604948	-2.599780
44	1	2.582048	2.183685	-1.187015
45	1	-0.716738	-0.822640	-2.821038
46	6	4.491786	-1.277941	-0.900449
47	1	4.637242	-1.240011	-1.984799
48	1	4.622850	-2.316778	-0.581030
49	6	5.478869	-0.351817	-0.177959
50	1	5.331068	-0.393971	0.904926
51	1	6.501336	-0.671063	-0.401702
52	1	5.359526	0.683940	-0.509597

TS(2a-3a)Et (E = -860.8296708 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-1.088382	-0.600065	-0.667447
2	7	-3.252503	1.305425	-2.383120
3	6	1.429833	-1.046048	-0.875748
4	6	1.263886	-0.232822	0.278307
5	6	1.026252	-0.284619	-2.015503
6	17	-1.382443	-2.588131	-2.145958
7	6	0.761163	1.040217	-0.144020
8	6	0.623129	1.008545	-1.563322

9	6	-2.611343	0.539510	-1.692236
10	6	-1.814351	0.108656	1.432562
11	6	-2.189010	-1.295859	1.456806
12	1	-2.616531	0.836708	1.302596
13	6	-3.641598	-0.715282	-0.436850
14	6	-3.044568	-1.733392	0.448439
15	1	-4.285666	-1.149658	-1.196127
16	1	-4.113067	0.117293	0.085291
17	6	-3.532804	-3.162223	0.320196
18	6	-1.626875	-2.221829	2.519709
19	1	-1.445869	-3.238039	2.156997
20	1	-2.336392	-2.290117	3.356904
21	1	-0.689221	-1.827244	2.922317
22	1	-4.463583	-3.292063	0.891836
23	1	-2.807412	-3.892914	0.688450
24	1	-3.741601	-3.403217	-0.725706
25	6	1.719230	-0.577544	1.676346
26	6	2.032250	-2.429930	-0.920054
27	6	1.176870	-0.707261	-3.456119
28	6	0.291113	2.189628	-2.445004
29	6	0.627640	2.274627	0.714919
30	1	2.753975	-0.241557	1.833436
31	1	1.696074	-1.656473	1.860635
32	1	1.102559	-0.093985	2.440516
33	1	3.099928	-2.374332	-1.175541
34	1	1.541026	-3.057136	-1.669997
35	1	1.952806	-2.940411	0.045330
36	1	2.184269	-0.461493	-3.821805
37	1	0.455972	-0.199970	-4.105316
38	1	1.025491	-1.783109	-3.576475
39	1	1.209473	2.727008	-2.721693
40	1	-0.370295	2.900065	-1.940285
41	1	-0.205896	1.881262	-3.369297
42	1	1.539845	2.885103	0.648772
43	1	0.475856	2.022821	1.768076
44	1	-0.211815	2.904117	0.400998
45	1	-1.116797	0.416412	2.204876
46	6	-4.691778	1.559367	-2.537597
47	1	-4.875189	2.572519	-2.161358
48	1	-5.276109	0.859317	-1.929720
49	6	-5.096401	1.470275	-4.013364
50	1	-4.923865	0.462271	-4.404464
51	1	-6.160225	1.705820	-4.122625
52	1	-4.519051	2.177381	-4.617207

3aEt (E = -860.8466177 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.284981	0.310182	-0.081854
2	7	2.470599	-1.384056	-0.159203
3	6	-2.091152	-1.253742	-0.905376
4	6	-2.591251	-0.573985	0.248259
5	6	-1.014638	-2.086983	-0.489229
6	17	-0.498947	1.419928	-2.247595
7	6	-1.841487	-1.009407	1.382772
8	6	-0.856270	-1.933668	0.923201
9	6	1.872996	-0.317541	0.214588
10	6	-0.146655	1.623607	1.743789
11	6	0.641675	2.547880	0.906915
12	1	0.428276	1.014950	2.448939
13	6	2.567380	0.908455	0.842066
14	6	1.860054	2.185267	0.398228
15	1	3.623513	0.965733	0.564790
16	1	2.531028	0.804334	1.935827

17	6	2.646716	3.022122	-0.586083
18	6	-0.036098	3.858957	0.524400
19	1	0.076137	4.108914	-0.533559
20	1	0.389437	4.682477	1.113692
21	1	-1.107850	3.817865	0.744618
22	1	3.548656	3.427596	-0.103382
23	1	2.078950	3.860114	-0.993476
24	1	2.986473	2.404642	-1.428360
25	6	-3.783606	0.354728	0.276780
26	6	-2.702169	-1.208111	-2.284617
27	6	-0.242316	-3.052213	-1.355539
28	6	0.056416	-2.759290	1.796687
29	6	-2.158649	-0.705856	2.826665
30	1	-4.711580	-0.214595	0.427490
31	1	-3.890155	0.909401	-0.661204
32	1	-3.712848	1.083116	1.091533
33	1	-3.506428	-1.953026	-2.363570
34	1	-1.966339	-1.426497	-3.063424
35	1	-3.129968	-0.226929	-2.508911
36	1	-0.616138	-4.075793	-1.210315
37	1	0.823227	-3.032979	-1.108644
38	1	-0.347997	-2.810311	-2.417710
39	1	-0.444002	-3.693146	2.090607
40	1	0.329035	-2.230156	2.716163
41	1	0.979268	-3.014556	1.270662
42	1	-2.842510	-1.464858	3.231998
43	1	-2.642079	0.268781	2.942580
44	1	-1.260342	-0.706615	3.452259
45	1	-1.006051	2.069213	2.238479
46	6	3.936390	-1.542892	0.022448
47	1	4.209654	-1.376184	1.075990
48	1	4.470641	-0.783246	-0.568913
49	6	4.376337	-2.941119	-0.416281
50	1	4.124482	-3.110709	-1.468993
51	1	5.458410	-3.067621	-0.295107
52	1	3.871629	-3.710656	0.178939

3bEt (E = -860.8640565 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.178944	-0.079879	0.285032
2	7	1.046984	1.712297	-0.056253
3	6	-2.605020	0.569772	0.068048
4	6	-2.582101	-0.834206	0.331886
5	6	-2.032019	0.785551	-1.220657
6	17	0.054428	-0.064986	2.721690
7	6	-1.990384	-1.484177	-0.792624
8	6	-1.648782	-0.480072	-1.751955
9	6	1.383721	0.801017	-0.890296
10	6	1.203905	-1.829798	-0.255732
11	6	2.666732	-1.538492	-0.022069
12	1	1.010618	-1.968494	-1.326255
13	6	2.671772	0.479175	-1.560754
14	6	3.359502	-0.546225	-0.634908
15	1	3.331782	1.342851	-1.704995
16	1	2.473437	0.046387	-2.548999
17	6	4.848706	-0.289544	-0.498202
18	6	3.307586	-2.474234	0.991255
19	1	4.312951	-2.181027	1.300956
20	1	3.355407	-3.497568	0.592522
21	1	2.680494	-2.513727	1.891901
22	1	5.329416	-0.292738	-1.487924
23	1	5.359560	-1.035660	0.113323
24	1	5.045281	0.699105	-0.056440

25	6	-3.194504	-1.516007	1.533768
26	6	-3.227388	1.623210	0.955568
27	6	-1.952631	2.107592	-1.946394
28	6	-1.129004	-0.737436	-3.146000
29	6	-1.904322	-2.975893	-1.009477
30	1	-4.259913	-1.720933	1.357492
31	1	-3.118477	-0.898188	2.433596
32	1	-2.707838	-2.472163	1.751439
33	1	-4.301711	1.718424	0.743565
34	1	-2.774710	2.607739	0.798628
35	1	-3.122065	1.374663	2.016330
36	1	-2.853081	2.265540	-2.556244
37	1	-1.088889	2.151082	-2.617730
38	1	-1.873791	2.948883	-1.251100
39	1	-1.960116	-0.952279	-3.832713
40	1	-0.450451	-1.596043	-3.176869
41	1	-0.588387	0.127422	-3.543035
42	1	-2.804746	-3.340295	-1.523831
43	1	-1.823948	-3.520640	-0.063336
44	1	-1.040497	-3.250676	-1.622542
45	1	0.923626	-2.764562	0.243703
46	6	1.779749	2.924518	0.366364
47	1	2.637054	3.090572	-0.297862
48	1	2.164677	2.729864	1.375056
49	6	0.858996	4.148219	0.384990
50	1	0.003239	3.976984	1.047010
51	1	1.402947	5.026301	0.749012
52	1	0.480845	4.371284	-0.618805

3cEt (E = -860.8585872 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.127362	-0.025941	-0.239875
2	7	-0.724078	1.941977	0.110626
3	6	2.287367	-1.487278	-0.005596
4	6	1.786405	-1.242249	1.304419
5	6	2.693343	-0.240089	-0.564817
6	17	-0.075001	-0.837133	-2.531397
7	6	1.863466	0.165791	1.548934
8	6	2.437310	0.782316	0.393606
9	6	-1.664028	1.120814	-0.200011
10	6	-0.844345	3.309508	0.663595
11	6	-1.407402	-1.178983	1.041155
12	6	-2.836207	-1.325503	0.547576
13	1	-1.392671	-0.590136	1.973787
14	6	-3.131145	1.119340	-0.017869
15	6	-3.636292	-0.314144	0.140292
16	1	-3.456051	1.769462	0.811544
17	1	-3.588168	1.550906	-0.921149
18	6	-5.106039	-0.438025	-0.216674
19	6	-3.310657	-2.771864	0.567321
20	1	-4.286940	-2.929057	0.103863
21	1	-3.353065	-3.153676	1.597555
22	1	-2.585454	-3.397205	0.028333
23	1	-5.531810	-1.417128	0.009540
24	1	-5.270685	-0.235963	-1.286532
25	1	-5.695011	0.308677	0.337321
26	6	1.445196	-2.290106	2.334889
27	6	2.463675	-2.835151	-0.662265
28	6	3.381460	-0.059793	-1.896172
29	6	2.857664	2.229235	0.269561
30	6	1.580293	0.838849	2.873573
31	1	2.335930	-2.539796	2.928783
32	1	1.089395	-3.216517	1.873169

33	1	0.671662	-1.949185	3.030220
34	1	3.492194	-3.200574	-0.531683
35	1	2.262933	-2.786412	-1.737585
36	1	1.791521	-3.585781	-0.234073
37	1	4.453558	-0.286643	-1.808437
38	1	3.292609	0.967874	-2.263595
39	1	2.961406	-0.721284	-2.660132
40	1	3.916828	2.344422	0.539702
41	1	2.279379	2.878896	0.933074
42	1	2.739428	2.606747	-0.751924
43	1	2.460337	0.785915	3.530224
44	1	0.749417	0.361902	3.404543
45	1	1.330680	1.897578	2.749603
46	1	-1.030937	-2.165777	1.324059
47	1	-0.080831	3.428964	1.439416
48	1	-1.829204	3.424187	1.134646
49	6	-0.650898	4.362275	-0.436412
50	1	-0.713757	5.369749	-0.011469
51	1	0.327877	4.250148	-0.914709
52	1	-1.422022	4.265227	-1.208353

TS(3c-4)Et (E = -860.8260575 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.809491	-0.160345	-0.872879
2	7	-0.384304	1.458045	-0.571027
3	6	3.126269	-1.207136	-0.506622
4	6	2.633162	-0.756737	0.756791
5	6	3.364637	-0.062321	-1.322060
6	17	0.627169	-1.291900	-3.050068
7	6	2.556505	0.670607	0.713046
8	6	3.002434	1.098769	-0.577371
9	6	-1.172024	0.335343	-0.586368
10	6	-0.722277	2.759718	0.020243
11	6	-0.847557	-0.902394	0.879509
12	6	-2.246476	-1.466304	0.909625
13	1	-0.583290	-0.391850	1.813508
14	6	-2.667246	0.295441	-0.666975
15	6	-3.165458	-0.883692	0.125863
16	1	-3.129835	1.218011	-0.279906
17	1	-2.972231	0.225407	-1.720526
18	6	-4.620296	-1.252819	-0.022869
19	6	-2.478941	-2.641134	1.835084
20	1	-3.518653	-2.980748	1.838629
21	1	-2.205795	-2.379501	2.867076
22	1	-1.847234	-3.493301	1.546312
23	1	-4.920824	-2.074757	0.631778
24	1	-4.839419	-1.548183	-1.058669
25	1	-5.263083	-0.389932	0.203217
26	6	2.443814	-1.604749	1.993944
27	6	3.458729	-2.632034	-0.883181
28	6	3.986358	-0.086352	-2.696778
29	6	3.209858	2.530698	-1.016441
30	6	2.271605	1.560330	1.901208
31	1	3.372451	-1.632468	2.581185
32	1	2.184132	-2.639647	1.747237
33	1	1.657825	-1.211798	2.647454
34	1	4.528243	-2.833249	-0.728718
35	1	3.232326	-2.833833	-1.935138
36	1	2.900922	-3.354716	-0.278358
37	1	5.079191	-0.178134	-2.621856
38	1	3.770003	0.829331	-3.255962
39	1	3.619057	-0.929382	-3.290089
40	1	4.226484	2.868213	-0.769870

41	1	2.508337	3.211598	-0.525414
42	1	3.079153	2.647007	-2.097255
43	1	3.162738	1.637035	2.540300
44	1	1.456954	1.175543	2.524572
45	1	2.002999	2.574504	1.593613
46	1	-0.144903	-1.755269	0.805943
47	1	0.188426	3.207063	0.436573
48	1	-1.421388	2.610072	0.857417
49	6	-1.333489	3.724217	-1.009325
50	1	-1.556641	4.693315	-0.547021
51	1	-0.636073	3.888347	-1.838354
52	1	-2.261733	3.318152	-1.426289

4Et (E = -860.8657895 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.546343	-0.455036	-0.081571
2	7	1.082712	-0.849893	0.919740
3	6	-2.397785	1.058682	-1.062563
4	6	-1.432570	1.906766	-0.433582
5	6	-3.006394	0.258567	-0.059422
6	17	-1.010332	-2.272517	-1.646866
7	6	-1.462844	1.639867	0.972542
8	6	-2.425485	0.612376	1.201536
9	6	1.580709	0.035185	-0.188212
10	6	1.997856	-1.401386	1.911892
11	6	2.360635	1.279979	0.283935
12	6	3.804135	1.015890	-0.097234
13	1	2.236375	1.448006	1.361779
14	6	2.553441	-0.678023	-1.165303
15	6	3.908996	-0.056469	-0.896009
16	1	2.547635	-1.764796	-1.012030
17	1	2.275261	-0.526644	-2.218635
18	6	5.144664	-0.630594	-1.537925
19	6	4.892461	1.942835	0.377320
20	1	5.880946	1.654556	0.005246
21	1	4.938751	1.964588	1.475784
22	1	4.697027	2.974472	0.049456
23	1	6.050011	-0.070212	-1.282555
24	1	5.048012	-0.634980	-2.633373
25	1	5.295817	-1.675473	-1.231185
26	6	-0.698703	3.039832	-1.112076
27	6	-2.762804	1.071415	-2.528015
28	6	-4.136566	-0.721067	-0.272599
29	6	-2.850229	0.074805	2.551165
30	6	-0.744814	2.430406	2.041080
31	1	-1.366596	3.903603	-1.239361
32	1	-0.333633	2.758652	-2.105515
33	1	0.161864	3.373145	-0.526294
34	1	-3.589228	1.771935	-2.714082
35	1	-3.081895	0.083454	-2.874389
36	1	-1.921336	1.386941	-3.153822
37	1	-5.105325	-0.202795	-0.243941
38	1	-4.158784	-1.495055	0.501951
39	1	-4.056739	-1.225746	-1.240177
40	1	-3.701021	0.648980	2.943995
41	1	-2.043651	0.141979	3.288512
42	1	-3.167991	-0.972529	2.496415
43	1	-1.358221	3.286551	2.356013
44	1	0.211366	2.823262	1.685131
45	1	-0.543489	1.825605	2.930925
46	1	2.015009	2.201039	-0.205736
47	1	2.534484	-0.587950	2.425743
48	1	2.764754	-2.009719	1.406727

49	6	1.257430	-2.261901	2.942471
50	1	1.955397	-2.671731	3.681404
51	1	0.506929	-1.667055	3.477708
52	1	0.748829	-3.100410	2.451953

8aEt (E = -1032.9718446 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.641935	0.055811	-0.276148
2	7	0.727961	1.352314	-0.896223
3	6	1.061197	1.247080	0.497714
4	7	0.953861	-1.550963	0.168021
5	6	-2.358894	1.332634	1.024469
6	6	-1.758523	0.435752	1.962818
7	6	-3.111970	0.552925	0.095087
8	17	-1.167470	-0.739170	-2.589935
9	6	-2.145234	-0.892780	1.610520
10	6	-2.980752	-0.820892	0.457432
11	6	1.412283	2.184848	-1.882360
12	6	2.085753	-1.066029	0.539913
13	6	0.856699	-3.001318	-0.173788
14	6	2.232262	0.373314	0.959697
15	1	0.968057	2.158361	1.098587
16	6	3.714999	0.632010	0.670916
17	1	2.133701	0.365896	2.061903
18	6	3.448227	-1.718187	0.522372
19	6	4.378228	-0.516225	0.456887
20	1	3.608848	-2.301640	1.442662
21	1	3.580718	-2.412529	-0.311027
22	6	5.847900	-0.736477	0.219458
23	6	4.270372	2.024897	0.761702
24	1	5.344091	2.060120	0.555219
25	1	4.103014	2.441642	1.765561
26	1	3.763077	2.693671	0.056013
27	1	6.405728	0.203803	0.187766
28	1	6.017779	-1.261615	-0.731106
29	1	6.285507	-1.361439	1.011496
30	6	-1.037885	0.834310	3.228030
31	6	-2.317857	2.841936	1.107379
32	6	-3.996197	1.081303	-1.010543
33	6	-3.699484	-1.967534	-0.212434
34	6	-1.838927	-2.133283	2.418860
35	1	-1.751152	0.947405	4.058014
36	1	-0.512513	1.786112	3.108542
37	1	-0.299407	0.084176	3.531358
38	1	-3.055544	3.210776	1.834458
39	1	-2.545763	3.306718	0.143097
40	1	-1.333858	3.203598	1.424356
41	1	-5.036602	1.162578	-0.664361
42	1	-3.984750	0.422794	-1.884455
43	1	-3.682491	2.076334	-1.342685
44	1	-4.751748	-2.003999	0.103554
45	1	-3.249227	-2.933198	0.041038
46	1	-3.681547	-1.870725	-1.303035
47	1	-2.545843	-2.235531	3.254439
48	1	-0.830959	-2.103888	2.847518
49	1	-1.918711	-3.043721	1.815662
50	1	1.504269	-3.570865	0.503966
51	1	-0.173971	-3.303003	0.035912
52	1	2.486039	1.935233	-1.894818
53	1	1.010980	1.924826	-2.870417
54	6	1.195240	-3.321996	-1.637639
55	1	2.225079	-3.046053	-1.885635
56	1	1.081460	-4.398735	-1.807228

57	1	0.526498	-2.788903	-2.316891
58	6	1.243532	3.694340	-1.638399
59	1	1.621493	3.977042	-0.648284
60	1	1.790904	4.274943	-2.391270
61	1	0.184559	3.974061	-1.689476

TS(8a-10)Et (E = -1032.9285334 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.473834	-0.159172	-0.276840
2	7	-0.231240	-0.412178	1.610230
3	6	-0.700924	0.888118	1.568076
4	7	-1.798675	-0.567159	-0.783202
5	6	2.839933	0.450595	0.521184
6	6	2.195974	1.666625	0.140669
7	6	3.026294	-0.330052	-0.650805
8	17	0.655320	-2.513224	-1.050835
9	6	1.990865	1.635641	-1.280180
10	6	2.494788	0.395335	-1.761213
11	6	-0.316338	-1.236447	2.818183
12	6	-2.345047	0.450251	-0.227318
13	6	-2.607067	-1.629933	-1.408326
14	6	-1.382148	1.406310	0.367489
15	1	-0.429301	1.611384	2.334231
16	6	-2.176570	2.690401	0.490641
17	1	-0.578740	1.529556	-0.669950
18	6	-3.734503	1.027190	-0.204771
19	6	-3.472027	2.469426	0.194553
20	1	-4.220766	0.943539	-1.184537
21	1	-4.393702	0.519605	0.511777
22	6	-4.624920	3.433887	0.263822
23	6	-1.548073	3.980612	0.938193
24	1	-2.292997	4.770093	1.069033
25	1	-0.812777	4.334204	0.203648
26	1	-1.018906	3.858128	1.891192
27	1	-4.313895	4.437713	0.565359
28	1	-5.381137	3.085853	0.981816
29	1	-5.125537	3.515147	-0.711090
30	6	2.071383	2.891709	1.016928
31	6	3.408622	0.137619	1.884318
32	6	3.815437	-1.612185	-0.731188
33	6	2.555374	-0.039966	-3.207062
34	6	1.555260	2.800042	-2.140389
35	1	3.010045	3.465418	0.998771
36	1	1.866448	2.632392	2.060199
37	1	1.276291	3.560396	0.678211
38	1	4.461560	0.450221	1.946093
39	1	3.370904	-0.934216	2.105759
40	1	2.864736	0.659739	2.676730
41	1	4.881598	-1.387320	-0.881318
42	1	3.481347	-2.242089	-1.559249
43	1	3.725007	-2.203482	0.185435
44	1	3.521145	0.231235	-3.657528
45	1	1.771264	0.436052	-3.806515
46	1	2.436918	-1.123981	-3.305594
47	1	2.429095	3.384983	-2.464175
48	1	0.886316	3.477715	-1.601289
49	1	1.029647	2.467790	-3.041730
50	1	-3.488284	-1.187208	-1.893839
51	1	-1.987787	-2.093952	-2.179402
52	1	-1.373614	-1.513877	2.967129
53	1	0.234915	-2.160798	2.613818
54	6	-3.041712	-2.692868	-0.387766
55	1	-3.673717	-2.255191	0.393699

56	1	-3.611388	-3.484035	-0.888233
57	1	-2.163807	-3.141928	0.084915
58	6	0.212182	-0.584017	4.105467
59	1	-0.340456	0.331536	4.346299
60	1	0.095545	-1.274625	4.948903
61	1	1.274101	-0.333804	4.014038

10Et (E = -1032.9807834 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.652357	-0.366154	-0.035439
2	7	0.502911	1.219264	-1.014859
3	6	1.776079	1.531501	-0.712670
4	7	1.396456	-1.365125	-0.231138
5	6	-2.636391	1.370632	0.090803
6	6	-1.837408	1.476196	1.275715
7	6	-3.250699	0.091452	0.091582
8	17	-1.453943	-1.936687	-1.729647
9	6	-1.995106	0.272954	2.020046
10	6	-2.839124	-0.598527	1.267494
11	6	-0.070832	1.955664	-2.178297
12	6	2.501463	-0.718505	0.024909
13	6	1.460402	-2.848806	-0.250214
14	6	2.676327	0.700509	-0.078473
15	1	2.143984	2.503236	-1.038003
16	6	4.053249	1.029367	0.329873
17	1	-0.180988	-1.245355	1.495593
18	6	3.832229	-1.305363	0.474283
19	6	4.721865	-0.096463	0.661570
20	1	3.709503	-1.880667	1.401860
21	1	4.242851	-2.002102	-0.265650
22	6	6.135879	-0.258673	1.145301
23	6	4.567334	2.444865	0.342980
24	1	5.585357	2.504524	0.738057
25	1	3.925762	3.090483	0.957885
26	1	4.578962	2.872459	-0.669326
27	1	6.647450	0.702722	1.253580
28	1	6.726809	-0.874305	0.451232
29	1	6.165737	-0.765547	2.120997
30	6	-1.138353	2.721962	1.769455
31	6	-3.055124	2.521691	-0.793788
32	6	-4.287011	-0.384625	-0.894165
33	6	-3.298824	-1.970560	1.698856
34	6	-1.516657	0.048857	3.433924
35	1	-1.814025	3.324619	2.393521
36	1	-0.800513	3.352268	0.942023
37	1	-0.260552	2.481703	2.379502
38	1	-3.973030	2.975610	-0.392199
39	1	-3.277290	2.204800	-1.818534
40	1	-2.300007	3.309789	-0.838494
41	1	-5.292196	-0.094124	-0.555815
42	1	-4.270775	-1.472168	-1.004423
43	1	-4.132696	0.045838	-1.888617
44	1	-4.202775	-1.905460	2.321256
45	1	-2.529276	-2.483869	2.285644
46	1	-3.535693	-2.603488	0.837338
47	1	-2.225220	0.495412	4.146925
48	1	-0.536414	0.502780	3.612448
49	1	-1.430805	-1.016645	3.663283
50	1	2.128689	-3.204301	0.544653
51	1	0.462751	-3.229508	-0.019706
52	1	0.361210	1.527428	-3.094998
53	1	-1.137162	1.728116	-2.212510
54	6	1.909277	-3.391580	-1.615874

55	1	2.913669	-3.041409	-1.879067
56	1	1.923699	-4.487794	-1.598130
57	1	1.215717	-3.068201	-2.397213
58	6	0.131160	3.481053	-2.196353
59	1	1.169106	3.764098	-2.399438
60	1	-0.484061	3.917064	-2.991621
61	1	-0.164996	3.938193	-1.246234

TS(10-11)Et (E = -1032.9485464 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-1.025537	-0.155027	0.340233
2	7	0.604186	-1.338585	0.553894
3	6	1.226533	-1.202349	-0.703007
4	7	0.241564	1.525901	-0.369213
5	6	-3.327280	-0.934506	1.085637
6	6	-2.932227	-1.773551	0.000055
7	6	-3.556685	0.378591	0.569380
8	17	-0.822050	0.841343	2.649973
9	6	-2.896474	-0.973275	-1.181432
10	6	-3.278993	0.359430	-0.824443
11	6	1.247593	-2.244798	1.524909
12	6	1.431151	1.260687	-0.891063
13	6	-0.187047	2.947986	-0.276771
14	6	1.908759	-0.053438	-1.125097
15	1	1.474271	-2.133719	-1.220381
16	6	3.018668	0.025484	-2.089605
17	1	-0.402511	-0.595870	-1.404366
18	6	2.369187	2.227219	-1.590397
19	6	3.321069	1.320555	-2.339041
20	1	1.820909	2.896424	-2.264130
21	1	2.902013	2.872000	-0.881205
22	6	4.442625	1.896773	-3.157268
23	6	3.709060	-1.201938	-2.623486
24	1	4.551832	-0.944521	-3.271190
25	1	3.017596	-1.822930	-3.208937
26	1	4.088927	-1.826900	-1.803791
27	1	5.061273	1.118071	-3.613696
28	1	5.099987	2.527502	-2.540856
29	1	4.059219	2.535077	-3.966450
30	6	-2.762864	-3.275655	0.048989
31	6	-3.623684	-1.380715	2.497556
32	6	-4.100647	1.538516	1.367332
33	6	-3.476475	1.493327	-1.804379
34	6	-2.739270	-1.487709	-2.592012
35	1	-3.714164	-3.777404	-0.179651
36	1	-2.444190	-3.617245	1.038946
37	1	-2.023289	-3.626572	-0.678018
38	1	-4.693309	-1.608116	2.612243
39	1	-3.362963	-0.606774	3.225282
40	1	-3.066491	-2.285188	2.763929
41	1	-5.185435	1.430156	1.507847
42	1	-3.930663	2.495935	0.863964
43	1	-3.637668	1.596151	2.357286
44	1	-4.432068	1.384619	-2.336645
45	1	-2.683638	1.520998	-2.560525
46	1	-3.494269	2.466290	-1.302869
47	1	-3.717579	-1.784025	-2.998579
48	1	-2.082048	-2.361405	-2.634289
49	1	-2.316881	-0.726801	-3.255011
50	1	0.769772	-2.057465	2.492314
51	1	2.304681	-1.958083	1.632727
52	1	-0.023844	3.442789	-1.244273
53	1	-1.267694	2.950787	-0.099119

54	6	1.148164	-3.738604	1.173105
55	1	1.630148	-3.964874	0.214667
56	1	1.644734	-4.340229	1.943676
57	1	0.101402	-4.054593	1.110854
58	6	0.504503	3.733837	0.848712
59	1	0.100626	4.752430	0.889832
60	1	0.328937	3.247888	1.811631
61	1	1.584888	3.805010	0.689163

11Et (E = -1033.0030799 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.693194	-0.044123	-0.379687
2	7	0.177822	1.678313	-1.012696
3	6	1.633238	1.772308	-1.079622
4	7	0.851793	-1.297003	-0.880971
5	6	-2.529261	0.607665	1.307395
6	6	-1.269429	0.790544	1.941710
7	6	-2.716084	-0.794635	1.090685
8	17	-2.236634	-0.469712	-2.220902
9	6	-0.668912	-0.499974	2.104690
10	6	-1.575423	-1.477483	1.596009
11	6	-0.519215	2.820364	-1.634880
12	6	2.039914	-0.718725	-0.435845
13	6	0.889599	-2.691555	-1.362846
14	6	2.360418	0.613489	-0.427100
15	1	1.954859	1.858058	-2.136423
16	6	3.663118	0.782334	0.260318
17	1	1.973594	2.694984	-0.594622
18	6	3.155203	-1.487851	0.249869
19	6	4.142527	-0.421777	0.650204
20	1	2.778447	-2.052735	1.110519
21	1	3.618677	-2.222471	-0.420923
22	6	5.442301	-0.766534	1.324439
23	6	4.322715	2.127136	0.439860
24	1	5.289911	2.034352	0.942514
25	1	3.699095	2.802820	1.040973
26	1	4.494623	2.622509	-0.525109
27	1	6.048409	0.122615	1.525457
28	1	6.045605	-1.445368	0.703807
29	1	5.276258	-1.278386	2.283432
30	6	-0.721736	2.072826	2.521955
31	6	-3.551172	1.679550	1.006635
32	6	-3.979019	-1.434257	0.569084
33	6	-1.398362	-2.976629	1.662863
34	6	0.598233	-0.768765	2.883227
35	1	-0.939090	2.125873	3.598538
36	1	-1.167236	2.953982	2.052096
37	1	0.364161	2.145654	2.401003
38	1	-4.300211	1.738898	1.809071
39	1	-4.089138	1.477529	0.073789
40	1	-3.089179	2.668302	0.918174
41	1	-4.719761	-1.529328	1.375801
42	1	-3.792602	-2.436462	0.170766
43	1	-4.430803	-0.844437	-0.234010
44	1	-1.817671	-3.376842	2.596802
45	1	-0.342520	-3.263864	1.628139
46	1	-1.907042	-3.483934	0.836040
47	1	0.410951	-0.666417	3.961637
48	1	1.402469	-0.072587	2.621699
49	1	0.967100	-1.783970	2.710835
50	1	-1.590988	2.587261	-1.666840
51	1	-0.191221	2.903918	-2.686343
52	1	1.412889	-3.335149	-0.639378

53	1	-0.143137	-3.053057	-1.418882
54	6	-0.322890	4.178753	-0.936904
55	1	0.724850	4.499148	-0.950368
56	1	-0.910521	4.950767	-1.448306
57	1	-0.651130	4.134055	0.107254
58	6	1.542642	-2.814919	-2.748948
59	1	1.552614	-3.860553	-3.079807
60	1	0.986244	-2.222642	-3.482933
61	1	2.576528	-2.450949	-2.732679

15Et (E = -836.3843591 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.189705	-0.115693	-0.607507
2	7	-0.861592	1.590265	-0.521034
3	6	-1.834769	-1.045102	1.029079
4	6	-0.573407	-1.081047	1.694198
5	6	-1.789128	-1.996285	-0.035010
6	17	0.079248	-0.762969	-2.980430
7	6	0.226523	-2.096665	1.073733
8	6	-0.522712	-2.661086	0.009955
9	6	-0.217684	-0.333812	2.960129
10	6	-3.040541	-0.244599	1.459032
11	6	-2.930516	-2.360668	-0.957890
12	6	-0.117723	-3.814164	-0.876412
13	6	1.564438	-2.577234	1.583732
14	1	-0.464631	-0.930911	3.850110
15	1	-0.764937	0.611295	3.035480
16	1	0.852625	-0.102906	3.013027
17	1	-3.614302	-0.789511	2.222791
18	1	-3.713596	-0.044731	0.619467
19	1	-2.752049	0.721962	1.883245
20	1	-3.507346	-3.202181	-0.547444
21	1	-2.569293	-2.658800	-1.947516
22	1	-3.624053	-1.524762	-1.096773
23	1	-0.637418	-4.736353	-0.580102
24	1	0.957808	-4.011827	-0.816107
25	1	-0.357932	-3.620287	-1.927566
26	1	1.427298	-3.291877	2.407707
27	1	2.178490	-1.755436	1.968697
28	1	2.140512	-3.088681	0.805363
29	7	2.037161	0.354565	-0.176722
30	6	3.014260	-0.436891	-0.684028
31	6	2.401269	1.464699	0.513126
32	6	4.369275	-0.153478	-0.519722
33	1	2.690052	-1.306727	-1.243096
34	6	3.736256	1.803925	0.729653
35	1	1.588063	2.083297	0.869632
36	6	4.740460	0.984470	0.203724
37	1	5.111829	-0.812500	-0.952409
38	1	3.977504	2.699489	1.288970
39	1	5.786580	1.229442	0.348938
40	6	-1.570417	2.843150	-0.406531
41	1	-2.466775	2.726332	0.228427
42	1	-1.937113	3.163036	-1.397106
43	6	-0.706672	3.978707	0.177564
44	1	-1.273292	4.917233	0.232670
45	1	-0.368325	3.723960	1.190267
46	1	0.177437	4.147212	-0.448960

14Et (E = -444.8549561 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	7	1.238661	0.918134	0.398652
2	6	0.075039	0.434738	0.239467
3	6	-1.160301	1.275873	0.181600
4	6	-2.296479	0.361318	-0.006071
5	6	-0.369281	-1.019356	0.083253
6	6	-1.870514	-0.920168	-0.063099
7	1	0.094533	-1.495992	-0.789800
8	1	-0.084949	-1.626116	0.952278
9	6	-2.684020	-2.169745	-0.243073
10	6	-3.708488	0.871455	-0.109676
11	1	-4.431295	0.062557	-0.244827
12	1	-3.811260	1.562874	-0.956696
13	1	-3.988050	1.428063	0.794809
14	1	-3.754157	-1.965233	-0.335280
15	1	-2.540530	-2.851775	0.607137
16	1	-2.363713	-2.715083	-1.142300
17	6	-1.190273	2.612837	0.285754
18	1	-2.118365	3.169758	0.236117
19	1	-0.271613	3.170001	0.422730
20	6	2.407222	0.030496	0.449417
21	1	2.755576	0.011725	1.492311
22	1	2.172256	-1.006269	0.165626
23	6	3.529366	0.574653	-0.445206
24	1	4.425938	-0.049901	-0.361389
25	1	3.215994	0.588505	-1.495344
26	1	3.788257	1.598272	-0.155158

TS(8a-16')Et (E = -1032.9270425 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.562049	-0.071648	-0.338479
2	7	0.819338	1.320170	-0.910348
3	6	1.553287	1.367585	0.243009
4	7	1.225062	-1.455717	-0.509810
5	6	-2.314452	1.667584	0.386813
6	6	-1.747483	1.087878	1.561489
7	6	-3.051089	0.655971	-0.283998
8	17	-1.256643	-0.988948	-2.502937
9	6	-2.156299	-0.288759	1.627663
10	6	-2.952860	-0.550168	0.479928
11	6	1.190124	2.148049	-2.067432
12	6	2.131098	-0.970193	0.286130
13	6	1.565595	-2.572570	-1.419036
14	6	1.663560	0.154608	1.126679
15	1	1.975033	2.298147	0.612663
16	6	2.727848	0.258341	2.211218
17	1	0.650579	-0.221081	1.600418
18	6	3.491960	-1.435307	0.725676
19	6	3.734045	-0.601098	1.970879
20	1	3.486304	-2.510913	0.953164
21	1	4.278882	-1.289350	-0.025657
22	6	5.013866	-0.779318	2.742959
23	6	2.607057	1.247607	3.338277
24	1	3.515525	1.284884	3.945861
25	1	1.771781	0.989739	4.002739
26	1	2.413011	2.259371	2.960528
27	1	5.073085	-0.119148	3.612687
28	1	5.884702	-0.574401	2.104316
29	1	5.116097	-1.814262	3.098049
30	6	-1.087975	1.856472	2.682770
31	6	-2.278322	3.132248	0.024311
32	6	-3.924330	0.851176	-1.497963
33	6	-3.667825	-1.843198	0.166850
34	6	-1.978776	-1.214577	2.810352

35	1	-1.848912	2.244618	3.375563
36	1	-0.511655	2.709550	2.312435
37	1	-0.412076	1.225027	3.266713
38	1	-3.112053	3.669466	0.500003
39	1	-2.361867	3.284755	-1.056527
40	1	-1.349773	3.606970	0.355874
41	1	-4.959912	1.058714	-1.192022
42	1	-3.932736	-0.037149	-2.135830
43	1	-3.584285	1.692243	-2.110594
44	1	-4.705712	-1.810253	0.528477
45	1	-3.182043	-2.700659	0.645092
46	1	-3.698161	-2.035785	-0.910475
47	1	-2.829794	-1.122414	3.501990
48	1	-1.069189	-0.985473	3.374311
49	1	-1.918431	-2.263655	2.501961
50	1	2.166925	-3.312897	-0.872582
51	1	2.194424	1.836668	-2.397427
52	1	0.487110	1.906871	-2.872141
53	1	0.628637	-3.051663	-1.711309
54	6	2.318161	-2.101787	-2.672652
55	1	3.266353	-1.619953	-2.408996
56	1	2.536698	-2.956218	-3.323639
57	1	1.709568	-1.386343	-3.232990
58	6	1.185600	3.663127	-1.809839
59	1	1.897748	3.940533	-1.024279
60	1	1.472159	4.198616	-2.722567
61	1	0.189744	4.005281	-1.510187

16'Et (E = -1032.9387451 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.651837	0.053475	-0.525922
2	7	0.950018	1.351444	-1.028968
3	6	2.012277	1.475106	-0.210581
4	7	1.016105	-1.167723	-0.033825
5	6	-2.276180	1.452947	0.822302
6	6	-1.821227	0.394780	1.674245
7	6	-3.074118	0.864162	-0.201814
8	17	-1.208111	-0.784771	-2.741939
9	6	-2.342492	-0.839977	1.176117
10	6	-3.121884	-0.545828	0.022621
11	6	1.096665	1.953017	-2.379943
12	6	2.006122	-0.609678	0.678342
13	6	1.246838	-2.519837	-0.607196
14	6	1.917020	0.818297	1.124261
15	1	2.925580	1.962740	-0.534696
16	6	3.116792	0.991620	2.032897
17	1	0.976594	1.091960	1.649160
18	6	3.223571	-1.258967	1.291118
19	6	3.831701	-0.141398	2.116707
20	1	2.940280	-2.111662	1.931914
21	1	3.945433	-1.665295	0.568270
22	6	5.099457	-0.391970	2.888999
23	6	3.377682	2.319624	2.693250
24	1	4.285122	2.307478	3.304322
25	1	2.538043	2.604691	3.342788
26	1	3.484150	3.115984	1.944632
27	1	5.429661	0.489939	3.445799
28	1	5.914664	-0.690110	2.214744
29	1	4.964343	-1.213772	3.606469
30	6	-1.156259	0.561032	3.022413
31	6	-2.106949	2.933820	1.077865
32	6	-3.837928	1.600942	-1.276999
33	6	-3.965330	-1.524674	-0.756821

34	6	-2.235028	-2.177729	1.870285
35	1	-1.910162	0.490256	3.819938
36	1	-0.670023	1.536162	3.120862
37	1	-0.403314	-0.210818	3.216156
38	1	-2.907139	3.306230	1.734133
39	1	-2.146815	3.511431	0.148899
40	1	-1.151395	3.159070	1.561960
41	1	-4.881054	1.763090	-0.969316
42	1	-3.856047	1.039509	-2.217158
43	1	-3.401161	2.583444	-1.483521
44	1	-5.006494	-1.495635	-0.405031
45	1	-3.606295	-2.552160	-0.639927
46	1	-3.967108	-1.296513	-1.826974
47	1	-3.033244	-2.291706	2.618735
48	1	-1.278232	-2.286655	2.390996
49	1	-2.326128	-3.010584	1.165350
50	1	1.640765	-3.185782	0.173795
51	1	2.062905	1.631256	-2.796919
52	1	0.312378	1.543611	-3.024083
53	1	0.273498	-2.922831	-0.905387
54	6	2.187068	-2.509327	-1.822448
55	1	3.171186	-2.106200	-1.563253
56	1	2.322729	-3.529249	-2.201965
57	1	1.764801	-1.895695	-2.624268
58	6	1.011809	3.486370	-2.371822
59	1	1.811318	3.923887	-1.763560
60	1	1.102806	3.879026	-3.391738
61	1	0.051429	3.816972	-1.959831

TS(16'-16)Et (E = -1032.9366009 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.492914	-0.160948	-0.623958
2	7	1.195009	0.379806	-2.102354
3	6	2.263816	0.356416	-1.367816
4	7	0.609330	-1.896032	-0.481598
5	6	-1.626267	1.411775	1.013376
6	6	-1.140521	0.302772	1.784526
7	6	-2.662682	0.924938	0.171913
8	17	-1.752523	-0.608291	-2.712911
9	6	-1.897681	-0.854483	1.428452
10	6	-2.828362	-0.475434	0.427389
11	6	1.321274	0.474023	-3.568536
12	6	1.543526	-1.269514	0.282140
13	6	0.600728	-3.355498	-0.639166
14	6	1.946463	0.145618	0.048994
15	1	3.281253	0.405407	-1.752858
16	6	2.945544	0.446887	1.135335
17	1	0.968757	1.014464	0.150076
18	6	2.254108	-1.777779	1.519799
19	6	3.112214	-0.610031	1.947943
20	1	1.560820	-2.082884	2.316595
21	1	2.869899	-2.663640	1.308520
22	6	4.011300	-0.730776	3.148110
23	6	3.593079	1.804592	1.207475
24	1	4.250377	1.900017	2.076344
25	1	2.831886	2.594530	1.268657
26	1	4.191930	2.009561	0.310025
27	1	4.579524	0.184643	3.336568
28	1	4.729526	-1.551823	3.015513
29	1	3.430625	-0.959914	4.052506
30	6	-0.209706	0.429836	2.967378
31	6	-1.268916	2.863424	1.236978
32	6	-3.537545	1.756796	-0.735827

33	6	-3.916645	-1.344737	-0.151804
34	6	-1.818645	-2.207886	2.094013
35	1	-0.750188	0.849352	3.828321
36	1	0.639284	1.089118	2.760361
37	1	0.192538	-0.538821	3.276818
38	1	-1.928746	3.310730	1.995897
39	1	-1.373591	3.455718	0.321899
40	1	-0.237921	2.976480	1.586224
41	1	-4.464092	2.046088	-0.219176
42	1	-3.815250	1.206899	-1.640111
43	1	-3.035656	2.678923	-1.048687
44	1	-4.856708	-1.197570	0.399462
45	1	-3.661061	-2.407705	-0.091828
46	1	-4.101178	-1.109525	-1.203801
47	1	-2.500229	-2.257474	2.955432
48	1	-0.810853	-2.423133	2.461779
49	1	-2.097345	-3.013413	1.407055
50	1	-0.376458	-3.629943	-1.048468
51	1	0.693982	-3.847207	0.341704
52	1	2.375435	0.340276	-3.851516
53	1	0.741567	-0.341534	-4.009864
54	6	1.716112	-3.847222	-1.575777
55	1	2.704119	-3.564834	-1.194040
56	1	1.683294	-4.939175	-1.668841
57	1	1.598719	-3.410919	-2.573376
58	6	0.799263	1.818646	-4.091316
59	1	0.898620	1.863478	-5.181953
60	1	-0.257984	1.943091	-3.838365
61	1	1.363803	2.652483	-3.657813

16Et (E = -1032.9836819 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.571792	0.173913	-0.618342
2	7	1.382051	0.699176	-1.690158
3	6	2.511583	0.626761	-1.032148
4	7	0.690002	-1.474666	0.032862
5	6	-2.475081	1.424112	0.556304
6	6	-1.743421	0.715914	1.559455
7	6	-3.119955	0.467630	-0.265245
8	17	-1.383313	-0.367050	-2.891783
9	6	-1.997981	-0.676317	1.391236
10	6	-2.816170	-0.840198	0.239670
11	6	1.449912	1.377615	-3.009893
12	6	1.916120	-1.214862	0.506763
13	6	0.248274	-2.892275	0.038217
14	6	2.728160	-0.133996	0.137868
15	1	3.380415	1.143413	-1.447274
16	6	3.982656	-0.192073	0.918767
17	1	-0.134983	1.897380	-0.212545
18	6	2.693313	-2.054649	1.508892
19	6	3.973364	-1.277417	1.722195
20	1	2.119437	-2.191501	2.434424
21	1	2.902533	-3.060814	1.125765
22	6	5.017079	-1.759909	2.691416
23	6	5.068711	0.841302	0.772035
24	1	5.883076	0.677055	1.483412
25	1	4.673270	1.852731	0.935408
26	1	5.503305	0.824296	-0.237188
27	1	5.878860	-1.086476	2.733054
28	1	5.388577	-2.757446	2.414301
29	1	4.610767	-1.844455	3.709770
30	6	-0.985626	1.335252	2.709586
31	6	-2.645199	2.921004	0.472202

32	6	-4.124502	0.763941	-1.351161
33	6	-3.466623	-2.108954	-0.260523
34	6	-1.619032	-1.727676	2.406828
35	1	-1.650278	1.509854	3.568372
36	1	-0.546776	2.296910	2.425821
37	1	-0.170606	0.688924	3.054340
38	1	-3.540937	3.235518	1.027201
39	1	-2.763168	3.261410	-0.562004
40	1	-1.783187	3.444930	0.893873
41	1	-5.141275	0.775677	-0.932047
42	1	-4.093670	0.012816	-2.144812
43	1	-3.946971	1.739764	-1.814702
44	1	-4.547498	-2.089431	-0.062878
45	1	-3.063738	-2.998758	0.233537
46	1	-3.333695	-2.234062	-1.341331
47	1	-2.184214	-1.562651	3.334379
48	1	-0.555035	-1.694722	2.664993
49	1	-1.850138	-2.737895	2.059986
50	1	-0.837882	-2.906704	-0.063233
51	1	0.491060	-3.369897	0.995952
52	1	2.500942	1.425043	-3.328108
53	1	0.913741	0.752767	-3.729044
54	6	0.868658	-3.682424	-1.126097
55	1	1.962797	-3.691974	-1.065152
56	1	0.516194	-4.720685	-1.111478
57	1	0.586091	-3.233537	-2.083710
58	6	0.852078	2.791608	-3.003265
59	1	0.965576	3.244524	-3.995559
60	1	-0.213256	2.774184	-2.756206
61	1	1.357958	3.427790	-2.268580

TS(16-10)Et (E = -1032.9718301 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.886241	-0.095131	-0.186287
2	7	0.450656	1.390417	0.632312
3	6	1.414794	0.995409	1.467510
4	7	0.821697	-1.493656	-0.221688
5	6	-3.179548	-0.464435	0.883772
6	6	-3.017256	-1.491816	-0.097472
7	6	-3.249988	0.784888	0.203127
8	17	-0.017766	0.592062	-2.510804
9	6	-3.010265	-0.876996	-1.382520
10	6	-3.142604	0.532338	-1.199104
11	6	1.672570	-1.426788	0.784373
12	6	1.889971	-0.304290	1.643838
13	1	1.926199	1.774048	2.036117
14	6	2.908603	-0.687852	2.644293
15	1	-0.789158	-0.677228	1.556472
16	6	2.611297	-2.533870	1.233198
17	6	3.322119	-1.955218	2.432574
18	1	2.033637	-3.434111	1.482899
19	1	3.314742	-2.829694	0.447290
20	6	4.336389	-2.768870	3.186902
21	6	3.374406	0.259408	3.718800
22	1	4.071191	-0.223912	4.409222
23	1	2.525823	0.638239	4.304047
24	1	3.886720	1.131324	3.288757
25	1	4.748041	-2.224038	4.041894
26	1	5.177511	-3.056620	2.539232
27	1	3.894625	-3.701829	3.566063
28	6	-2.987013	-2.974772	0.195420
29	6	-3.443273	-0.685083	2.351985
30	6	-3.579173	2.117474	0.838453

31	6	-3.337184	1.545547	-2.300346
32	6	-2.977142	-1.579082	-2.719246
33	1	-4.003793	-3.360982	0.354681
34	1	-2.406860	-3.195588	1.098208
35	1	-2.549406	-3.544425	-0.631048
36	1	-4.523853	-0.783869	2.533213
37	1	-3.076086	0.147429	2.959633
38	1	-2.953176	-1.592781	2.713922
39	1	-4.667369	2.272518	0.863076
40	1	-3.146378	2.956696	0.283565
41	1	-3.218200	2.175063	1.870339
42	1	-4.392521	1.574643	-2.607779
43	1	-2.731532	1.305485	-3.178056
44	1	-3.061066	2.555005	-1.977749
45	1	-3.994915	-1.682909	-3.121371
46	1	-2.554515	-2.586467	-2.641516
47	1	-2.382737	-1.022016	-3.449861
48	6	0.960018	-2.599966	-1.203018
49	1	1.072832	-3.555980	-0.672829
50	1	0.022601	-2.653632	-1.764772
51	6	0.387443	2.845723	0.332148
52	1	1.365675	3.180249	-0.039324
53	1	-0.317009	2.969307	-0.496946
54	6	2.113627	-2.387654	-2.196896
55	1	3.083119	-2.337398	-1.690380
56	1	2.146849	-3.217653	-2.912674
57	1	1.962814	-1.454681	-2.745477
58	6	-0.053173	3.705963	1.526192
59	1	0.654625	3.634608	2.359729
60	1	-0.112667	4.759273	1.228376
61	1	-1.037094	3.394414	1.891126

TS(8a-17)Et (E = -1032.9292688 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.145410	-0.276677	0.417359
2	7	1.676573	0.563234	-0.150453
3	6	1.321874	1.127639	-1.329845
4	7	-1.617265	1.013412	-0.284438
5	6	-0.118120	-2.296903	-1.091686
6	6	-1.495884	-2.145824	-0.740970
7	6	0.601274	-2.672882	0.085278
8	17	-0.117249	0.222450	2.823561
9	6	-1.625510	-2.384521	0.653079
10	6	-0.327466	-2.703143	1.166173
11	6	-0.773681	2.080161	-0.348375
12	6	0.288427	2.207573	-1.416466
13	1	1.879332	0.878215	-2.233284
14	6	0.817198	3.628922	-1.249254
15	1	-0.212769	2.109047	-2.396301
16	6	-0.928365	3.413628	0.357614
17	6	0.137069	4.277256	-0.290320
18	1	-1.934408	3.842680	0.220814
19	1	-0.780950	3.344166	1.444971
20	6	0.310001	5.698944	0.173882
21	6	1.931610	4.143375	-2.120763
22	1	2.211544	5.170789	-1.869941
23	1	1.641727	4.122584	-3.181440
24	1	2.829229	3.518778	-2.022303
25	1	1.118413	6.217705	-0.349738
26	1	0.529903	5.726583	1.250665
27	1	-0.614832	6.274348	0.024404
28	6	-2.606246	-1.916040	-1.737952
29	6	0.416326	-2.297238	-2.506252

30	6	2.021448	-3.185925	0.139472
31	6	-0.040478	-3.196077	2.564013
32	6	-2.903922	-2.435514	1.456933
33	1	-2.685025	-2.772314	-2.421865
34	1	-2.436435	-1.020628	-2.346844
35	1	-3.575581	-1.805691	-1.243274
36	1	0.273796	-3.284750	-2.969617
37	1	1.486584	-2.071655	-2.539531
38	1	-0.096655	-1.561659	-3.134440
39	1	2.032484	-4.280781	0.036759
40	1	2.512204	-2.946816	1.089108
41	1	2.635878	-2.777777	-0.667745
42	1	-0.243153	-4.274507	2.637198
43	1	-0.658542	-2.685251	3.307881
44	1	1.004954	-3.035112	2.845570
45	1	-3.227654	-3.475869	1.603908
46	1	-3.721167	-1.904721	0.959052
47	1	-2.775298	-1.991822	2.450323
48	6	-3.064915	1.218465	-0.026782
49	1	-3.408674	2.063369	-0.640754
50	1	-3.571518	0.323064	-0.400259
51	6	3.097562	0.226789	0.115331
52	1	3.524027	1.096489	0.637919
53	1	3.113484	-0.604314	0.826207
54	6	-3.464564	1.444382	1.440556
55	1	-4.555407	1.532458	1.515238
56	1	-3.140922	0.608699	2.067821
57	1	-3.020573	2.356936	1.848707
58	6	3.976396	-0.103271	-1.099314
59	1	4.088947	0.754297	-1.770901
60	1	4.976468	-0.383974	-0.751085
61	1	3.573839	-0.941064	-1.679032

17Et (E = -1032.9600554 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.409761	-0.084802	0.215140
2	7	-0.725127	1.840853	-0.423028
3	6	-1.894442	1.642388	-0.914134
4	7	-0.623317	-1.425781	-0.829732
5	6	2.466082	0.897718	-1.002442
6	6	2.390450	-0.486711	-1.340804
7	6	2.787496	0.997597	0.386597
8	17	0.094536	-0.018450	2.675552
9	6	2.658480	-1.243307	-0.163079
10	6	2.909439	-0.323737	0.899899
11	6	-1.683831	-0.734738	-0.148577
12	6	-2.516540	0.281037	-0.955898
13	1	-2.475412	2.488745	-1.282340
14	6	-3.895771	0.270675	-0.294729
15	1	-2.631951	0.022245	-2.029118
16	6	-2.677205	-1.475023	0.758627
17	6	-3.961199	-0.688561	0.641672
18	1	-2.866278	-2.512256	0.438449
19	1	-2.339996	-1.539080	1.801852
20	6	-5.142383	-1.055639	1.501758
21	6	-4.988352	1.206081	-0.751052
22	1	-5.945621	0.978251	-0.272379
23	1	-5.133746	1.135457	-1.839024
24	1	-4.755504	2.256876	-0.527000
25	1	-6.028136	-0.447249	1.294253
26	1	-4.891443	-0.936723	2.564954
27	1	-5.412518	-2.111310	1.357116
28	6	2.297528	-1.007079	-2.755423

29	6	2.498613	2.002965	-2.036210
30	6	3.101022	2.252906	1.168083
31	6	3.392996	-0.682484	2.283112
32	6	2.837343	-2.742211	-0.078711
33	1	3.231382	-0.797045	-3.297625
34	1	1.481561	-0.541634	-3.319880
35	1	2.144045	-2.089049	-2.779587
36	1	3.327048	1.829879	-2.737166
37	1	2.668395	2.982362	-1.579033
38	1	1.581439	2.060168	-2.635750
39	1	4.183566	2.344279	1.334574
40	1	2.620617	2.248188	2.153519
41	1	2.775534	3.155830	0.642214
42	1	4.492276	-0.666581	2.317110
43	1	3.066641	-1.684023	2.579872
44	1	3.020478	0.017158	3.036556
45	1	3.903127	-3.006996	-0.131196
46	1	2.328197	-3.255846	-0.898829
47	1	2.446505	-3.150742	0.859633
48	6	-0.220180	3.229395	-0.224738
49	1	0.042899	3.295060	0.837695
50	1	0.711923	3.317785	-0.784981
51	6	-0.827519	-2.516444	-1.788673
52	1	-1.778680	-2.352183	-2.320577
53	1	-0.033847	-2.476246	-2.545049
54	6	-1.155799	4.383766	-0.591619
55	1	-2.092012	4.352180	-0.022978
56	1	-0.654479	5.327168	-0.350366
57	1	-1.395466	4.402228	-1.660932
58	6	-0.835826	-3.924026	-1.160262
59	1	-1.662697	-4.041698	-0.453381
60	1	-0.938750	-4.691369	-1.938679
61	1	0.097733	-4.107353	-0.617442

TS(17-18)Et (E = -1032.9465078 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.069225	-0.662935	-0.488241
2	7	-1.514895	0.853944	-0.021356
3	6	-0.887705	1.978955	-0.290465
4	7	1.707199	0.182361	0.277388
5	6	-0.098466	-2.329093	1.404741
6	6	0.795620	-2.897401	0.449187
7	6	-1.408445	-2.314516	0.829852
8	17	-0.102122	-0.657241	-2.960710
9	6	0.042973	-3.201475	-0.723224
10	6	-1.321817	-2.852280	-0.483695
11	6	1.253431	1.304567	-0.468758
12	6	0.443516	2.390131	0.264297
13	1	-1.340791	2.653829	-1.030146
14	6	0.935510	3.704255	-0.301810
15	1	0.468745	2.328096	1.360482
16	6	2.075900	2.026556	-1.542970
17	6	1.816612	3.498435	-1.295945
18	1	3.146046	1.795552	-1.460149
19	1	1.791256	1.747384	-2.566559
20	6	2.513264	4.532353	-2.140843
21	6	0.410564	5.009239	0.239365
22	1	0.830184	5.875939	-0.280575
23	1	0.645585	5.111004	1.308565
24	1	-0.684677	5.065176	0.150924
25	1	2.229344	5.555844	-1.877049
26	1	2.283632	4.379705	-3.204624
27	1	3.604178	4.445695	-2.038089

28	6	2.237070	-3.290534	0.676920
29	6	0.195545	-2.000492	2.850580
30	6	-2.661194	-1.971593	1.600924
31	6	-2.458774	-3.139584	-1.435383
32	6	0.554395	-3.940289	-1.936680
33	1	2.304608	-4.360635	0.919057
34	1	2.685456	-2.736590	1.505346
35	1	2.855459	-3.115525	-0.209566
36	1	-0.221246	-2.775190	3.510242
37	1	-0.243605	-1.043682	3.156322
38	1	1.269917	-1.949893	3.045707
39	1	-2.859960	-2.743654	2.357465
40	1	-3.540923	-1.919435	0.953132
41	1	-2.573069	-1.014355	2.126273
42	1	-2.661278	-4.218786	-1.478602
43	1	-2.226512	-2.805645	-2.452769
44	1	-3.386123	-2.647533	-1.125049
45	1	0.396822	-5.022241	-1.818329
46	1	1.626322	-3.778480	-2.089939
47	1	0.039991	-3.621516	-2.847600
48	6	2.754386	0.281693	1.302564
49	1	2.600998	1.206690	1.883513
50	1	2.627164	-0.552676	2.001348
51	6	-2.895382	0.745673	-0.571778
52	1	-2.920388	1.183364	-1.580927
53	1	-3.141827	-0.312985	-0.672154
54	6	4.193813	0.257537	0.757367
55	1	4.404548	1.135233	0.138607
56	1	4.913611	0.248651	1.585806
57	1	4.358611	-0.637423	0.146886
58	6	-3.922348	1.440889	0.331602
59	1	-3.710413	2.514074	0.408859
60	1	-4.932120	1.321409	-0.077492
61	1	-3.905938	1.017612	1.341380

18Et (E = -1032.9816054 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.600955	-0.037392	-0.295999
2	7	0.543018	1.628923	-0.260783
3	6	1.801413	0.956053	-0.424822
4	7	0.787945	-1.137057	0.680953
5	6	-2.242054	0.058651	1.631572
6	6	-2.609492	-1.099480	0.883456
7	6	-2.504655	1.207791	0.822541
8	17	-0.456757	-0.728386	-2.656343
9	6	-3.071405	-0.669425	-0.395062
10	6	-3.011504	0.757008	-0.430761
11	6	1.942135	-0.518608	0.082848
12	6	2.723221	0.612842	0.747268
13	1	2.313587	1.144739	-1.371316
14	6	4.158176	0.401060	0.390563
15	1	2.429009	0.982075	1.723774
16	6	2.978374	-1.341874	-0.700010
17	6	4.301755	-0.646309	-0.442697
18	1	3.007774	-2.375961	-0.338172
19	1	2.727411	-1.395680	-1.765003
20	6	5.557920	-1.165307	-1.089739
21	6	5.217655	1.336569	0.912771
22	1	6.223183	1.041086	0.598247
23	1	5.203060	1.366622	2.011210
24	1	5.042086	2.364009	0.563957
25	1	6.446485	-0.604264	-0.784080
26	1	5.488768	-1.114411	-2.185508

27	1	5.720048	-2.222169	-0.832269
28	6	-2.674297	-2.517075	1.402020
29	6	-1.847473	0.105150	3.089027
30	6	-2.453581	2.634863	1.313669
31	6	-3.490242	1.624456	-1.572230
32	6	-3.670803	-1.553262	-1.462375
33	1	-3.681094	-2.731605	1.787800
34	1	-1.968045	-2.688789	2.218838
35	1	-2.463959	-3.251608	0.617989
36	1	-2.728044	0.302199	3.717247
37	1	-1.118277	0.897372	3.289236
38	1	-1.412044	-0.840031	3.426027
39	1	-3.311836	2.836374	1.970122
40	1	-2.501172	3.351061	0.488443
41	1	-1.544811	2.843311	1.887082
42	1	-4.575005	1.788016	-1.505116
43	1	-3.286111	1.161789	-2.543171
44	1	-3.009251	2.608007	-1.567251
45	1	-4.758377	-1.634009	-1.323927
46	1	-3.256955	-2.566100	-1.431420
47	1	-3.487218	-1.157177	-2.464982
48	6	0.583040	3.083364	-0.444009
49	1	1.071654	3.310237	-1.407609
50	1	-0.449172	3.437889	-0.525082
51	6	1.041547	-2.122528	1.744431
52	1	2.028456	-1.924151	2.188933
53	1	0.305423	-1.963470	2.542252
54	6	0.962128	-3.590190	1.287238
55	1	1.100005	-4.263797	2.142665
56	1	-0.013512	-3.801307	0.837425
57	1	1.729567	-3.823274	0.542678
58	6	1.305526	3.849253	0.677654
59	1	2.355432	3.546311	0.751620
60	1	1.277009	4.927886	0.481141
61	1	0.828503	3.662477	1.646680

7aEt (E = -1032.9711202 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.757354	0.130037	-0.341188
2	7	-0.936511	2.038962	-1.377807
3	6	-0.075058	2.227377	-0.454717
4	7	1.103213	-0.822397	-0.603260
5	6	-1.116726	0.589980	2.100938
6	6	-0.884712	-0.813928	1.977176
7	6	-2.384045	0.883870	1.502339
8	17	-2.028787	-0.852332	-2.240623
9	6	-1.987709	-1.377535	1.269696
10	6	-2.921770	-0.327070	0.995298
11	6	2.353493	-0.464676	-0.114332
12	6	2.765411	0.726250	0.412515
13	1	0.420577	3.192174	-0.300406
14	6	4.164740	0.637363	0.843870
15	1	2.161977	1.615715	0.513559
16	6	3.536440	-1.425848	-0.017349
17	6	4.642671	-0.605757	0.601786
18	1	3.283798	-2.291929	0.609134
19	1	3.830821	-1.830326	-0.992187
20	6	6.013542	-1.176811	0.843698
21	6	4.888324	1.814114	1.447773
22	1	5.924926	1.573075	1.703661
23	1	4.386616	2.157489	2.363260
24	1	4.902118	2.664573	0.751828
25	1	6.685312	-0.437723	1.293647

26	1	6.480641	-1.520697	-0.091553
27	1	5.980048	-2.045708	1.518104
28	6	0.261918	-1.567690	2.607651
29	6	-0.272015	1.544849	2.911274
30	6	-3.069419	2.229766	1.510286
31	6	-4.289787	-0.515755	0.388754
32	6	-2.229536	-2.843543	0.995275
33	1	0.058999	-1.748948	3.672594
34	1	1.202076	-1.011848	2.536132
35	1	0.416098	-2.539902	2.130372
36	1	-0.554144	1.498015	3.972810
37	1	-0.400462	2.580387	2.581295
38	1	0.793022	1.303196	2.839908
39	1	-3.658891	2.359453	2.428643
40	1	-3.754284	2.342639	0.663402
41	1	-2.348212	3.052882	1.467470
42	1	-5.001987	-0.849085	1.157050
43	1	-4.278084	-1.264426	-0.408220
44	1	-4.676855	0.414340	-0.039194
45	1	-2.896784	-3.271843	1.756435
46	1	-1.299201	-3.419887	1.015127
47	1	-2.699087	-2.998614	0.018366
48	6	-1.465904	2.961751	-2.401528
49	6	1.025570	-2.158502	-1.264675
50	1	-2.550162	3.014486	-2.243603
51	1	-1.320912	2.463526	-3.367048
52	1	-0.015966	-2.499160	-1.243232
53	1	1.598220	-2.894442	-0.684644
54	6	-0.840508	4.355552	-2.398553
55	1	-1.285892	4.959932	-3.195510
56	1	-1.012151	4.874515	-1.448314
57	1	0.240209	4.310179	-2.575271
58	6	1.496283	-2.143175	-2.727963
59	1	2.522706	-1.771105	-2.814468
60	1	1.459845	-3.154042	-3.153252
61	1	0.846090	-1.496324	-3.325758

TS(7a-7c)Et (E = -1032.9606686 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.646442	0.065934	-0.501736
2	7	-0.703726	2.079912	-1.298127
3	6	0.503221	1.676209	-1.472110
4	7	1.154817	-1.060521	-0.336011
5	6	-1.245474	0.594394	1.857296
6	6	-1.097850	-0.832231	1.855385
7	6	-2.440953	0.912399	1.135616
8	17	-1.682443	-1.048745	-2.401756
9	6	-2.157161	-1.377324	1.084745
10	6	-2.984259	-0.296532	0.635302
11	6	2.396648	-0.560980	-0.015216
12	6	2.694550	0.632769	0.585686
13	1	1.246097	2.283502	-2.001619
14	6	4.145526	0.800309	0.702527
15	1	1.976895	1.346299	0.967831
16	6	3.726035	-1.251666	-0.309262
17	6	4.773581	-0.290337	0.201109
18	1	3.803489	-2.234745	0.174235
19	1	3.839548	-1.427120	-1.384703
20	6	6.242495	-0.608978	0.135029
21	6	4.761362	2.025365	1.329611
22	1	5.854126	1.969230	1.357139
23	1	4.405102	2.159761	2.360626
24	1	4.484920	2.932656	0.774463

25	1	6.851608	0.201066	0.550784
26	1	6.576891	-0.775214	-0.899990
27	1	6.483933	-1.524870	0.695737
28	6	-0.073513	-1.593586	2.661287
29	6	-0.450778	1.555378	2.714867
30	6	-3.092299	2.272123	1.078971
31	6	-4.287259	-0.462804	-0.106274
32	6	-2.491194	-2.836291	0.878916
33	1	-0.355203	-1.600096	3.723595
34	1	0.922962	-1.148177	2.580617
35	1	0.004737	-2.634388	2.335186
36	1	-0.933199	1.683052	3.694768
37	1	-0.372540	2.548841	2.259474
38	1	0.564584	1.189837	2.896019
39	1	-3.737182	2.417721	1.957189
40	1	-3.721332	2.389341	0.190993
41	1	-2.354979	3.080459	1.080683
42	1	-5.080533	-0.793321	0.579489
43	1	-4.203268	-1.207988	-0.903730
44	1	-4.616602	0.475220	-0.564402
45	1	-3.401623	-3.099327	1.435429
46	1	-1.691140	-3.492142	1.234596
47	1	-2.675870	-3.069171	-0.176202
48	6	-1.298620	3.349258	-1.788077
49	6	1.047552	-2.533806	-0.508942
50	1	-2.373690	3.311613	-1.597838
51	1	-1.151385	3.384231	-2.874862
52	1	0.007200	-2.816804	-0.306371
53	1	1.657916	-3.045916	0.250145
54	6	-0.669470	4.581575	-1.125524
55	1	-1.121130	5.494893	-1.526860
56	1	-0.825448	4.571429	-0.041461
57	1	0.408358	4.623396	-1.316908
58	6	1.411409	-3.053079	-1.911789
59	1	2.464261	-2.880502	-2.151234
60	1	1.224675	-4.133149	-1.969450
61	1	0.799455	-2.558141	-2.671822

7cEt (E = -1032.9618122 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.653320	0.054065	-0.549819
2	7	-0.188059	2.021424	-1.333288
3	6	0.676006	1.224634	-1.852957
4	7	0.950559	-1.260222	-0.084120
5	6	-1.360246	0.788997	1.736418
6	6	-1.435237	-0.639623	1.822740
7	6	-2.421133	1.233376	0.884081
8	17	-1.722260	-1.078649	-2.429849
9	6	-2.485457	-1.073987	0.975889
10	6	-3.091764	0.086135	0.390599
11	6	2.226471	-0.839752	0.210066
12	6	2.647231	0.420420	0.551960
13	1	1.412478	1.585032	-2.580484
14	6	4.099293	0.435401	0.752528
15	1	2.017892	1.285711	0.718974
16	6	3.466233	-1.730039	0.190664
17	6	4.603063	-0.806752	0.558460
18	1	3.380299	-2.570396	0.892689
19	1	3.615327	-2.171878	-0.800341
20	6	6.019322	-1.301568	0.672826
21	6	4.840113	1.691244	1.135885
22	1	5.911402	1.511963	1.270845
23	1	4.447757	2.108288	2.073992

24	1	4.723603	2.467138	0.366301
25	1	6.708291	-0.496530	0.950769
26	1	6.378702	-1.730333	-0.274803
27	1	6.112413	-2.092678	1.432449
28	6	-0.619585	-1.476557	2.776901
29	6	-0.490595	1.659110	2.617318
30	6	-2.869013	2.662557	0.695539
31	6	-4.341176	0.070447	-0.454091
32	6	-3.020203	-2.476755	0.810066
33	1	-0.943518	-1.293358	3.810897
34	1	0.448054	-1.241918	2.715254
35	1	-0.736423	-2.545789	2.580845
36	1	-0.962257	1.804734	3.599923
37	1	-0.329979	2.651171	2.183344
38	1	0.492090	1.208047	2.789978
39	1	-3.652049	2.909988	1.426175
40	1	-3.289137	2.836533	-0.300658
41	1	-2.050152	3.371509	0.846144
42	1	-5.229089	-0.074595	0.178111
43	1	-4.317718	-0.739374	-1.189811
44	1	-4.474754	1.009949	-0.999960
45	1	-4.019176	-2.559212	1.260331
46	1	-2.380307	-3.217807	1.298356
47	1	-3.114162	-2.754578	-0.246273
48	6	-0.316805	3.471830	-1.612740
49	6	0.695193	-2.723027	-0.089281
50	1	-1.372264	3.742601	-1.526040
51	1	-0.002910	3.645358	-2.649953
52	1	-0.370109	-2.874176	0.119671
53	1	1.240943	-3.202581	0.736728
54	6	1.023917	-3.432284	-1.415764
55	1	2.086251	-3.359727	-1.665563
56	1	0.765497	-4.496647	-1.343145
57	1	0.448224	-2.993944	-2.236345
58	6	0.537552	4.311307	-0.653878
59	1	1.597774	4.053763	-0.751431
60	1	0.420616	5.375982	-0.882193
61	1	0.240896	4.152152	0.388097

TS(7c-8b)Et (E = -1032.9442662 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.605509	0.002209	-0.394950
2	7	0.190073	1.840598	-0.916248
3	6	1.161947	0.962420	-1.221840
4	7	0.986165	-1.429842	0.223708
5	6	-1.558659	0.711959	1.804196
6	6	-1.695889	-0.712174	1.824980
7	6	-2.482462	1.230305	0.841754
8	17	-1.480029	-0.941882	-2.479986
9	6	-2.657844	-1.073319	0.841541
10	6	-3.147315	0.129257	0.240557
11	6	2.189370	-0.908029	0.377880
12	6	2.456460	0.499536	0.336264
13	1	1.896159	1.186302	-1.997950
14	6	3.931782	0.648566	0.270959
15	1	1.910627	1.190247	0.967635
16	6	3.509230	-1.657181	0.402963
17	6	4.541515	-0.556628	0.274148
18	1	3.631374	-2.208690	1.347251
19	1	3.576241	-2.401746	-0.396859
20	6	6.006609	-0.889544	0.194711
21	6	4.577096	2.007809	0.203410
22	1	5.669633	1.948345	0.198742

23	1	4.276274	2.624205	1.062223
24	1	4.264433	2.546337	-0.701374
25	1	6.627837	0.009863	0.137489
26	1	6.232035	-1.505228	-0.688491
27	1	6.332391	-1.465440	1.073671
28	6	-1.071537	-1.610496	2.867048
29	6	-0.764698	1.518823	2.807833
30	6	-2.821693	2.687236	0.636603
31	6	-4.279898	0.199275	-0.753136
32	6	-3.199726	-2.453119	0.551405
33	1	-1.523137	-1.413259	3.849303
34	1	0.007876	-1.450447	2.963970
35	1	-1.233568	-2.668504	2.642879
36	1	-1.343417	1.663743	3.731717
37	1	-0.509694	2.510435	2.421776
38	1	0.170460	1.020043	3.086111
39	1	-3.658031	2.978707	1.287839
40	1	-3.122647	2.897945	-0.394913
41	1	-1.977014	3.338495	0.878271
42	1	-5.246497	0.090630	-0.240358
43	1	-4.206697	-0.594501	-1.502968
44	1	-4.293659	1.155494	-1.285705
45	1	-4.211402	-2.566643	0.965514
46	1	-2.577074	-3.238231	0.992102
47	1	-3.263059	-2.642182	-0.526168
48	6	0.194705	3.280340	-1.211799
49	6	0.835317	-2.907264	0.270649
50	1	-0.842858	3.627995	-1.250447
51	1	0.626676	3.424265	-2.214009
52	1	-0.156927	-3.124655	0.675800
53	1	1.564067	-3.335414	0.971366
54	6	0.969036	-3.574390	-1.108984
55	1	1.954857	-3.393793	-1.549542
56	1	0.831204	-4.658029	-1.013042
57	1	0.215584	-3.188393	-1.801688
58	6	0.987711	4.107674	-0.188161
59	1	2.030435	3.775388	-0.142329
60	1	0.979514	5.168272	-0.465510
61	1	0.555555	4.014134	0.814713

8bEt (E = -1032.9660284 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.549991	0.131766	-0.258793
2	7	0.339408	1.916185	-0.258892
3	6	1.370573	1.092088	-0.817906
4	7	1.106218	-1.355507	0.437948
5	6	-1.893312	0.764021	1.782191
6	6	-1.891705	-0.665646	1.781777
7	6	-2.683113	1.203976	0.678657
8	17	-1.027006	-0.775974	-2.499103
9	6	-2.666523	-1.107015	0.666881
10	6	-3.151164	0.047909	-0.010202
11	6	2.290125	-0.851963	0.437709
12	6	2.506450	0.609050	0.105451
13	1	1.690210	1.325146	-1.839494
14	6	3.962159	0.608205	-0.350633
15	1	2.437305	1.177229	1.048554
16	6	3.621783	-1.551940	0.568274
17	6	4.567843	-0.563481	-0.093107
18	1	3.876592	-1.713652	1.627035
19	1	3.632105	-2.538413	0.094725
20	6	5.994883	-0.969810	-0.343827
21	6	4.569430	1.845044	-0.952966

22	1	5.597368	1.681327	-1.289201
23	1	4.579587	2.667110	-0.223229
24	1	3.979093	2.190382	-1.810121
25	1	6.569346	-0.179971	-0.835881
26	1	6.040894	-1.865750	-0.979176
27	1	6.504723	-1.220598	0.597636
28	6	-1.376451	-1.509636	2.927831
29	6	-1.332770	1.624040	2.891422
30	6	-3.136792	2.619570	0.404342
31	6	-4.120855	0.045364	-1.165937
32	6	-3.037747	-2.528194	0.312684
33	1	-1.951901	-1.293533	3.838618
34	1	-0.321893	-1.318452	3.160039
35	1	-1.487435	-2.579079	2.725951
36	1	-2.052925	1.707149	3.718915
37	1	-1.105071	2.635878	2.544934
38	1	-0.409373	1.203177	3.304785
39	1	-4.187688	2.744551	0.701758
40	1	-3.064123	2.886500	-0.655828
41	1	-2.549051	3.346149	0.971743
42	1	-5.152418	-0.064540	-0.800571
43	1	-3.919284	-0.775814	-1.860014
44	1	-4.069913	0.977909	-1.737290
45	1	-4.070204	-2.748997	0.618403
46	1	-2.389300	-3.258615	0.807578
47	1	-2.971630	-2.702686	-0.767214
48	6	0.382709	3.377133	-0.248385
49	6	0.945863	-2.820717	0.650253
50	1	-0.613424	3.753610	0.010172
51	1	0.606025	3.734984	-1.268799
52	1	-0.003524	-2.973303	1.164636
53	1	1.736757	-3.195431	1.310479
54	6	0.940977	-3.590392	-0.680002
55	1	1.895356	-3.483600	-1.206671
56	1	0.769770	-4.656090	-0.491642
57	1	0.152817	-3.221184	-1.342347
58	6	1.418091	3.971963	0.723278
59	1	2.430776	3.645627	0.463015
60	1	1.396684	5.068312	0.685798
61	1	1.211472	3.658959	1.753784

TS(8b-18)Et (E = -1032.9511061 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.472130	0.053644	-0.229508
2	7	0.474408	1.818914	-0.182508
3	6	1.646305	1.080643	-0.459024
4	7	0.840344	-1.294102	0.867631
5	6	-2.277125	1.074539	1.210085
6	6	-2.211399	-0.292996	1.616844
7	6	-2.776120	1.113148	-0.125912
8	17	-0.393530	-0.714594	-2.568759
9	6	-2.678822	-1.099648	0.536848
10	6	-3.016876	-0.230726	-0.540216
11	6	2.040941	-0.857778	0.467285
12	6	2.534696	0.546755	0.656262
13	1	2.116269	1.172435	-1.440978
14	6	4.010397	0.473266	0.348099
15	1	2.287773	0.982862	1.630320
16	6	3.167036	-1.689379	-0.125546
17	6	4.354519	-0.746884	-0.095372
18	1	3.333418	-2.596700	0.472543
19	1	2.936671	-2.034285	-1.140612
20	6	5.698888	-1.239411	-0.557227

21	6	4.877755	1.693765	0.496179
22	1	5.913904	1.507295	0.198692
23	1	4.881841	2.046263	1.536963
24	1	4.493260	2.518207	-0.119241
25	1	6.470567	-0.467288	-0.488587
26	1	5.652260	-1.578774	-1.601813
27	1	6.027293	-2.100686	0.042059
28	6	-1.889270	-0.751443	3.020536
29	6	-2.035536	2.252104	2.124739
30	6	-3.169064	2.339752	-0.917869
31	6	-3.702328	-0.639452	-1.820348
32	6	-2.992025	-2.578048	0.575962
33	1	-2.715622	-0.502665	3.701354
34	1	-0.984931	-0.274638	3.414479
35	1	-1.741175	-1.833868	3.071904
36	1	-2.918259	2.433077	2.755016
37	1	-1.835176	3.169635	1.565491
38	1	-1.184313	2.081039	2.792056
39	1	-4.263103	2.442991	-0.941679
40	1	-2.824016	2.291813	-1.956902
41	1	-2.765289	3.254114	-0.474714
42	1	-4.793099	-0.652251	-1.679215
43	1	-3.394722	-1.637064	-2.147072
44	1	-3.478052	0.052499	-2.637339
45	1	-4.056218	-2.732857	0.804726
46	1	-2.416935	-3.105086	1.342654
47	1	-2.794652	-3.065763	-0.384367
48	6	0.452133	3.267592	-0.416895
49	6	0.651390	-2.751169	1.109410
50	1	-0.588765	3.605249	-0.378993
51	1	0.818804	3.469821	-1.437927
52	1	-0.224479	-2.834233	1.757232
53	1	1.504786	-3.125456	1.691234
54	6	0.446436	-3.627644	-0.136046
55	1	0.228654	-4.658060	0.170002
56	1	-0.389918	-3.262835	-0.739172
57	1	1.332532	-3.645634	-0.776784
58	6	1.295842	4.064696	0.591065
59	1	2.342637	3.742108	0.560771
60	1	1.263604	5.136438	0.359459
61	1	0.922732	3.919715	1.611406

TS(8b-19)Et (E = -1032.9152699 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.885955	-0.135948	0.302964
2	7	-0.288486	1.674093	-0.389220
3	6	0.795451	0.872715	-0.801158
4	7	2.181441	-1.750204	-1.075342
5	6	-1.616314	-0.401876	2.697032
6	6	-2.341883	-1.398608	1.970835
7	6	-2.081559	0.877360	2.261346
8	17	-1.529310	-1.505326	-1.613123
9	6	-3.248759	-0.737689	1.096920
10	6	-3.072658	0.670892	1.252577
11	6	2.611550	-0.785166	-0.379810
12	6	1.655377	0.244942	0.202127
13	1	0.935558	0.607773	-1.848363
14	6	2.515206	1.042622	1.169242
15	1	0.936088	-0.493859	1.020660
16	6	4.019622	-0.438480	0.078968
17	6	3.805305	0.675086	1.075337
18	1	4.526574	-1.301294	0.527582
19	1	4.646493	-0.117570	-0.764500

20	6	4.995473	1.244908	1.799842
21	6	1.938981	2.101518	2.063113
22	1	2.717309	2.629702	2.620822
23	1	1.249115	1.657554	2.791891
24	1	1.364649	2.832534	1.487600
25	1	4.723076	2.035741	2.503876
26	1	5.720931	1.662863	1.087205
27	1	5.519761	0.458521	2.361212
28	6	-2.235827	-2.892928	2.167879
29	6	-0.694587	-0.672886	3.865522
30	6	-1.747745	2.214619	2.880221
31	6	-3.944661	1.741967	0.639068
32	6	-4.314669	-1.401999	0.262489
33	1	-2.965298	-3.240478	2.913389
34	1	-1.241861	-3.186162	2.522125
35	1	-2.431314	-3.437234	1.238096
36	1	-1.276364	-0.802689	4.789302
37	1	0.007666	0.148908	4.034842
38	1	-0.105594	-1.583765	3.716796
39	1	-2.556539	2.529344	3.554899
40	1	-1.621686	2.997544	2.125961
41	1	-0.828913	2.172904	3.471001
42	1	-4.872942	1.862610	1.216281
43	1	-4.227814	1.499158	-0.390486
44	1	-3.439858	2.712688	0.625730
45	1	-5.226410	-1.542601	0.860757
46	1	-3.994725	-2.382287	-0.101075
47	1	-4.578653	-0.800578	-0.612416
48	6	-0.634357	2.890566	-1.126877
49	6	0.323732	4.065868	-0.877272
50	1	0.284439	4.393885	0.167681
51	1	1.355508	3.777832	-1.109535
52	1	0.054840	4.918538	-1.512193
53	6	3.114881	-2.719490	-1.665121
54	6	2.843633	-2.861720	-3.169988
55	1	1.798357	-3.134622	-3.345442
56	1	3.038904	-1.916938	-3.690176
57	1	3.487359	-3.634467	-3.605179
58	1	-1.655148	3.174150	-0.848121
59	1	-0.645977	2.661595	-2.206703
60	1	2.932187	-3.685162	-1.173976
61	1	4.170031	-2.456635	-1.497393

19Et (E = -1032.9533754 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.706792	-0.293124	-0.162004
2	7	-0.131521	0.196356	1.678824
3	6	-1.427582	-0.150027	1.315520
4	7	-3.758550	-1.341799	0.061551
5	6	2.530605	1.319453	-0.880576
6	6	2.697938	0.147674	-1.676859
7	6	2.802016	0.976241	0.477837
8	17	0.181357	-2.627419	-0.468244
9	6	3.058393	-0.923479	-0.814227
10	6	3.114241	-0.416499	0.523389
11	6	-3.419794	-0.139117	-0.178369
12	6	-2.208790	0.510646	0.403281
13	1	-1.831003	-1.084146	1.716841
14	6	-2.219627	1.915542	-0.044889
15	1	-0.093349	0.527530	-1.592484
16	6	-4.099266	0.892801	-1.067196
17	6	-3.279970	2.140223	-0.854972
18	1	-4.101583	0.568584	-2.117002

19	1	-5.151582	1.040517	-0.791277
20	6	-3.701896	3.424361	-1.510789
21	6	-1.248548	2.956013	0.447700
22	1	-1.605994	3.966486	0.229169
23	1	-0.262426	2.844769	-0.016572
24	1	-1.104764	2.866580	1.529457
25	1	-3.039647	4.260515	-1.270512
26	1	-4.723296	3.701656	-1.212336
27	1	-3.713542	3.310203	-2.604663
28	6	2.604190	0.081911	-3.181280
29	6	2.287937	2.710711	-1.414256
30	6	2.901735	1.960037	1.619985
31	6	3.619336	-1.197340	1.715313
32	6	3.487297	-2.305682	-1.242680
33	1	3.584117	0.285599	-3.636139
34	1	1.893961	0.816971	-3.570591
35	1	2.281433	-0.905894	-3.525545
36	1	3.226996	3.142213	-1.789041
37	1	1.908185	3.383391	-0.639291
38	1	1.568939	2.709630	-2.239371
39	1	3.865870	2.485724	1.582433
40	1	2.836968	1.465794	2.592849
41	1	2.111720	2.716724	1.581990
42	1	4.709663	-1.318757	1.652702
43	1	3.182622	-2.200669	1.767319
44	1	3.402921	-0.689512	2.659215
45	1	4.571501	-2.323875	-1.422939
46	1	2.989587	-2.618175	-2.165195
47	1	3.260809	-3.056004	-0.480030
48	6	0.217609	-0.083992	3.085432
49	6	-0.361238	0.954866	4.057345
50	1	0.027767	1.955127	3.836206
51	1	-1.454340	0.989012	3.982374
52	1	-0.097784	0.702486	5.091396
53	6	-4.968399	-1.888098	-0.570161
54	6	-5.510234	-3.069889	0.239769
55	1	-4.747203	-3.849324	0.336384
56	1	-5.796048	-2.748572	1.247965
57	1	-6.391898	-3.503342	-0.246477
58	1	1.306255	-0.109908	3.174206
59	1	-0.156733	-1.086321	3.355777
60	1	-4.701875	-2.229884	-1.582655
61	1	-5.753547	-1.124147	-0.688252

2aAr (E = -1091.8459213 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.948274	-0.067468	-0.325760
2	7	-2.460086	-0.095104	-0.010288
3	6	2.879989	0.648705	1.175696
4	6	1.858171	0.233414	2.080823
5	6	2.413426	1.828628	0.508188
6	17	0.689853	1.477776	-2.299527
7	6	0.756834	1.127521	1.947792
8	6	1.108645	2.125563	0.986959
9	6	-1.293565	-0.065843	-0.073582
10	6	0.631054	-2.261093	0.525080
11	6	1.811590	-2.362247	-0.331486
12	1	-0.281304	-2.740846	0.171240
13	6	0.314999	-1.653270	-2.094227
14	6	1.623021	-2.045361	-1.692301
15	1	0.192951	-1.262568	-3.097253
16	1	-0.539817	-2.200474	-1.712669
17	6	2.762329	-2.027154	-2.697388

18	6	3.104594	-2.970763	0.180030
19	1	4.002605	-2.545885	-0.279011
20	1	3.105226	-4.050752	-0.033094
21	1	3.189943	-2.862129	1.264592
22	1	2.876137	-3.025242	-3.144893
23	1	3.726465	-1.751491	-2.257483
24	1	2.541007	-1.328084	-3.510421
25	6	2.007173	-0.778650	3.189321
26	6	4.311549	0.162615	1.151644
27	6	3.250186	2.705288	-0.392343
28	6	0.298509	3.349904	0.639596
29	6	-0.460069	1.143860	2.843310
30	1	2.390419	-0.283842	4.093760
31	1	2.708086	-1.577636	2.934118
32	1	1.052115	-1.244567	3.450282
33	1	4.945254	0.823104	1.761075
34	1	4.730916	0.156454	0.139513
35	1	4.405920	-0.847619	1.555999
36	1	3.825795	3.423288	0.209979
37	1	2.630343	3.268364	-1.093957
38	1	3.967440	2.123011	-0.980661
39	1	0.604748	4.202297	1.262656
40	1	-0.771639	3.188400	0.806001
41	1	0.430951	3.630379	-0.409035
42	1	-0.228490	1.647830	3.792551
43	1	-0.803014	0.132171	3.084402
44	1	-1.296685	1.678843	2.384139
45	1	0.815567	-2.486929	1.571317
46	6	-3.849438	-0.147106	0.029300
47	6	-4.581033	0.779099	-0.751092
48	6	-4.467483	-1.126345	0.841885
49	6	-5.978682	0.701341	-0.697506
50	6	-5.867815	-1.156443	0.860687
51	6	-6.617350	-0.253916	0.099630
52	1	-6.565806	1.397180	-1.287537
53	1	-6.368965	-1.896901	1.475211
54	1	-7.701120	-0.296023	0.126523
55	6	-3.876653	1.802717	-1.606276
56	1	-3.249188	2.470073	-1.002338
57	1	-3.214137	1.329920	-2.340936
58	1	-4.600907	2.417056	-2.146888
59	6	-3.644536	-2.098261	1.650351
60	1	-2.982298	-2.694665	1.010341
61	1	-3.002765	-1.579990	2.373865
62	1	-4.291039	-2.784706	2.202760

TS(2a-3a)Ar (E = -1091.8390436 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-3.191473	1.446431	-2.400302
2	6	1.464109	-0.985898	-0.868840
3	6	1.239137	-0.303513	0.358633
4	6	1.115724	-0.103972	-1.936652
5	17	-1.286458	-2.372583	-2.424790
6	6	0.757796	1.010688	0.053226
7	6	0.687795	1.133621	-1.365933
8	6	-2.533330	0.662242	-1.755406
9	6	-1.918493	-0.011495	1.364527
10	6	-2.265239	-1.421030	1.270551
11	1	-2.729505	0.709596	1.248544
12	6	-3.616707	-0.734327	-0.652263
13	6	-3.057674	-1.801485	0.188640
14	1	-4.197371	-1.102804	-1.492207
15	1	-4.126041	0.063316	-0.113873

16	6	-3.497456	-3.228366	-0.071869
17	6	-1.752838	-2.409117	2.302231
18	1	-1.532823	-3.396643	1.885641
19	1	-2.512524	-2.542907	3.085860
20	1	-0.849407	-2.031386	2.789809
21	1	-4.449987	-3.424903	0.441559
22	1	-2.769644	-3.967444	0.274715
23	1	-3.650940	-3.391578	-1.142038
24	6	1.627926	-0.799836	1.730958
25	6	2.070062	-2.358968	-1.034610
26	6	1.335757	-0.370000	-3.405430
27	6	0.399978	2.407105	-2.126772
28	6	0.589408	2.148374	1.031300
29	1	2.655977	-0.492873	1.969935
30	1	1.590646	-1.891917	1.797726
31	1	0.979138	-0.394062	2.513619
32	1	3.151043	-2.279900	-1.217602
33	1	1.626077	-2.893575	-1.879686
34	1	1.933470	-2.976178	-0.140596
35	1	2.368837	-0.120774	-3.687204
36	1	0.668173	0.231436	-4.030720
37	1	1.160259	-1.420048	-3.653841
38	1	1.330291	2.969110	-2.291837
39	1	-0.288170	3.059897	-1.581201
40	1	-0.044935	2.206498	-3.105765
41	1	1.497378	2.768174	1.052844
42	1	0.413426	1.787847	2.048357
43	1	-0.247769	2.801340	0.762569
44	1	-1.269280	0.250120	2.194114
45	6	-4.558942	1.731031	-2.636181
46	6	-5.197265	1.116765	-3.736976
47	6	-5.213080	2.676918	-1.816114
48	6	-6.540694	1.441341	-3.976236
49	6	-6.555852	2.969172	-2.098736
50	6	-7.219823	2.355458	-3.164806
51	1	-7.050721	0.973671	-4.812826
52	1	-7.077136	3.689427	-1.475597
53	1	-8.258167	2.595608	-3.368382
54	6	-4.450245	0.151876	-4.627829
55	1	-3.558301	0.620911	-5.062516
56	1	-4.102693	-0.732501	-4.080005
57	1	-5.088651	-0.189417	-5.447292
58	6	-4.488227	3.352175	-0.675662
59	1	-4.204191	2.638624	0.109297
60	1	-3.563400	3.833052	-1.018067
61	1	-5.119766	4.117187	-0.215694
62	72	-1.061773	-0.558794	-0.735265

3aAr (E = -1091.8581161 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-1.963514	-0.696823	0.266284
2	6	2.584489	-1.399976	1.207154
3	6	3.216578	-1.064834	-0.031317
4	6	1.371459	-2.081470	0.907288
5	17	1.413451	1.677952	1.998476
6	6	2.408650	-1.568194	-1.094681
7	6	1.260769	-2.185382	-0.514046
8	6	-1.120603	0.041668	-0.354692
9	6	1.361523	1.280565	-1.962233
10	6	0.699452	2.455425	-1.360598
11	1	0.742308	0.683967	-2.639533
12	6	-1.502323	1.214172	-1.272036
13	6	-0.606460	2.407495	-0.951338

14	1	-2.555683	1.486464	-1.159710
15	1	-1.356131	0.898908	-2.313579
16	6	-1.302937	3.528275	-0.212449
17	6	1.585854	3.668257	-1.103961
18	1	1.406203	4.135801	-0.133101
19	1	1.412965	4.424248	-1.882033
20	1	2.643852	3.389585	-1.147769
21	1	-2.039885	4.012950	-0.870268
22	1	-0.620276	4.297871	0.151352
23	1	-1.859007	3.134629	0.648177
24	6	4.563489	-0.396003	-0.178787
25	6	3.177502	-1.197652	2.580207
26	6	0.410934	-2.686377	1.903230
27	6	0.225452	-2.999196	-1.249488
28	6	2.786940	-1.612811	-2.554723
29	1	5.368577	-1.143591	-0.151727
30	1	4.755040	0.317733	0.629288
31	1	4.648660	0.141372	-1.128825
32	1	3.805797	-2.058873	2.847293
33	1	2.404759	-1.095836	3.346991
34	1	3.800998	-0.300413	2.627369
35	1	0.580897	-3.768882	1.988665
36	1	-0.627906	-2.525552	1.598835
37	1	0.540595	-2.252739	2.899623
38	1	0.561702	-4.041822	-1.342324
39	1	0.047926	-2.619779	-2.260926
40	1	-0.728599	-2.996828	-0.717728
41	1	3.318105	-2.548294	-2.779668
42	1	3.446047	-0.784785	-2.831652
43	1	1.908480	-1.570115	-3.206625
44	1	2.329504	1.483074	-2.414501
45	6	-3.380866	-0.535759	0.169770
46	6	-4.054783	0.005699	1.293686
47	6	-4.110039	-1.014221	-0.946392
48	6	-5.453678	0.098119	1.265165
49	6	-5.511070	-0.911678	-0.927463
50	6	-6.184333	-0.354272	0.162436
51	1	-5.969674	0.521141	2.122557
52	1	-6.073702	-1.279964	-1.780984
53	1	-7.267345	-0.282731	0.157073
54	6	-3.273000	0.473948	2.499386
55	1	-2.602607	-0.314247	2.863759
56	1	-2.635955	1.337574	2.268022
57	1	-3.946291	0.762371	3.312215
58	6	-3.415931	-1.645869	-2.133122
59	1	-2.810151	-0.922077	-2.693301
60	1	-2.742484	-2.452601	-1.822686
61	1	-4.150239	-2.066274	-2.826998
62	72	1.104959	0.267093	0.027204

TS(3a-3b)Ar (E = -1091.8572578 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-1.506993	-0.737557	0.819782
2	6	2.686044	-1.733515	1.161977
3	6	3.427317	-1.131411	0.099496
4	6	1.580682	-2.426924	0.585070
5	17	1.761058	1.603228	1.943838
6	6	2.781394	-1.452938	-1.132732
7	6	1.630672	-2.243611	-0.828246
8	6	-0.952340	-0.215469	-0.213791
9	6	1.248990	1.189823	-1.769781
10	6	0.325992	2.272982	-1.319070
11	1	0.806820	0.507811	-2.503894

12	6	-1.615881	0.666251	-1.262174
13	6	-0.998188	2.052451	-1.077582
14	1	-2.702444	0.714129	-1.151653
15	1	-1.393896	0.267928	-2.259911
16	6	-1.979060	3.096109	-0.587477
17	6	0.995125	3.624680	-1.124588
18	1	0.414321	4.322642	-0.519170
19	1	1.177805	4.091336	-2.102916
20	1	1.969490	3.500050	-0.637754
21	1	-2.744554	3.286359	-1.354304
22	1	-1.513641	4.050887	-0.337633
23	1	-2.512594	2.735879	0.302271
24	6	4.727052	-0.374850	0.245663
25	6	3.084960	-1.748770	2.618918
26	6	0.604084	-3.309580	1.322307
27	6	0.733405	-2.914259	-1.840158
28	6	3.327758	-1.188481	-2.514118
29	1	5.579605	-1.065896	0.187279
30	1	4.788246	0.145108	1.206324
31	1	4.857103	0.370395	-0.546111
32	1	3.762489	-2.590686	2.818228
33	1	2.218248	-1.859450	3.277697
34	1	3.600604	-0.828558	2.907838
35	1	0.907944	-4.362017	1.233118
36	1	-0.410193	-3.210677	0.927973
37	1	0.561848	-3.064598	2.387311
38	1	1.169669	-3.869413	-2.165359
39	1	0.593575	-2.298468	-2.734869
40	1	-0.254738	-3.125545	-1.422784
41	1	3.970002	-2.021616	-2.832077
42	1	3.931184	-0.276292	-2.548096
43	1	2.531023	-1.085964	-3.257265
44	1	2.190199	1.575134	-2.163888
45	6	-2.906434	-0.684091	1.113031
46	6	-3.315782	0.069583	2.240979
47	6	-3.840347	-1.459555	0.382422
48	6	-4.672784	0.072301	2.594824
49	6	-5.187710	-1.435341	0.779266
50	6	-5.609251	-0.671015	1.870154
51	1	-4.990295	0.656465	3.453944
52	1	-5.907632	-2.030226	0.224017
53	1	-6.654999	-0.664549	2.160647
54	6	-2.304854	0.850876	3.048105
55	1	-1.483785	0.205339	3.383702
56	1	-1.842746	1.657163	2.464648
57	1	-2.774294	1.300235	3.928399
58	6	-3.411526	-2.323547	-0.783644
59	1	-3.094365	-1.728555	-1.649553
60	1	-2.567260	-2.969579	-0.514259
61	1	-4.236601	-2.964260	-1.109141
62	72	1.230878	0.048086	0.154299

3bAr (E = -1091.8674491 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.397333	-0.244621	0.107215
2	6	-2.084304	-2.048721	-0.591775
3	6	-3.072282	-1.059750	-0.304055
4	6	-1.293636	-2.238702	0.580413
5	17	-1.045924	0.864827	-2.549901
6	6	-2.886407	-0.629548	1.041855
7	6	-1.779994	-1.354909	1.590053
8	6	0.899384	0.573834	0.964555
9	6	-1.329746	2.116842	0.760646

10	6	-0.215863	3.088943	0.482798
11	1	-1.399520	1.889579	1.829693
12	6	1.472965	1.697197	1.753101
13	6	1.050882	2.945132	0.953836
14	1	2.562817	1.669289	1.853393
15	1	1.037044	1.701588	2.759911
16	6	2.195589	3.915720	0.736658
17	6	-0.633819	4.251935	-0.402686
18	1	0.198106	4.852271	-0.777039
19	1	-1.318710	4.917618	0.141569
20	1	-1.184384	3.866553	-1.270439
21	1	2.601583	4.253767	1.701687
22	1	1.904110	4.805336	0.175243
23	1	3.025681	3.434615	0.198129
24	6	-4.185145	-0.625600	-1.228399
25	6	-1.967836	-2.838474	-1.874578
26	6	-0.229983	-3.298097	0.748511
27	6	-1.353544	-1.323165	3.039508
28	6	-3.821592	0.265816	1.816558
29	1	-5.060611	-1.279340	-1.108218
30	1	-3.879010	-0.667217	-2.277750
31	1	-4.509237	0.399306	-1.020767
32	1	-2.610186	-3.729715	-1.835599
33	1	-0.942995	-3.182770	-2.049431
34	1	-2.273059	-2.247696	-2.743540
35	1	-0.694394	-4.271701	0.958768
36	1	0.443301	-3.070673	1.579027
37	1	0.383445	-3.414224	-0.150955
38	1	-2.002525	-1.970254	3.646572
39	1	-1.412762	-0.313734	3.459838
40	1	-0.325958	-1.675260	3.169622
41	1	-4.632159	-0.328494	2.261493
42	1	-4.282186	1.026217	1.178392
43	1	-3.309292	0.786287	2.631035
44	1	-2.291095	2.536935	0.447323
45	6	2.772445	-0.605613	-0.109762
46	6	3.310148	-0.496285	-1.415244
47	6	3.547494	-1.123725	0.958855
48	6	4.639447	-0.888877	-1.627704
49	6	4.869573	-1.518002	0.691769
50	6	5.418428	-1.397838	-0.585577
51	1	5.059822	-0.794991	-2.624335
52	1	5.466718	-1.925893	1.501922
53	1	6.442748	-1.705200	-0.769816
54	6	2.490968	0.048791	-2.559997
55	1	1.594794	-0.553521	-2.745151
56	1	2.140508	1.068711	-2.365920
57	1	3.082433	0.065186	-3.480069
58	6	3.005201	-1.284937	2.362815
59	1	3.059313	-0.350155	2.935513
60	1	1.957981	-1.601346	2.364786
61	1	3.586016	-2.033885	2.909429
62	72	-0.824017	0.108629	-0.230270

TS(3b-3c)Ar (E = -1091.8613129 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-0.912045	1.378680	-0.802027
2	6	2.606110	-1.473576	0.186380
3	6	2.080306	-0.887844	1.372919
4	6	2.829429	-0.432586	-0.762204
5	17	0.122091	-1.833312	-2.370691
6	6	1.952180	0.518838	1.147934
7	6	2.424783	0.799914	-0.173625

8	6	-1.667600	0.445570	-0.348261
9	6	-1.006775	-1.640913	1.171804
10	6	-2.379524	-2.068310	0.693843
11	1	-1.095211	-0.911113	1.992309
12	6	-3.087781	0.256113	0.021490
13	6	-3.344611	-1.236133	0.232154
14	1	-3.296510	0.838627	0.932307
15	1	-3.764444	0.665324	-0.742638
16	6	-4.761220	-1.638217	-0.130737
17	6	-2.582006	-3.574325	0.781680
18	1	-3.489220	-3.933018	0.290799
19	1	-2.606474	-3.902831	1.830720
20	1	-1.728999	-4.081695	0.310652
21	1	-4.982418	-2.688734	0.065856
22	1	-4.966564	-1.443386	-1.194811
23	1	-5.486851	-1.040052	0.441723
24	6	1.899082	-1.577627	2.702245
25	6	2.959090	-2.927884	-0.014336
26	6	3.477500	-0.610157	-2.113744
27	6	2.618201	2.176288	-0.768522
28	6	1.605001	1.544328	2.204580
29	1	2.812507	-1.477979	3.305759
30	1	1.698491	-2.646644	2.584106
31	1	1.074011	-1.149652	3.280421
32	1	4.023380	-3.104253	0.196924
33	1	2.769372	-3.248986	-1.043938
34	1	2.380709	-3.580154	0.648021
35	1	4.569603	-0.679116	-2.009918
36	1	3.263890	0.230674	-2.781354
37	1	3.131760	-1.522005	-2.610891
38	1	3.598819	2.582996	-0.483808
39	1	1.855985	2.882587	-0.425670
40	1	2.578983	2.156583	-1.862475
41	1	2.483703	1.763849	2.827962
42	1	0.812639	1.194964	2.876202
43	1	1.277930	2.489559	1.760809
44	1	-0.486723	-2.504618	1.597709
45	6	-1.206416	2.732769	-1.195943
46	6	-1.002938	3.072309	-2.555195
47	6	-1.637762	3.691775	-0.251513
48	6	-1.259624	4.390195	-2.957883
49	6	-1.866258	5.004621	-0.700371
50	6	-1.686620	5.353919	-2.039352
51	1	-1.119504	4.657436	-4.000765
52	1	-2.187965	5.753723	0.017032
53	1	-1.872543	6.371960	-2.365731
54	6	-1.852999	3.359521	1.209067
55	1	-2.866001	2.977180	1.391292
56	1	-1.150745	2.602874	1.570312
57	1	-1.731412	4.255024	1.826193
58	6	-0.544313	2.038913	-3.558427
59	1	0.425460	1.608437	-3.282105
60	1	-1.247104	1.200943	-3.633598
61	1	-0.444762	2.486122	-4.551540
62	72	0.252442	-0.476268	-0.367634

3cAr (E = -1091.8631072 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-0.762590	-0.015235	-0.269734
2	7	1.419507	0.044909	-0.336362
3	6	-2.892844	-1.365929	0.401532
4	6	-2.237632	-0.975164	1.603998
5	6	-2.041274	-2.275975	-0.292823
6	17	-1.779261	0.345714	-2.461847
7	6	-0.965081	-1.627512	1.641724
8	6	-0.848708	-2.437183	0.469319
9	6	0.939120	1.200533	-0.646176
10	6	-1.034001	1.921574	0.943851
11	6	-0.651854	3.285365	0.380293
12	1	-0.414317	1.715002	1.833238
13	6	1.504319	2.554232	-0.754761
14	6	0.477853	3.592329	-0.297838
15	1	2.471372	2.669971	-0.243306
16	1	1.714002	2.735944	-1.820956
17	6	0.899280	4.988640	-0.722018
18	6	-1.704671	4.340993	0.694654
19	1	-1.515362	5.316404	0.242111
20	1	-1.801291	4.478529	1.781192
21	1	-2.682700	3.994261	0.332974
22	1	0.290049	5.784479	-0.291135
23	1	0.867863	5.092696	-1.817647
24	1	1.940633	5.175900	-0.420127
25	6	-2.853158	-0.194668	2.739152
26	6	-4.287357	-0.976671	-0.027422
27	6	-2.406659	-3.018780	-1.554767
28	6	0.263881	-3.421942	0.190749
29	6	-0.031040	-1.663079	2.830049
30	1	-3.312059	-0.880911	3.464902
31	1	-3.637225	0.484113	2.389504
32	1	-2.112953	0.406333	3.277087
33	1	-5.014365	-1.748163	0.263408
34	1	-4.352856	-0.851735	-1.113204
35	1	-4.605235	-0.035741	0.433384
36	1	-3.045826	-3.881474	-1.319266
37	1	-1.521624	-3.398247	-2.075554
38	1	-2.952660	-2.379029	-2.254828
39	1	0.072136	-4.372374	0.708678
40	1	1.235316	-3.051492	0.532896
41	1	0.350651	-3.646577	-0.877218
42	1	-0.314866	-2.478493	3.511001
43	1	-0.066952	-0.733319	3.407370
44	1	1.007838	-1.835577	2.531698
45	1	-2.054524	1.985046	1.334764
46	6	2.778910	-0.366322	-0.085979
47	6	3.412623	-1.158106	-1.071460
48	6	3.430224	-0.021717	1.119541
49	6	4.719752	-1.604678	-0.826641
50	6	4.736226	-0.499653	1.323507
51	6	5.378948	-1.283138	0.363187
52	1	5.217924	-2.209634	-1.578044
53	1	5.246271	-0.249092	2.248827
54	1	6.387257	-1.642693	0.540784
55	6	2.711557	-1.501608	-2.366558
56	1	1.771226	-2.036610	-2.189360
57	1	2.459090	-0.603348	-2.943385
58	1	3.347561	-2.134266	-2.992030
59	6	2.773193	0.843405	2.173164
60	1	2.790275	1.905390	1.897169
61	1	1.725669	0.574127	2.333791
62	1	3.297397	0.746326	3.128426

TS(3c-5)Ar (E = -1091.833824 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.623358	-0.196862	-0.831712
2	7	-0.679768	1.367480	-0.574910
3	6	3.050016	-1.029223	-0.705013
4	6	2.612645	-0.723269	0.619730
5	6	3.111023	0.189970	-1.446144
6	17	0.403661	-1.396946	-2.960143
7	6	2.391766	0.688216	0.689785
8	6	2.700518	1.250449	-0.588552
9	6	-1.371329	0.181422	-0.487675
10	6	-0.874327	-0.998957	1.002503
11	6	-2.268930	-1.542349	1.201901
12	1	-0.492881	-0.515804	1.909236
13	6	-2.857188	0.024923	-0.528997
14	6	-3.257833	-1.062186	0.432965
15	1	-3.377038	0.962818	-0.281282
16	1	-3.163169	-0.229758	-1.553361
17	6	-4.708908	-1.474858	0.434833
18	6	-2.411147	-2.610031	2.265982
19	1	-3.442839	-2.949421	2.393776
20	1	-2.056500	-2.235986	3.236603
21	1	-1.795277	-3.486855	2.020241
22	1	-4.935747	-2.231884	1.189516
23	1	-4.995812	-1.879679	-0.545948
24	1	-5.357449	-0.607232	0.621577
25	6	2.581462	-1.679732	1.790503
26	6	3.498436	-2.378724	-1.213932
27	6	3.624491	0.319200	-2.859687
28	6	2.759264	2.729757	-0.890629
29	6	2.119567	1.485664	1.943921
30	1	3.544304	-1.666643	2.319911
31	1	2.399716	-2.711348	1.471207
32	1	1.806863	-1.416389	2.518551
33	1	4.593472	-2.462425	-1.168949
34	1	3.194936	-2.538171	-2.253535
35	1	3.083471	-3.198073	-0.617833
36	1	4.723275	0.297746	-2.872841
37	1	3.308353	1.259256	-3.322622
38	1	3.267230	-0.498609	-3.493670
39	1	3.678942	3.167087	-0.476972
40	1	1.912718	3.271326	-0.457021
41	1	2.762778	2.922853	-1.967508
42	1	3.066657	1.813954	2.395817
43	1	1.588830	0.896454	2.698487
44	1	1.527458	2.382384	1.737078
45	1	-0.211234	-1.869368	0.835012
46	6	-1.139155	2.690725	-0.319318
47	6	-1.086696	3.617402	-1.395759
48	6	-1.653280	3.090947	0.941704
49	6	-1.530559	4.931330	-1.185429
50	6	-2.090910	4.416732	1.102624
51	6	-2.030087	5.336671	0.054700
52	1	-1.492914	5.635645	-2.011478
53	1	-2.478930	4.723057	2.070037
54	1	-2.372517	6.356140	0.200815
55	6	-0.595020	3.201443	-2.764703
56	1	0.472227	2.952440	-2.761642
57	1	-1.123519	2.312645	-3.128378
58	1	-0.746695	4.010070	-3.486418
59	6	-1.725084	2.145014	2.120033
60	1	-2.393584	1.296683	1.936171
61	1	-0.741898	1.727692	2.362491

62	1	-2.092371	2.671765	3.006056

5Ar (E = -1091.8869782 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.757970	-0.610198	0.004011
2	7	-0.991067	0.482898	0.179735
3	6	3.261994	-0.520198	-0.192136
4	6	2.971472	-0.395712	1.198131
5	6	2.770047	0.643695	-0.855613
6	17	0.607974	-1.873699	-2.056493
7	6	2.283344	0.839098	1.390368
8	6	2.170122	1.491460	0.125604
9	6	-1.879408	-0.607777	0.232230
10	6	-1.864902	-1.614461	1.153297
11	6	-2.828976	-2.659486	0.778509
12	1	-1.294260	-1.618245	2.070656
13	6	-2.923938	-0.951004	-0.814952
14	6	-3.476776	-2.276567	-0.347464
15	1	-3.700986	-0.180078	-0.891250
16	1	-2.464665	-1.039419	-1.805553
17	6	-4.583655	-2.973730	-1.088021
18	6	-3.015649	-3.908343	1.599905
19	1	-3.811374	-4.545019	1.201989
20	1	-3.268548	-3.662260	2.640140
21	1	-2.090654	-4.499619	1.624247
22	1	-4.873015	-3.910950	-0.602518
23	1	-4.284679	-3.209712	-2.118927
24	1	-5.478751	-2.338934	-1.152807
25	6	3.474035	-1.306331	2.291728
26	6	4.053460	-1.636433	-0.830889
27	6	3.009145	0.981156	-2.308409
28	6	1.720882	2.917695	-0.083251
29	6	1.891840	1.420895	2.728310
30	1	4.472973	-0.985205	2.620680
31	1	3.549983	-2.343125	1.952130
32	1	2.813944	-1.293609	3.163760
33	1	5.130022	-1.419762	-0.781259
34	1	3.787408	-1.768479	-1.883457
35	1	3.886331	-2.593136	-0.325194
36	1	4.031618	1.360407	-2.443808
37	1	2.324014	1.754760	-2.667108
38	1	2.890619	0.105826	-2.954380
39	1	2.552773	3.602657	0.133787
40	1	0.887686	3.189521	0.569856
41	1	1.403659	3.103767	-1.112422
42	1	2.762407	1.883893	3.214179
43	1	1.508398	0.654648	3.411281
44	1	1.124503	2.193183	2.624303
45	1	0.890783	-1.934709	1.258902
46	6	-1.565011	1.792942	0.018940
47	6	-1.577452	2.437085	-1.242594
48	6	-2.125544	2.430949	1.155013
49	6	-2.135717	3.723054	-1.339990
50	6	-2.670275	3.717787	1.014014
51	6	-2.676137	4.365144	-0.223386
52	1	-2.147499	4.217675	-2.306907
53	1	-3.092640	4.208741	1.886095
54	1	-3.101171	5.359367	-0.318196
55	6	-1.018032	1.776410	-2.483238
56	1	0.052228	1.564107	-2.390185
57	1	-1.506798	0.820348	-2.696778
58	1	-1.153201	2.424494	-3.354574

59	6	-2.148705	1.748070	2.503843
60	1	-2.854421	0.907936	2.517308
61	1	-1.168206	1.334568	2.762171
62	1	-2.447369	2.450800	3.287551

6aAr (E = -1494.9484914 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.065109	-0.427335	-0.440348
2	7	1.776150	0.699151	0.113579
3	6	-0.935953	-2.815439	-0.542541
4	6	0.408361	-2.919933	-0.072904
5	6	-0.901064	-2.338928	-1.883060
6	17	-0.697994	1.133776	-2.252058
7	6	1.277072	-2.497898	-1.120923
8	6	0.461907	-2.127450	-2.242129
9	6	2.747996	0.273497	1.029674
10	6	2.623783	-0.613218	2.052480
11	6	3.923549	-0.814553	2.709207
12	1	1.696931	-1.069915	2.370368
13	6	4.199742	0.728656	0.989547
14	6	4.858920	-0.038326	2.111293
15	1	4.654923	0.510833	0.015723
16	1	4.292475	1.812173	1.130882
17	6	6.313373	0.143938	2.451102
18	6	4.088888	-1.736532	3.890638
19	1	5.114610	-1.735683	4.272662
20	1	3.830073	-2.770904	3.624772
21	1	3.422263	-1.441926	4.713070
22	1	6.613176	-0.478303	3.301225
23	1	6.537410	1.189487	2.710047
24	1	6.964003	-0.117718	1.603618
25	6	0.821722	-3.586896	1.215855
26	6	-2.148706	-3.301398	0.212275
27	6	-2.078380	-2.178462	-2.812938
28	6	0.946065	-1.784776	-3.630638
29	6	2.783159	-2.619138	-1.118125
30	1	0.749543	-4.679397	1.112189
31	1	0.182060	-3.287667	2.052254
32	1	1.853727	-3.345364	1.481653
33	1	-2.236636	-4.394114	0.130616
34	1	-3.074333	-2.868035	-0.178248
35	1	-2.083404	-3.054036	1.276860
36	1	-2.176644	-3.060992	-3.460927
37	1	-1.963991	-1.300547	-3.455732
38	1	-3.018246	-2.067860	-2.262794
39	1	0.884816	-2.669553	-4.280122
40	1	1.987656	-1.452076	-3.627254
41	1	0.343328	-0.992544	-4.084992
42	1	3.079875	-3.650411	-1.356017
43	1	3.210335	-2.362690	-0.143924
44	1	3.242455	-1.964489	-1.864328
45	1	-0.356576	-0.697607	1.339291
46	7	-3.231821	0.275163	0.485476
47	6	-2.155145	0.021683	0.116723
48	6	-4.510497	0.580877	0.942562
49	6	-4.829099	0.298170	2.291467
50	6	-5.428949	1.161797	0.037201
51	6	-6.122832	0.614201	2.725285
52	6	-6.708562	1.458095	0.524450
53	6	-7.053276	1.187284	1.852454
54	1	-6.397003	0.409665	3.754757
55	1	-7.435217	1.905389	-0.145283
56	1	-8.049927	1.425278	2.209078

57	6	1.951916	2.080582	-0.307601
58	6	2.574073	2.396225	-1.538080
59	6	1.512843	3.114693	0.558429
60	6	2.746779	3.747174	-1.884270
61	6	1.699809	4.451833	0.173608
62	6	2.313449	4.771710	-1.040119
63	1	3.226647	3.989849	-2.828292
64	1	1.360087	5.243326	0.835811
65	1	2.453739	5.809957	-1.324758
66	6	0.850107	2.799819	1.881507
67	1	0.542612	3.721163	2.385737
68	1	-0.036680	2.168044	1.751026
69	1	1.521738	2.248595	2.550612
70	6	3.027416	1.323530	-2.500765
71	1	3.513448	0.489148	-1.986467
72	1	2.171677	0.915205	-3.051712
73	1	3.730300	1.734061	-3.233082
74	6	-5.040517	1.444598	-1.392584
75	1	-4.151545	2.083013	-1.452672
76	1	-4.800277	0.520926	-1.934083
77	1	-5.856319	1.943136	-1.921810
78	6	-3.810457	-0.316477	3.218684
79	1	-3.484509	-1.301651	2.862713
80	1	-2.909220	0.303459	3.296000
81	1	-4.226599	-0.439142	4.221641

TS(6a-7a)Ar (E = -1494.9388281 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	0.754098	-1.502723	-0.324199
2	6	-2.471607	1.386702	1.103300
3	6	-1.650031	0.657767	2.024598
4	6	-3.346820	0.462721	0.469440
5	17	-1.996485	-0.712740	-2.389476
6	6	-2.006912	-0.720561	1.941033
7	6	-3.058270	-0.838351	0.967543
8	6	1.847808	-1.564883	0.539070
9	6	2.119159	-0.807765	1.640959
10	6	3.392631	-1.223779	2.240390
11	1	1.511930	0.001372	2.020248
12	6	2.991646	-2.556462	0.378317
13	6	3.922954	-2.243452	1.523843
14	1	2.634033	-3.592617	0.410752
15	1	3.485654	-2.444166	-0.594320
16	6	5.203216	-3.004379	1.737175
17	6	3.951001	-0.557875	3.472386
18	1	4.908948	-0.991899	3.775454
19	1	3.256926	-0.650704	4.319432
20	1	4.107176	0.516482	3.302326
21	1	5.750228	-2.640208	2.613543
22	1	5.874065	-2.918769	0.869369
23	1	5.016340	-4.078253	1.886693
24	6	-0.779819	1.277858	3.091994
25	6	-2.548663	2.890918	1.003174
26	6	-4.458480	0.809100	-0.488103
27	6	-3.847298	-2.082956	0.633748
28	6	-1.500291	-1.808761	2.861509
29	1	-1.405143	1.623304	3.927807
30	1	-0.220972	2.142349	2.720210
31	1	-0.060848	0.560658	3.497413
32	1	-3.267457	3.283869	1.736174
33	1	-2.875540	3.215673	0.010917
34	1	-1.582124	3.362824	1.204348
35	1	-5.392891	0.987386	0.063206

36	1	-4.637779	0.003038	-1.204591
37	1	-4.232697	1.713541	-1.061170
38	1	-4.828908	-2.051078	1.126543
39	1	-3.342188	-2.991051	0.974514
40	1	-4.020880	-2.177749	-0.443298
41	1	-1.954255	-1.705936	3.856910
42	1	-0.412462	-1.769662	2.987131
43	1	-1.752407	-2.804233	2.486689
44	1	0.358557	1.123533	0.295964
45	7	0.147872	2.766834	-1.379447
46	6	-0.233751	1.719126	-0.914377
47	6	0.992840	3.876796	-1.411907
48	6	2.127609	4.000233	-0.568087
49	6	0.667855	4.878551	-2.365155
50	6	2.924387	5.146459	-0.700836
51	6	1.490043	6.008217	-2.452281
52	6	2.611516	6.143267	-1.628482
53	1	3.798177	5.251966	-0.065487
54	1	1.250269	6.781519	-3.174880
55	1	3.242216	7.022545	-1.711174
56	6	0.814099	-2.450717	-1.427750
57	6	0.269493	-3.748673	-1.284166
58	6	1.451220	-2.068715	-2.634154
59	6	0.356058	-4.645281	-2.362147
60	6	1.517914	-2.993750	-3.687675
61	6	0.971506	-4.273476	-3.559323
62	1	-0.060995	-5.642438	-2.253187
63	1	2.003820	-2.702305	-4.614355
64	1	1.030058	-4.976849	-4.384061
65	6	2.042292	-0.687979	-2.810747
66	1	2.658475	-0.647712	-3.714341
67	1	1.256450	0.071251	-2.910276
68	1	2.663320	-0.395194	-1.957104
69	6	-0.403484	-4.188287	-0.002646
70	1	0.162912	-3.884249	0.883411
71	1	-1.407779	-3.755837	0.092139
72	1	-0.516222	-5.276795	0.017624
73	6	-0.537024	4.726901	-3.262105
74	1	-0.486924	3.800622	-3.845695
75	1	-1.466772	4.680690	-2.682326
76	1	-0.609606	5.568978	-3.955931
77	6	2.483868	2.942846	0.444666
78	1	1.717021	2.854771	1.223849
79	1	2.578235	1.949155	-0.008532
80	1	3.432340	3.184572	0.932769
81	72	-0.936488	-0.201651	-0.238772

7aAr (E = -1494.9750253 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.452347	-0.396222	0.370918
2	6	-1.453650	2.602241	-1.322676
3	6	-0.108624	2.438434	-1.780905
4	6	-1.407582	3.089912	0.006500
5	17	-1.100723	0.669328	2.408690
6	6	0.771089	2.851036	-0.734342
7	6	-0.033361	3.239669	0.379974
8	6	2.357132	-0.762842	-0.632093
9	6	2.203352	-0.725899	-1.985687
10	6	3.439620	-1.161808	-2.649280
11	1	1.305116	-0.443965	-2.515103
12	6	3.765618	-1.267217	-0.349806
13	6	4.365963	-1.487317	-1.717255
14	1	4.336781	-0.542487	0.242204

15	1	3.753652	-2.190908	0.241037
16	6	5.762547	-2.018056	-1.895342
17	6	3.558230	-1.229932	-4.150673
18	1	4.539949	-1.594200	-4.469087
19	1	3.403490	-0.241092	-4.604447
20	1	2.796981	-1.899596	-4.574917
21	1	6.023258	-2.126577	-2.953645
22	1	5.882529	-3.003898	-1.421873
23	1	6.510539	-1.354556	-1.436708
24	6	0.295115	2.156320	-3.208102
25	6	-2.683348	2.431799	-2.181209
26	6	-2.570849	3.540289	0.854839
27	6	0.415086	3.921088	1.650602
28	6	2.264986	3.022512	-0.885712
29	1	0.203266	3.071180	-3.811373
30	1	-0.337061	1.393036	-3.673970
31	1	1.332679	1.818606	-3.274673
32	1	-2.850884	3.332306	-2.788606
33	1	-3.583701	2.270523	-1.581350
34	1	-2.587765	1.586931	-2.871522
35	1	-2.623409	4.638336	0.869859
36	1	-2.472162	3.196914	1.889374
37	1	-3.524795	3.171415	0.468026
38	1	0.007442	4.940620	1.688886
39	1	1.503624	4.003622	1.705273
40	1	0.065745	3.394151	2.545737
41	1	2.480189	3.863791	-1.558971
42	1	2.741909	2.130625	-1.306889
43	1	2.744711	3.235324	0.072375
44	1	-1.301847	-0.988190	-2.511156
45	7	-1.942696	-0.751334	-0.544895
46	6	-1.150633	-0.530176	-1.531059
47	6	-3.055336	-1.659936	-0.494697
48	6	-2.969131	-2.953750	-1.077896
49	6	-4.227126	-1.249782	0.191467
50	6	-4.072152	-3.814772	-0.945795
51	6	-5.305211	-2.141329	0.276107
52	6	-5.232878	-3.418523	-0.282915
53	1	-4.006615	-4.811194	-1.372221
54	1	-6.205481	-1.824826	0.793393
55	1	-6.071956	-4.101245	-0.196576
56	6	1.792372	-0.930089	1.686113
57	6	2.540971	-0.162629	2.608232
58	6	1.401415	-2.251245	2.015358
59	6	2.874552	-0.723865	3.852300
60	6	1.753980	-2.777847	3.267820
61	6	2.484237	-2.021741	4.187141
62	1	3.447380	-0.130292	4.559031
63	1	1.449321	-3.790242	3.517052
64	1	2.748692	-2.440528	5.153051
65	6	0.607701	-3.097806	1.048913
66	1	0.517651	-4.123591	1.419194
67	1	-0.405404	-2.701481	0.916166
68	1	1.075791	-3.130198	0.058638
69	6	2.977676	1.247364	2.293893
70	1	3.486199	1.313548	1.326738
71	1	2.117924	1.923109	2.253060
72	1	3.658872	1.620815	3.064781
73	6	-4.358423	0.128689	0.792651
74	1	-3.524986	0.362488	1.459973
75	1	-4.381773	0.902116	0.014928
76	1	-5.288925	0.207476	1.362607
77	6	-1.754353	-3.476161	-1.819080

78	1	-1.786122	-3.221174	-2.886507
79	1	-0.813128	-3.088505	-1.421735
80	1	-1.720608	-4.567996	-1.751898
81	72	-0.333281	0.718810	0.067051

TS(7a-8a)Ar (E = -1494.9469832 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.910312	-0.385524	-0.037412
2	7	-2.201974	1.237237	-0.301166
3	6	-2.105179	1.067974	1.039381
4	7	0.784926	1.002897	0.479911
5	6	-1.925590	-2.739876	0.062821
6	6	-2.084777	-2.158626	1.351197
7	6	-0.527805	-2.949820	-0.155267
8	17	-0.882282	-0.645512	-2.524053
9	6	-0.783085	-2.006159	1.930483
10	6	0.171948	-2.525012	1.004723
11	6	0.470747	1.985661	1.316129
12	6	-0.687631	1.999878	2.151420
13	1	-2.951390	1.299310	1.685981
14	6	-0.755102	3.363562	2.751497
15	1	-0.829582	1.170977	2.833925
16	6	1.176532	3.322722	1.418110
17	6	0.280657	4.123114	2.339812
18	1	2.184851	3.207038	1.835983
19	1	1.312667	3.781884	0.432416
20	6	0.608695	5.552468	2.674195
21	6	-1.872208	3.739792	3.687620
22	1	-1.744801	4.743014	4.105073
23	1	-1.933800	3.030028	4.524616
24	1	-2.841730	3.708919	3.171680
25	1	-0.101010	5.978278	3.390315
26	1	0.596384	6.186970	1.775776
27	1	1.615482	5.637219	3.108110
28	6	-3.389876	-1.930392	2.075455
29	6	-3.016010	-3.243273	-0.852589
30	6	0.076991	-3.691018	-1.321131
31	6	1.642474	-2.775477	1.254574
32	6	-0.523054	-1.618941	3.368119
33	1	-3.632911	-2.798604	2.704482
34	1	-4.222378	-1.787856	1.380186
35	1	-3.347825	-1.050831	2.725221
36	1	-3.097503	-4.336701	-0.773407
37	1	-2.808593	-3.002845	-1.900501
38	1	-3.992239	-2.822861	-0.596717
39	1	0.005904	-4.776953	-1.160939
40	1	1.135263	-3.442672	-1.451977
41	1	-0.434097	-3.451868	-2.257586
42	1	1.860407	-3.844642	1.133211
43	1	1.925917	-2.497554	2.272646
44	1	2.298245	-2.231682	0.564771
45	1	-0.540281	-2.509841	4.012533
46	1	-1.288643	-0.933498	3.745298
47	1	0.449819	-1.137122	3.504493
48	6	-3.139684	2.062398	-1.009444
49	6	-4.312389	1.466313	-1.538336
50	6	-2.901659	3.445171	-1.196130
51	6	-5.234454	2.268912	-2.227680
52	6	-3.850052	4.211819	-1.893236
53	6	-5.013335	3.635974	-2.404838
54	1	-6.131259	1.807049	-2.630445
55	1	-3.659716	5.271689	-2.037523
56	1	-5.734714	4.242736	-2.943075

57	6	2.121325	1.013612	-0.097024
58	6	2.348129	1.437262	-1.429159
59	6	3.202881	0.573240	0.712377
60	6	3.648848	1.327964	-1.953882
61	6	4.483000	0.483701	0.144990
62	6	4.707104	0.843152	-1.185934
63	1	3.822299	1.639033	-2.979712
64	1	5.306786	0.133176	0.759808
65	1	5.700237	0.758549	-1.615237
66	6	-4.578577	-0.011702	-1.385393
67	1	-3.787799	-0.603513	-1.858247
68	1	-4.625319	-0.309346	-0.331142
69	1	-5.531090	-0.281396	-1.852063
70	6	-1.650275	4.108027	-0.676586
71	1	-1.659974	4.207830	0.414232
72	1	-0.761594	3.526572	-0.934706
73	1	-1.540366	5.109929	-1.104144
74	6	3.031071	0.262140	2.183321
75	1	3.095010	1.175828	2.790747
76	1	2.064647	-0.194241	2.398737
77	1	3.819163	-0.412576	2.530860
78	6	1.284648	2.088864	-2.284442
79	1	0.275240	1.772760	-2.028590
80	1	1.333817	3.182483	-2.182696
81	1	1.441664	1.854608	-3.341568

8aAr (E = -1494.9757154 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.180576	-0.935668	0.145814
2	7	1.684956	-0.191017	0.053299
3	6	1.179728	0.063375	-1.283727
4	7	-1.184689	1.194943	-0.192716
5	6	-1.339923	-2.282138	-1.722144
6	6	-2.277846	-2.299054	-0.647229
7	6	-0.183299	-3.012593	-1.308309
8	17	-0.041988	-1.104513	2.632555
9	6	-1.690341	-3.011962	0.436854
10	6	-0.396490	-3.458570	0.028037
11	6	-0.411111	1.985547	-0.858592
12	6	0.758584	1.483271	-1.655191
13	1	1.696805	-0.436117	-2.106284
14	6	1.667856	2.717264	-1.687942
15	1	0.352417	1.375755	-2.680598
16	6	-0.433279	3.491773	-0.905901
17	6	1.001049	3.816798	-1.298425
18	1	-1.149548	3.853864	-1.657834
19	1	-0.746913	3.928453	0.047638
20	6	1.471556	5.245084	-1.250160
21	6	3.072392	2.610252	-2.209128
22	1	3.588264	3.574897	-2.212867
23	1	3.073219	2.219839	-3.237281
24	1	3.657355	1.909941	-1.601680
25	1	2.517701	5.343887	-1.553212
26	1	1.374422	5.655959	-0.235249
27	1	0.865948	5.882237	-1.910823
28	6	-3.710678	-1.817025	-0.674888
29	6	-1.572313	-1.824210	-3.142812
30	6	0.920410	-3.442297	-2.243328
31	6	0.509249	-4.362177	0.832549
32	6	-2.394148	-3.394773	1.715335
33	1	-4.395530	-2.676027	-0.657915
34	1	-3.928020	-1.243416	-1.579022
35	1	-3.962381	-1.186533	0.185354

36	1	-1.679177	-2.693087	-3.808298
37	1	-0.736496	-1.224761	-3.521082
38	1	-2.484900	-1.230016	-3.239111
39	1	0.529679	-4.172797	-2.966499
40	1	1.743751	-3.921653	-1.708069
41	1	1.332078	-2.604082	-2.814982
42	1	0.205039	-5.412369	0.717837
43	1	0.472784	-4.119027	1.898759
44	1	1.553009	-4.283827	0.512235
45	1	-2.892894	-4.368120	1.598761
46	1	-3.159574	-2.662099	1.992020
47	1	-1.695857	-3.469949	2.553122
48	6	3.019845	0.070193	0.486699
49	6	4.113810	-0.667998	-0.042687
50	6	3.269543	1.074418	1.461009
51	6	5.419646	-0.373161	0.381493
52	6	4.590715	1.337601	1.858063
53	6	5.666925	0.627839	1.322078
54	1	6.245337	-0.949279	-0.027716
55	1	4.768368	2.112220	2.599079
56	1	6.681777	0.844029	1.641417
57	6	-2.443636	1.741382	0.306327
58	6	-3.514761	1.841725	-0.616616
59	6	-2.601720	2.149636	1.651347
60	6	-4.764010	2.284426	-0.153718
61	6	-3.870399	2.591972	2.065486
62	6	-4.948969	2.646459	1.181611
63	1	-5.590535	2.348348	-0.854971
64	1	-3.999013	2.904252	3.097061
65	1	-5.921154	2.982558	1.527046
66	6	3.899608	-1.791153	-1.027400
67	1	3.080123	-2.438697	-0.702779
68	1	3.636278	-1.423770	-2.027574
69	1	4.805056	-2.398711	-1.124684
70	6	2.145914	1.877045	2.070208
71	1	1.610172	2.452872	1.306302
72	1	1.417230	1.226896	2.561310
73	1	2.536309	2.582788	2.811232
74	6	-3.339815	1.535485	-2.088311
75	1	-4.305656	1.316981	-2.553485
76	1	-2.910561	2.392789	-2.625683
77	1	-2.674337	0.687792	-2.259450
78	6	-1.454018	2.184708	2.630876
79	1	-1.786681	2.599661	3.586620
80	1	-1.039862	1.190850	2.820601
81	1	-0.631090	2.809918	2.265848

8a'Ar (E = -1494.9624281 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.870395	-0.485253	-0.015674
2	7	-0.523510	1.513317	-0.126135
3	6	-0.182218	1.183915	1.247231
4	7	1.480932	-0.755731	0.009862
5	6	-3.092988	-0.775214	1.170129
6	6	-2.100489	-1.167130	2.116304
7	6	-3.093775	-1.740533	0.113790
8	17	-0.829432	-1.013457	-2.452820
9	6	-1.506524	-2.381629	1.659842
10	6	-2.117702	-2.734499	0.420158
11	6	2.041252	0.034175	0.859554
12	6	1.225035	0.839814	1.824766
13	1	-0.808014	1.664251	2.002578
14	6	2.258316	1.785977	2.439978

15	1	0.956029	0.156237	2.650477
16	6	3.504165	0.365555	1.015406
17	6	3.500339	1.500161	2.021459
18	1	4.057483	-0.513329	1.376492
19	1	3.968235	0.629834	0.058792
20	6	4.805325	2.127348	2.432815
21	6	1.831130	2.765135	3.498428
22	1	2.642357	3.433996	3.800453
23	1	1.483094	2.230745	4.394982
24	1	0.990008	3.380171	3.154932
25	1	4.664262	2.938535	3.152876
26	1	5.334768	2.537862	1.561189
27	1	5.474406	1.383879	2.889492
28	6	-1.927577	-0.583620	3.496338
29	6	-4.119025	0.308245	1.421936
30	6	-4.061941	-1.810915	-1.043646
31	6	-1.876314	-3.983823	-0.393359
32	6	-0.608266	-3.245375	2.517624
33	1	-2.573868	-1.109438	4.215398
34	1	-2.196046	0.476214	3.524349
35	1	-0.897479	-0.676711	3.857040
36	1	-4.761739	0.023387	2.266800
37	1	-4.770598	0.459312	0.557152
38	1	-3.662544	1.273181	1.671772
39	1	-4.882683	-2.504715	-0.812135
40	1	-3.571495	-2.162617	-1.956282
41	1	-4.506136	-0.835705	-1.264542
42	1	-2.693588	-4.704326	-0.248163
43	1	-0.944344	-4.482593	-0.108795
44	1	-1.817331	-3.760413	-1.463908
45	1	-1.148433	-3.551629	3.424252
46	1	0.302087	-2.729705	2.844297
47	1	-0.308229	-4.158419	1.997505
48	6	-0.762044	2.787351	-0.715655
49	6	-1.971183	2.999924	-1.447422
50	6	0.177553	3.856343	-0.649359
51	6	-2.238297	4.259357	-2.005375
52	6	-0.131536	5.098248	-1.226685
53	6	-1.337276	5.317716	-1.890664
54	1	-3.172060	4.400146	-2.542835
55	1	0.604969	5.895190	-1.163912
56	1	-1.561169	6.285553	-2.328011
57	6	2.337320	-1.439656	-0.952335
58	6	2.724735	-0.775171	-2.139246
59	6	2.763447	-2.757527	-0.677910
60	6	3.532033	-1.472796	-3.053520
61	6	3.575184	-3.411746	-1.617770
62	6	3.955275	-2.778864	-2.802755
63	1	3.824261	-0.975613	-3.973364
64	1	3.904426	-4.425524	-1.411093
65	1	4.575591	-3.299605	-3.525018
66	6	2.364057	-3.469706	0.591732
67	1	2.608266	-2.889787	1.489824
68	1	1.286453	-3.656937	0.616502
69	1	2.872896	-4.434834	0.667744
70	6	2.331991	0.652882	-2.443116
71	1	1.310545	0.876981	-2.131805
72	1	2.997060	1.368159	-1.938918
73	1	2.408948	0.845128	-3.517097
74	6	-2.983840	1.902421	-1.662679
75	1	-2.607156	1.128862	-2.341137
76	1	-3.249328	1.410242	-0.723049
77	1	-3.903081	2.308870	-2.097389

78	6	1.538979	3.690146	-0.025272
79	1	1.506434	3.742315	1.065327
80	1	1.984081	2.727540	-0.286123
81	1	2.214632	4.480133	-0.370580

TS(8a'-9)Ar (E = -1494.9371235 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.579812	-0.348510	-0.497276
2	7	-0.025151	-0.834199	1.456727
3	6	-0.263889	0.538044	1.469863
4	7	-1.830715	-0.589883	-0.810024
5	6	3.009125	0.033801	0.216027
6	6	2.404283	1.319940	0.060501
7	6	3.083407	-0.570630	-1.069505
8	17	0.475692	-2.392436	-1.909909
9	6	2.097197	1.503778	-1.328975
10	6	2.507841	0.328146	-2.019392
11	6	-2.208070	0.398262	-0.091429
12	6	-1.102319	1.219434	0.463230
13	1	0.207688	1.160875	2.220177
14	6	-1.784339	2.524568	0.832291
15	1	-0.434453	1.414559	-0.616408
16	6	-3.534819	1.036472	0.198533
17	6	-3.120888	2.406724	0.704888
18	1	-4.165218	1.074218	-0.697065
19	1	-4.106374	0.478107	0.952280
20	6	-4.184990	3.417246	1.036946
21	6	-1.019509	3.721239	1.323501
22	1	-1.688715	4.536920	1.609033
23	1	-0.342600	4.102247	0.548047
24	1	-0.404958	3.472619	2.197392
25	1	-3.770046	4.363860	1.392887
26	1	-4.859112	3.030973	1.814405
27	1	-4.805941	3.630945	0.155905
28	6	2.469058	2.414459	1.098918
29	6	3.649270	-0.457291	1.493283
30	6	3.794020	-1.853691	-1.420913
31	6	2.474780	0.117537	-3.514407
32	6	1.677797	2.801615	-1.982038
33	1	3.452351	2.906687	1.056487
34	1	2.344094	2.026024	2.114354
35	1	1.713488	3.186373	0.937542
36	1	4.556091	0.123929	1.713533
37	1	3.944599	-1.507510	1.421451
38	1	2.978972	-0.362518	2.354189
39	1	4.787922	-1.628140	-1.832806
40	1	3.239830	-2.429551	-2.167206
41	1	3.936569	-2.495951	-0.547017
42	1	3.430260	0.418268	-3.968040
43	1	1.686374	0.710530	-3.990914
44	1	2.299094	-0.932362	-3.766749
45	1	2.563542	3.380016	-2.283309
46	1	1.090327	3.429060	-1.305081
47	1	1.075989	2.631903	-2.880768
48	6	0.079082	-1.566743	2.661928
49	6	0.813121	-2.792881	2.657684
50	6	-0.555842	-1.154032	3.878683
51	6	1.005365	-3.494200	3.855031
52	6	-0.332481	-1.900097	5.048537
53	6	0.460651	-3.046958	5.059407
54	1	1.582759	-4.414084	3.828774
55	1	-0.819012	-1.575815	5.964668
56	1	0.620814	-3.599570	5.979496

57	6	-2.786552	-1.457457	-1.444620
58	6	-3.414573	-2.481298	-0.701799
59	6	-3.044749	-1.277776	-2.821943
60	6	-4.324151	-3.319245	-1.368119
61	6	-3.966249	-2.133413	-3.444013
62	6	-4.604003	-3.148272	-2.725854
63	1	-4.807624	-4.115579	-0.810149
64	1	-4.174372	-2.002055	-4.501619
65	1	-5.308374	-3.807183	-3.223463
66	6	-2.341042	-0.200644	-3.615217
67	1	-2.502702	0.798627	-3.191339
68	1	-1.258326	-0.374669	-3.630714
69	1	-2.697270	-0.188774	-4.649427
70	6	-3.117912	-2.694704	0.765803
71	1	-2.043085	-2.674956	0.967155
72	1	-3.572325	-1.917490	1.395348
73	1	-3.516135	-3.657249	1.099557
74	6	1.354631	-3.382348	1.381613
75	1	0.554158	-3.625811	0.674848
76	1	2.022522	-2.694421	0.854303
77	1	1.911005	-4.301711	1.590499
78	6	-1.551077	-0.007285	3.989711
79	1	-1.076447	0.976211	4.081399
80	1	-2.222594	0.040917	3.128450
81	1	-2.165876	-0.153662	4.884632

9Ar (E = -1494.9718699 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.268512	-0.865473	0.106901
2	7	-0.957817	1.218975	-0.213774
3	6	-0.577760	1.623261	1.030127
4	7	1.772315	0.320415	-0.274482
5	6	-2.796325	-1.461595	0.333371
6	6	-2.301280	-1.178103	1.643803
7	6	-2.154598	-2.642601	-0.127606
8	17	0.663006	-2.236347	-1.713671
9	6	-1.373365	-2.199489	1.998856
10	6	-1.260696	-3.088457	0.894162
11	6	1.852902	1.098232	0.753645
12	6	0.692158	1.435055	1.551004
13	1	-1.296384	2.105939	1.677318
14	6	1.191408	1.956661	2.840985
15	1	0.800177	-1.238020	1.513376
16	6	3.070824	1.689481	1.428224
17	6	2.532194	2.118506	2.779098
18	1	3.887195	0.964014	1.494392
19	1	3.463254	2.543420	0.859603
20	6	3.465588	2.672203	3.817965
21	6	0.275770	2.297960	3.985784
22	1	0.831547	2.660066	4.854729
23	1	-0.303634	1.419747	4.298038
24	1	-0.444506	3.078345	3.705109
25	1	2.948391	2.933624	4.745561
26	1	3.973370	3.575346	3.449838
27	1	4.252568	1.945364	4.064378
28	6	-2.895550	-0.164723	2.594191
29	6	-2.496858	-3.414887	-1.377234
30	6	-0.454716	-4.364078	0.865164
31	6	-0.778222	-2.404635	3.369554
32	1	-3.753871	-0.602374	3.124739
33	1	-3.260193	0.724833	2.070802
34	1	-2.175716	0.158731	3.352255
35	1	-3.168857	-4.248872	-1.129605

36	1	-1.603513	-3.830281	-1.852115
37	1	-3.007627	-2.791036	-2.117362
38	1	-1.041767	-5.202965	1.266411
39	1	0.455500	-4.279286	1.468413
40	1	-0.152606	-4.621607	-0.153815
41	1	-1.482904	-2.955553	4.009722
42	1	-0.552428	-1.453304	3.861067
43	1	0.152239	-2.976902	3.321295
44	6	2.939627	0.162036	-1.110237
45	6	3.872596	-0.870326	-0.862755
46	6	3.115847	1.069830	-2.180412
47	6	4.983330	-0.979023	-1.716097
48	6	4.235090	0.915622	-3.013723
49	6	5.165183	-0.101341	-2.787068
50	1	5.706604	-1.768199	-1.533142
51	1	4.371778	1.603406	-3.843035
52	1	6.025867	-0.208824	-3.439602
53	6	-1.934870	1.934103	-0.963774
54	6	-2.531454	3.180819	-0.577431
55	6	-2.263708	1.402585	-2.249945
56	6	-3.510594	3.749676	-1.413434
57	6	-3.237195	2.018664	-3.044297
58	6	-3.890933	3.176435	-2.623913
59	1	-3.962990	4.686820	-1.102040
60	1	-3.468002	1.584433	-4.012570
61	1	-4.648800	3.644039	-3.243445
62	6	2.140285	2.200887	-2.424224
63	1	2.223629	2.981928	-1.655802
64	1	2.333069	2.671235	-3.392870
65	1	1.102534	1.856381	-2.406076
66	6	-1.550946	0.198348	-2.809334
67	1	-1.798354	-0.729274	-2.282581
68	1	-1.824117	0.042824	-3.857561
69	1	-0.462741	0.310818	-2.768991
70	6	3.704462	-1.852003	0.274678
71	1	3.489920	-1.357723	1.228296
72	1	2.867703	-2.531790	0.082274
73	1	4.611951	-2.451283	0.396948
74	6	-3.996125	-0.796391	-0.297130
75	1	-4.918253	-1.240544	0.105540
76	1	-4.030688	0.276765	-0.093801
77	1	-4.020039	-0.925705	-1.382387
78	6	-2.158116	4.020327	0.637801
79	1	-2.598232	3.656032	1.574995
80	1	-1.074765	4.087890	0.783073
81	1	-2.529736	5.039575	0.493209

TS(9-9')Ar (E = -1494.9719189 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.100298	-0.937394	-0.204101
2	7	-1.070383	0.909890	0.177557
3	6	-0.760885	0.949056	1.503130
4	7	1.804781	0.725249	-0.019875
5	6	-2.209249	-2.131115	-0.386660
6	6	-1.791103	-2.206790	0.978085
7	6	-1.305452	-2.906725	-1.161741
8	17	1.295549	-1.340520	-2.318466
9	6	-0.643762	-3.048510	1.045028
10	6	-0.325690	-3.457646	-0.280268
11	6	1.721574	1.105361	1.212654
12	6	0.529514	0.891305	2.003916
13	1	-1.552153	1.012839	2.235190
14	6	0.917788	1.047195	3.421699

15	1	1.243868	-1.523617	1.062808
16	6	2.786516	1.683205	2.118456
17	6	2.186586	1.507276	3.499499
18	1	3.744759	1.170624	1.990421
19	1	2.971007	2.741513	1.889447
20	6	2.986640	1.871277	4.717860
21	6	-0.035077	0.781123	4.556263
22	1	0.446170	0.914575	5.528760
23	1	-0.422696	-0.244544	4.509646
24	1	-0.900692	1.456630	4.520647
25	1	2.439870	1.683870	5.646409
26	1	3.266857	2.934420	4.701493
27	1	3.923778	1.298062	4.756718
28	6	-2.601825	-1.732923	2.161891
29	6	-1.460520	-3.261158	-2.619391
30	6	0.766565	-4.424574	-0.667443
31	6	-0.010214	-3.567839	2.311544
32	1	-3.328908	-2.503894	2.456030
33	1	-3.169303	-0.825345	1.932953
34	1	-1.973505	-1.528979	3.034480
35	1	-1.945470	-4.243013	-2.716384
36	1	-0.493569	-3.309605	-3.127672
37	1	-2.080492	-2.534764	-3.154174
38	1	0.403323	-5.461320	-0.617475
39	1	1.630221	-4.344331	0.001327
40	1	1.119508	-4.240445	-1.686068
41	1	-0.559559	-4.448398	2.675864
42	1	-0.016360	-2.816741	3.107359
43	1	1.029849	-3.862740	2.148023
44	6	2.966588	1.125512	-0.779893
45	6	4.113175	0.301112	-0.838568
46	6	2.920042	2.366632	-1.456874
47	6	5.209417	0.742387	-1.598378
48	6	4.035113	2.761216	-2.213051
49	6	5.174507	1.956889	-2.286850
50	1	6.095645	0.116623	-1.647735
51	1	4.002431	3.708749	-2.742756
52	1	6.029491	2.274649	-2.875200
53	6	-2.211669	1.583823	-0.348252
54	6	-3.119308	2.405667	0.401071
55	6	-2.399713	1.495489	-1.763371
56	6	-4.216091	2.983866	-0.265394
57	6	-3.503902	2.101951	-2.372974
58	6	-4.435466	2.826588	-1.631146
59	1	-4.901073	3.593063	0.317162
60	1	-3.618101	2.009714	-3.448976
61	1	-5.291571	3.288968	-2.110819
62	6	1.711954	3.273266	-1.361207
63	1	1.623663	3.728850	-0.365183
64	1	1.784617	4.086531	-2.089197
65	1	0.778845	2.731483	-1.538993
66	6	-1.408822	0.783945	-2.648077
67	1	-1.422173	-0.303463	-2.516810
68	1	-1.632201	0.970955	-3.702942
69	1	-0.382076	1.117390	-2.468446
70	6	4.188622	-1.027241	-0.120480
71	1	3.859049	-0.960227	0.921729
72	1	3.543020	-1.768669	-0.603209
73	1	5.214715	-1.407639	-0.131535
74	6	-3.536824	-1.585397	-0.855155
75	1	-4.318540	-2.346209	-0.714202
76	1	-3.839245	-0.694473	-0.299537
77	1	-3.526612	-1.322854	-1.916401

78	6	-2.992167	2.785857	1.870516
79	1	-3.275504	1.978778	2.558454
80	1	-1.979068	3.108972	2.133546
81	1	-3.663166	3.624514	2.080145

9'Ar (E = -1494.9854885 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.305650	-0.744127	-0.222963
2	7	1.032638	1.290030	0.218153
3	6	0.329203	2.364105	-0.228872
4	7	-1.810867	0.251133	0.096379
5	6	2.117913	-1.386246	-1.947194
6	6	1.132230	-2.420151	-1.971288
7	6	2.799050	-1.457208	-0.697406
8	17	-0.567331	-2.029290	1.731046
9	6	1.175131	-3.097350	-0.726872
10	6	2.192535	-2.485337	0.074825
11	6	-2.013339	1.479867	-0.302242
12	6	-1.000437	2.453128	-0.573726
13	1	0.883760	3.297921	-0.266761
14	6	-1.667216	3.686843	-1.044356
15	1	-0.500596	-0.568679	-1.832306
16	6	-3.360306	2.143709	-0.535029
17	6	-3.006725	3.522469	-1.039149
18	1	-3.959337	1.566716	-1.249348
19	1	-3.951798	2.180760	0.387291
20	6	-4.086923	4.490341	-1.433803
21	6	-0.893609	4.916169	-1.441313
22	1	-1.551743	5.701555	-1.822910
23	1	-0.156575	4.683496	-2.221742
24	1	-0.341140	5.333514	-0.587827
25	1	-3.680315	5.439303	-1.796406
26	1	-4.749090	4.713136	-0.584483
27	1	-4.721871	4.071759	-2.228010
28	6	0.346006	-2.838756	-3.188829
29	6	2.486496	-0.552868	-3.151127
30	6	4.118669	-0.809567	-0.356872
31	6	2.704026	-3.011541	1.392816
32	6	0.437347	-4.371130	-0.392021
33	1	0.933904	-3.545522	-3.793032
34	1	0.096007	-1.980611	-3.818892
35	1	-0.589975	-3.338760	-2.920609
36	1	2.839355	-1.198957	-3.966988
37	1	3.287242	0.154564	-2.924040
38	1	1.630465	0.015775	-3.535307
39	1	4.925418	-1.538742	-0.521654
40	1	4.177190	-0.484798	0.685091
41	1	4.325856	0.058531	-0.983923
42	1	3.396473	-3.850011	1.228379
43	1	1.885396	-3.368439	2.024074
44	1	3.246621	-2.241857	1.951646
45	1	1.027706	-5.241155	-0.714398
46	1	-0.533536	-4.428475	-0.895656
47	1	0.256480	-4.460534	0.681397
48	6	2.307734	1.670684	0.803116
49	6	3.292648	2.346385	0.036015
50	6	2.531303	1.409519	2.179469
51	6	4.499083	2.714728	0.655480
52	6	3.756714	1.788159	2.752401
53	6	4.740423	2.433698	2.000419
54	1	5.257270	3.219302	0.063074
55	1	3.924236	1.588584	3.806600
56	1	5.680002	2.722510	2.460413

57	6	-3.009133	-0.451301	0.532641
58	6	-3.726812	-1.277717	-0.360238
59	6	-3.455695	-0.256359	1.861690
60	6	-4.882105	-1.927195	0.110147
61	6	-4.612985	-0.924439	2.288500
62	6	-5.323060	-1.761173	1.423741
63	1	-5.437905	-2.563607	-0.572329
64	1	-4.952343	-0.785427	3.310680
65	1	-6.214988	-2.274132	1.769399
66	6	3.113102	2.683791	-1.431259
67	1	4.071075	2.611266	-1.957752
68	1	2.399455	2.022441	-1.924757
69	1	2.752221	3.711966	-1.570753
70	6	1.473573	0.779656	3.057321
71	1	1.344839	-0.292720	2.869269
72	1	1.739771	0.896123	4.112403
73	1	0.495349	1.244436	2.897846
74	6	-3.309915	-1.469164	-1.801943
75	1	-3.116353	-0.516599	-2.306938
76	1	-2.385364	-2.049259	-1.889716
77	1	-4.092737	-1.997423	-2.355034
78	6	-2.708264	0.641109	2.821173
79	1	-1.678729	0.293620	2.951603
80	1	-2.659732	1.679370	2.468654
81	1	-3.196512	0.644836	3.800264

TS(9'-10)Ar (E = -1494.9737012 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.873936	0.015875	-0.122601
2	7	0.510870	1.389660	0.969460
3	6	1.467010	0.850059	1.727564
4	7	0.899279	-1.353916	-0.361955
5	6	-3.275554	0.004684	0.843193
6	6	-3.092787	-1.290687	0.264951
7	6	-3.254914	0.962677	-0.206330
8	17	-0.149441	1.249038	-2.224815
9	6	-2.962223	-1.131215	-1.141160
10	6	-3.055781	0.262699	-1.435510
11	6	1.773062	-1.405737	0.637735
12	6	1.971689	-0.448864	1.670025
13	1	1.951557	1.521042	2.437872
14	6	3.042196	-0.951549	2.561742
15	1	-0.781286	-0.751330	1.554168
16	6	2.786126	-2.517169	0.843253
17	6	3.514472	-2.130337	2.106128
18	1	2.279683	-3.484887	0.928679
19	1	3.461203	-2.605678	-0.016479
20	6	4.600148	-3.006733	2.666001
21	6	3.494823	-0.190933	3.780504
22	1	4.235170	-0.754837	4.354636
23	1	2.647949	0.029113	4.444308
24	1	3.950709	0.771078	3.508059
25	1	5.018858	-2.602597	3.592735
26	1	5.426662	-3.122067	1.949677
27	1	4.224333	-4.017448	2.881318
28	6	-3.265247	-2.574023	1.038727
29	6	-3.682280	0.219861	2.279787
30	6	-3.540265	2.442822	-0.092144
31	6	-3.236499	0.844104	-2.813977
32	6	-2.907134	-2.221859	-2.186334
33	1	-4.292734	-2.639363	1.424063
34	1	-2.586863	-2.626078	1.897317
35	1	-3.093977	-3.454008	0.414718

36	1	-4.669766	-0.231384	2.453709
37	1	-3.760426	1.280722	2.528051
38	1	-2.979684	-0.245993	2.979138
39	1	-4.591475	2.648729	-0.339106
40	1	-2.921932	3.030236	-0.779012
41	1	-3.358840	2.817190	0.918999
42	1	-4.296355	0.781538	-3.102994
43	1	-2.648246	0.307791	-3.563272
44	1	-2.933468	1.892922	-2.856246
45	1	-3.879122	-2.309376	-2.691908
46	1	-2.674959	-3.194722	-1.746656
47	1	-2.156963	-2.018565	-2.958324
48	6	0.423356	2.838824	1.059787
49	6	-0.465587	3.427922	1.989469
50	6	1.265981	3.648222	0.256328
51	6	-0.592600	4.827886	2.013252
52	6	1.108887	5.042472	0.315585
53	6	0.171474	5.632469	1.167685
54	1	-1.286693	5.280673	2.715703
55	1	1.739927	5.666202	-0.310356
56	1	0.057663	6.711734	1.189860
57	6	1.104140	-2.298589	-1.450730
58	6	0.467898	-3.561167	-1.430427
59	6	1.974708	-1.944982	-2.514370
60	6	0.633783	-4.420296	-2.531736
61	6	2.113345	-2.834943	-3.590488
62	6	1.435440	-4.057408	-3.613611
63	1	0.135001	-5.385432	-2.523772
64	1	2.768411	-2.562925	-4.412575
65	1	1.548574	-4.727927	-4.459584
66	6	-1.194783	2.602373	3.025533
67	1	-2.134087	3.080663	3.321768
68	1	-1.405552	1.589416	2.682347
69	1	-0.583548	2.503028	3.934287
70	6	2.356118	3.056072	-0.607242
71	1	1.949911	2.343701	-1.328122
72	1	2.878626	3.846363	-1.154698
73	1	3.099853	2.521683	-0.001716
74	6	-0.306231	-4.056167	-0.228771
75	1	0.321957	-4.712462	0.390086
76	1	-0.647468	-3.242881	0.412686
77	1	-1.173047	-4.650617	-0.535316
78	6	2.786981	-0.671013	-2.488624
79	1	2.144086	0.209550	-2.422442
80	1	3.466380	-0.643483	-1.626421
81	1	3.395915	-0.590307	-3.394003

10Ar (E = -1494.9775824 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.262641	-0.761352	-0.202933
2	7	1.643355	1.100829	-0.139811
3	6	1.208248	2.265112	-0.569952
4	7	-1.387687	0.689211	0.089883
5	6	0.541305	-2.830265	-1.695344
6	6	-0.861733	-2.559883	-1.708786
7	6	0.900685	-3.231755	-0.383158
8	17	1.458083	-1.047928	1.998565
9	6	-1.373113	-2.830219	-0.406214
10	6	-0.283553	-3.213719	0.422110
11	6	-1.278039	1.955776	-0.370008
12	6	-0.125915	2.642488	-0.791696
13	1	1.952072	3.051368	-0.702095
14	6	-0.513367	4.011980	-1.209381

15	1	0.690388	-0.316088	-1.915358
16	6	-2.434146	2.941384	-0.437923
17	6	-1.832461	4.199060	-1.007996
18	1	-3.257642	2.567746	-1.049051
19	1	-2.852245	3.099364	0.564860
20	6	-2.680695	5.415305	-1.258383
21	6	0.484183	5.001790	-1.752205
22	1	-0.006071	5.920459	-2.086543
23	1	1.033598	4.582235	-2.605586
24	1	1.229028	5.282642	-0.994701
25	1	-2.101671	6.237046	-1.691011
26	1	-3.133739	5.783154	-0.326199
27	1	-3.508764	5.191485	-1.946386
28	6	-1.637510	-2.290976	-2.975463
29	6	1.412149	-2.886844	-2.926124
30	6	2.247441	-3.763587	0.046628
31	6	-0.411431	-3.781641	1.812953
32	6	-2.819838	-2.997643	-0.009975
33	1	-1.490571	-3.114957	-3.687296
34	1	-1.308861	-1.370258	-3.472905
35	1	-2.709411	-2.208959	-2.785806
36	1	1.251541	-3.837730	-3.455392
37	1	2.476340	-2.827585	-2.679591
38	1	1.182561	-2.072299	-3.619310
39	1	2.270446	-4.858331	-0.052804
40	1	2.463751	-3.512590	1.088184
41	1	3.060840	-3.362295	-0.567237
42	1	-0.596860	-4.864879	1.762719
43	1	-1.243947	-3.329144	2.361827
44	1	0.496927	-3.617897	2.397099
45	1	-3.046543	-4.070138	0.076150
46	1	-3.500168	-2.576153	-0.751024
47	1	-3.052338	-2.536021	0.953795
48	6	3.039460	1.125142	0.271028
49	6	4.039346	0.600970	-0.578666
50	6	3.381090	1.719699	1.510712
51	6	5.375507	0.624749	-0.142597
52	6	4.728401	1.725431	1.904644
53	6	5.721828	1.172534	1.093212
54	1	6.145182	0.217657	-0.791974
55	1	4.992331	2.165643	2.861655
56	1	6.757759	1.177991	1.417385
57	6	-2.673034	0.373809	0.702258
58	6	-3.819103	0.108545	-0.084877
59	6	-2.761452	0.388768	2.119272
60	6	-5.032421	-0.182312	0.564143
61	6	-3.990383	0.079145	2.723409
62	6	-5.121607	-0.210340	1.955538
63	1	-5.910721	-0.393265	-0.039732
64	1	-4.057123	0.084800	3.807112
65	1	-6.064807	-0.444054	2.438874
66	6	3.721762	0.087205	-1.964415
67	1	2.858591	-0.581138	-1.975477
68	1	3.468418	0.912022	-2.645025
69	1	4.582545	-0.440544	-2.386566
70	6	2.336144	2.342681	2.409605
71	1	1.515056	1.644801	2.594133
72	1	2.778030	2.618752	3.371771
73	1	1.903577	3.251441	1.971252
74	6	-3.810230	0.139647	-1.598792
75	1	-4.366283	1.006802	-1.979142
76	1	-2.800527	0.185385	-2.008517
77	1	-4.306736	-0.746743	-2.008242

78	6	-1.585733	0.780376	2.985768
79	1	-0.761287	0.062599	2.926159
80	1	-1.175710	1.752526	2.686327
81	1	-1.894939	0.852563	4.032738

TS(10-11)Ar (E = -1494.9511358 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-1.401988	-0.400107	-0.396594
2	7	-0.281599	0.836037	0.800932
3	6	0.276360	-0.075259	1.732725
4	7	0.440598	-1.711960	-0.705076
5	6	-3.746723	-0.535009	0.585060
6	6	-3.469543	-1.873452	0.155192
7	6	-3.857349	0.283563	-0.575771
8	17	-0.885085	1.022372	-2.401229
9	6	-3.402213	-1.876699	-1.265636
10	6	-3.633907	-0.544218	-1.716655
11	6	1.398252	-1.675423	0.216468
12	6	1.316890	-0.956398	1.432156
13	1	0.132647	0.180356	2.785660
14	6	2.352797	-1.475420	2.343405
15	1	-1.073997	-1.305737	1.257967
16	6	2.631946	-2.553432	0.274934
17	6	3.138484	-2.360067	1.687150
18	1	2.400105	-3.597690	0.048082
19	1	3.373490	-2.239912	-0.472143
20	6	4.380640	-3.061914	2.160164
21	6	2.489782	-0.987944	3.761454
22	1	3.355755	-1.431212	4.260949
23	1	1.599397	-1.238355	4.354098
24	1	2.600700	0.104313	3.792234
25	1	4.632918	-2.800707	3.192383
26	1	5.244825	-2.806751	1.529610
27	1	4.264692	-4.154208	2.110752
28	6	-3.539607	-3.074061	1.067465
29	6	-4.127359	-0.186436	2.004920
30	6	-4.269811	1.736114	-0.639304
31	6	-3.847841	-0.135008	-3.151448
32	6	-3.292088	-3.082788	-2.168879
33	1	-4.576971	-3.227656	1.398766
34	1	-2.921564	-2.946385	1.962027
35	1	-3.219663	-3.989328	0.563850
36	1	-5.040995	-0.728746	2.286964
37	1	-4.332549	0.879810	2.122415
38	1	-3.349219	-0.462671	2.725209
39	1	-5.302892	1.822475	-1.004006
40	1	-3.632496	2.311538	-1.319677
41	1	-4.228667	2.215561	0.342721
42	1	-4.899113	-0.296360	-3.432447
43	1	-3.225738	-0.715874	-3.839211
44	1	-3.610849	0.919667	-3.310162
45	1	-4.282602	-3.355106	-2.560360
46	1	-2.895473	-3.952904	-1.640452
47	1	-2.642245	-2.896363	-3.030496
48	6	0.101864	2.212072	1.044336
49	6	-0.648905	3.013012	1.940014
50	6	1.255791	2.742744	0.412084
51	6	-0.253755	4.341531	2.168232
52	6	1.612033	4.078216	0.664969
53	6	0.866561	4.877956	1.532463
54	1	-0.835671	4.952314	2.852492
55	1	2.490924	4.485374	0.173743
56	1	1.159679	5.906931	1.715965

57	6	0.611773	-2.691465	-1.769580
58	6	0.137508	-4.011194	-1.566518
59	6	1.268893	-2.336022	-2.973299
60	6	0.247956	-4.937868	-2.616824
61	6	1.358789	-3.297459	-3.994351
62	6	0.839350	-4.583759	-3.830295
63	1	-0.126360	-5.946641	-2.468123
64	1	1.853527	-3.027088	-4.922291
65	1	0.912771	-5.308569	-4.634797
66	6	-1.874325	2.478985	2.642216
67	1	-2.693700	2.318841	1.934742
68	1	-1.690606	1.518483	3.134679
69	1	-2.221835	3.187047	3.400868
70	6	2.107108	1.917514	-0.523489
71	1	1.522451	1.570853	-1.379618
72	1	2.949188	2.510653	-0.894085
73	1	2.509123	1.028948	-0.024242
74	6	-0.406936	-4.470678	-0.231658
75	1	0.404750	-4.820508	0.422694
76	1	-0.920175	-3.672280	0.306123
77	1	-1.095928	-5.311503	-0.360848
78	6	1.915755	-0.984416	-3.168240
79	1	1.178748	-0.177281	-3.163609
80	1	2.635259	-0.763119	-2.370605
81	1	2.453585	-0.956356	-4.120580

11Ar (E = -1495.0024408 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.006049	-0.849399	-0.123871
2	7	-1.710703	0.119834	0.415816
3	6	-1.414641	1.165343	1.448900
4	7	1.129429	0.953634	-0.108413
5	6	0.213327	-2.606321	1.656574
6	6	1.535580	-2.069397	1.530015
7	6	-0.074546	-3.331614	0.460576
8	17	-0.662463	-1.358768	-2.412169
9	6	2.061672	-2.473437	0.267999
10	6	1.066976	-3.244077	-0.391520
11	6	0.476849	2.172869	0.170260
12	6	-0.674179	2.334138	0.868348
13	1	-2.343405	1.468328	1.938008
14	6	-1.049984	3.759689	0.884075
15	1	-0.795424	0.713395	2.243087
16	6	0.918566	3.526471	-0.344827
17	6	-0.131227	4.474402	0.189995
18	1	1.928192	3.808223	-0.027954
19	1	0.935346	3.523373	-1.443165
20	6	-0.057928	5.956783	-0.057240
21	6	-2.278845	4.267889	1.593999
22	1	-2.384724	5.352257	1.493909
23	1	-2.245452	4.033010	2.667060
24	1	-3.189980	3.804126	1.192153
25	1	-0.903013	6.486808	0.394610
26	1	-0.059577	6.187310	-1.132541
27	1	0.864532	6.389452	0.357642
28	6	2.333432	-1.501357	2.677886
29	6	-0.562983	-2.633859	2.954523
30	6	-1.297403	-4.169994	0.168654
31	6	1.244185	-3.993548	-1.687195
32	6	3.487333	-2.299749	-0.196315
33	1	2.760245	-2.324772	3.269624
34	1	1.716802	-0.902469	3.355109
35	1	3.161705	-0.878960	2.333298

36	1	-0.033669	-3.256857	3.689093
37	1	-1.559657	-3.058877	2.821550
38	1	-0.683976	-1.639871	3.399883
39	1	-1.055678	-5.238209	0.259056
40	1	-1.673336	-4.004469	-0.847020
41	1	-2.114066	-3.959361	0.864362
42	1	1.612886	-5.009871	-1.486769
43	1	1.967478	-3.502893	-2.345692
44	1	0.303552	-4.078646	-2.237963
45	1	4.086963	-3.172715	0.099895
46	1	3.954998	-1.412252	0.235811
47	1	3.556884	-2.212141	-1.284930
48	6	-3.064758	0.162783	-0.089048
49	6	-4.086571	-0.530822	0.611421
50	6	-3.395405	0.922272	-1.244658
51	6	-5.405868	-0.491555	0.132766
52	6	-4.728463	0.925304	-1.692984
53	6	-5.729631	0.224455	-1.020215
54	1	-6.178338	-1.030478	0.674000
55	1	-4.975397	1.496640	-2.583110
56	1	-6.751478	0.242757	-1.386188
57	6	2.562491	1.107199	-0.261423
58	6	3.351946	1.506497	0.852201
59	6	3.173353	0.904440	-1.524277
60	6	4.743238	1.619951	0.696593
61	6	4.567908	1.041344	-1.638002
62	6	5.355214	1.382127	-0.536802
63	1	5.345247	1.908559	1.553820
64	1	5.031560	0.886690	-2.608023
65	1	6.431361	1.477655	-0.641272
66	6	-3.785351	-1.320919	1.863583
67	1	-3.188801	-2.210263	1.636836
68	1	-3.216710	-0.737661	2.595939
69	1	-4.712676	-1.653376	2.340266
70	6	-2.386080	1.758619	-2.001111
71	1	-1.478008	1.197029	-2.227173
72	1	-2.816729	2.099104	-2.948457
73	1	-2.089058	2.645128	-1.429423
74	6	2.734715	1.864312	2.187495
75	1	2.398003	2.909588	2.201347
76	1	1.860097	1.251583	2.412221
77	1	3.464386	1.744305	2.994987
78	6	2.362598	0.577493	-2.757547
79	1	1.979817	-0.449274	-2.749843
80	1	1.487500	1.229048	-2.849229
81	1	2.974840	0.694159	-3.657257

TS(11-12)Ar (E = -1494.9738143 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.448250	-0.449890	-0.111942
2	7	0.498471	-0.676961	1.785498
3	6	-0.257124	1.417512	1.774596
4	7	-1.690291	0.328247	-0.452830
5	6	2.604810	0.829027	-0.491981
6	6	1.731741	1.398128	-1.471499
7	6	2.869805	-0.521387	-0.871844
8	17	0.072461	-2.795932	-0.712690
9	6	1.467406	0.404885	-2.459623
10	6	2.171270	-0.772836	-2.091316
11	6	-2.302360	0.967279	0.541712
12	6	-1.642760	1.393464	1.713599
13	1	0.267892	1.666079	2.685636
14	6	-2.660126	1.680320	2.737529

15	1	0.276639	1.733958	0.874607
16	6	-3.787749	1.181855	0.727559
17	6	-3.892947	1.590808	2.184825
18	1	-4.176924	1.959082	0.057942
19	1	-4.351779	0.271549	0.497114
20	6	-5.232069	1.874050	2.804886
21	6	-2.290369	2.064969	4.143983
22	1	-3.172501	2.259494	4.760189
23	1	-1.665783	2.969124	4.152006
24	1	-1.710174	1.267325	4.625729
25	1	-5.144173	2.161303	3.856979
26	1	-5.888681	0.993840	2.752036
27	1	-5.750510	2.687999	2.277231
28	6	1.457372	2.882110	-1.576283
29	6	3.356915	1.649750	0.528566
30	6	3.853409	-1.470743	-0.226607
31	6	2.310999	-2.006808	-2.944960
32	6	0.721703	0.589638	-3.759925
33	1	2.405043	3.421498	-1.715279
34	1	0.983268	3.304502	-0.681287
35	1	0.821341	3.115909	-2.432628
36	1	4.078615	2.302063	0.015250
37	1	3.917680	1.021584	1.222107
38	1	2.702271	2.299844	1.120313
39	1	4.806410	-1.469520	-0.774941
40	1	3.479226	-2.499977	-0.219609
41	1	4.066798	-1.192155	0.808833
42	1	3.144052	-1.880051	-3.652016
43	1	1.405726	-2.205075	-3.526618
44	1	2.512248	-2.896240	-2.342361
45	1	1.429271	0.710316	-4.592726
46	1	0.079147	1.472963	-3.741383
47	1	0.086796	-0.271244	-3.996018
48	6	0.477956	-1.127869	3.099052
49	6	-0.618674	-1.923510	3.564011
50	6	1.525824	-0.808811	4.018317
51	6	-0.642614	-2.359516	4.896017
52	6	1.456597	-1.263825	5.342476
53	6	0.380223	-2.032988	5.790655
54	1	-1.478339	-2.967923	5.230961
55	1	2.264017	-1.012871	6.025230
56	1	0.342079	-2.378763	6.818928
57	6	-2.483159	0.158825	-1.666081
58	6	-3.148656	-1.060924	-1.939681
59	6	-2.611883	1.258830	-2.554748
60	6	-3.840178	-1.189637	-3.158209
61	6	-3.307080	1.082390	-3.760344
62	6	-3.903769	-0.140975	-4.074800
63	1	-4.345697	-2.127122	-3.371517
64	1	-3.387879	1.919404	-4.447904
65	1	-4.434815	-0.265567	-5.013082
66	6	-2.085032	2.634349	-2.210162
67	1	-2.833898	3.211478	-1.649376
68	1	-1.189737	2.592206	-1.591322
69	1	-1.856704	3.203422	-3.117157
70	6	-3.221748	-2.206341	-0.955084
71	1	-2.605365	-3.052156	-1.274527
72	1	-2.875187	-1.919784	0.037228
73	1	-4.256926	-2.558942	-0.871775
74	6	2.720124	-0.001410	3.579058
75	1	3.246384	-0.495647	2.755279
76	1	2.435425	0.992462	3.216112
77	1	3.425728	0.130230	4.405443

78	6	-1.744272	-2.320539	2.638416
79	1	-2.310662	-1.446456	2.298239
80	1	-1.365541	-2.827918	1.745965
81	1	-2.441189	-2.992446	3.150259

12Ar (E = -1494.9924115 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.596251	-0.601209	-0.205852
2	7	1.662354	0.821088	0.364992
3	6	-1.202380	2.203271	-1.777385
4	7	-1.588388	0.168672	0.464354
5	6	0.912431	-0.600229	-2.721936
6	6	-0.091664	-1.609692	-2.535674
7	6	2.130307	-1.076726	-2.147871
8	17	0.799737	-2.307775	1.549461
9	6	0.505135	-2.694904	-1.843300
10	6	1.873127	-2.359357	-1.590937
11	6	-2.478910	0.976186	-0.012967
12	6	-2.358166	1.842733	-1.202772
13	1	-1.173989	2.897302	-2.608288
14	6	-3.708783	2.347640	-1.508876
15	1	-0.251046	1.855833	-1.398343
16	6	-3.874804	1.191067	0.544418
17	6	-4.569660	1.991460	-0.532282
18	1	-4.376911	0.247021	0.772387
19	1	-3.829922	1.742283	1.492825
20	6	-6.028279	2.316215	-0.397639
21	6	-3.976856	3.183538	-2.729766
22	1	-5.034797	3.440892	-2.824006
23	1	-3.673610	2.653366	-3.642006
24	1	-3.404907	4.120654	-2.695884
25	1	-6.408176	2.891225	-1.246060
26	1	-6.214033	2.896648	0.516970
27	1	-6.624645	1.396959	-0.314123
28	6	-1.475947	-1.578384	-3.143769
29	6	0.822203	0.552541	-3.695268
30	6	3.478239	-0.410520	-2.279282
31	6	2.898420	-3.294332	-0.996466
32	6	-0.115432	-4.031558	-1.518006
33	1	-1.434823	-1.847098	-4.209149
34	1	-1.932521	-0.584860	-3.075831
35	1	-2.151200	-2.287869	-2.655627
36	1	1.223069	0.244412	-4.672289
37	1	1.400828	1.422614	-3.368600
38	1	-0.211042	0.874278	-3.853384
39	1	3.935355	-0.655710	-3.249156
40	1	4.168690	-0.737205	-1.496040
41	1	3.400782	0.678266	-2.209506
42	1	3.301001	-3.960589	-1.773441
43	1	2.465541	-3.915975	-0.207982
44	1	3.741480	-2.748765	-0.560866
45	1	0.357069	-4.826281	-2.111986
46	1	-1.185899	-4.049411	-1.744841
47	1	0.012302	-4.290980	-0.460620
48	6	2.676011	1.678032	0.759552
49	6	3.634115	1.254859	1.740351
50	6	2.802017	2.999289	0.222952
51	6	4.659517	2.123041	2.135040
52	6	3.842943	3.834849	0.653139
53	6	4.775887	3.410159	1.601179
54	1	5.375209	1.780183	2.878238
55	1	3.917948	4.834165	0.231052
56	1	5.577287	4.069435	1.920374

57	6	-1.960033	-0.439501	1.745215
58	6	-1.621499	0.243412	2.933372
59	6	-2.649036	-1.669594	1.759093
60	6	-1.982464	-0.348862	4.154736
61	6	-2.994111	-2.219942	3.002398
62	6	-2.661474	-1.569066	4.193393
63	1	-1.719494	0.156251	5.078972
64	1	-3.517396	-3.170732	3.029821
65	1	-2.925742	-2.013551	5.147396
66	6	-3.008880	-2.385895	0.478400
67	1	-3.755617	-1.836624	-0.110941
68	1	-2.131605	-2.520154	-0.162190
69	1	-3.420992	-3.375319	0.694596
70	6	-0.893965	1.569621	2.910749
71	1	0.024695	1.513255	2.316366
72	1	-1.509949	2.367903	2.474064
73	1	-0.630901	1.876482	3.926733
74	6	1.821095	3.517140	-0.797433
75	1	1.789072	2.879381	-1.689538
76	1	0.799471	3.549889	-0.396503
77	1	2.091161	4.529669	-1.115988
78	6	3.544813	-0.120260	2.351549
79	1	2.566308	-0.297431	2.810395
80	1	3.666298	-0.910785	1.599911
81	1	4.318784	-0.255497	3.114685

13Ar (E = -819.1030003 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.039080	0.677371	-0.542215
2	7	1.783067	0.496715	-0.296810
3	6	-0.667484	-1.362049	0.747872
4	6	-0.902358	-1.647844	-0.630168
5	6	-1.591082	-0.344269	1.142547
6	17	-0.729499	2.854390	-1.436126
7	6	-2.014775	-0.847976	-1.067295
8	6	-2.444598	-0.052039	0.025666
9	6	-0.243501	-2.754874	-1.423915
10	6	0.290627	-2.107759	1.644071
11	6	-1.772641	0.193325	2.545751
12	6	-3.637559	0.872929	0.039983
13	6	-2.670156	-0.914622	-2.428104
14	1	-0.793797	-3.697462	-1.295060
15	1	0.787075	-2.926409	-1.099180
16	1	-0.223649	-2.536808	-2.497185
17	1	-0.157850	-3.056275	1.971421
18	1	0.538550	-1.533980	2.541566
19	1	1.229231	-2.339511	1.132259
20	1	-2.525537	-0.398021	3.084787
21	1	-2.116621	1.233327	2.547415
22	1	-0.845388	0.145905	3.125147
23	1	-4.553421	0.314773	0.279527
24	1	-3.788639	1.359321	-0.928621
25	1	-3.530589	1.663319	0.789493
26	1	-3.441857	-1.696630	-2.443366
27	1	-1.952891	-1.156183	-3.220414
28	1	-3.154813	0.030585	-2.692092
29	6	3.118821	0.240763	-0.043740
30	6	3.679244	0.524231	1.237445
31	6	3.956677	-0.289808	-1.069188
32	6	5.035341	0.257701	1.468689
33	6	5.307702	-0.538530	-0.793289
34	6	5.853438	-0.273677	0.466766
35	1	5.452856	0.476113	2.448365

36	1	5.938425	-0.941311	-1.581759
37	1	6.902249	-0.472884	0.663435
38	6	3.391448	-0.565020	-2.441479
39	1	2.588496	-1.314330	-2.408349
40	1	2.959598	0.342830	-2.884596
41	1	4.168579	-0.935477	-3.117705
42	6	2.821813	1.121242	2.326806
43	1	2.386607	2.080150	2.013238
44	1	1.982879	0.463607	2.590682
45	1	3.408445	1.296862	3.234303

14Ar (E = -675.8655679 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.297305	0.837606	0.006404
2	6	0.111476	0.378815	0.002419
3	6	-1.113310	1.230516	-0.011293
4	6	-2.267266	0.317981	-0.011666
5	6	-0.346816	-1.072842	0.010098
6	6	-1.854569	-0.969819	0.000288
7	1	0.040081	-1.618135	-0.859368
8	1	0.029361	-1.605788	0.891803
9	6	-2.687949	-2.218766	0.004789
10	6	-3.679313	0.837689	-0.023938
11	1	-4.416303	0.030424	-0.022146
12	1	-3.858101	1.457626	-0.912669
13	1	-3.868515	1.471116	0.853043
14	1	-3.760925	-2.008892	-0.001838
15	1	-2.466045	-2.829166	0.891653
16	1	-2.457579	-2.841383	-0.871358
17	6	-1.117490	2.571956	-0.020604
18	1	-2.039266	3.141298	-0.030320
19	1	-0.183875	3.121441	-0.018547
20	6	2.406678	-0.056993	0.020760
21	6	2.990778	-0.457076	-1.204089
22	6	2.970403	-0.443070	1.259580
23	6	4.126141	-1.281036	-1.166847
24	6	4.106171	-1.267279	1.250468
25	6	4.681326	-1.691523	0.048863
26	1	4.578993	-1.593526	-2.103642
27	1	4.543472	-1.568979	2.198120
28	1	5.561662	-2.326273	0.059750
29	6	2.369855	0.037665	2.561562
30	1	2.270914	1.130171	2.572716
31	1	1.363995	-0.369556	2.730090
32	1	2.993885	-0.259812	3.409537
33	6	2.411498	0.008643	-2.521058
34	1	1.408325	-0.400304	-2.700907
35	1	2.313106	1.100981	-2.546441
36	1	3.048960	-0.298734	-3.355397

15Ar (E = -1067.4049257 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.109976	0.007236	-0.511896
2	7	-0.734255	1.752760	-0.366089
3	6	-1.770432	-0.876646	1.132285
4	6	-0.497269	-0.992273	1.767353
5	6	-1.792437	-1.798339	0.041622
6	17	0.084337	-0.609485	-2.893392
7	6	0.243030	-2.021388	1.096761
8	6	-0.555622	-2.518230	0.035192
9	6	-0.095294	-0.314142	3.057732
10	6	-2.926949	-0.039197	1.622624

11	6	-2.971290	-2.094900	-0.857540
12	6	-0.224825	-3.666668	-0.886650
13	6	1.574530	-2.574053	1.547178
14	1	-0.398641	-0.919508	3.924024
15	1	-0.568815	0.667187	3.162041
16	1	0.989058	-0.172452	3.128121
17	1	-3.471571	-0.566458	2.419037
18	1	-3.639588	0.176068	0.821073
19	1	-2.591215	0.921821	2.022859
20	1	-3.550323	-2.942685	-0.464129
21	1	-2.651690	-2.355159	-1.871871
22	1	-3.651590	-1.240820	-0.932457
23	1	-0.764883	-4.574970	-0.584132
24	1	0.844488	-3.901948	-0.871297
25	1	-0.499475	-3.446324	-1.923710
26	1	1.429113	-3.358592	2.302966
27	1	2.207406	-1.802669	1.999183
28	1	2.134627	-3.020965	0.718988
29	7	2.171985	0.269598	-0.170260
30	6	3.046131	-0.440944	-0.927465
31	6	2.673546	1.130559	0.749808
32	6	4.427857	-0.316875	-0.790414
33	1	2.611677	-1.105452	-1.664792
34	6	4.042655	1.300328	0.948507
35	1	1.948306	1.698302	1.316877
36	6	4.939519	0.566474	0.165194
37	1	5.083109	-0.900579	-1.425093
38	1	4.392499	2.001982	1.695720
39	1	6.009640	0.683861	0.292828
40	6	-1.455186	2.928299	-0.267779
41	6	-1.095163	3.947090	0.666756
42	6	-2.583540	3.152528	-1.119713
43	6	-1.851596	5.124587	0.741224
44	6	-3.310396	4.344796	-1.011333
45	6	-2.957746	5.333702	-0.087201
46	1	-1.562867	5.887917	1.460090
47	1	-4.163797	4.498682	-1.667424
48	1	-3.532530	6.252105	-0.017171
49	6	-2.984370	2.109655	-2.133795
50	1	-2.141963	1.834066	-2.779079
51	1	-3.320825	1.180969	-1.651430
52	1	-3.802696	2.472026	-2.764965
53	6	0.106437	3.769066	1.562081
54	1	0.050727	2.830795	2.129511
55	1	1.036173	3.737160	0.977784
56	1	0.188499	4.595082	2.276527

TS(9'-18)Ar (E = -1494.9224018 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.091490	-0.000396	-0.029215
2	7	0.129033	-0.014677	2.151350
3	6	1.398689	-0.066370	2.608682
4	7	1.647209	1.614461	0.096686
5	6	-1.211564	-2.182579	-0.481879
6	6	0.153614	-2.454606	-0.775633
7	6	-1.676862	-1.216321	-1.419949
8	17	-1.446110	1.900729	-0.474866
9	6	0.528991	-1.673292	-1.916365
10	6	-0.607365	-0.916098	-2.319306
11	6	2.587790	1.295499	0.970448
12	6	2.480367	0.010019	1.653649
13	1	1.591274	-0.287755	3.653011
14	6	3.881122	-0.294096	2.125405

15	1	2.009450	-0.762677	0.604620
16	6	3.971090	1.863088	1.152815
17	6	4.708733	0.727905	1.837802
18	1	4.417559	2.137612	0.188879
19	1	3.996857	2.775336	1.764177
20	6	6.171808	0.869320	2.157404
21	6	4.201719	-1.591727	2.818021
22	1	5.260008	-1.663838	3.085000
23	1	3.954427	-2.446805	2.174391
24	1	3.616439	-1.708083	3.739769
25	1	6.577103	-0.017974	2.652530
26	1	6.344867	1.731207	2.817351
27	1	6.759382	1.045767	1.245540
28	6	1.010600	-3.559505	-0.205538
29	6	-2.099485	-2.901952	0.506500
30	6	-3.111368	-0.779172	-1.581790
31	6	-0.745382	-0.054765	-3.552218
32	6	1.818341	-1.874077	-2.678961
33	1	1.109244	-4.372121	-0.940062
34	1	0.576759	-3.990016	0.700338
35	1	2.020051	-3.209841	0.036738
36	1	-2.823301	-3.530152	-0.031080
37	1	-2.671252	-2.212815	1.137469
38	1	-1.524500	-3.553537	1.167697
39	1	-3.645181	-1.476416	-2.244291
40	1	-3.180807	0.221931	-2.014351
41	1	-3.640664	-0.760389	-0.623670
42	1	-1.341135	-0.577038	-4.313936
43	1	0.224693	0.179598	-3.999830
44	1	-1.249524	0.891547	-3.329510
45	1	1.835808	-2.880724	-3.121459
46	1	2.699044	-1.783051	-2.034291
47	1	1.925223	-1.158068	-3.497596
48	6	1.812969	2.881988	-0.591576
49	6	2.374436	2.883972	-1.890127
50	6	1.466570	4.096874	0.043322
51	6	2.554239	4.109877	-2.551116
52	6	1.669476	5.301477	-0.650702
53	6	2.202160	5.315045	-1.941043
54	1	2.984143	4.110096	-3.548469
55	1	1.400779	6.234845	-0.164687
56	1	2.348026	6.255658	-2.462654
57	6	-0.907843	-0.280583	3.133029
58	6	-1.011131	-1.583136	3.692574
59	6	-1.804012	0.738416	3.541158
60	6	-2.062424	-1.861214	4.581882
61	6	-2.838778	0.413987	4.434828
62	6	-2.983375	-0.877434	4.943197
63	1	-2.148909	-2.863170	4.992531
64	1	-3.525756	1.197272	4.740773
65	1	-3.793224	-1.109634	5.627522
66	6	2.804931	1.603623	-2.565919
67	1	1.955843	0.935941	-2.735867
68	1	3.267549	1.817068	-3.534429
69	1	3.526527	1.041322	-1.960743
70	6	0.863457	4.131087	1.425722
71	1	1.388388	3.470337	2.123736
72	1	0.885584	5.147708	1.830309
73	1	-0.177987	3.798572	1.391662
74	6	-1.641160	2.169833	3.096364
75	1	-0.624208	2.524339	3.291698
76	1	-1.822716	2.291956	2.024758
77	1	-2.337522	2.817572	3.637930

78	6	-0.011704	-2.680317	3.396015
79	1	-0.482585	-3.664854	3.486843
80	1	0.415289	-2.587745	2.396470
81	1	0.826396	-2.657386	4.105373

18Ar (E = -1494.9944024 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.127020	-0.813063	-0.386318
2	7	-1.508206	0.623187	-0.011093
3	6	-0.706899	1.700135	-0.556916
4	7	1.444635	0.398749	0.075251
5	6	-0.178615	-2.343799	1.629193
6	6	0.890065	-2.832342	0.815889
7	6	-1.405256	-2.560467	0.927588
8	17	-0.083755	-0.943529	-2.838158
9	6	0.326258	-3.336258	-0.390942
10	6	-1.088936	-3.164042	-0.324703
11	6	0.865792	1.616509	-0.458094
12	6	0.078796	2.657176	0.331722
13	1	-1.059609	2.128610	-1.494840
14	6	0.389973	3.982368	-0.285167
15	1	-0.070406	2.561917	1.396645
16	6	1.594878	2.394399	-1.563038
17	6	1.191807	3.840952	-1.355438
18	1	2.679716	2.277312	-1.452266
19	1	1.334309	2.023181	-2.560056
20	6	1.698068	4.900736	-2.296457
21	6	-0.220288	5.240298	0.275369
22	1	0.102904	6.134333	-0.266385
23	1	0.053632	5.369398	1.331836
24	1	-1.317564	5.195381	0.233818
25	1	1.366035	5.903455	-2.010340
26	1	1.355456	4.713371	-3.323889
27	1	2.797262	4.903124	-2.324593
28	6	2.327283	-2.974981	1.257122
29	6	-0.045402	-1.917412	3.072112
30	6	-2.793267	-2.369246	1.491317
31	6	-2.079972	-3.659129	-1.351585
32	6	1.060888	-4.062188	-1.492015
33	1	2.451766	-3.902668	1.833744
34	1	2.648909	-2.144365	1.891197
35	1	3.014374	-3.022350	0.407798
36	1	-0.066297	-2.799548	3.728097
37	1	-0.862222	-1.260528	3.383341
38	1	0.897467	-1.394796	3.258511
39	1	-3.126804	-3.290929	1.988897
40	1	-3.525402	-2.130420	0.714310
41	1	-2.828463	-1.563034	2.228345
42	1	-2.281905	-4.729429	-1.203099
43	1	-1.704154	-3.528873	-2.371052
44	1	-3.037223	-3.132972	-1.279116
45	1	0.966411	-5.148986	-1.357780
46	1	2.129006	-3.824490	-1.495516
47	1	0.661325	-3.810269	-2.478968
48	6	-2.868683	0.939852	0.319943
49	6	-3.226341	1.305105	1.642123
50	6	-3.866721	0.868912	-0.689919
51	6	-4.573857	1.580950	1.934638
52	6	-5.198479	1.159873	-0.356144
53	6	-5.556614	1.513759	0.947588
54	1	-4.845017	1.850682	2.951794
55	1	-5.958225	1.103507	-1.130374
56	1	-6.592134	1.730803	1.190342

57	6	2.812060	0.424328	0.512291
58	6	3.156314	0.910941	1.800229
59	6	3.828701	-0.077614	-0.345880
60	6	4.501954	0.885765	2.206088
61	6	5.161537	-0.075633	0.096825
62	6	5.503323	0.402002	1.363804
63	1	4.756923	1.250070	3.197393
64	1	5.934357	-0.455371	-0.565227
65	1	6.538059	0.392750	1.691629
66	6	-2.208988	1.412875	2.757189
67	1	-1.305670	0.845721	2.528092
68	1	-1.909115	2.456362	2.923617
69	1	-2.625245	1.045308	3.702176
70	6	-3.525927	0.483366	-2.112392
71	1	-2.855457	1.209548	-2.586984
72	1	-3.014295	-0.482984	-2.168742
73	1	-4.434529	0.424894	-2.719517
74	6	2.121512	1.453693	2.759913
75	1	2.459988	1.341293	3.795269
76	1	1.939289	2.522245	2.589211
77	1	1.163603	0.940340	2.647595
78	6	3.515642	-0.625613	-1.720955
79	1	2.900717	-1.531377	-1.674436
80	1	2.957868	0.085418	-2.336587
81	1	4.440993	-0.880295	-2.247205

TS(8a-17)Ar (E = -1494.930217 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.123505	-0.369749	0.327510
2	7	1.771734	0.461263	-0.097713
3	6	1.454748	1.106427	-1.263279
4	7	-1.519595	0.974633	-0.491991
5	6	-0.424821	-2.442760	-1.092182
6	6	-1.703443	-2.263909	-0.470430
7	6	0.515216	-2.799768	-0.071172
8	17	-0.292635	0.183224	2.720376
9	6	-1.546038	-2.463233	0.923760
10	6	-0.173727	-2.772566	1.173946
11	6	-0.725877	2.083929	-0.473196
12	6	0.495774	2.238307	-1.331565
13	1	2.067048	0.938088	-2.144563
14	6	1.014049	3.635071	-0.988126
15	1	0.127111	2.257418	-2.375638
16	6	-1.040599	3.406110	0.188984
17	6	0.147011	4.272433	-0.185440
18	1	-1.996461	3.825500	-0.163410
19	1	-1.137773	3.318625	1.280007
20	6	0.230820	5.677621	0.347912
21	6	2.303518	4.140717	-1.575264
22	1	2.515890	5.170731	-1.274431
23	1	2.273634	4.109452	-2.674145
24	1	3.149986	3.516681	-1.260914
25	1	1.139850	6.194783	0.027229
26	1	0.212522	5.673520	1.447062
27	1	-0.632609	6.272830	0.018384
28	6	-3.010714	-2.128491	-1.210843
29	6	-0.216560	-2.547153	-2.587280
30	6	1.890132	-3.401009	-0.258404
31	6	0.403514	-3.213382	2.497187
32	6	-2.642176	-2.507356	1.959611
33	1	-3.381067	-3.124288	-1.495384
34	1	-2.905449	-1.543852	-2.128245
35	1	-3.782504	-1.648437	-0.603903

36	1	-0.576176	-3.519987	-2.952963
37	1	0.837533	-2.464018	-2.864461
38	1	-0.763522	-1.771990	-3.133854
39	1	1.885172	-4.438664	0.102679
40	1	2.674403	-2.867754	0.288109
41	1	2.177258	-3.424888	-1.311665
42	1	0.249859	-4.293497	2.638396
43	1	-0.068191	-2.693808	3.335761
44	1	1.480490	-3.023626	2.552795
45	1	-2.891509	-3.549984	2.203115
46	1	-3.557585	-2.025659	1.603622
47	1	-2.339412	-2.015231	2.889935
48	6	3.155702	0.123677	0.160043
49	6	3.963805	-0.613085	-0.746482
50	6	3.715184	0.609043	1.374416
51	6	5.286725	-0.918301	-0.380171
52	6	5.042981	0.281481	1.691581
53	6	5.826429	-0.489781	0.831871
54	1	5.893975	-1.500762	-1.067484
55	1	5.463611	0.655905	2.620181
56	1	6.849606	-0.738391	1.095000
57	6	-2.948609	1.172429	-0.679614
58	6	-3.393457	1.288242	-2.023477
59	6	-3.876882	1.250165	0.386890
60	6	-4.766087	1.431662	-2.280800
61	6	-5.241941	1.401572	0.080259
62	6	-5.691732	1.484330	-1.237805
63	1	-5.102454	1.502042	-3.311177
64	1	-5.953179	1.461773	0.898653
65	1	-6.750516	1.595584	-1.448855
66	6	3.493801	-1.076001	-2.109519
67	1	2.419382	-1.256629	-2.140862
68	1	3.721683	-0.330626	-2.884224
69	1	4.006210	-2.000397	-2.395197
70	6	2.942627	1.516587	2.303042
71	1	2.442785	2.320217	1.750890
72	1	2.156331	0.983003	2.845009
73	1	3.618319	1.967368	3.036878
74	6	-2.429382	1.261219	-3.189136
75	1	-2.954982	1.019388	-4.118096
76	1	-1.947396	2.237972	-3.332167
77	1	-1.629112	0.530718	-3.037520
78	6	-3.467766	1.216500	1.841125
79	1	-4.350769	1.306268	2.481413
80	1	-2.945922	0.297140	2.110977
81	1	-2.787496	2.036319	2.093290

17Ar (E = -1494.9737042 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.052351	-0.535300	-0.517499
2	7	-1.516062	1.132063	0.337598
3	6	-0.945884	2.266096	0.563560
4	7	1.615210	0.208418	0.291715
5	6	-0.640241	-2.302020	1.233290
6	6	0.546077	-2.761756	0.584126
7	6	-1.719792	-2.388102	0.296665
8	17	0.071839	-0.551160	-2.992984
9	6	0.206501	-3.095481	-0.757629
10	6	-1.192068	-2.863350	-0.933443
11	6	1.136497	1.347226	-0.480943
12	6	0.480267	2.531795	0.249254
13	1	-1.545929	3.070127	0.998457
14	6	0.655677	3.714311	-0.710555

15	1	0.952500	2.811678	1.211260
16	6	2.028252	1.978245	-1.554911
17	6	1.510587	3.389236	-1.690359
18	1	3.088051	2.019538	-1.248725
19	1	1.998523	1.441516	-2.509429
20	6	2.003459	4.264559	-2.812339
21	6	-0.018482	5.038155	-0.451000
22	1	0.327472	5.810557	-1.144403
23	1	0.187354	5.390846	0.570356
24	1	-1.111184	4.973526	-0.554014
25	1	1.596151	5.279546	-2.772054
26	1	1.732811	3.828600	-3.783843
27	1	3.100080	4.336289	-2.791653
28	6	1.848762	-3.065322	1.282869
29	6	-0.772193	-2.088566	2.724061
30	6	-3.190662	-2.297064	0.628625
31	6	-1.983234	-3.235463	-2.162949
32	6	1.101522	-3.755104	-1.779319
33	1	1.794234	-4.053230	1.763397
34	1	2.079880	-2.330523	2.058514
35	1	2.694095	-3.082035	0.589990
36	1	-0.795891	-3.057462	3.244151
37	1	-1.695641	-1.561763	2.978650
38	1	0.067489	-1.520883	3.138367
39	1	-3.567040	-3.293156	0.903847
40	1	-3.786838	-1.946961	-0.218725
41	1	-3.389566	-1.626763	1.467513
42	1	-2.176128	-4.317995	-2.182680
43	1	-1.445125	-2.973494	-3.079107
44	1	-2.953727	-2.729071	-2.190742
45	1	0.881916	-4.830829	-1.837438
46	1	2.159635	-3.651088	-1.521824
47	1	0.955021	-3.330076	-2.777504
48	6	-2.933818	1.068091	0.655607
49	6	-3.367825	1.114439	2.000167
50	6	-3.852523	0.983767	-0.415497
51	6	-4.748339	1.032111	2.253649
52	6	-5.221467	0.918925	-0.113215
53	6	-5.670210	0.932197	1.210141
54	1	-5.093921	1.052892	3.282773
55	1	-5.935904	0.861632	-0.928589
56	1	-6.731975	0.872774	1.425614
57	6	2.892024	0.141608	0.924463
58	6	3.053031	0.548451	2.276331
59	6	4.017825	-0.355047	0.206962
60	6	4.324005	0.482731	2.871990
61	6	5.270089	-0.400563	0.840685
62	6	5.432827	0.022205	2.162055
63	1	4.434434	0.790945	3.908569
64	1	6.123278	-0.782925	0.286975
65	1	6.408472	-0.022780	2.635984
66	6	-2.410625	1.273283	3.164003
67	1	-1.461664	0.758387	2.998043
68	1	-2.175487	2.329526	3.353091
69	1	-2.856693	0.876049	4.080748
70	6	-3.393202	0.992160	-1.855672
71	1	-2.758717	1.857358	-2.079451
72	1	-2.805923	0.102435	-2.113067
73	1	-4.253696	1.021753	-2.529997
74	6	1.890010	1.037000	3.113845
75	1	1.972478	0.670481	4.143690
76	1	1.859868	2.133889	3.166479
77	1	0.937409	0.701477	2.698815

78	6	3.901171	-0.863057	-1.213901
79	1	4.768376	-1.480631	-1.469945
80	1	2.997175	-1.460482	-1.358048
81	1	3.850205	-0.045938	-1.942308

TS(17-18)Ar (E = -1494.9514245 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.006264	-0.663091	-0.421316
2	7	-1.533587	0.844995	0.086372
3	6	-0.931970	1.996757	-0.214889
4	7	1.668200	0.192432	0.310532
5	6	-0.418554	-2.333653	1.440481
6	6	0.719682	-2.817697	0.726184
7	6	-1.562365	-2.457429	0.590132
8	17	0.257827	-0.746315	-2.881093
9	6	0.285605	-3.199809	-0.574424
10	6	-1.124305	-2.979128	-0.656972
11	6	1.206628	1.357870	-0.384873
12	6	0.394624	2.438162	0.323950
13	1	-1.470887	2.691116	-0.872842
14	6	0.854251	3.746099	-0.284879
15	1	0.405838	2.424489	1.419127
16	6	2.056231	2.061261	-1.444375
17	6	1.746534	3.531434	-1.264793
18	1	3.125741	1.876165	-1.267590
19	1	1.856266	1.724911	-2.468788
20	6	2.426428	4.550951	-2.139195
21	6	0.285509	5.051143	0.209024
22	1	0.668986	5.909983	-0.350242
23	1	0.526233	5.205610	1.270608
24	1	-0.811619	5.064652	0.128753
25	1	2.117798	5.575610	-1.910334
26	1	2.208219	4.358935	-3.198944
27	1	3.518010	4.491882	-2.025238
28	6	2.076038	-3.099402	1.324860
29	6	-0.448707	-2.008883	2.915840
30	6	-2.998700	-2.309409	1.030759
31	6	-1.999744	-3.390393	-1.816068
32	6	1.119759	-3.893265	-1.624355
33	1	2.076057	-4.093962	1.794122
34	1	2.349528	-2.369574	2.090872
35	1	2.867151	-3.090421	0.570599
36	1	-0.664800	-2.914520	3.501168
37	1	-1.221258	-1.273397	3.160950
38	1	0.510516	-1.615684	3.264470
39	1	-3.366080	-3.269556	1.421169
40	1	-3.658670	-2.012599	0.211038
41	1	-3.111140	-1.568129	1.825645
42	1	-2.163222	-4.477501	-1.805730
43	1	-1.543097	-3.133199	-2.777512
44	1	-2.983135	-2.911736	-1.771441
45	1	1.015293	-4.984027	-1.532643
46	1	2.182679	-3.653948	-1.523030
47	1	0.811923	-3.609047	-2.634643
48	6	-2.986844	0.885372	0.043179
49	6	-3.642888	1.182231	1.263347
50	6	-3.725109	0.674293	-1.144086
51	6	-5.045926	1.202375	1.290594
52	6	-5.129442	0.712088	-1.071361
53	6	-5.789416	0.961284	0.133040
54	1	-5.551308	1.416745	2.227411
55	1	-5.702399	0.549482	-1.979254
56	1	-6.873938	0.980919	0.166485

57	6	2.990351	0.109452	0.862489
58	6	3.218991	0.522161	2.204793
59	6	4.071642	-0.396683	0.092106
60	6	4.507613	0.412728	2.749162
61	6	5.348972	-0.477662	0.675873
62	6	5.573928	-0.079107	1.992518
63	1	4.669960	0.717062	3.779601
64	1	6.170921	-0.866661	0.080462
65	1	6.565525	-0.155511	2.427693
66	6	-2.861976	1.489138	2.522590
67	1	-2.120605	0.714413	2.743143
68	1	-2.308994	2.433543	2.435149
69	1	-3.534933	1.577823	3.380246
70	6	-3.061192	0.439246	-2.480744
71	1	-2.365935	1.243833	-2.744725
72	1	-2.478286	-0.486088	-2.505947
73	1	-3.814345	0.378506	-3.271798
74	6	2.112533	1.079531	3.073487
75	1	2.316987	0.886011	4.132000
76	1	2.021883	2.167547	2.955155
77	1	1.143491	0.644177	2.817554
78	6	3.917346	-0.864938	-1.340143
79	1	4.341969	-1.868693	-1.468301
80	1	2.876641	-0.891145	-1.659824
81	1	4.454675	-0.202431	-2.031848

TS(7a-7a')Ar (E = -1494.9682937 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.274515	-0.582381	-0.373295
2	7	2.004982	0.657329	0.546200
3	6	1.157396	1.373702	-0.106728
4	7	-1.637878	0.156828	0.241267
5	6	-0.307181	-1.036647	-2.771151
6	6	0.129008	-2.292635	-2.250998
7	6	0.828767	-0.164731	-2.806282
8	17	0.299249	-2.463715	1.210077
9	6	1.529310	-2.197980	-1.977792
10	6	1.959309	-0.891706	-2.323063
11	6	-2.288277	1.301306	-0.226543
12	6	-1.874409	2.226026	-1.140262
13	1	1.198545	2.452175	-0.191152
14	6	-2.908133	3.250861	-1.332170
15	1	-0.922013	2.239451	-1.648045
16	6	-3.677977	1.721810	0.237649
17	6	-3.971683	2.981555	-0.539242
18	1	-4.418842	0.936784	0.046270
19	1	-3.704103	1.895593	1.320087
20	6	-5.259569	3.740210	-0.366468
21	6	-2.719952	4.405123	-2.283884
22	1	-3.584252	5.076671	-2.291337
23	1	-2.563157	4.048127	-3.311452
24	1	-1.835446	4.998579	-2.012588
25	1	-5.294293	4.630013	-1.004540
26	1	-5.396766	4.073262	0.673241
27	1	-6.133164	3.119951	-0.616741
28	6	-0.655863	-3.580368	-2.178212
29	6	-1.658896	-0.732908	-3.376168
30	6	0.892387	1.174333	-3.502815
31	6	3.379329	-0.382547	-2.310589
32	6	2.396395	-3.352291	-1.540629
33	1	-0.258672	-4.299918	-2.907661
34	1	-1.712078	-3.427144	-2.413866
35	1	-0.590807	-4.044783	-1.188230

36	1	-1.597814	-0.765143	-4.472952
37	1	-2.026994	0.257434	-3.089231
38	1	-2.410208	-1.463308	-3.065238
39	1	1.313114	1.052698	-4.511129
40	1	1.525039	1.892812	-2.970129
41	1	-0.100348	1.618555	-3.614395
42	1	3.858466	-0.560720	-3.283542
43	1	3.986955	-0.879651	-1.548341
44	1	3.422073	0.693882	-2.116876
45	1	2.563621	-4.039042	-2.382675
46	1	1.930983	-3.923130	-0.731132
47	1	3.377792	-3.015109	-1.193703
48	6	3.196398	1.046766	1.256199
49	6	3.713573	2.379083	1.271273
50	6	3.892738	0.015898	1.948430
51	6	4.889274	2.633341	1.997329
52	6	5.061603	0.328569	2.656955
53	6	5.560834	1.628788	2.691195
54	1	5.278380	3.646669	2.008590
55	1	5.579734	-0.466694	3.183196
56	1	6.466108	1.856732	3.244333
57	6	-2.311780	-0.463024	1.374088
58	6	-3.279836	-1.472215	1.167934
59	6	-2.016764	-0.011697	2.683502
60	6	-3.935839	-2.023703	2.280886
61	6	-2.693004	-0.586582	3.770797
62	6	-3.646629	-1.588982	3.576367
63	1	-4.678764	-2.800308	2.122449
64	1	-2.465227	-0.241611	4.775401
65	1	-4.161236	-2.025792	4.426581
66	6	3.107111	3.565623	0.549454
67	1	2.994335	3.389402	-0.527368
68	1	2.122375	3.842903	0.945017
69	1	3.758966	4.435712	0.669175
70	6	3.419777	-1.415703	1.955486
71	1	2.468065	-1.531774	2.480413
72	1	3.257465	-1.801124	0.945459
73	1	4.159433	-2.053597	2.448474
74	6	-3.608807	-1.975089	-0.217881
75	1	-4.472393	-2.646863	-0.189962
76	1	-3.833395	-1.156327	-0.910115
77	1	-2.766515	-2.531277	-0.643226
78	6	-0.981886	1.063939	2.927675
79	1	-1.005492	1.389760	3.972187
80	1	0.030892	0.697768	2.716641
81	1	-1.143495	1.940060	2.289423

7a'Ar (E = -1494.9742062 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.261382	-0.606721	-0.406174
2	7	-2.078402	0.203812	0.700316
3	6	-1.268227	-0.360421	1.524076
4	7	1.331258	0.736689	-0.052896
5	6	1.385835	-2.543890	-0.728360
6	6	0.579628	-2.515842	-1.905547
7	6	0.545204	-2.895341	0.368909
8	17	-1.231571	0.262010	-2.509961
9	6	-0.751748	-2.883303	-1.540027
10	6	-0.774873	-3.112340	-0.141251
11	6	2.351937	0.529331	0.887511
12	6	2.290812	-0.113611	2.080402
13	1	-1.468220	-0.386237	2.599589
14	6	3.621301	-0.151129	2.706713

15	1	1.394173	-0.512409	2.534255
16	6	3.787182	0.985996	0.681710
17	6	4.511426	0.488638	1.910597
18	1	4.202866	0.567499	-0.242958
19	1	3.862063	2.075452	0.581853
20	6	5.974278	0.759187	2.135061
21	6	3.857280	-0.789565	4.051927
22	1	4.898557	-0.693879	4.374721
23	1	3.609055	-1.859768	4.032521
24	1	3.222640	-0.328047	4.821211
25	1	6.324597	0.340567	3.084443
26	1	6.184347	1.838734	2.150122
27	1	6.592527	0.328083	1.334287
28	6	1.063458	-2.359272	-3.325875
29	6	2.891111	-2.437027	-0.688625
30	6	0.998087	-3.276914	1.758068
31	6	-1.915429	-3.727387	0.631430
32	6	-1.887049	-3.130490	-2.502290
33	1	1.121359	-3.342674	-3.813601
34	1	2.059613	-1.911256	-3.369757
35	1	0.385444	-1.734492	-3.916040
36	1	3.340492	-3.431006	-0.824734
37	1	3.247913	-2.035271	0.263082
38	1	3.274170	-1.793734	-1.486048
39	1	1.042084	-4.371895	1.848787
40	1	0.315665	-2.911165	2.533034
41	1	1.992860	-2.883812	1.978772
42	1	-1.879736	-4.822836	0.542162
43	1	-2.891546	-3.404614	0.255612
44	1	-1.862535	-3.487193	1.697326
45	1	-1.826190	-4.152247	-2.904370
46	1	-1.858957	-2.434090	-3.344381
47	1	-2.863128	-3.024706	-2.017806
48	6	-3.355364	0.802387	0.996441
49	6	-4.294406	0.145818	1.836527
50	6	-3.663834	2.056797	0.408594
51	6	-5.534930	0.764828	2.064141
52	6	-4.909135	2.639843	0.685936
53	6	-5.844110	2.003180	1.503341
54	1	-6.262194	0.256824	2.690397
55	1	-5.141142	3.604372	0.245367
56	1	-6.807208	2.464944	1.695678
57	6	1.380628	2.059080	-0.660868
58	6	1.836285	2.238293	-1.990029
59	6	1.014340	3.186440	0.123795
60	6	1.876950	3.537239	-2.525635
61	6	1.068880	4.465829	-0.451567
62	6	1.490208	4.645720	-1.770942
63	1	2.226098	3.671694	-3.545369
64	1	0.778633	5.324281	0.147645
65	1	1.526076	5.640871	-2.203055
66	6	-4.050383	-1.202170	2.482000
67	1	-3.456097	-1.863531	1.849160
68	1	-3.527629	-1.112054	3.443071
69	1	-5.005377	-1.698070	2.681915
70	6	-2.687415	2.795265	-0.473403
71	1	-1.765195	3.050170	0.058792
72	1	-2.394393	2.198792	-1.341368
73	1	-3.132766	3.728590	-0.830702
74	6	2.290808	1.080535	-2.846918
75	1	2.905533	1.438774	-3.679086
76	1	2.878098	0.359355	-2.271054
77	1	1.435130	0.543850	-3.270326

78	6	0.594443	3.045443	1.570943
79	1	0.143173	3.975223	1.931199
80	1	-0.124428	2.232682	1.710136
81	1	1.450734	2.813598	2.216701

TS(7a'-7c')Ar (E = -1494.966574 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.031359	-0.772856	-0.150422
2	7	-2.108564	-0.133708	0.237782
3	6	-1.501256	-0.345074	1.350229
4	7	1.295564	0.844938	0.447740
5	6	-0.109869	-3.052906	1.013621
6	6	1.275480	-2.704735	0.937339
7	6	-0.580253	-3.291714	-0.311986
8	17	-0.241828	-0.285009	-2.558049
9	6	1.656236	-2.722678	-0.437901
10	6	0.509674	-3.090930	-1.202558
11	6	1.267256	1.480980	1.695118
12	6	0.806235	1.030055	2.894559
13	1	-1.997078	-0.225807	2.316391
14	6	0.931604	2.079842	3.915010
15	1	0.423040	0.041241	3.099995
16	6	1.745559	2.911954	1.902637
17	6	1.479973	3.187549	3.362949
18	1	2.805328	3.034770	1.651603
19	1	1.199363	3.601890	1.247536
20	6	1.830717	4.504711	3.999883
21	6	0.503619	1.858661	5.343469
22	1	0.692281	2.736248	5.969639
23	1	1.038989	1.007413	5.786941
24	1	-0.569393	1.628508	5.402318
25	1	1.585392	4.517172	5.067309
26	1	1.292624	5.339598	3.527128
27	1	2.904126	4.725851	3.903854
28	6	2.182267	-2.638741	2.146659
29	6	-0.810320	-3.387574	2.309025
30	6	-1.936213	-3.814354	-0.727166
31	6	0.513424	-3.424695	-2.671621
32	6	3.048514	-2.593122	-1.011465
33	1	2.036739	-3.536318	2.762619
34	1	1.992534	-1.771117	2.788668
35	1	3.234778	-2.613124	1.854467
36	1	-0.406499	-4.325127	2.717609
37	1	-1.883980	-3.533185	2.170849
38	1	-0.670292	-2.613475	3.070880
39	1	-1.861208	-4.866602	-1.034726
40	1	-2.350808	-3.256616	-1.574516
41	1	-2.661275	-3.765486	0.088969
42	1	0.783906	-4.481996	-2.810228
43	1	1.233312	-2.816235	-3.225060
44	1	-0.467433	-3.264605	-3.127257
45	1	3.396601	-3.571206	-1.371438
46	1	3.763628	-2.239380	-0.266742
47	1	3.085891	-1.902124	-1.860695
48	6	-3.504692	0.187916	0.053344
49	6	-4.520666	-0.538452	0.729518
50	6	-3.843476	1.239016	-0.835775
51	6	-5.862547	-0.210607	0.471572
52	6	-5.197271	1.539144	-1.044162
53	6	-6.206081	0.818060	-0.404106
54	1	-6.641109	-0.778621	0.971877
55	1	-5.452876	2.349494	-1.719633
56	1	-7.249207	1.055049	-0.586738

57	6	2.332175	1.356353	-0.445215
58	6	3.686941	0.974390	-0.238928
59	6	2.019180	2.279816	-1.475107
60	6	4.670151	1.404380	-1.142799
61	6	3.036469	2.695534	-2.353006
62	6	4.348276	2.244638	-2.211296
63	1	5.698452	1.088106	-0.990531
64	1	2.786462	3.393907	-3.146949
65	1	5.117292	2.567132	-2.906311
66	6	-4.247449	-1.658560	1.709597
67	1	-3.359566	-2.232894	1.443268
68	1	-4.097444	-1.283358	2.730182
69	1	-5.098067	-2.346561	1.740766
70	6	-2.788847	2.073983	-1.514347
71	1	-2.223693	2.665586	-0.783855
72	1	-2.068234	1.455578	-2.054566
73	1	-3.249368	2.770871	-2.220986
74	6	4.113083	0.196442	0.983821
75	1	5.030368	-0.370106	0.791468
76	1	4.320669	0.877097	1.821797
77	1	3.335744	-0.484014	1.323284
78	6	0.646910	2.888780	-1.637330
79	1	0.109740	2.444943	-2.481144
80	1	0.035531	2.737856	-0.746843
81	1	0.732003	3.966379	-1.821950

7c'Ar (E = -1494.9729006 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.015747	-0.758956	-0.120506
2	7	-2.125635	-0.183539	0.268122
3	6	-1.507609	-0.283255	1.388751
4	7	1.358862	0.840903	0.099451
5	6	0.064103	-2.917183	1.222398
6	6	1.403500	-2.425202	1.262080
7	6	-0.232398	-3.273261	-0.127010
8	17	-0.559953	-0.611336	-2.549483
9	6	1.948650	-2.516833	-0.052205
10	6	0.936997	-3.029265	-0.910625
11	6	0.751739	2.118711	0.245351
12	6	-0.087998	2.556591	1.212904
13	1	-2.011118	-0.089806	2.342325
14	6	-0.484229	3.950008	0.961225
15	1	-0.406266	1.985873	2.075271
16	6	0.954269	3.261085	-0.735998
17	6	0.128287	4.387917	-0.164952
18	1	2.009554	3.535782	-0.849227
19	1	0.598294	2.970309	-1.732379
20	6	0.069691	5.741446	-0.817793
21	6	-1.412814	4.699882	1.881444
22	1	-1.568166	5.732466	1.554318
23	1	-1.014581	4.727473	2.905062
24	1	-2.395906	4.211994	1.932158
25	1	-0.571914	6.434267	-0.263613
26	1	-0.319716	5.674845	-1.843794
27	1	1.069134	6.194360	-0.886622
28	6	2.177481	-2.136590	2.524729
29	6	-0.760872	-3.230425	2.447784
30	6	-1.482970	-3.949127	-0.641424
31	6	1.130633	-3.458968	-2.342444
32	6	3.408683	-2.385338	-0.409336
33	1	2.557830	-3.074853	2.954796
34	1	1.554605	-1.658190	3.287426
35	1	3.036284	-1.488371	2.335783

36	1	-0.392300	-4.154286	2.915994
37	1	-1.814674	-3.386945	2.206635
38	1	-0.702650	-2.436799	3.199705
39	1	-1.298659	-5.020429	-0.803486
40	1	-1.812682	-3.523838	-1.595300
41	1	-2.312871	-3.864969	0.065517
42	1	1.481036	-4.501018	-2.374691
43	1	1.872184	-2.841912	-2.858197
44	1	0.200640	-3.394481	-2.912392
45	1	3.901086	-3.361532	-0.288876
46	1	3.929314	-1.668917	0.228893
47	1	3.554629	-2.072607	-1.446396
48	6	-3.511537	0.153372	0.055604
49	6	-4.540173	-0.584943	0.694030
50	6	-3.819686	1.230196	-0.812507
51	6	-5.874671	-0.224748	0.445994
52	6	-5.169257	1.559361	-1.014436
53	6	-6.193361	0.841364	-0.395362
54	1	-6.666115	-0.797252	0.920213
55	1	-5.408940	2.388988	-1.672242
56	1	-7.230926	1.105320	-0.572974
57	6	2.806911	0.940667	0.073672
58	6	3.503648	1.168921	1.290611
59	6	3.523569	0.861986	-1.148248
60	6	4.906460	1.256415	1.270297
61	6	4.924698	0.970461	-1.123474
62	6	5.618826	1.155862	0.074016
63	1	5.435771	1.415591	2.205708
64	1	5.470162	0.910310	-2.060918
65	1	6.701756	1.230756	0.072974
66	6	-4.267711	-1.762561	1.605129
67	1	-3.481387	-2.407935	1.205750
68	1	-3.956378	-1.452666	2.610237
69	1	-5.172438	-2.366955	1.718593
70	6	-2.747740	2.046600	-1.494182
71	1	-2.135309	2.599044	-0.772300
72	1	-2.072164	1.411757	-2.074304
73	1	-3.203646	2.775398	-2.171573
74	6	2.778147	1.353528	2.605169
75	1	3.439244	1.123159	3.447121
76	1	2.434738	2.389243	2.723004
77	1	1.890829	0.720179	2.668934
78	6	2.828987	0.682010	-2.479345
79	1	2.281441	-0.263018	-2.545304
80	1	2.089725	1.467498	-2.664367
81	1	3.559876	0.706062	-3.293914

TS(7c'-7c)Ar (E = -1494.958347 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.221236	-0.407328	-0.282805
2	7	-2.201602	0.628748	-0.212392
3	6	-1.276715	1.514389	-0.120463
4	7	1.630159	0.615262	-0.009716
5	6	-0.639186	-1.921161	1.681872
6	6	0.640027	-2.373889	1.217623
7	6	-1.617764	-2.315316	0.717560
8	17	-0.241132	-0.624610	-2.717593
9	6	0.454289	-2.979594	-0.050893
10	6	-0.938494	-2.936176	-0.365444
11	6	1.766399	2.020919	-0.228968
12	6	1.279642	3.062929	0.479685
13	1	-1.510574	2.578805	-0.021881
14	6	1.678549	4.340361	-0.134634

15	1	0.670975	2.989795	1.372132
16	6	2.545809	2.595041	-1.402100
17	6	2.427149	4.090610	-1.234259
18	1	3.591299	2.265251	-1.413792
19	1	2.100284	2.261721	-2.348166
20	6	3.079218	5.054875	-2.187643
21	6	1.279024	5.671871	0.448785
22	1	1.678388	6.509853	-0.131064
23	1	1.641451	5.774752	1.481153
24	1	0.185473	5.777441	0.480777
25	1	2.884266	6.096435	-1.910555
26	1	2.715813	4.911150	-3.215542
27	1	4.169937	4.916752	-2.214641
28	6	1.867901	-2.505527	2.081745
29	6	-0.922373	-1.410515	3.078345
30	6	-3.113202	-2.280259	0.915114
31	6	-1.574546	-3.617128	-1.551722
32	6	1.491924	-3.730337	-0.848319
33	1	1.808485	-3.450246	2.643050
34	1	1.951035	-1.697141	2.810951
35	1	2.790120	-2.522237	1.498205
36	1	-0.969485	-2.246842	3.790768
37	1	-1.880319	-0.884595	3.133141
38	1	-0.144153	-0.726571	3.433638
39	1	-3.445989	-3.223360	1.371561
40	1	-3.655860	-2.161808	-0.026323
41	1	-3.425595	-1.468122	1.576311
42	1	-1.581533	-4.706741	-1.406089
43	1	-1.032373	-3.406295	-2.478893
44	1	-2.611310	-3.298252	-1.694869
45	1	1.441896	-4.804555	-0.617577
46	1	2.505897	-3.390869	-0.620015
47	1	1.331689	-3.621744	-1.926177
48	6	-3.622631	0.863830	-0.144412
49	6	-4.181176	1.464973	1.009604
50	6	-4.431081	0.464549	-1.233830
51	6	-5.574849	1.638783	1.054941
52	6	-5.815183	0.675216	-1.147132
53	6	-6.388404	1.251864	-0.011050
54	1	-6.017384	2.084995	1.940402
55	1	-6.442584	0.381027	-1.982811
56	1	-7.462297	1.397910	0.042923
57	6	2.941512	0.063764	0.310798
58	6	3.477025	0.278786	1.611123
59	6	3.716793	-0.628111	-0.658466
60	6	4.749841	-0.224910	1.927042
61	6	4.982309	-1.123892	-0.294454
62	6	5.502048	-0.929434	0.986715
63	1	5.144233	-0.063203	2.926553
64	1	5.569289	-1.652036	-1.040578
65	1	6.483406	-1.315148	1.244798
66	6	-3.346307	1.915587	2.190980
67	1	-2.510232	1.239294	2.393974
68	1	-2.919590	2.914107	2.031969
69	1	-3.964546	1.968391	3.092122
70	6	-3.831394	-0.134302	-2.483504
71	1	-3.178749	0.578542	-3.000544
72	1	-3.209469	-1.007626	-2.265312
73	1	-4.619566	-0.437818	-3.178581
74	6	2.711755	1.025018	2.680266
75	1	3.092408	0.770136	3.674854
76	1	2.801744	2.110343	2.551699
77	1	1.642188	0.796455	2.641941

78	6	3.259978	-0.813014	-2.089493
79	1	4.045333	-1.304963	-2.672691
80	1	2.353886	-1.416247	-2.174133
81	1	3.031671	0.142899	-2.569734

7cAr (E = -1494.9638696 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.203154	-0.615908	-0.305511
2	7	-2.012376	0.600217	-0.315420
3	6	-1.154116	1.208452	-1.062497
4	7	1.634994	0.482266	-0.097043
5	6	-0.312447	-1.785059	1.962480
6	6	0.763803	-2.472630	1.310903
7	6	-1.522463	-2.121115	1.278129
8	17	-0.298083	-1.444250	-2.625241
9	6	0.228382	-3.166040	0.198277
10	6	-1.186662	-2.950381	0.174952
11	6	1.616130	1.890646	-0.154205
12	6	0.795599	2.765219	0.480459
13	1	-1.413321	2.132476	-1.587886
14	6	1.106387	4.145730	0.079435
15	1	0.052561	2.506088	1.222520
16	6	2.554255	2.701810	-1.034164
17	6	2.135764	4.134872	-0.800219
18	1	3.608926	2.536860	-0.785457
19	1	2.435922	2.406486	-2.084507
20	6	2.836628	5.288160	-1.465069
21	6	0.359520	5.330638	0.637131
22	1	0.753996	6.279276	0.260142
23	1	0.421390	5.353277	1.734169
24	1	-0.707260	5.284466	0.376867
25	1	2.411555	6.251227	-1.162830
26	1	2.768062	5.224743	-2.560792
27	1	3.907623	5.304303	-1.215252
28	6	2.150707	-2.667666	1.870096
29	6	-0.243581	-1.127089	3.322561
30	6	-2.919032	-1.843280	1.778133
31	6	-2.156108	-3.659204	-0.738878
32	6	0.974202	-4.111520	-0.709921
33	1	2.180671	-3.604293	2.446101
34	1	2.441762	-1.858336	2.541388
35	1	2.912422	-2.734501	1.089145
36	1	-0.460443	-1.863287	4.110193
37	1	-0.972886	-0.317506	3.431372
38	1	0.746613	-0.712799	3.527372
39	1	-3.244273	-2.660885	2.437463
40	1	-3.644979	-1.768637	0.964081
41	1	-2.975909	-0.916688	2.355042
42	1	-2.325905	-4.687059	-0.387273
43	1	-1.776169	-3.713276	-1.763215
44	1	-3.128948	-3.158409	-0.768623
45	1	0.806062	-5.153073	-0.400518
46	1	2.053190	-3.930050	-0.683827
47	1	0.641185	-4.014681	-1.748318
48	6	-3.392222	0.956103	-0.082810
49	6	-3.750474	1.659124	1.087356
50	6	-4.359713	0.562716	-1.036204
51	6	-5.107925	1.950789	1.298550
52	6	-5.704378	0.876562	-0.782047
53	6	-6.080952	1.561501	0.375858
54	1	-5.395023	2.488182	2.197327
55	1	-6.457065	0.577071	-1.504896
56	1	-7.125934	1.790922	0.557098

57	6	2.991792	-0.012407	0.073361
58	6	3.672727	0.232030	1.299346
59	6	3.671496	-0.674830	-0.982065
60	6	4.983731	-0.239382	1.467372
61	6	4.984416	-1.135005	-0.767960
62	6	5.639650	-0.930690	0.446347
63	1	5.488759	-0.060555	2.412704
64	1	5.498800	-1.638241	-1.581968
65	1	6.653866	-1.290073	0.590006
66	6	-2.715652	2.121777	2.087333
67	1	-1.973794	1.345132	2.300784
68	1	-2.165431	2.996543	1.718159
69	1	-3.190625	2.405366	3.031044
70	6	-3.974127	-0.164949	-2.304754
71	1	-3.395589	0.475572	-2.982008
72	1	-3.350542	-1.042632	-2.106487
73	1	-4.868212	-0.493292	-2.842197
74	6	3.025624	0.991821	2.436100
75	1	3.517492	0.755866	3.385708
76	1	3.092054	2.076639	2.285237
77	1	1.961491	0.759418	2.520920
78	6	3.062749	-0.861954	-2.353759
79	1	3.853304	-0.958620	-3.105582
80	1	2.437479	-1.758972	-2.417883
81	1	2.421054	-0.022270	-2.629992

TS(7c-8b)Ar (E = -1494.9485309 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.018563	-0.646544	-0.302670
2	7	-1.684612	0.601954	-0.218373
3	6	-0.720404	1.351662	-0.800254
4	7	1.836196	0.586670	0.167062
5	6	-0.174742	-2.019488	1.830292
6	6	0.920235	-2.622397	1.128739
7	6	-1.371021	-2.296002	1.096576
8	17	0.036142	-1.247943	-2.685678
9	6	0.404785	-3.224679	-0.047387
10	6	-1.010667	-3.021532	-0.070190
11	6	1.631525	1.905902	0.270541
12	6	0.382533	2.521970	0.516074
13	1	-0.981735	2.161850	-1.479522
14	6	0.557369	3.978056	0.296531
15	1	-0.262849	2.175228	1.308025
16	6	2.645018	2.978482	-0.081521
17	6	1.826432	4.252323	-0.075794
18	1	3.464447	3.022619	0.647106
19	1	3.116615	2.765724	-1.048327
20	6	2.457726	5.573078	-0.422382
21	6	-0.586053	4.941074	0.480644
22	1	-0.296697	5.973242	0.261642
23	1	-0.960503	4.909509	1.513673
24	1	-1.429800	4.678941	-0.171546
25	1	1.743515	6.399313	-0.348763
26	1	2.858716	5.570011	-1.446382
27	1	3.300877	5.799053	0.247034
28	6	2.318100	-2.822934	1.662168
29	6	-0.136397	-1.494368	3.248575
30	6	-2.778951	-2.067099	1.589448
31	6	-1.962508	-3.630936	-1.070143
32	6	1.177590	-4.077994	-1.021947
33	1	2.395776	-3.815636	2.128750
34	1	2.579819	-2.082286	2.419914
35	1	3.077319	-2.768598	0.876599

36	1	-0.424372	-2.288313	3.952674
37	1	-0.827384	-0.659967	3.406460
38	1	0.863390	-1.156660	3.532650
39	1	-3.131761	-2.955545	2.132886
40	1	-3.479416	-1.880453	0.770812
41	1	-2.841658	-1.217526	2.273443
42	1	-2.165392	-4.680558	-0.813111
43	1	-1.549463	-3.607453	-2.082953
44	1	-2.922825	-3.105843	-1.088234
45	1	1.051127	-5.143375	-0.781289
46	1	2.249832	-3.859023	-0.990658
47	1	0.834516	-3.923780	-2.049497
48	6	-3.073911	0.937023	-0.079601
49	6	-3.577798	1.451367	1.138917
50	6	-3.939395	0.737989	-1.186624
51	6	-4.947841	1.749928	1.235141
52	6	-5.299814	1.053324	-1.047169
53	6	-5.807625	1.555313	0.153811
54	1	-5.334881	2.138060	2.173200
55	1	-5.962376	0.899461	-1.893912
56	1	-6.863421	1.789768	0.245453
57	6	3.226365	0.172749	0.238852
58	6	3.880866	0.208037	1.498956
59	6	3.931431	-0.232611	-0.920005
60	6	5.211793	-0.225703	1.589175
61	6	5.266314	-0.656747	-0.783349
62	6	5.902899	-0.667751	0.457980
63	1	5.705770	-0.211968	2.556438
64	1	5.808459	-0.964928	-1.672659
65	1	6.932291	-1.001467	0.541650
66	6	-2.688691	1.708734	2.335095
67	1	-1.868910	0.988073	2.394514
68	1	-2.238847	2.709526	2.293527
69	1	-3.263512	1.651045	3.265273
70	6	-3.424991	0.198359	-2.501979
71	1	-2.693827	0.872074	-2.963619
72	1	-2.915609	-0.763145	-2.380890
73	1	-4.250210	0.064087	-3.207836
74	6	3.186899	0.722336	2.741768
75	1	3.714636	0.392606	3.641995
76	1	3.157485	1.820283	2.764693
77	1	2.149705	0.383486	2.801774
78	6	3.320457	-0.186098	-2.301877
79	1	4.104177	-0.062893	-3.056457
80	1	2.770722	-1.101969	-2.545105
81	1	2.607115	0.635373	-2.407949

8bAr (E = -1494.9782064 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.183468	-0.720226	-0.487718
2	7	-1.718699	0.453651	0.003321
3	6	-0.950824	1.310924	-0.893290
4	7	1.579128	0.790052	0.154811
5	6	0.091118	-2.236817	1.551769
6	6	1.050887	-2.749290	0.618488
7	6	-1.212335	-2.489912	1.027799
8	17	-0.253780	-1.154243	-2.931938
9	6	0.340073	-3.297944	-0.480631
10	6	-1.057047	-3.122470	-0.238432
11	6	1.243921	2.032646	0.049041
12	6	-0.175069	2.449500	-0.231279
13	1	-1.450600	1.597302	-1.819426
14	6	0.036969	3.782195	-0.945454

15	1	-0.636395	2.680020	0.746196
16	6	2.148689	3.236796	-0.018414
17	6	1.301408	4.217652	-0.813242
18	1	2.376278	3.624767	0.984764
19	1	3.112217	2.997935	-0.480093
20	6	1.918713	5.502616	-1.294021
21	6	-1.120183	4.477311	-1.607367
22	1	-0.848318	5.469925	-1.978085
23	1	-1.955117	4.590540	-0.902187
24	1	-1.500290	3.891197	-2.453133
25	1	1.204806	6.123928	-1.842034
26	1	2.771168	5.303239	-1.958651
27	1	2.304200	6.093691	-0.450694
28	6	2.529578	-2.924817	0.876248
29	6	0.389941	-1.811154	2.971206
30	6	-2.509324	-2.328102	1.781811
31	6	-2.165402	-3.672824	-1.104215
32	6	0.931552	-4.077265	-1.628278
33	1	2.713161	-3.898399	1.353638
34	1	2.931161	-2.153060	1.537317
35	1	3.114390	-2.901464	-0.048224
36	1	0.275296	-2.666274	3.653440
37	1	-0.286039	-1.025422	3.322606
38	1	1.415352	-1.447325	3.077169
39	1	-2.738113	-3.249982	2.336337
40	1	-3.351907	-2.124505	1.115211
41	1	-2.462503	-1.509603	2.504229
42	1	-2.309162	-4.745430	-0.909227
43	1	-1.939304	-3.554447	-2.168612
44	1	-3.119144	-3.173200	-0.906841
45	1	0.858244	-5.157094	-1.433767
46	1	1.990310	-3.841462	-1.777761
47	1	0.410703	-3.866775	-2.566946
48	6	-3.009231	0.791689	0.500899
49	6	-3.184057	1.252976	1.832079
50	6	-4.142871	0.668619	-0.353029
51	6	-4.475559	1.582392	2.281911
52	6	-5.411972	1.008246	0.136204
53	6	-5.585568	1.465893	1.446406
54	1	-4.601735	1.932180	3.303587
55	1	-6.272200	0.906461	-0.519907
56	1	-6.575720	1.722476	1.810308
57	6	2.967603	0.499061	0.463481
58	6	3.437435	0.671515	1.786289
59	6	3.821440	0.039954	-0.566155
60	6	4.776570	0.347043	2.064981
61	6	5.155808	-0.253611	-0.244151
62	6	5.632638	-0.111103	1.061440
63	1	5.144037	0.464297	3.080096
64	1	5.821018	-0.596604	-1.030632
65	1	6.664895	-0.351702	1.293683
66	6	-2.025583	1.409034	2.796207
67	1	-1.114379	0.963502	2.394334
68	1	-1.818249	2.467740	3.004579
69	1	-2.248380	0.934496	3.760308
70	6	-3.999086	0.170731	-1.773016
71	1	-3.476976	0.896358	-2.408881
72	1	-3.414389	-0.753662	-1.822476
73	1	-4.981830	-0.016345	-2.217338
74	6	2.561349	1.215236	2.895908
75	1	2.919478	0.870023	3.870622
76	1	2.578406	2.313421	2.918921
77	1	1.517420	0.911610	2.789959

78	6	3.332864	-0.126931	-1.986610
79	1	4.173426	-0.316262	-2.660293
80	1	2.638623	-0.971030	-2.087552
81	1	2.800467	0.758680	-2.350332

TS(8b-18)Ar (E = -1494.9614203 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.205637	-0.553035	-0.389110
2	7	-1.598340	0.827592	0.051672
3	6	-0.661580	1.736288	-0.524031
4	7	1.660582	0.394152	0.283398
5	6	-0.667942	-2.200918	1.477636
6	6	0.508816	-2.713394	0.845159
7	6	-1.755275	-2.327040	0.558968
8	17	-0.110040	-0.629354	-2.862282
9	6	0.157715	-3.119123	-0.470147
10	6	-1.240789	-2.879873	-0.647972
11	6	1.478034	1.680970	-0.062790
12	6	0.311438	2.520033	0.348572
13	1	-0.871768	2.184229	-1.494977
14	6	0.662304	3.908569	-0.127413
15	1	0.071172	2.456168	1.412818
16	6	2.451658	2.535088	-0.850191
17	6	1.827155	3.915865	-0.796642
18	1	3.448373	2.493311	-0.389108
19	1	2.579249	2.167166	-1.875407
20	6	2.522981	5.070220	-1.464374
21	6	-0.279861	5.051669	0.135285
22	1	0.054656	5.983488	-0.329988
23	1	-0.385027	5.230953	1.214556
24	1	-1.282484	4.820142	-0.248052
25	1	1.968340	6.006869	-1.357514
26	1	2.657157	4.876820	-2.538073
27	1	3.526361	5.220126	-1.040827
28	6	1.813213	-3.003777	1.546882
29	6	-0.788566	-1.862294	2.945639
30	6	-3.216086	-2.121570	0.880288
31	6	-2.052604	-3.314420	-1.844034
32	6	1.053695	-3.816748	-1.464830
33	1	1.768842	-3.999494	2.011800
34	1	2.023842	-2.281251	2.339428
35	1	2.665314	-2.996502	0.862136
36	1	-0.851077	-2.783415	3.543067
37	1	-1.687796	-1.276291	3.152208
38	1	0.072642	-1.295651	3.315691
39	1	-3.646609	-3.050631	1.280861
40	1	-3.795508	-1.845309	-0.005310
41	1	-3.368764	-1.335210	1.623495
42	1	-2.329102	-4.374482	-1.749600
43	1	-1.492935	-3.193340	-2.775692
44	1	-2.979839	-2.740419	-1.938361
45	1	0.889228	-4.903356	-1.435473
46	1	2.111988	-3.638526	-1.250162
47	1	0.858218	-3.478808	-2.487759
48	6	-2.934898	1.235612	0.372016
49	6	-3.272240	1.627150	1.692323
50	6	-3.928409	1.240621	-0.643780
51	6	-4.599814	1.992643	1.978634
52	6	-5.238099	1.623722	-0.317450
53	6	-5.580082	1.994535	0.986183
54	1	-4.856921	2.280956	2.994473
55	1	-5.994607	1.624704	-1.097209
56	1	-6.599838	2.280973	1.223936

57	6	3.024710	-0.048326	0.514520
58	6	3.511737	0.112289	1.839525
59	6	3.845594	-0.616452	-0.486141
60	6	4.800903	-0.340510	2.153077
61	6	5.131934	-1.062505	-0.124164
62	6	5.609076	-0.934594	1.179377
63	1	5.168004	-0.225564	3.168567
64	1	5.761247	-1.507799	-0.889486
65	1	6.603045	-1.287638	1.434794
66	6	-2.246699	1.687843	2.803959
67	1	-1.417088	1.002278	2.621742
68	1	-1.822144	2.697036	2.897571
69	1	-2.701642	1.440434	3.769623
70	6	-3.599699	0.837337	-2.063157
71	1	-2.844302	1.492469	-2.511712
72	1	-3.192166	-0.178022	-2.116179
73	1	-4.495600	0.878634	-2.690579
74	6	2.667612	0.769476	2.909536
75	1	3.159966	0.701105	3.883859
76	1	2.498826	1.833318	2.696832
77	1	1.678080	0.306753	2.987668
78	6	3.437071	-0.718414	-1.938004
79	1	3.833454	-1.634310	-2.389381
80	1	2.357564	-0.711340	-2.083595
81	1	3.842324	0.123880	-2.516239

TS(8b-19)Ar (E = -1494.9223873 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.422771	-0.961622	0.693594
2	7	-1.710988	0.488829	-0.015882
3	6	-0.469037	0.888742	-0.575045
4	7	2.387036	0.520605	-1.184688
5	6	-1.164656	-1.340100	3.058476
6	6	0.109120	-1.982235	2.940649
7	6	-2.100688	-2.055441	2.243409
8	17	0.229878	-2.390795	-1.175478
9	6	-0.044536	-3.094383	2.064289
10	6	-1.403692	-3.135012	1.630816
11	6	1.951444	1.453609	-0.446736
12	6	0.621655	1.346389	0.284832
13	1	-0.238165	0.760962	-1.624473
14	6	0.589668	2.591943	1.156520
15	1	0.906079	0.411854	1.186209
16	6	2.599598	2.774685	-0.091615
17	6	1.668191	3.364410	0.935335
18	1	3.618906	2.629609	0.286323
19	1	2.697209	3.414621	-0.978363
20	6	1.996081	4.703484	1.538868
21	6	-0.558083	2.897933	2.069729
22	1	-0.356517	3.773348	2.693000
23	1	-0.774773	2.053337	2.732074
24	1	-1.466519	3.092278	1.491821
25	1	1.277490	5.011858	2.302739
26	1	2.018507	5.483104	0.764056
27	1	2.994120	4.685161	1.998547
28	6	1.339432	-1.665697	3.761427
29	6	-1.501340	-0.299649	4.101900
30	6	-3.599322	-1.867399	2.213370
31	6	-2.026179	-4.220440	0.788133
32	6	1.010773	-4.124252	1.743338
33	1	1.332280	-2.238577	4.699859
34	1	1.392990	-0.604584	4.023923
35	1	2.261013	-1.922162	3.228978

36	1	-1.723808	-0.794044	5.058641
37	1	-2.377742	0.294888	3.833382
38	1	-0.668800	0.388218	4.282465
39	1	-4.085821	-2.617943	2.852393
40	1	-4.010273	-1.978014	1.204703
41	1	-3.891388	-0.882043	2.580621
42	1	-2.300992	-5.079626	1.416663
43	1	-1.337498	-4.574828	0.015903
44	1	-2.935920	-3.872515	0.288676
45	1	0.932206	-4.977695	2.431734
46	1	2.021942	-3.715826	1.841112
47	1	0.904480	-4.503624	0.723204
48	6	-2.986505	0.790031	-0.601933
49	6	-4.015791	1.353213	0.200430
50	6	-3.261555	0.498542	-1.972380
51	6	-5.274428	1.617708	-0.366056
52	6	-4.531891	0.788804	-2.494230
53	6	-5.539517	1.346911	-1.706071
54	1	-6.048546	2.047293	0.264433
55	1	-4.728913	0.554575	-3.536603
56	1	-6.516596	1.557087	-2.129461
57	6	3.635437	0.672750	-1.857826
58	6	4.808776	0.161500	-1.255739
59	6	3.665338	1.237873	-3.154196
60	6	6.020173	0.262906	-1.956499
61	6	4.898437	1.317704	-3.819726
62	6	6.072114	0.841562	-3.227899
63	1	6.925748	-0.125023	-1.498710
64	1	4.929780	1.751014	-4.815386
65	1	7.016582	0.909287	-3.758281
66	6	-3.817276	1.715910	1.654662
67	1	-2.909362	1.272009	2.054402
68	1	-3.742539	2.804068	1.783607
69	1	-4.670238	1.384299	2.258679
70	6	-2.251488	-0.142315	-2.898495
71	1	-1.530858	0.587667	-3.290905
72	1	-1.675896	-0.930498	-2.406607
73	1	-2.761119	-0.584278	-3.760698
74	6	4.753009	-0.492322	0.106686
75	1	5.727810	-0.909588	0.376101
76	1	4.464520	0.215800	0.895080
77	1	4.014344	-1.303599	0.123717
78	6	2.395469	1.722620	-3.817700
79	1	2.595943	2.050294	-4.841996
80	1	1.640319	0.927812	-3.853803
81	1	1.941446	2.566355	-3.281762

19Ar (E = -1494.9646212 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-1.389013	-0.775608	-0.153573
2	7	-0.676457	1.143802	0.296317
3	6	0.713467	0.957428	0.299265
4	7	3.437756	0.395412	-0.361661
5	6	-3.697471	-0.477393	0.845426
6	6	-3.426986	-1.879267	0.846513
7	6	-3.781494	-0.039894	-0.509185
8	17	-0.206214	-1.688605	-2.041627
9	6	-3.348834	-2.310168	-0.511541
10	6	-3.561780	-1.177854	-1.349222
11	6	2.901914	-0.078289	0.692908
12	6	1.493455	0.185622	1.115234
13	1	1.261559	1.443401	-0.508471
14	6	1.339127	-0.424639	2.453979

15	1	-0.814513	-1.934342	1.122456
16	6	3.533057	-0.979947	1.737741
17	6	2.475837	-1.072174	2.805833
18	1	3.782804	-1.958486	1.307837
19	1	4.475206	-0.565797	2.115509
20	6	2.785900	-1.803629	4.081076
21	6	0.149688	-0.221735	3.354252
22	1	0.278843	-0.745894	4.304821
23	1	-0.773377	-0.587836	2.895884
24	1	0.011799	0.841967	3.572475
25	1	1.937953	-1.842365	4.769584
26	1	3.628609	-1.331939	4.607365
27	1	3.090643	-2.837242	3.863225
28	6	-3.436083	-2.777314	2.059529
29	6	-4.029417	0.345931	2.066735
30	6	-4.261438	1.314748	-0.972536
31	6	-3.695595	-1.203734	-2.853356
32	6	-3.142021	-3.733437	-0.969828
33	1	-4.461528	-3.109298	2.276699
34	1	-3.057988	-2.264059	2.948667
35	1	-2.819756	-3.667315	1.906200
36	1	-5.076015	0.179909	2.358855
37	1	-3.905842	1.415794	1.880332
38	1	-3.406480	0.078230	2.926824
39	1	-5.359315	1.319687	-1.027687
40	1	-3.883627	1.566895	-1.967146
41	1	-3.957987	2.115496	-0.293822
42	1	-4.730536	-1.441877	-3.135688
43	1	-3.042645	-1.955083	-3.305919
44	1	-3.447710	-0.237133	-3.302841
45	1	-4.098292	-4.275075	-0.980246
46	1	-2.462029	-4.277968	-0.306328
47	1	-2.723755	-3.775560	-1.979330
48	6	-1.094036	2.487209	-0.068597
49	6	-1.432223	3.396709	0.964067
50	6	-1.137905	2.902456	-1.424866
51	6	-1.866125	4.688776	0.623660
52	6	-1.560009	4.210977	-1.718607
53	6	-1.934680	5.098340	-0.708716
54	1	-2.135636	5.377850	1.418685
55	1	-1.591803	4.528494	-2.756709
56	1	-2.264802	6.101943	-0.957134
57	6	4.798662	0.106097	-0.662172
58	6	5.110041	-1.002282	-1.485447
59	6	5.810245	0.992920	-0.221784
60	6	6.452557	-1.226101	-1.828523
61	6	7.139299	0.732001	-0.588808
62	6	7.465622	-0.371989	-1.382117
63	1	6.697853	-2.075876	-2.459616
64	1	7.919852	1.408889	-0.252370
65	1	8.498280	-0.558205	-1.660049
66	6	-1.298817	3.024531	2.422321
67	1	-1.753068	2.055946	2.641037
68	1	-0.242660	2.955220	2.713027
69	1	-1.768110	3.781569	3.058119
70	6	-0.756344	1.992486	-2.573613
71	1	0.195550	1.479419	-2.412785
72	1	-1.509401	1.214967	-2.753331
73	1	-0.668453	2.570997	-3.498071
74	6	4.015971	-1.913760	-1.993600
75	1	4.412169	-2.624407	-2.725313
76	1	3.550715	-2.493582	-1.185612
77	1	3.208514	-1.342297	-2.466094

78	6	5.459673	2.203074	0.614700
79	1	6.338969	2.835604	0.769852
80	1	4.680930	2.806280	0.131731
81	1	5.071028	1.924457	1.603357

2aAd (E = -1171.657922 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-1.403238	0.253497	-0.202688
2	7	2.017969	0.043106	0.037760
3	6	-3.349357	-1.225085	0.538789
4	6	-2.341139	-1.434638	1.526239
5	6	-2.864387	-1.765893	-0.696356
6	17	-1.167553	0.214514	-2.718222
7	6	-1.229575	-2.066925	0.898374
8	6	-1.561392	-2.288349	-0.474155
9	6	0.856179	0.076995	-0.018372
10	6	-1.128452	1.487667	1.796503
11	6	-2.293409	2.095069	1.149665
12	1	-0.213642	2.080168	1.823428
13	6	-0.751175	2.568064	-0.649621
14	6	-2.074329	2.656653	-0.122878
15	1	-0.605365	2.860256	-1.682975
16	1	0.086508	2.786520	0.004501
17	6	-3.188239	3.256776	-0.963333
18	6	-3.600726	2.280182	1.898004
19	1	-4.485489	2.232076	1.255474
20	1	-3.601679	3.266530	2.386981
21	1	-3.711386	1.534365	2.689974
22	1	-3.293796	4.326296	-0.729385
23	1	-4.162240	2.784862	-0.796297
24	1	-2.943977	3.177850	-2.027633
25	6	-2.511742	-1.291765	3.018009
26	6	-4.785397	-0.824211	0.790503
27	6	-3.686289	-1.926297	-1.952567
28	6	-0.735132	-3.055325	-1.477216
29	6	-0.019998	-2.609624	1.623345
30	1	-2.903601	-2.229887	3.437914
31	1	-3.214664	-0.497851	3.283828
32	1	-1.563304	-1.078262	3.520259
33	1	-5.418275	-1.719507	0.876406
34	1	-5.195247	-0.216262	-0.023540
35	1	-4.894250	-0.255472	1.716703
36	1	-4.290447	-2.843482	-1.893298
37	1	-3.053466	-1.990319	-2.840548
38	1	-4.375716	-1.088290	-2.101390
39	1	-1.031720	-4.113875	-1.489875
40	1	0.332825	-3.015395	-1.238721
41	1	-0.862456	-2.655113	-2.486928
42	1	-0.260930	-3.568352	2.104585
43	1	0.327029	-1.926626	2.406088
44	1	0.816037	-2.786787	0.940262
45	1	-1.337370	1.044325	2.765896
46	6	3.465492	0.058618	0.067489
47	6	3.972518	1.334424	-0.660836
48	6	3.947775	0.071312	1.544150
49	6	4.009059	-1.206379	-0.651669
50	6	5.520897	1.350260	-0.627969
51	1	3.605460	1.332755	-1.694252
52	1	3.565202	2.222890	-0.162807
53	6	5.496477	0.092896	1.567550
54	1	3.540389	0.953948	2.052460
55	1	3.566128	-0.818422	2.060459
56	6	5.557288	-1.179433	-0.618928

57	1	3.628308	-2.103684	-0.147458
58	1	3.643116	-1.221573	-1.685593
59	6	6.067128	0.090427	-1.344700
60	6	6.006849	1.363197	0.842720
61	1	5.873367	2.252411	-1.143230
62	6	6.042490	-1.167901	0.852054
63	1	5.831858	0.101471	2.612217
64	1	5.935668	-2.074888	-1.127669
65	1	7.164952	0.106002	-1.343937
66	1	5.743396	0.081908	-2.394263
67	1	7.103836	1.395936	0.874148
68	1	5.640790	2.263707	1.354314
69	1	7.139928	-1.170011	0.884033
70	1	5.701473	-2.074774	1.370088

TS(2a-3a)Ad (E = -1171.6453536 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-1.049478	-0.629971	-0.583544
2	7	-3.286148	1.274458	-2.151263
3	6	1.467935	-0.803666	-0.988540
4	6	1.302773	-0.203453	0.290621
5	6	0.940108	0.090738	-1.968330
6	17	-1.238749	-2.470602	-2.248823
7	6	0.681945	1.073575	0.104191
8	6	0.462899	1.255115	-1.293590
9	6	-2.712535	0.458930	-1.439804
10	6	-1.754812	-0.257295	1.595877
11	6	-2.132509	-1.649458	1.413179
12	1	-2.555834	0.484356	1.577236
13	6	-3.647940	-0.798357	-0.346440
14	6	-2.996614	-1.933986	0.361622
15	1	-4.355812	-1.152520	-1.088745
16	1	-4.094785	-0.071215	0.330124
17	6	-3.486996	-3.328534	0.029260
18	6	-1.535615	-2.721008	2.308222
19	1	-1.359697	-3.669010	1.791537
20	1	-2.218270	-2.920995	3.146588
21	1	-0.587249	-2.382250	2.737505
22	1	-4.430693	-3.530811	0.557197
23	1	-2.771696	-4.106092	0.309646
24	1	-3.671797	-3.425166	-1.044481
25	6	1.844905	-0.738712	1.595173
26	6	2.179104	-2.102890	-1.281628
27	6	1.019410	-0.093308	-3.463806
28	6	-0.013141	2.526282	-1.955613
29	6	0.498406	2.137336	1.159795
30	1	2.863321	-0.363665	1.769620
31	1	1.896515	-1.832553	1.598918
32	1	1.234781	-0.430121	2.450047
33	1	3.232153	-1.912600	-1.533192
34	1	1.721833	-2.629046	-2.124404
35	1	2.164880	-2.779506	-0.420729
36	1	1.994522	0.247092	-3.840883
37	1	0.245119	0.481540	-3.981944
38	1	0.895164	-1.142658	-3.745716
39	1	0.846197	3.146008	-2.249235
40	1	-0.637598	3.121528	-1.282772
41	1	-0.605502	2.324053	-2.852151
42	1	1.343264	2.840821	1.143127
43	1	0.447693	1.707858	2.164128
44	1	-0.416296	2.718843	1.002547
45	1	-1.050805	-0.065749	2.399362
46	6	-4.674593	1.640563	-2.504096

47	6	-5.600077	1.828834	-1.270535
48	6	-4.600665	2.984272	-3.280078
49	6	-5.274012	0.555943	-3.444458
50	6	-7.012873	2.264829	-1.740494
51	1	-5.679774	0.894017	-0.707101
52	1	-5.167018	2.585940	-0.602878
53	6	-6.008361	3.419424	-3.748418
54	1	-4.157786	3.749166	-2.628274
55	1	-3.928502	2.858710	-4.138349
56	6	-6.689497	0.990115	-3.902698
57	1	-4.612568	0.423828	-4.309906
58	1	-5.325237	-0.406461	-2.920873
59	6	-7.603002	1.170567	-2.664923
60	6	-6.923742	3.602304	-2.513437
61	1	-7.655317	2.388675	-0.858623
62	6	-6.599131	2.328794	-4.675766
63	1	-5.930036	4.367846	-4.295930
64	1	-7.103085	0.211643	-4.557193
65	1	-8.614754	1.455065	-2.984170
66	1	-7.691746	0.221157	-2.118036
67	1	-7.926520	3.920841	-2.829318
68	1	-6.523806	4.390378	-1.860318
69	1	-7.597078	2.628904	-5.023365
70	1	-5.967682	2.208139	-5.566701

3aAd (E = -1171.6591008 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-1.547763	0.215296	-0.111087
2	7	1.520374	-0.416511	-0.117616
3	6	-2.828650	-1.822463	-0.876343
4	6	-3.484479	-1.327609	0.293433
5	6	-1.537431	-2.282285	-0.491029
6	17	-1.969021	1.167826	-2.315087
7	6	-2.607907	-1.504190	1.403894
8	6	-1.396327	-2.082424	0.917743
9	6	0.655656	0.380101	0.383853
10	6	-2.051879	1.593306	1.588645
11	6	-1.449309	2.704067	0.818721
12	1	-1.449491	1.221546	2.423121
13	6	0.856710	1.715340	1.131841
14	6	-0.112235	2.733830	0.532740
15	1	1.872108	2.107393	1.081371
16	1	0.630566	1.547485	2.192585
17	6	0.551404	3.756686	-0.363175
18	6	-2.437253	3.733302	0.289392
19	1	-2.091477	4.260527	-0.600868
20	1	-2.637115	4.478266	1.072407
21	1	-3.394037	3.259913	0.041652
22	1	1.222615	4.399413	0.225835
23	1	-0.154709	4.402202	-0.887099
24	1	1.171857	3.257189	-1.118969
25	6	-4.902817	-0.810608	0.353153
26	6	-3.457187	-1.965823	-2.241485
27	6	-0.525883	-2.965497	-1.379703
28	6	-0.257158	-2.602895	1.759082
29	6	-2.962309	-1.290610	2.855066
30	1	-5.609477	-1.640589	0.493883
31	1	-5.188132	-0.294328	-0.569661
32	1	-5.046415	-0.114079	1.185384
33	1	-3.995863	-2.921482	-2.309096
34	1	-2.708729	-1.946530	-3.038385
35	1	-4.172054	-1.164039	-2.448306
36	1	-0.570476	-4.055158	-1.240922

37	1	0.488411	-2.628738	-1.147793
38	1	-0.715940	-2.759557	-2.437741
39	1	-0.411104	-3.667009	1.989058
40	1	-0.176994	-2.068173	2.711232
41	1	0.696812	-2.499288	1.236170
42	1	-3.388005	-2.210208	3.280564
43	1	-3.702472	-0.494979	2.982302
44	1	-2.086067	-1.027457	3.456283
45	1	-3.073381	1.776172	1.917210
46	6	3.008597	-0.288920	-0.049542
47	6	3.549573	-0.197994	1.407315
48	6	3.571247	-1.593074	-0.684577
49	6	3.539622	0.911620	-0.885440
50	6	5.100602	-0.181337	1.400066
51	1	3.176752	0.703342	1.905792
52	1	3.182185	-1.061860	1.978803
53	6	5.117014	-1.594228	-0.691853
54	1	3.189989	-2.453735	-0.118129
55	1	3.180290	-1.681013	-1.706892
56	6	5.090011	0.922824	-0.879804
57	1	3.160438	0.824697	-1.912656
58	1	3.165598	1.858418	-0.480685
59	6	5.598860	1.034824	0.579416
60	6	5.635471	-1.486171	0.762711
61	1	5.462167	-0.100192	2.434379
62	6	5.625187	-0.384093	-1.512707
63	1	5.479413	-2.526835	-1.145331
64	1	5.443609	1.786048	-1.460030
65	1	6.697018	1.070578	0.591871
66	1	5.240642	1.969796	1.034045
67	1	6.734380	-1.488227	0.774728
68	1	5.302890	-2.355248	1.347575
69	1	6.723982	-0.372107	-1.529661
70	1	5.285079	-0.465031	-2.554468

3bAd (E = -1171.6819022 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-1.144519	0.015338	-0.257872
2	7	0.955111	-0.020219	0.385277
3	6	-2.184118	-2.285238	-0.095777
4	6	-3.249062	-1.391751	-0.422404
5	6	-1.721495	-1.960799	1.214682
6	17	-0.726174	-0.036255	-2.670292
7	6	-3.443799	-0.514645	0.684993
8	6	-2.492323	-0.861420	1.696213
9	6	0.333474	0.902997	1.019431
10	6	-1.851835	2.182459	0.005193
11	6	-0.766227	3.214646	-0.162670
12	1	-2.207747	2.179879	1.042697
13	6	0.693356	2.202856	1.651893
14	6	0.351262	3.281736	0.603163
15	1	1.743029	2.299994	1.947097
16	1	0.086254	2.334555	2.557347
17	6	1.388578	4.387869	0.553800
18	6	-1.042969	4.198774	-1.289001
19	1	-0.194192	4.835580	-1.548005
20	1	-1.894416	4.846277	-1.034972
21	1	-1.327388	3.640864	-2.191144
22	1	1.503451	4.846862	1.547325
23	1	1.130324	5.186458	-0.144269
24	1	2.379416	4.002016	0.270164
25	6	-4.091782	-1.444092	-1.675305
26	6	-1.708003	-3.436156	-0.951632

27	6	-0.688529	-2.726540	2.007518
28	6	-2.443456	-0.284691	3.091827
29	6	-4.577922	0.468687	0.841663
30	1	-4.926685	-2.147933	-1.549259
31	1	-3.508910	-1.770760	-2.541888
32	1	-4.520646	-0.466186	-1.917287
33	1	-2.329555	-4.326239	-0.779328
34	1	-0.672590	-3.711062	-0.725678
35	1	-1.761304	-3.196914	-2.018296
36	1	-1.171327	-3.502810	2.617660
37	1	-0.130303	-2.074115	2.686517
38	1	0.036398	-3.224112	1.356035
39	1	-3.171945	-0.787624	3.743780
40	1	-2.680949	0.784222	3.100235
41	1	-1.455325	-0.407855	3.546354
42	1	-5.454590	-0.029071	1.279710
43	1	-4.886521	0.893031	-0.119025
44	1	-4.310102	1.301798	1.498360
45	1	-2.711892	2.434491	-0.626013
46	6	2.406099	-0.314772	0.197076
47	6	3.131277	-0.450990	1.562249
48	6	2.528367	-1.651209	-0.575611
49	6	3.075235	0.811867	-0.638244
50	6	4.625768	-0.789603	1.325890
51	1	3.044397	0.483191	2.130638
52	1	2.649047	-1.242122	2.152436
53	6	4.018690	-1.996527	-0.811371
54	1	2.039981	-2.448263	0.001743
55	1	1.997141	-1.563714	-1.531754
56	6	4.568921	0.469710	-0.869466
57	1	2.549706	0.913135	-1.595951
58	1	2.985627	1.768758	-0.110744
59	6	5.285811	0.341281	0.497676
60	6	4.738516	-2.127175	0.553778
61	1	5.130007	-0.878881	2.297244
62	6	4.681362	-0.868432	-1.640135
63	1	4.087246	-2.945914	-1.358431
64	1	5.031849	1.274336	-1.455782
65	1	6.350598	0.119519	0.343838
66	1	5.229893	1.292938	1.044993
67	1	5.795646	-2.382859	0.399379
68	1	4.290787	-2.941205	1.141013
69	1	5.737496	-1.107762	-1.824890
70	1	4.191455	-0.782043	-2.619580

3cAd (E = -1171.6728623 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-1.086543	-0.050716	-0.233983
2	7	1.098593	0.289770	-0.249939
3	6	-3.170222	-1.460730	0.428412
4	6	-2.288002	-1.433593	1.548042
5	6	-2.537616	-2.196084	-0.613358
6	17	-2.012485	0.585063	-2.405679
7	6	-1.096285	-2.133221	1.187788
8	6	-1.251601	-2.604116	-0.154601
9	6	0.461368	1.403206	-0.312005
10	6	-1.668506	1.642935	1.218535
11	6	-1.581589	3.071992	0.719275
12	1	-0.950242	1.483235	2.039823
13	6	0.768570	2.848091	-0.179520
14	6	-0.492761	3.639799	0.154500
15	1	1.576008	3.041743	0.543016
16	1	1.155755	3.205395	-1.145463

17	6	-0.356477	5.102269	-0.226646
18	6	-2.880342	3.838922	0.924699
19	1	-2.896136	4.825417	0.456495
20	1	-3.093310	3.963205	1.996333
21	1	-3.713218	3.260185	0.501873
22	1	-1.188780	5.723284	0.109166
23	1	-0.266163	5.218479	-1.318006
24	1	0.561405	5.524925	0.209928
25	6	-2.628801	-0.970695	2.943696
26	6	-4.570893	-0.897767	0.382891
27	6	-3.168750	-2.588749	-1.925712
28	6	-0.330315	-3.546338	-0.896735
29	6	-0.008407	-2.519174	2.165351
30	1	-2.972532	-1.822301	3.548302
31	1	-3.429144	-0.225518	2.943459
32	1	-1.767824	-0.530015	3.457612
33	1	-5.306784	-1.650730	0.699019
34	1	-4.841789	-0.576811	-0.628361
35	1	-4.681900	-0.032915	1.045398
36	1	-3.761708	-3.506651	-1.803606
37	1	-2.416008	-2.780257	-2.696793
38	1	-3.833212	-1.807690	-2.306424
39	1	-0.710631	-4.576003	-0.839061
40	1	0.678442	-3.544962	-0.476669
41	1	-0.246864	-3.290760	-1.959199
42	1	-0.357869	-3.330237	2.820294
43	1	0.284253	-1.684829	2.813043
44	1	0.890422	-2.875999	1.656002
45	1	-2.653705	1.484062	1.665417
46	6	2.569357	0.031463	-0.116480
47	6	2.850399	-1.447417	-0.470763
48	6	3.379814	0.935822	-1.084025
49	6	3.024074	0.298659	1.344666
50	6	4.361012	-1.756696	-0.330840
51	1	2.271872	-2.094306	0.197968
52	1	2.510097	-1.646165	-1.495943
53	6	4.893505	0.633400	-0.942675
54	1	3.046779	0.753828	-2.114824
55	1	3.195680	1.992100	-0.859542
56	6	4.538886	-0.001832	1.481739
57	1	2.820262	1.343101	1.613377
58	1	2.445716	-0.336390	2.028739
59	6	4.806585	-1.485529	1.127845
60	6	5.163580	-0.849216	-1.294220
61	1	4.537647	-2.810954	-0.581391
62	6	5.336421	0.909639	0.516010
63	1	5.452054	1.284529	-1.627788
64	1	4.849457	0.194101	2.516472
65	1	5.875362	-1.711349	1.242528
66	1	4.261152	-2.143462	1.818980
67	1	6.236993	-1.066724	-1.210704
68	1	4.871719	-1.050260	-2.334248
69	1	6.412566	0.718279	0.624039
70	1	5.169348	1.966269	0.768384

TS(3c-4)Ad (E = -1171.6377754 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.616200	-0.017124	-0.813814
2	7	-0.627580	1.615897	-0.549615
3	6	2.837899	-1.294353	-0.573943
4	6	2.462620	-0.808799	0.714138
5	6	3.159144	-0.172909	-1.392130
6	17	0.287794	-1.130861	-2.981367

7	6	2.544848	0.619622	0.687064
8	6	2.978330	1.011707	-0.620467
9	6	-1.365303	0.471437	-0.567535
10	6	-1.111405	-0.736242	0.942005
11	6	-2.289124	-1.620267	0.640214
12	1	-1.266835	-0.057298	1.783965
13	6	-2.824523	0.220232	-0.812943
14	6	-3.169577	-1.138507	-0.251080
15	1	-3.481681	0.978840	-0.359852
16	1	-3.014005	0.264721	-1.894607
17	6	-4.458150	-1.770718	-0.712197
18	6	-2.379883	-2.945353	1.364656
19	1	-3.256529	-3.530604	1.072300
20	1	-2.422115	-2.792506	2.452364
21	1	-1.488124	-3.556735	1.165066
22	1	-4.663906	-2.724795	-0.219877
23	1	-4.435685	-1.945967	-1.797100
24	1	-5.309461	-1.102254	-0.517005
25	6	2.268107	-1.646365	1.958494
26	6	2.989375	-2.742504	-0.975903
27	6	3.711440	-0.241597	-2.794541
28	6	3.405754	2.395200	-1.056242
29	6	2.451694	1.497660	1.915148
30	1	3.234211	-1.816041	2.454930
31	1	1.843486	-2.630631	1.732870
32	1	1.611801	-1.157398	2.686349
33	1	4.034485	-3.065907	-0.868346
34	1	2.697779	-2.902548	-2.018759
35	1	2.377774	-3.404720	-0.353816
36	1	4.792458	-0.440890	-2.772822
37	1	3.560192	0.698386	-3.334878
38	1	3.234947	-1.036702	-3.376112
39	1	4.501029	2.481510	-1.022121
40	1	2.993329	3.172238	-0.409193
41	1	3.093121	2.619910	-2.081884
42	1	3.335390	1.350487	2.552322
43	1	1.570075	1.272123	2.525789
44	1	2.410475	2.557717	1.653933
45	1	-0.237422	-1.342005	1.216557
46	6	-1.050535	2.983180	-0.163523
47	6	-1.656307	3.007874	1.268245
48	6	0.177201	3.924726	-0.196414
49	6	-2.102102	3.536038	-1.172375
50	6	-2.070770	4.452363	1.649008
51	1	-2.527324	2.341730	1.316427
52	1	-0.912829	2.626200	1.981852
53	6	-0.224756	5.370082	0.186227
54	1	0.931503	3.551437	0.504911
55	1	0.620142	3.901677	-1.201047
56	6	-2.518510	4.977092	-0.786184
57	1	-1.666196	3.518060	-2.180426
58	1	-2.985381	2.888310	-1.188037
59	6	-3.124197	4.972498	0.639571
60	6	-0.826589	5.373457	1.613309
61	1	-2.499115	4.449206	2.660541
62	6	-1.276666	5.899393	-0.817850
63	1	0.666603	6.011693	0.160438
64	1	-3.267147	5.340056	-1.503275
65	1	-3.440447	5.987423	0.917512
66	1	-4.020033	4.335974	0.667094
67	1	-1.106749	6.396004	1.901713
68	1	-0.078696	5.025713	2.340150
69	1	-1.561836	6.928385	-0.558427

70	1	-0.852427	5.925588	-1.831229

4Ad (E = -1171.6616613 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-1.085125	-0.057818	-0.138692
2	7	0.921942	0.226098	0.100239
3	6	-3.248129	-1.394970	0.013763
4	6	-2.665544	-1.345256	1.316281
5	6	-2.392451	-2.164683	-0.823903
6	17	-1.881119	0.926763	-2.232992
7	6	-1.448384	-2.095916	1.280693
8	6	-1.279647	-2.606391	-0.046605
9	6	0.441637	1.552357	0.155128
10	6	-0.449715	1.968252	1.240259
11	6	-0.812383	3.402117	0.951367
12	1	-0.179987	1.728219	2.273705
13	6	0.693799	2.746380	-0.753452
14	6	-0.181864	3.826892	-0.157314
15	1	1.742362	3.079286	-0.735237
16	1	0.448216	2.556023	-1.805755
17	6	-0.252181	5.185254	-0.801075
18	6	-1.760092	4.148085	1.852180
19	1	-1.904668	5.183273	1.529618
20	1	-1.388380	4.166610	2.886348
21	1	-2.746588	3.663403	1.874502
22	1	-0.879767	5.882868	-0.238281
23	1	-0.658335	5.110712	-1.819053
24	1	0.750359	5.626657	-0.888842
25	6	-3.317235	-0.784745	2.561218
26	6	-4.581241	-0.810413	-0.387955
27	6	-2.681815	-2.564497	-2.250275
28	6	-0.302991	-3.675041	-0.480755
29	6	-0.628689	-2.466184	2.495988
30	1	-3.935332	-1.552307	3.048774
31	1	-3.967945	0.065305	2.332498
32	1	-2.577017	-0.448620	3.295075
33	1	-5.378587	-1.560039	-0.283973
34	1	-4.575009	-0.472970	-1.428900
35	1	-4.854276	0.046929	0.236297
36	1	-3.309633	-3.466767	-2.275783
37	1	-1.762655	-2.786308	-2.802087
38	1	-3.209117	-1.773645	-2.791759
39	1	-0.801530	-4.655161	-0.486981
40	1	0.550658	-3.745406	0.196690
41	1	0.084894	-3.500803	-1.490062
42	1	-1.088340	-3.316783	3.019712
43	1	-0.559610	-1.641803	3.214124
44	1	0.390417	-2.755071	2.227426
45	1	-1.551581	1.325903	1.224489
46	6	2.360545	-0.107897	0.044076
47	6	2.991026	0.299199	-1.323578
48	6	3.131547	0.611890	1.186032
49	6	2.545723	-1.634047	0.211796
50	6	4.494533	-0.072737	-1.362484
51	1	2.445496	-0.212658	-2.128338
52	1	2.873413	1.376403	-1.483556
53	6	4.634633	0.241041	1.144275
54	1	3.003413	1.697862	1.086286
55	1	2.693306	0.319861	2.150902
56	6	4.045582	-2.018129	0.179038
57	1	2.098854	-1.946205	1.164082
58	1	2.008030	-2.148273	-0.593284
59	6	4.655103	-1.600821	-1.181034

60	6	5.235724	0.663910	-0.219063
61	1	4.916158	0.230781	-2.330453
62	6	4.791447	-1.289079	1.323384
63	1	5.159156	0.763301	1.956155
64	1	4.142519	-3.104831	0.309393
65	1	5.717909	-1.877698	-1.219635
66	1	4.151169	-2.132847	-2.000248
67	1	6.307504	0.422810	-0.248309
68	1	5.145235	1.751593	-0.350131
69	1	5.855442	-1.563775	1.314914
70	1	4.384641	-1.598041	2.296782

8aAd (E = -1654.5929963 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.383053	-0.716423	-0.099426
2	7	-0.041021	-0.493094	1.835925
3	6	-0.224891	0.842282	1.330066
4	7	-1.856377	-0.231128	-0.760668
5	6	2.748609	0.138022	-0.102885
6	6	2.016508	1.041542	-0.933305
7	6	2.806115	-1.119924	-0.772799
8	17	0.071265	-3.219770	-0.109532
9	6	1.638429	0.343205	-2.120193
10	6	2.125151	-0.992724	-2.020529
11	6	-2.426199	0.566847	0.079431
12	6	-1.606700	1.431379	1.017992
13	1	0.459075	1.606940	1.708553
14	6	-2.620173	1.875920	2.068418
15	1	-1.364834	2.334923	0.426295
16	6	-3.894155	0.794618	0.400308
17	6	-3.865592	1.512618	1.733605
18	1	-4.362361	1.437794	-0.355620
19	1	-4.470426	-0.133317	0.416595
20	6	-5.163762	1.788039	2.443890
21	6	-2.189592	2.738215	3.221760
22	1	-3.029139	3.021257	3.863717
23	1	-1.719985	3.661450	2.851302
24	1	-1.441497	2.233328	3.842380
25	1	-5.014197	2.331241	3.381395
26	1	-5.687709	0.850566	2.678738
27	1	-5.841498	2.382226	1.813638
28	6	1.885437	2.531860	-0.733027
29	6	3.483787	0.511921	1.162875
30	6	3.574803	-2.340120	-0.322985
31	6	2.068585	-2.067746	-3.079578
32	6	1.036986	1.007595	-3.338802
33	1	2.692995	3.062183	-1.259858
34	1	1.944421	2.804736	0.324255
35	1	0.934736	2.914002	-1.121222
36	1	4.461364	0.954936	0.923192
37	1	3.664239	-0.359662	1.799194
38	1	2.926157	1.244051	1.755372
39	1	4.577231	-2.349241	-0.775115
40	1	3.066349	-3.264552	-0.612076
41	1	3.704023	-2.362090	0.763924
42	1	3.050599	-2.188818	-3.558269
43	1	1.347693	-1.826572	-3.866785
44	1	1.786532	-3.037486	-2.654501
45	1	1.762140	1.702122	-3.785998
46	1	0.137973	1.589267	-3.102056
47	1	0.770839	0.277876	-4.108651
48	6	-0.017542	-0.925014	3.247749
49	6	0.677084	-2.310238	3.341997

50	6	0.768284	0.067917	4.150097
51	6	-1.464805	-1.075643	3.803902
52	6	0.708693	-2.814317	4.805539
53	1	0.148046	-3.023536	2.701186
54	1	1.700832	-2.223574	2.950525
55	6	0.790669	-0.426033	5.618291
56	1	1.793912	0.162335	3.767926
57	1	0.311261	1.063818	4.096972
58	6	-1.438909	-1.569320	5.271875
59	1	-1.989199	-0.115431	3.734798
60	1	-2.009018	-1.789238	3.170296
61	6	-0.739466	-2.948613	5.337715
62	6	1.486677	-1.807101	5.686438
63	1	1.204932	-3.794022	4.838777
64	6	-0.660150	-0.554525	6.144861
65	1	1.343245	0.296615	6.235174
66	1	-2.469368	-1.659866	5.643542
67	1	-0.728854	-3.318929	6.372799
68	1	-1.294997	-3.681041	4.735547
69	1	1.523031	-2.161078	6.726568
70	1	2.525380	-1.722748	5.336106
71	1	-0.651768	-0.886401	7.192781
72	1	-1.158440	0.425568	6.120592
73	6	-2.632592	-1.019268	-1.805896
74	6	-3.353534	-2.242630	-1.170803
75	6	-3.658739	-0.148724	-2.587575
76	6	-1.597709	-1.536608	-2.841359
77	6	-4.052225	-3.074082	-2.278284
78	1	-2.619846	-2.857031	-0.639105
79	1	-4.098830	-1.910422	-0.439108
80	6	-4.352710	-0.995308	-3.688409
81	1	-4.434190	0.243146	-1.927139
82	1	-3.138864	0.709961	-3.035467
83	6	-2.278815	-2.391291	-3.937940
84	1	-1.097341	-0.675900	-3.298896
85	1	-0.842502	-2.145755	-2.334482
86	6	-2.994944	-3.595553	-3.280890
87	6	-5.081275	-2.191304	-3.025975
88	1	-4.565422	-3.923155	-1.808140
89	6	-3.306820	-1.521827	-4.696280
90	1	-5.082673	-0.359832	-4.207531
91	1	-1.509802	-2.752772	-4.633559
92	1	-3.478127	-4.211365	-4.051783
93	1	-2.266234	-4.232206	-2.762579
94	1	-5.599545	-2.783932	-3.791988
95	1	-5.847839	-1.827397	-2.326552
96	1	-3.800978	-2.112452	-5.479645
97	1	-2.801833	-0.681457	-5.193248

TS(8a-9)Ad (E = -1654.5530296 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.474173	-0.236027	-0.238752
2	7	-0.206574	-0.468553	1.666927
3	6	-0.575144	0.868454	1.563520
4	7	-2.012028	-0.550334	-0.724825
5	6	2.910052	0.255515	0.349389
6	6	2.279466	1.514112	0.094804
7	6	2.985619	-0.449893	-0.882524
8	17	0.682228	-2.621544	-0.946313
9	6	1.952011	1.569965	-1.299945
10	6	2.373346	0.345592	-1.893683
11	6	-2.406548	0.515852	-0.136793
12	6	-1.308810	1.379733	0.408002

13	1	-0.189065	1.607650	2.260846
14	6	-1.934874	2.750565	0.549465
15	1	-0.555000	1.384216	-0.713420
16	6	-3.717070	1.264740	0.039759
17	6	-3.265455	2.668527	0.378850
18	1	-4.336709	1.250266	-0.855999
19	1	-4.323056	0.833751	0.847941
20	6	-4.301082	3.751336	0.519230
21	6	-1.146784	3.976579	0.918344
22	1	-1.800457	4.837667	1.081375
23	1	-0.436713	4.244664	0.126494
24	1	-0.566317	3.820950	1.835394
25	1	-3.863582	4.723773	0.760458
26	1	-5.021470	3.500478	1.310991
27	1	-4.877196	3.862676	-0.410160
28	6	2.317164	2.688855	1.044913
29	6	3.625092	-0.131457	1.622334
30	6	3.755494	-1.725613	-1.106532
31	6	2.275302	-0.008788	-3.359494
32	6	1.491931	2.789264	-2.065140
33	1	3.314766	3.152683	1.024931
34	1	2.117293	2.392158	2.079497
35	1	1.594456	3.460761	0.773689
36	1	4.678320	0.185291	1.584840
37	1	3.614054	-1.214321	1.783196
38	1	3.172391	0.338852	2.499825
39	1	4.817478	-1.491290	-1.272451
40	1	3.389040	-2.274359	-1.977348
41	1	3.689807	-2.398807	-0.246900
42	1	3.180383	0.301126	-3.901666
43	1	1.423315	0.485896	-3.839593
44	1	2.157458	-1.087808	-3.504361
45	1	2.358679	3.342946	-2.455592
46	1	0.919508	3.476344	-1.436241
47	1	0.860618	2.521337	-2.918783
48	6	-0.247440	-1.178748	2.963039
49	6	0.481133	-2.536243	2.818500
50	6	0.418976	-0.371509	4.114192
51	6	-1.730252	-1.450899	3.353502
52	6	0.410288	-3.333309	4.143671
53	1	0.023160	-3.104905	2.000985
54	1	1.527124	-2.357920	2.536891
55	6	0.349934	-1.167305	5.442328
56	1	1.464420	-0.163061	3.852548
57	1	-0.090694	0.593244	4.239824
58	6	-1.806034	-2.243265	4.681580
59	1	-2.258746	-0.491595	3.446127
60	1	-2.210279	-2.015564	2.544281
61	6	-1.070667	-3.595834	4.513086
62	6	1.085068	-2.519327	5.274707
63	1	0.932811	-4.290882	4.015918
64	6	-1.131399	-1.427070	5.810809
65	1	0.830210	-0.581557	6.238228
66	1	-2.859566	-2.424573	4.935912
67	1	-1.130493	-4.176108	5.444603
68	1	-1.554413	-4.192446	3.727097
69	1	1.054886	-3.083451	6.217471
70	1	2.143685	-2.345901	5.034827
71	1	-1.192064	-1.975651	6.761093
72	1	-1.657823	-0.472463	5.953563
73	6	-2.879073	-1.585508	-1.373013
74	6	-2.834256	-2.867851	-0.492137
75	6	-4.371864	-1.200665	-1.584063

76	6	-2.270474	-1.887471	-2.772642
77	6	-3.589703	-4.025992	-1.188007
78	1	-1.793074	-3.143231	-0.310570
79	1	-3.296954	-2.644924	0.479832
80	6	-5.140196	-2.362121	-2.271498
81	1	-4.850814	-0.979638	-0.623080
82	1	-4.442309	-0.306044	-2.215806
83	6	-3.028553	-3.051655	-3.455327
84	1	-2.334265	-0.979003	-3.389631
85	1	-1.214545	-2.143449	-2.659470
86	6	-2.939842	-4.315724	-2.564121
87	6	-5.071195	-3.629972	-1.388003
88	1	-3.526637	-4.921812	-0.555602
89	6	-4.510935	-2.659448	-3.652451
90	1	-6.187846	-2.057088	-2.399885
91	1	-2.564661	-3.255146	-4.429823
92	1	-3.454092	-5.155430	-3.052261
93	1	-1.890202	-4.607636	-2.429949
94	1	-5.624924	-4.450290	-1.865340
95	1	-5.546944	-3.440712	-0.415071
96	1	-5.058821	-3.472941	-4.147849
97	1	-4.585730	-1.775375	-4.301560

9Ad (E = -1654.587228 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.280017	-0.998769	-0.558202
2	7	-1.186123	0.567952	0.682100
3	6	-1.031324	0.002233	1.878527
4	7	1.601647	0.100072	0.503137
5	6	-2.586238	-1.770774	-1.492294
6	6	-2.433607	-2.372951	-0.203992
7	6	-1.629887	-2.365779	-2.363712
8	17	0.415549	0.016881	-2.686217
9	6	-1.365801	-3.307968	-0.279156
10	6	-0.860075	-3.292438	-1.614845
11	6	1.428862	-0.440903	1.670287
12	6	0.101242	-0.756013	2.195778
13	1	-1.801841	0.118742	2.644327
14	6	0.264599	-1.525912	3.447518
15	1	0.918017	-2.270698	-0.027576
16	6	2.423558	-0.977157	2.702154
17	6	1.572161	-1.682650	3.728456
18	1	3.146967	-1.643656	2.220312
19	1	2.995418	-0.177493	3.179870
20	6	2.222749	-2.382410	4.889151
21	6	-0.905841	-1.982111	4.279908
22	1	-0.580614	-2.569404	5.143116
23	1	-1.600540	-2.598580	3.696536
24	1	-1.480366	-1.127007	4.662330
25	1	1.491714	-2.854622	5.552285
26	1	2.818238	-1.681459	5.492467
27	1	2.912642	-3.164304	4.540324
28	6	-3.407515	-2.245144	0.942548
29	6	-3.759257	-0.939100	-1.953274
30	6	-1.584909	-2.185853	-3.858891
31	6	0.220921	-4.191828	-2.163056
32	6	-0.949940	-4.273767	0.801953
33	1	-4.258188	-2.925188	0.789526
34	1	-3.810133	-1.233500	1.035726
35	1	-2.947916	-2.510236	1.898734
36	1	-4.549361	-1.590311	-2.356113
37	1	-3.479624	-0.240137	-2.748455
38	1	-4.201234	-0.360511	-1.138072

39	1	-2.303251	-2.868705	-4.336106
40	1	-0.593649	-2.404885	-4.265239
41	1	-1.840135	-1.165327	-4.156946
42	1	-0.206776	-5.128535	-2.549128
43	1	0.952907	-4.448700	-1.391520
44	1	0.763983	-3.714784	-2.986056
45	1	-1.566246	-5.183956	0.761414
46	1	-1.057968	-3.842762	1.801349
47	1	0.096944	-4.568515	0.688172
48	6	-2.003811	1.814249	0.568663
49	6	-2.065400	2.250151	-0.915074
50	6	-3.452964	1.670138	1.115120
51	6	-1.285522	2.939653	1.375421
52	6	-2.831215	3.588756	-1.057141
53	1	-1.044487	2.353980	-1.300727
54	1	-2.557326	1.473110	-1.510036
55	6	-4.214839	3.014091	0.976587
56	1	-3.979351	0.888058	0.556760
57	1	-3.439150	1.367848	2.170819
58	6	-2.045727	4.280569	1.240683
59	1	-1.223006	2.645182	2.432813
60	1	-0.258587	3.037845	1.002467
61	6	-2.102352	4.691049	-0.250995
62	6	-4.271956	3.423105	-0.515401
63	1	-2.865198	3.869010	-2.118176
64	6	-3.484427	4.112589	1.786284
65	1	-5.234470	2.886110	1.364374
66	1	-1.518622	5.052269	1.817751
67	1	-2.629843	5.648865	-0.358583
68	1	-1.085584	4.834345	-0.641957
69	1	-4.827711	4.364473	-0.625430
70	1	-4.809853	2.660656	-1.096179
71	1	-4.031438	5.062105	1.708423
72	1	-3.456112	3.841992	2.851517
73	6	2.883892	0.704869	0.008405
74	6	2.487952	2.026056	-0.717942
75	6	3.925735	1.086590	1.102478
76	6	3.579952	-0.259031	-0.994892
77	6	3.718180	2.694450	-1.373876
78	1	1.729949	1.807775	-1.471370
79	1	2.037836	2.705031	0.020455
80	6	5.160377	1.783108	0.467558
81	1	3.459445	1.747712	1.846638
82	1	4.287961	0.195534	1.620710
83	6	4.815260	0.428263	-1.631285
84	1	3.883313	-1.173188	-0.465293
85	1	2.872721	-0.551375	-1.775033
86	6	4.367965	1.709828	-2.377935
87	6	4.738557	3.069189	-0.276127
88	1	3.392514	3.599297	-1.905139
89	6	5.831995	0.806617	-0.528654
90	1	5.866872	2.033861	1.270996
91	1	5.281452	-0.267720	-2.341955
92	1	5.234208	2.183303	-2.861305
93	1	3.651851	1.453309	-3.169606
94	1	5.619905	3.554757	-0.718076
95	1	4.290939	3.786083	0.426922
96	1	6.719554	1.276076	-0.975235
97	1	6.173388	-0.096141	-0.001906

TS(9-10)Ad (E = -1654.577824 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	0.297568	-0.010540	-0.208882
2	7	-0.201974	-0.184108	1.836622
3	6	-1.192351	0.718481	2.117263
4	7	-2.049731	-0.119493	-0.737790
5	6	2.722883	0.792659	0.235689
6	6	2.106247	1.769184	-0.598481
7	6	2.837947	-0.414255	-0.511392
8	17	0.231918	-2.542098	-0.617496
9	6	1.886143	1.184235	-1.880980
10	6	2.316667	-0.165289	-1.824218
11	6	-2.772001	0.572848	0.095873
12	6	-2.280167	1.097821	1.367492
13	1	-1.156540	1.167601	3.106255
14	6	-3.291275	2.030459	1.909356
15	1	-0.400123	1.618814	-0.661529
16	6	-4.207564	1.093747	-0.032874
17	6	-4.398241	2.011119	1.145096
18	1	-4.347755	1.642892	-0.963671
19	1	-4.936434	0.274463	-0.030096
20	6	-5.698773	2.742692	1.324491
21	6	-3.072597	2.823125	3.171585
22	1	-3.899643	3.513752	3.357806
23	1	-2.147728	3.412015	3.112705
24	1	-2.985560	2.168649	4.049905
25	1	-5.685549	3.405803	2.194536
26	1	-6.533372	2.038192	1.454521
27	1	-5.934406	3.352144	0.440051
28	6	1.915808	3.225504	-0.253743
29	6	3.372074	1.110652	1.562260
30	6	3.614694	-1.654530	-0.142767
31	6	2.420965	-1.134142	-2.977009
32	6	1.378726	1.927196	-3.091923
33	1	2.832231	3.796757	-0.464179
34	1	1.677127	3.365316	0.806054
35	1	1.100114	3.665482	-0.834488
36	1	4.318566	1.643765	1.391749
37	1	3.604100	0.212412	2.139193
38	1	2.744367	1.756434	2.184897
39	1	4.502102	-1.746579	-0.784872
40	1	3.013788	-2.560994	-0.271942
41	1	3.963629	-1.623835	0.893182
42	1	3.456061	-1.171246	-3.346456
43	1	1.783791	-0.840356	-3.817127
44	1	2.135640	-2.146614	-2.675728
45	1	2.160021	2.591040	-3.488619
46	1	0.508563	2.546185	-2.847441
47	1	1.091205	1.244454	-3.897155
48	6	-2.588531	-0.734380	-2.021605
49	6	-3.077988	-2.179330	-1.711298
50	6	-3.752293	0.016168	-2.743903
51	6	-1.410156	-0.775953	-3.037182
52	6	-3.471928	-2.907373	-3.022165
53	1	-2.286548	-2.726392	-1.194127
54	1	-3.943859	-2.123710	-1.035436
55	6	-4.144569	-0.710796	-4.061156
56	1	-4.648605	0.037242	-2.124327
57	1	-3.456088	1.051966	-2.958442
58	6	-1.796187	-1.533976	-4.329831
59	1	-1.122434	0.255907	-3.280358
60	1	-0.552809	-1.280965	-2.586767
61	6	-2.247975	-2.971066	-3.969586
62	6	-4.620731	-2.144407	-3.722401
63	1	-3.798798	-3.926464	-2.775528

64	6	-2.946279	-0.779971	-5.030327
65	1	-4.966558	-0.149458	-4.526360
66	1	-0.919440	-1.578354	-4.990290
67	1	-2.510802	-3.519990	-4.884607
68	1	-1.425957	-3.513864	-3.485798
69	1	-4.920809	-2.667622	-4.640835
70	1	-5.504027	-2.105489	-3.068854
71	1	-3.237609	-1.295036	-5.956100
72	1	-2.621777	0.232557	-5.309413
73	6	0.262919	-0.954923	3.057676
74	6	1.381678	-1.949938	2.672080
75	6	0.799388	-0.034286	4.194808
76	6	-0.943850	-1.777076	3.601818
77	6	1.811955	-2.798874	3.894733
78	1	1.027740	-2.600251	1.867798
79	1	2.243939	-1.396890	2.289085
80	6	1.219995	-0.885365	5.422448
81	1	1.654312	0.542372	3.822738
82	1	0.035688	0.684127	4.516902
83	6	-0.522401	-2.619431	4.830401
84	1	-1.760699	-1.096880	3.879140
85	1	-1.317185	-2.424623	2.798147
86	6	0.598716	-3.603450	4.419206
87	6	2.339293	-1.871643	5.014604
88	1	2.605214	-3.490916	3.581508
89	6	-0.002369	-1.679246	5.945304
90	1	1.586956	-0.212999	6.209864
91	1	-1.392939	-3.180609	5.196014
92	1	0.896247	-4.218943	5.279569
93	1	0.233865	-4.286602	3.640231
94	1	2.653372	-2.465903	5.883919
95	1	3.222553	-1.317987	4.665603
96	1	0.282043	-2.264764	6.830404
97	1	-0.797394	-0.986939	6.257676

10Ad (E = -1654.5777353 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.084063	-0.758936	0.343197
2	7	-1.647213	0.649104	0.184618
3	6	-1.281190	1.804037	0.829607
4	7	1.566420	0.892826	-0.097717
5	6	-1.456482	-2.630024	1.478348
6	6	-0.329667	-2.388610	2.316087
7	6	-0.980338	-3.172958	0.248140
8	17	0.058522	-0.997492	-2.217727
9	6	0.839368	-2.825223	1.625642
10	6	0.442968	-3.296704	0.346559
11	6	1.208149	2.096174	0.251210
12	6	-0.068237	2.442578	0.872953
13	1	-2.087164	2.345840	1.318998
14	6	0.085011	3.773763	1.500843
15	1	0.592757	-0.086038	1.909286
16	6	1.998304	3.407231	0.202491
17	6	1.251030	4.333807	1.127525
18	1	3.050066	3.316031	0.461610
19	1	1.964621	3.800265	-0.822881
20	6	1.806338	5.693725	1.444435
21	6	-0.978028	4.384325	2.375831
22	1	-0.641987	5.328841	2.812581
23	1	-1.248342	3.708936	3.198054
24	1	-1.896604	4.590846	1.809285
25	1	1.164242	6.253846	2.130647
26	1	1.923535	6.295506	0.530975

27	1	2.802881	5.617265	1.902682
28	6	-0.385241	-1.969113	3.763919
29	6	-2.886116	-2.590101	1.966791
30	6	-1.794433	-3.780969	-0.868614
31	6	1.297007	-3.998013	-0.681443
32	6	2.217295	-2.875133	2.240730
33	1	-0.556695	-2.841967	4.411698
34	1	-1.193943	-1.254915	3.949806
35	1	0.548847	-1.493091	4.074605
36	1	-3.085796	-3.472815	2.591497
37	1	-3.609523	-2.601634	1.148192
38	1	-3.088006	-1.706604	2.580902
39	1	-1.636983	-4.868392	-0.899024
40	1	-1.508691	-3.374900	-1.844931
41	1	-2.865664	-3.610284	-0.731287
42	1	1.085196	-5.076842	-0.672336
43	1	2.365361	-3.871983	-0.483360
44	1	1.094014	-3.625850	-1.690725
45	1	2.239543	-3.605254	3.061702
46	1	2.513419	-1.905332	2.657851
47	1	2.977627	-3.178773	1.515419
48	6	-3.054086	0.717969	-0.376163
49	6	-3.362090	-0.553322	-1.200751
50	6	-4.131360	0.856068	0.739933
51	6	-3.161319	1.940230	-1.337851
52	6	-4.779820	-0.481216	-1.820959
53	1	-2.608290	-0.665798	-1.985994
54	1	-3.290927	-1.431331	-0.552782
55	6	-5.547800	0.942522	0.113588
56	1	-4.066503	-0.006395	1.413470
57	1	-3.955892	1.754828	1.344817
58	6	-4.578787	2.026708	-1.955511
59	1	-2.941108	2.867441	-0.792724
60	1	-2.402260	1.837102	-2.123947
61	6	-4.868804	0.740880	-2.765328
62	6	-5.835110	-0.343069	-0.697881
63	1	-4.963391	-1.402010	-2.390950
64	6	-5.625703	2.172482	-0.823646
65	1	-6.287618	1.045141	0.919165
66	1	-4.627187	2.901193	-2.618326
67	1	-5.867952	0.796599	-3.219379
68	1	-4.143584	0.638784	-3.583991
69	1	-6.844629	-0.298782	-1.129624
70	1	-5.804804	-1.221234	-0.037222
71	1	-6.634349	2.254611	-1.251530
72	1	-5.440641	3.094271	-0.253551
73	6	2.995170	0.599279	-0.538067
74	6	3.975821	0.827441	0.658420
75	6	3.118328	-0.902407	-0.915203
76	6	3.433476	1.416669	-1.786636
77	6	5.431108	0.498616	0.238907
78	1	3.934212	1.854052	1.027150
79	1	3.663620	0.181669	1.489020
80	6	4.569566	-1.278976	-1.308316
81	1	2.806590	-1.514019	-0.058336
82	1	2.450894	-1.127709	-1.746899
83	6	4.893279	1.060367	-2.173201
84	1	2.749744	1.184538	-2.613032
85	1	3.374085	2.491475	-1.605454
86	6	5.832906	1.366711	-0.979874
87	6	5.533732	-0.996825	-0.135256
88	1	6.098397	0.717956	1.083394
89	6	4.990945	-0.438688	-2.536516

90	1	4.595400	-2.346713	-1.564943
91	1	5.185693	1.670980	-3.037979
92	1	6.874415	1.157281	-1.259686
93	1	5.778345	2.433841	-0.719543
94	1	6.564200	-1.249179	-0.421137
95	1	5.275558	-1.620658	0.731964
96	1	6.018232	-0.691269	-2.833430
97	1	4.339086	-0.663524	-3.391354

TS(10-11)Ad (E = -1654.5633852 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.749594	0.374196	0.137956
2	7	0.033822	0.112123	-1.735433
3	6	-1.006280	-0.803549	-1.442095
4	7	-1.347638	0.830904	0.980711
5	6	2.907958	-0.933134	-0.275404
6	6	2.233081	-1.606020	0.786351
7	6	3.314220	0.344677	0.204271
8	17	1.009950	2.905149	-0.081376
9	6	2.266379	-0.760139	1.938733
10	6	2.922450	0.446307	1.578082
11	6	-2.373252	0.443814	0.227796
12	6	-2.227774	-0.445396	-0.877416
13	1	-0.987092	-1.742085	-1.997770
14	6	-3.529387	-1.069004	-1.160045
15	1	-0.225304	-1.236247	0.235116
16	6	-3.878777	0.624967	0.420175
17	6	-4.495261	-0.442141	-0.453725
18	1	-4.221530	0.562730	1.450305
19	1	-4.170055	1.619957	0.056887
20	6	-5.986871	-0.618471	-0.508843
21	6	-3.693852	-2.178126	-2.165665
22	1	-4.741383	-2.473812	-2.272564
23	1	-3.125024	-3.069576	-1.868960
24	1	-3.324740	-1.874647	-3.154674
25	1	-6.282428	-1.403058	-1.212182
26	1	-6.485439	0.312177	-0.817878
27	1	-6.394761	-0.883379	0.477372
28	6	1.823296	-3.059088	0.786053
29	6	3.314699	-1.585041	-1.575725
30	6	4.190212	1.347352	-0.507271
31	6	3.308010	1.589577	2.485069
32	6	1.834056	-1.198820	3.319109
33	1	2.673680	-3.695987	1.072709
34	1	1.483249	-3.384205	-0.201995
35	1	1.009354	-3.247601	1.492367
36	1	4.187061	-2.234436	-1.412807
37	1	3.592788	-0.849704	-2.335019
38	1	2.515564	-2.207245	-1.990758
39	1	5.222618	1.284174	-0.134168
40	1	3.836934	2.371293	-0.349942
41	1	4.218553	1.168991	-1.586205
42	1	4.385748	1.557242	2.698952
43	1	2.781663	1.548179	3.443185
44	1	3.090589	2.558761	2.023423
45	1	2.487965	-2.005433	3.679166
46	1	0.807684	-1.585123	3.333122
47	1	1.896903	-0.382960	4.044837
48	6	0.196733	0.480776	-3.180441
49	6	1.462508	1.359239	-3.337147
50	6	0.340282	-0.760895	-4.108849
51	6	-1.034206	1.312005	-3.649720
52	6	1.642718	1.805778	-4.808799

53	1	1.379105	2.232019	-2.682098
54	1	2.340459	0.787579	-3.013383
55	6	0.517156	-0.314039	-5.583550
56	1	1.202775	-1.358843	-3.787042
57	1	-0.549628	-1.399626	-4.036684
58	6	-0.860474	1.755060	-5.123789
59	1	-1.947462	0.712208	-3.543607
60	1	-1.140417	2.185165	-2.993763
61	6	0.409958	2.629412	-5.253739
62	6	1.786947	0.560421	-5.715201
63	1	2.546500	2.425522	-4.884124
64	6	-0.720719	0.504748	-6.025902
65	1	0.614878	-1.206340	-6.216989
66	1	-1.741524	2.335042	-5.430698
67	1	0.534282	2.963866	-6.293264
68	1	0.313502	3.529278	-4.631089
69	1	1.926870	0.866049	-6.761475
70	1	2.675727	-0.018129	-5.425360
71	1	-0.614340	0.807254	-7.076940
72	1	-1.626994	-0.114022	-5.957595
73	6	-1.596167	1.505194	2.317885
74	6	-2.291088	0.522235	3.313228
75	6	-0.225961	1.865993	2.952508
76	6	-2.403278	2.828161	2.186270
77	6	-2.500830	1.202450	4.690327
78	1	-3.255036	0.176351	2.934434
79	1	-1.655956	-0.367234	3.421400
80	6	-0.394250	2.525793	4.344906
81	1	0.366767	0.949102	3.056652
82	1	0.313598	2.551131	2.295514
83	6	-2.594489	3.479292	3.581005
84	1	-1.856495	3.504089	1.516873
85	1	-3.385796	2.652191	1.742661
86	6	-3.341020	2.492282	4.513253
87	6	-1.128056	1.561033	5.302927
88	1	-3.032123	0.504634	5.351583
89	6	-1.217107	3.826428	4.191250
90	1	0.601226	2.763241	4.744005
91	1	-3.188498	4.395469	3.463294
92	1	-3.516476	2.959919	5.491753
93	1	-4.327129	2.247183	4.092499
94	1	-1.260897	2.031793	6.286753
95	1	-0.534405	0.648988	5.457214
96	1	-1.346253	4.308984	5.169868
97	1	-0.685771	4.537117	3.544109

11Ad (E = -1654.6084934 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.112427	-0.919715	0.069725
2	7	-1.648936	-0.013593	0.327287
3	6	-1.234533	0.731511	1.555647
4	7	1.265955	0.906073	0.113779
5	6	-0.762926	-2.937709	1.413572
6	6	0.274670	-2.347765	2.197664
7	6	-0.164322	-3.498052	0.253426
8	17	0.162526	-1.324474	-2.349130
9	6	1.524576	-2.599971	1.544348
10	6	1.251877	-3.296554	0.338762
11	6	0.618128	2.055072	0.590909
12	6	-0.554454	2.029697	1.296008
13	1	-2.048702	0.788568	2.280559
14	6	-0.988253	3.387296	1.650404
15	1	-0.484892	0.089099	2.077626

16	6	0.946437	3.530726	0.364109
17	6	-0.118333	4.281713	1.129179
18	1	1.951257	3.834181	0.664926
19	1	0.856776	3.763747	-0.703113
20	6	-0.102925	5.783022	1.226113
21	6	-2.201426	3.667814	2.500769
22	1	-2.319136	4.738649	2.692884
23	1	-2.129684	3.160501	3.473115
24	1	-3.123482	3.313439	2.021140
25	1	-0.957192	6.161782	1.797436
26	1	-0.137419	6.252888	0.232027
27	1	0.811453	6.148695	1.717174
28	6	0.141712	-1.856877	3.622752
29	6	-2.199735	-3.096941	1.846714
30	6	-0.854682	-4.324875	-0.804124
31	6	2.253778	-3.872649	-0.632123
32	6	2.868141	-2.394142	2.206161
33	1	0.358560	-2.675578	4.324540
34	1	-0.870060	-1.501700	3.841923
35	1	0.840432	-1.043424	3.848171
36	1	-2.303944	-3.975335	2.499887
37	1	-2.868346	-3.240323	0.993406
38	1	-2.558610	-2.225776	2.402851
39	1	-0.744198	-5.396699	-0.585002
40	1	-0.433492	-4.140922	-1.797171
41	1	-1.926236	-4.107764	-0.855189
42	1	2.315484	-4.963843	-0.516404
43	1	3.257266	-3.467630	-0.471864
44	1	1.972923	-3.667382	-1.671145
45	1	2.961774	-3.069092	3.068891
46	1	3.005283	-1.372554	2.578407
47	1	3.697217	-2.618705	1.529505
48	6	-2.977490	0.269265	-0.274905
49	6	-3.298569	-0.852236	-1.301169
50	6	-4.123754	0.295096	0.778978
51	6	-2.968902	1.631167	-1.034866
52	6	-4.662372	-0.603220	-1.989443
53	1	-2.502211	-0.893888	-2.051223
54	1	-3.312563	-1.819739	-0.781545
55	6	-5.491202	0.549075	0.093306
56	1	-4.141876	-0.661106	1.319191
57	1	-3.947845	1.087805	1.517248
58	6	-4.336975	1.885045	-1.716238
59	1	-2.738489	2.445895	-0.338365
60	1	-2.165205	1.608680	-1.782105
61	6	-4.626210	0.754351	-2.732640
62	6	-5.782997	-0.579605	-0.923662
63	1	-4.851719	-1.412090	-2.708221
64	6	-5.453187	1.910466	-0.643558
65	1	-6.276693	0.567196	0.861312
66	1	-4.305034	2.851369	-2.237829
67	1	-5.586389	0.934182	-3.236347
68	1	-3.849234	0.738025	-3.509319
69	1	-6.758727	-0.413666	-1.401231
70	1	-5.835346	-1.549041	-0.407786
71	1	-6.425858	2.109104	-1.114840
72	1	-5.269998	2.723439	0.073741
73	6	2.700775	1.031243	-0.347345
74	6	3.628950	1.552435	0.791387
75	6	3.220288	-0.378770	-0.741807
76	6	2.852491	1.927295	-1.614881
77	6	5.101764	1.623592	0.313206
78	1	3.309656	2.540437	1.134340

79	1	3.541909	0.873518	1.650955
80	6	4.700017	-0.345083	-1.202191
81	1	3.129518	-1.043232	0.121156
82	1	2.607412	-0.782784	-1.554624
83	6	4.333373	1.982782	-2.073234
84	1	2.216844	1.517318	-2.410874
85	1	2.514611	2.945846	-1.420073
86	6	5.204226	2.549885	-0.924179
87	6	5.590397	0.206027	-0.064648
88	1	5.722510	2.024764	1.126026
89	6	4.825319	0.565975	-2.444435
90	1	5.013216	-1.366647	-1.458230
91	1	4.407242	2.640967	-2.949623
92	1	6.251357	2.626760	-1.248320
93	1	4.871736	3.565381	-0.664596
94	1	6.639641	0.238793	-0.389405
95	1	5.543299	-0.454955	0.812403
96	1	5.869799	0.601671	-2.784035
97	1	4.226564	0.162728	-3.272616

14Ad (E = -755.667076 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.249133	0.708974	0.069182
2	6	0.060997	0.263766	0.105792
3	6	-1.117243	1.195434	0.151040
4	6	-2.321304	0.374760	0.338151
5	6	-0.518361	-1.154909	0.156711
6	6	-2.000525	-0.937157	0.356943
7	1	-0.329579	-1.694775	-0.778114
8	1	-0.076366	-1.756771	0.957478
9	6	-2.908848	-2.121888	0.522644
10	6	-3.685590	0.995194	0.476451
11	1	-4.468079	0.245196	0.619548
12	1	-3.938424	1.581850	-0.416946
13	1	-3.714917	1.683760	1.331396
14	1	-3.955928	-1.833982	0.650660
15	1	-2.611809	-2.719273	1.396437
16	1	-2.843823	-2.786706	-0.350641
17	6	-1.044467	2.529572	0.036809
18	1	-1.926406	3.157544	0.079866
19	1	-0.083270	3.009001	-0.102482
20	6	2.488134	-0.100445	0.069081
21	6	2.531622	-1.233552	-0.996165
22	6	3.643115	0.895295	-0.239824
23	6	2.742179	-0.711567	1.479073
24	6	3.908210	-1.947515	-0.961382
25	1	1.746769	-1.973448	-0.808107
26	1	2.348198	-0.802129	-1.990050
27	6	5.016793	0.188577	-0.204479
28	1	3.465781	1.345084	-1.226153
29	1	3.606160	1.708829	0.496016
30	6	4.112985	-1.434015	1.508638
31	1	2.716609	0.092527	2.226318
32	1	1.942948	-1.419759	1.732785
33	6	4.128657	-2.559649	0.444738
34	6	5.038636	-0.936516	-1.266933
35	1	3.913235	-2.746613	-1.715209
36	6	5.242768	-0.421013	1.200975
37	1	5.807999	0.918723	-0.421724
38	1	4.266860	-1.867326	2.506284
39	1	5.089017	-3.092453	0.476191
40	1	3.342835	-3.297300	0.662906
41	1	6.011692	-1.447178	-1.260385

42	1	4.902621	-0.510184	-2.270660
43	1	6.219246	-0.923311	1.243564
44	1	5.253126	0.373925	1.959507

15Ad (E = -1147.2052187 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.182853	-0.034684	-0.520081
2	7	-0.734820	1.708481	-0.333183
3	6	-1.958442	-1.127193	0.864819
4	6	-0.783924	-1.109685	1.677369
5	6	-1.733668	-2.050054	-0.201823
6	17	0.080615	-0.541934	-2.929986
7	6	0.145545	-2.050513	1.128511
8	6	-0.440837	-2.629935	-0.028957
9	6	-0.638524	-0.391892	3.000776
10	6	-3.266728	-0.444187	1.187826
11	6	-2.736898	-2.458969	-1.255716
12	6	0.142973	-3.720414	-0.894689
13	6	1.447915	-2.465056	1.772258
14	1	-1.011001	-1.015088	3.826972
15	1	-1.202482	0.545960	3.012114
16	1	0.407433	-0.151371	3.222673
17	1	-3.879701	-1.079308	1.844254
18	1	-3.852201	-0.239747	0.286011
19	1	-3.107437	0.510040	1.697789
20	1	-3.283047	-3.359985	-0.940706
21	1	-2.249397	-2.681578	-2.210219
22	1	-3.477707	-1.673621	-1.438142
23	1	-0.337086	-4.686943	-0.685424
24	1	1.216573	-3.846349	-0.717350
25	1	0.004711	-3.506798	-1.960657
26	1	1.274503	-3.255814	2.515815
27	1	1.932360	-1.631657	2.292806
28	1	2.161228	-2.859647	1.040834
29	7	2.062389	0.297040	-0.038377
30	6	3.012990	-0.461857	-0.637010
31	6	2.461748	1.288060	0.797382
32	6	4.376102	-0.261502	-0.423731
33	1	2.659023	-1.232867	-1.311545
34	6	3.806114	1.537554	1.069982
35	1	1.669521	1.887727	1.226673
36	6	4.783365	0.752981	0.448501
37	1	5.097025	-0.888369	-0.933917
38	1	4.076113	2.339453	1.746112
39	1	5.836402	0.931401	0.634834
40	6	-1.285446	3.040225	-0.266251
41	6	-1.440113	3.530385	1.205992
42	6	-0.357252	4.048164	-1.013896
43	6	-2.690205	3.093309	-0.943187
44	6	-2.024480	4.963735	1.257467
45	1	-2.093131	2.831343	1.747021
46	1	-0.455491	3.502342	1.695574
47	6	-0.938473	5.482264	-0.967343
48	1	0.638943	4.024402	-0.549305
49	1	-0.240480	3.710624	-2.052259
50	6	-3.277711	4.524809	-0.896010
51	1	-2.590257	2.751270	-1.982214
52	1	-3.357845	2.388703	-0.428656
53	6	-3.416911	4.976898	0.578942
54	6	-1.078771	5.934393	0.507326
55	1	-2.123129	5.282490	2.305048
56	6	-2.331428	5.496013	-1.644168
57	1	-0.264395	6.168146	-1.499922

58	1	-4.265960	4.530799	-1.377178
59	1	-3.849019	5.986783	0.625706
60	1	-4.102931	4.305648	1.115167
61	1	-1.476461	6.958389	0.552818
62	1	-0.091933	5.948460	0.992342
63	1	-2.747307	6.513786	-1.631561
64	1	-2.240316	5.195162	-2.697246

TS(8a-16)Ad (E = -1654.5427612 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.961156	0.106583	-0.087351
2	7	-0.289691	-1.433305	-0.749353
3	6	-1.312746	-1.409780	0.147353
4	7	-0.862374	1.405632	-0.555699
5	6	2.703405	-1.314898	1.172343
6	6	1.731108	-0.855441	2.111827
7	6	3.439571	-0.184886	0.727485
8	17	2.248018	0.711816	-2.080674
9	6	1.868694	0.567468	2.244966
10	6	2.915710	0.975764	1.372509
11	6	-1.900743	0.885559	0.080257
12	6	-1.552380	-0.217631	1.018965
13	1	-1.948964	-2.272222	0.304310
14	6	-2.777880	-0.389098	1.902390
15	1	-0.659766	0.124382	1.645175
16	6	-3.356784	1.260002	0.300360
17	6	-3.774831	0.394249	1.469112
18	1	-3.471811	2.315387	0.567484
19	1	-4.004434	1.096445	-0.570865
20	6	-5.182747	0.494640	1.992921
21	6	-2.798503	-1.371420	3.043277
22	1	-3.810573	-1.521496	3.430603
23	1	-2.172861	-1.027148	3.878015
24	1	-2.406843	-2.348083	2.732683
25	1	-5.367594	-0.186088	2.828884
26	1	-5.909092	0.263190	1.201165
27	1	-5.401442	1.515842	2.335641
28	6	0.914428	-1.758457	3.006850
29	6	3.041510	-2.759196	0.889703
30	6	4.673824	-0.224835	-0.136311
31	6	3.465228	2.376340	1.235703
32	6	1.210539	1.441423	3.289258
33	1	1.542856	-2.150638	3.819684
34	1	0.502565	-2.615875	2.465293
35	1	0.080994	-1.225728	3.471021
36	1	3.784852	-3.130590	1.611223
37	1	3.464043	-2.889120	-0.111942
38	1	2.160321	-3.403456	0.965266
39	1	5.565623	-0.371755	0.490293
40	1	4.806106	0.703697	-0.697969
41	1	4.636853	-1.042610	-0.862364
42	1	4.338065	2.518425	1.889413
43	1	2.721657	3.130616	1.513417
44	1	3.786628	2.586610	0.209866
45	1	1.847301	1.512984	4.183933
46	1	0.241621	1.043905	3.606793
47	1	1.042085	2.459007	2.921252
48	6	-0.977181	2.541539	-1.550995
49	6	-2.253024	3.425091	-1.411751
50	6	0.242226	3.486433	-1.345084
51	6	-0.966238	1.963083	-2.995454
52	6	-2.251140	4.573446	-2.456829
53	1	-3.152304	2.825399	-1.574948

54	1	-2.303570	3.850081	-0.400732
55	6	0.257865	4.613590	-2.406472
56	1	0.183957	3.916869	-0.334835
57	1	1.171282	2.916987	-1.410210
58	6	-0.954160	3.106635	-4.040699
59	1	-0.088967	1.326044	-3.129015
60	1	-1.858064	1.334180	-3.128544
61	6	-2.226351	3.971111	-3.881699
62	6	-1.014407	5.476760	-2.255802
63	1	-3.167741	5.164283	-2.321665
64	6	0.299902	3.990248	-3.824435
65	1	1.150566	5.234743	-2.251556
66	1	-0.926047	2.668865	-5.047941
67	1	-2.237700	4.775145	-4.630685
68	1	-3.123763	3.358613	-4.049791
69	1	-1.016436	6.290176	-2.994668
70	1	-1.040794	5.941854	-1.260096
71	1	0.332989	4.786147	-4.581705
72	1	1.209579	3.387390	-3.943699
73	6	-0.350354	-2.490672	-1.814124
74	6	-0.431929	-3.917565	-1.192650
75	6	-1.597519	-2.261935	-2.715546
76	6	0.911533	-2.427563	-2.707396
77	6	-0.502888	-4.992283	-2.306225
78	1	0.450069	-4.081719	-0.559217
79	1	-1.316956	-4.005884	-0.550794
80	6	-1.667164	-3.339216	-3.825826
81	1	-2.505485	-2.291024	-2.099967
82	1	-1.535906	-1.258114	-3.155467
83	6	0.851237	-3.502025	-3.821488
84	1	0.992318	-1.432861	-3.155608
85	1	1.806968	-2.576631	-2.089563
86	6	0.766166	-4.910011	-3.186855
87	6	-1.757133	-4.744001	-3.180292
88	1	-0.568222	-5.985646	-1.841501
89	6	-0.396095	-3.258317	-4.705524
90	1	-2.557342	-3.160488	-4.444451
91	1	1.758602	-3.426930	-4.435749
92	1	0.732560	-5.678835	-3.971396
93	1	1.660873	-5.105917	-2.579043
94	1	-1.828985	-5.513547	-3.961392
95	1	-2.666048	-4.820233	-2.566366
96	1	-0.443201	-4.007209	-5.508565
97	1	-0.331226	-2.271531	-5.184755

16Ad (E = -1654.5918017 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.901792	-0.312844	0.091622
2	7	-0.645330	-1.720257	-1.057464
3	6	-1.650724	-1.649472	-0.247296
4	7	-0.632285	1.129646	-0.540845
5	6	3.178559	-0.238509	1.324856
6	6	2.207256	-0.547491	2.307338
7	6	2.948435	1.102192	0.872205
8	17	2.416322	-0.717455	-1.822139
9	6	1.341520	0.582257	2.438117
10	6	1.834866	1.615493	1.584733
11	6	-1.592777	0.779072	0.322074
12	6	-1.835282	-0.569679	0.678602
13	1	-2.428048	-2.411089	-0.239783
14	6	-2.821207	-0.600768	1.784244
15	1	0.588586	-1.800088	1.086058
16	6	-2.544503	1.637468	1.151619

17	6	-3.225381	0.652408	2.073471
18	1	-2.010652	2.429447	1.685007
19	1	-3.285237	2.138062	0.515796
20	6	-4.216359	1.123027	3.102167
21	6	-3.257362	-1.889121	2.432316
22	1	-3.912913	-1.710205	3.289542
23	1	-2.387461	-2.462240	2.778600
24	1	-3.804739	-2.531118	1.728477
25	1	-4.625779	0.293167	3.686318
26	1	-5.060684	1.645858	2.629616
27	1	-3.757816	1.832935	3.805482
28	6	2.202914	-1.762375	3.201242
29	6	4.362141	-1.097257	0.950520
30	6	3.879837	1.876571	-0.027123
31	6	1.410066	3.060445	1.640289
32	6	0.277358	0.730223	3.500351
33	1	2.829901	-1.582771	4.087388
34	1	2.595068	-2.645361	2.687620
35	1	1.193173	-2.004133	3.544999
36	1	5.223391	-0.864569	1.593900
37	1	4.663256	-0.934303	-0.087861
38	1	4.142456	-2.163928	1.067609
39	1	4.797492	2.147327	0.514692
40	1	3.423628	2.805203	-0.384258
41	1	4.169955	1.289243	-0.904093
42	1	1.938485	3.570349	2.459163
43	1	0.338511	3.170379	1.828384
44	1	1.646917	3.595939	0.717088
45	1	0.734334	0.946489	4.477179
46	1	-0.319227	-0.181260	3.608705
47	1	-0.413544	1.547804	3.275158
48	6	-0.764694	2.270538	-1.507583
49	6	-1.136140	3.654587	-0.894698
50	6	0.576871	2.420981	-2.270494
51	6	-1.869702	1.882198	-2.538098
52	6	-1.246308	4.727827	-2.011543
53	1	-2.095128	3.600251	-0.372210
54	1	-0.377916	3.955400	-0.166080
55	6	0.465168	3.490202	-3.384012
56	1	1.370213	2.699467	-1.565488
57	1	0.856115	1.455355	-2.704817
58	6	-1.988939	2.955191	-3.647760
59	1	-1.615928	0.908076	-2.972391
60	1	-2.831225	1.767688	-2.017527
61	6	-2.352814	4.318903	-3.013399
62	6	0.103464	4.855816	-2.754670
63	1	-1.505969	5.689368	-1.547981
64	6	-0.636059	3.076762	-4.390452
65	1	1.429837	3.563936	-3.903210
66	1	-2.773815	2.654006	-4.354863
67	1	-2.454625	5.083998	-3.795248
68	1	-3.322393	4.251042	-2.499286
69	1	0.033241	5.627157	-3.533995
70	1	0.891780	5.171983	-2.056796
71	1	-0.712594	3.822865	-5.193432
72	1	-0.376058	2.118546	-4.860988
73	6	-0.624926	-2.779041	-2.120299
74	6	-1.927687	-3.625957	-2.198170
75	6	-0.426070	-2.079462	-3.494874
76	6	0.558500	-3.752828	-1.853057
77	6	-1.828792	-4.672877	-3.338703
78	1	-2.096326	-4.155865	-1.250356
79	1	-2.794444	-2.972203	-2.372999

80	6	-0.311007	-3.128691	-4.626766
81	1	-1.282490	-1.415573	-3.680272
82	1	0.473101	-1.459645	-3.454553
83	6	0.664306	-4.796484	-2.992713
84	1	1.488862	-3.184983	-1.776729
85	1	0.394831	-4.253843	-0.888759
86	6	-0.639876	-5.624346	-3.063364
87	6	-1.614750	-3.957696	-4.693466
88	1	-2.764241	-5.248118	-3.367352
89	6	0.887601	-4.067594	-4.341381
90	1	-0.152431	-2.608724	-5.581284
91	1	1.514711	-5.460896	-2.788245
92	1	-0.570284	-6.378161	-3.859865
93	1	-0.797561	-6.163903	-2.118744
94	1	-1.555725	-4.698495	-5.502916
95	1	-2.468881	-3.302153	-4.915252
96	1	0.990965	-4.801995	-5.152492
97	1	1.819177	-3.487352	-4.305354

TS(8a-17)Ad (E = -1654.542044 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.269235	-0.477675	0.220144
2	7	1.670001	0.220295	-0.225300
3	6	1.462340	0.481931	-1.542658
4	7	-1.558450	0.946881	-0.621597
5	6	-0.528145	-2.559436	-1.202990
6	6	-1.788972	-2.499683	-0.527962
7	6	0.471284	-2.896737	-0.236555
8	17	-0.501639	0.191297	2.584144
9	6	-1.553006	-2.691416	0.855967
10	6	-0.153326	-2.936895	1.039189
11	6	-0.475083	1.761826	-0.811387
12	6	0.504686	1.555438	-1.966642
13	1	2.117785	0.030713	-2.289323
14	6	1.163867	2.910865	-2.169375
15	1	-0.052601	1.238380	-2.859510
16	6	-0.103306	3.094765	-0.152596
17	6	0.815160	3.743423	-1.176159
18	1	-0.948383	3.735948	0.093207
19	1	0.431660	2.942108	0.796275
20	6	1.231818	5.175508	-0.974097
21	6	2.065876	3.168167	-3.346463
22	1	2.510556	4.168166	-3.322143
23	1	1.513178	3.067608	-4.291797
24	1	2.887546	2.439195	-3.379238
25	1	1.916674	5.528823	-1.751022
26	1	1.729030	5.296802	-0.000480
27	1	0.356331	5.840229	-0.964986
28	6	-3.116568	-2.570887	-1.243032
29	6	-0.360859	-2.616811	-2.705699
30	6	1.845259	-3.408162	-0.593067
31	6	0.466811	-3.356957	2.350850
32	6	-2.580906	-2.798620	1.956282
33	1	-3.220916	-3.561408	-1.709982
34	1	-3.209691	-1.828237	-2.040254
35	1	-3.962968	-2.445511	-0.562966
36	1	-0.574973	-3.629507	-3.080767
37	1	0.657925	-2.360487	-3.011797
38	1	-1.041515	-1.927492	-3.216275
39	1	1.774521	-4.460078	-0.906911
40	1	2.541627	-3.367418	0.247876
41	1	2.287594	-2.852917	-1.425365
42	1	0.103335	-4.352453	2.643225

43	1	0.214786	-2.662403	3.159934
44	1	1.557274	-3.412342	2.286035
45	1	-2.715932	-3.847899	2.255946
46	1	-3.556669	-2.416568	1.642226
47	1	-2.275378	-2.237398	2.846124
48	6	3.073564	0.148537	0.315086
49	6	4.121061	-0.438639	-0.669270
50	6	3.477710	1.623751	0.629791
51	6	3.100790	-0.648426	1.639487
52	6	5.534317	-0.394380	-0.030232
53	1	3.861782	-1.471552	-0.925666
54	1	4.132816	0.141234	-1.601193
55	6	4.891329	1.678037	1.258690
56	1	3.444269	2.210417	-0.297049
57	1	2.738308	2.054719	1.316675
58	6	4.515047	-0.602335	2.271123
59	1	2.363022	-0.226186	2.331637
60	1	2.815383	-1.688373	1.452761
61	6	5.540517	-1.211315	1.284460
62	6	5.919043	1.073950	0.272126
63	1	6.254892	-0.826729	-0.737576
64	6	4.900051	0.865403	2.575848
65	1	5.148791	2.725424	1.467398
66	1	4.508052	-1.182912	3.203236
67	1	6.545471	-1.200150	1.728505
68	1	5.290498	-2.261803	1.078204
69	1	6.928322	1.117233	0.704052
70	1	5.939579	1.658346	-0.658699
71	1	5.895940	0.906206	3.038293
72	1	4.190128	1.300238	3.292748
73	6	-2.996485	1.400255	-0.581522
74	6	-3.790699	0.529130	0.420461
75	6	-3.214071	2.888454	-0.185678
76	6	-3.579070	1.213603	-2.016061
77	6	-5.300377	0.872266	0.377380
78	1	-3.640030	-0.524509	0.181287
79	1	-3.391522	0.693554	1.429415
80	6	-4.723587	3.249234	-0.212181
81	1	-2.812587	3.068940	0.818909
82	1	-2.684876	3.541128	-0.889571
83	6	-5.088123	1.562664	-2.048293
84	1	-3.022096	1.858310	-2.710644
85	1	-3.420391	0.178910	-2.336561
86	6	-5.849234	0.650685	-1.054188
87	6	-5.496796	2.351841	0.781529
88	1	-5.836037	0.221741	1.082282
89	6	-5.281268	3.041991	-1.640065
90	1	-4.834988	4.302973	0.077853
91	1	-5.473352	1.404209	-3.065027
92	1	-6.923883	0.878640	-1.083251
93	1	-5.734987	-0.402800	-1.345489
94	1	-6.564491	2.611709	0.773382
95	1	-5.129659	2.515141	1.804258
96	1	-6.346774	3.308772	-1.671895
97	1	-4.760520	3.700930	-2.349221

17Ad (E = -1654.5702106 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	0.029526	-0.616611	0.698816
2	7	1.442269	1.117956	-0.237834
3	6	0.881373	2.264952	-0.098933
4	7	-1.643342	0.242897	-0.035598
5	6	-0.061148	-2.921444	-0.667416
6	6	-0.916417	-3.010739	0.469458
7	6	1.288778	-2.906100	-0.196352
8	17	0.936919	-0.119943	2.979190
9	6	-0.094422	-2.995561	1.637244
10	6	1.270164	-2.949377	1.220722
11	6	-1.174844	1.204635	0.922821
12	6	-0.478416	2.488692	0.461662
13	1	1.400844	3.161283	-0.430463
14	6	-0.496416	3.380740	1.706507
15	1	-0.999852	3.051756	-0.339664
16	6	-1.958991	1.580717	2.188332
17	6	-1.317606	2.872667	2.635376
18	1	-3.033236	1.756976	2.012913
19	1	-1.904343	0.815495	2.975151
20	6	-1.654492	3.449381	3.985151
21	6	0.287750	4.667236	1.752859
22	1	0.044534	5.259866	2.639936
23	1	0.080734	5.288534	0.868763
24	1	1.371458	4.482254	1.769999
25	1	-1.182243	4.420669	4.162904
26	1	-1.330776	2.765908	4.782243
27	1	-2.741382	3.574294	4.093870
28	6	-2.377861	-3.392514	0.474525
29	6	-0.432167	-3.170566	-2.113680
30	6	2.482020	-3.188552	-1.076323
31	6	2.461041	-3.105393	2.133071
32	6	-0.572283	-3.247041	3.049593
33	1	-2.473588	-4.483151	0.583923
34	1	-2.886454	-3.108951	-0.449204
35	1	-2.922102	-2.935383	1.306719
36	1	0.065934	-4.081335	-2.475611
37	1	-0.137316	-2.353372	-2.782965
38	1	-1.507590	-3.321147	-2.233954
39	1	2.515547	-4.262776	-1.314388
40	1	3.426548	-2.940312	-0.585999
41	1	2.441765	-2.653589	-2.029976
42	1	2.570952	-4.153212	2.447985
43	1	2.355235	-2.491335	3.032715
44	1	3.393535	-2.811161	1.640065
45	1	-0.623476	-4.327824	3.249060
46	1	-1.572342	-2.835434	3.225911
47	1	0.101717	-2.797813	3.783465
48	6	2.831350	1.078932	-0.838766
49	6	2.739402	0.451001	-2.255297
50	6	3.506148	2.474250	-0.972268
51	6	3.726896	0.192057	0.064728
52	6	4.157488	0.312006	-2.871102
53	1	2.250476	-0.528201	-2.192114
54	1	2.110044	1.088739	-2.891756
55	6	4.925391	2.335672	-1.577566
56	1	2.918484	3.127510	-1.630539
57	1	3.565477	2.957548	0.012667
58	6	5.141733	0.047446	-0.553420
59	1	3.789287	0.640060	1.064356
60	1	3.263812	-0.793698	0.183441
61	6	5.043246	-0.580271	-1.966377
62	6	4.812021	1.709029	-2.988145
63	1	4.069270	-0.141588	-3.867145

64	6	5.797968	1.442920	-0.665726
65	1	5.370568	3.336462	-1.652757
66	1	5.748182	-0.596889	0.096529
67	1	6.047189	-0.667540	-2.403782
68	1	4.630695	-1.593147	-1.908599
69	1	5.807512	1.619938	-3.443212
70	1	4.213530	2.358551	-3.642275
71	1	6.810311	1.353299	-1.082183
72	1	5.894801	1.899350	0.328887
73	6	-2.894042	0.362417	-0.829738
74	6	-4.135334	-0.134422	-0.022402
75	6	-3.167505	1.833234	-1.263906
76	6	-2.774858	-0.490413	-2.118144
77	6	-5.425181	-0.046022	-0.876131
78	1	-3.962964	-1.167078	0.297295
79	1	-4.246344	0.472126	0.883881
80	6	-4.461087	1.931587	-2.112112
81	1	-3.255604	2.471138	-0.375891
82	1	-2.315005	2.199997	-1.851608
83	6	-4.062603	-0.404134	-2.973846
84	1	-1.908163	-0.140082	-2.696818
85	1	-2.580622	-1.529554	-1.842362
86	6	-5.267944	-0.915675	-2.146842
87	6	-5.668232	1.426210	-1.286011
88	1	-6.276251	-0.409811	-0.283779
89	6	-4.310462	1.066360	-3.386218
90	1	-4.622931	2.980808	-2.395975
91	1	-3.942406	-1.024710	-3.872976
92	1	-6.185091	-0.871848	-2.751007
93	1	-5.115733	-1.968100	-1.867363
94	1	-6.590795	1.508389	-1.877819
95	1	-5.801086	2.049806	-0.390575
96	1	-5.216993	1.139780	-4.003252
97	1	-3.472511	1.434070	-3.995617

TS(17-18)Ad (E = -1654.5480594 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.010876	-0.654766	-0.336771
2	7	-1.539391	0.967188	0.191784
3	6	-0.822235	2.020048	-0.168985
4	7	1.735959	0.179545	0.317336
5	6	-0.061658	-2.699231	1.267303
6	6	0.824781	-3.064458	0.210306
7	6	-1.387991	-2.648795	0.728285
8	17	-0.222444	-0.469026	-2.802366
9	6	0.054579	-3.177620	-0.980843
10	6	-1.315302	-2.953254	-0.657286
11	6	1.238098	1.294046	-0.411044
12	6	0.520707	2.420539	0.343144
13	1	-1.219751	2.683383	-0.938277
14	6	1.012436	3.705631	-0.283583
15	1	0.586031	2.370451	1.434517
16	6	1.960239	1.961647	-1.591733
17	6	1.780255	3.447856	-1.355825
18	1	3.024926	1.694721	-1.626471
19	1	1.551124	1.664681	-2.565505
20	6	2.430186	4.436022	-2.288110
21	6	0.589960	5.038841	0.277308
22	1	0.986698	5.880047	-0.299772
23	1	0.932658	5.150800	1.316021
24	1	-0.506060	5.132453	0.295441
25	1	2.209445	5.474835	-2.023130
26	1	2.095638	4.270788	-3.321813

27	1	3.522473	4.310508	-2.286658
28	6	2.230497	-3.604385	0.330244
29	6	0.218480	-2.719611	2.755144
30	6	-2.620107	-2.635602	1.602214
31	6	-2.451002	-3.218666	-1.616857
32	6	0.556996	-3.706568	-2.302252
33	1	2.195362	-4.703842	0.324943
34	1	2.726243	-3.299490	1.252984
35	1	2.865562	-3.299039	-0.506825
36	1	-0.390090	-3.497097	3.237938
37	1	-0.016903	-1.770378	3.250907
38	1	1.264985	-2.949684	2.965754
39	1	-2.738321	-3.618005	2.083659
40	1	-3.535059	-2.440276	1.038785
41	1	-2.552549	-1.892828	2.403616
42	1	-2.394934	-4.253570	-1.980835
43	1	-2.411255	-2.561619	-2.493337
44	1	-3.427489	-3.094465	-1.140685
45	1	0.492168	-4.804981	-2.321338
46	1	1.602163	-3.434770	-2.481646
47	1	-0.030163	-3.316545	-3.137395
48	6	-3.044146	1.090173	-0.016245
49	6	-3.673704	0.994473	1.403758
50	6	-3.495150	2.443811	-0.643310
51	6	-3.598590	-0.043180	-0.905845
52	6	-5.219123	1.058224	1.325598
53	1	-3.352247	0.061389	1.876681
54	1	-3.287985	1.819329	2.018749
55	6	-5.042897	2.520059	-0.718552
56	1	-3.121887	3.285721	-0.043319
57	1	-3.088341	2.551206	-1.657421
58	6	-5.145817	0.019266	-0.979408
59	1	-3.165805	0.037118	-1.910646
60	1	-3.286374	-1.003336	-0.495250
61	6	-5.744183	-0.101766	0.444044
62	6	-5.643361	2.408628	0.702525
63	1	-5.633196	0.969861	2.339021
64	6	-5.575390	1.367469	-1.601904
65	1	-5.320609	3.485176	-1.162775
66	1	-5.506024	-0.809173	-1.604182
67	1	-6.841154	-0.067187	0.393249
68	1	-5.474446	-1.068520	0.890817
69	1	-6.738665	2.477979	0.654558
70	1	-5.292860	3.241240	1.328497
71	1	-6.670245	1.422205	-1.673319
72	1	-5.177809	1.457354	-2.622191
73	6	3.052674	0.228839	1.036925
74	6	4.180014	-0.402774	0.166311
75	6	3.474240	1.686195	1.395449
76	6	2.952986	-0.552966	2.371651
77	6	5.532598	-0.396336	0.921428
78	1	3.896216	-1.426620	-0.097934
79	1	4.271180	0.158310	-0.772061
80	6	4.833892	1.699925	2.141233
81	1	3.546697	2.296761	0.490666
82	1	2.706436	2.141306	2.033394
83	6	4.306080	-0.555493	3.126153
84	1	2.171771	-0.093807	2.993103
85	1	2.641670	-1.577312	2.167456
86	6	5.396216	-1.202236	2.236293
87	6	5.927643	1.063370	1.250498
88	1	6.303775	-0.854139	0.286632
89	6	4.712036	0.899117	3.458890

90	1	5.102708	2.741423	2.365901
91	1	4.198806	-1.132083	4.055694
92	1	6.356478	-1.218012	2.770671
93	1	5.134400	-2.246387	2.013348
94	1	6.896509	1.086667	1.768912
95	1	6.043165	1.640864	0.322294
96	1	5.667641	0.912604	4.001532
97	1	3.959938	1.361151	4.114090

18Ad (E = -1654.5919628 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.070257	-0.950155	0.525354
2	7	1.539808	0.402075	0.101000
3	6	0.797309	1.479160	0.697578
4	7	-1.456623	0.355231	0.099171
5	6	-0.417315	-2.887038	-1.156922
6	6	-1.085774	-3.245349	0.051364
7	6	0.991089	-2.914090	-0.906042
8	17	0.175209	-0.860757	2.987869
9	6	-0.093373	-3.478992	1.045408
10	6	1.189347	-3.283870	0.455961
11	6	-0.775955	1.473029	0.701931
12	6	0.005659	2.520941	-0.086608
13	1	1.185873	1.846763	1.645470
14	6	-0.202386	3.824047	0.611400
15	1	0.049581	2.459904	-1.167418
16	6	-1.322989	2.212778	1.942536
17	6	-0.898127	3.655621	1.751585
18	1	-2.411039	2.130930	2.016257
19	1	-0.923583	1.775016	2.862549
20	6	-1.271674	4.686492	2.783341
21	6	0.371721	5.096242	0.042894
22	1	0.098178	5.974534	0.635594
23	1	0.014826	5.258133	-0.983894
24	1	1.468643	5.049596	-0.005533
25	1	-0.941835	5.692669	2.506198
26	1	-0.829681	4.445410	3.760445
27	1	-2.361476	4.715526	2.928651
28	6	-2.548730	-3.580264	0.231740
29	6	-0.991883	-2.850596	-2.555622
30	6	2.015445	-2.914195	-2.018661
31	6	2.496117	-3.597470	1.147320
32	6	-0.349709	-4.064126	2.412075
33	1	-2.675802	-4.670630	0.289726
34	1	-3.161402	-3.223651	-0.599456
35	1	-2.961519	-3.158143	1.154534
36	1	-0.585108	-3.689861	-3.137747
37	1	-0.743645	-1.931205	-3.096745
38	1	-2.078868	-2.954212	-2.555588
39	1	1.794966	-3.735590	-2.715413
40	1	3.027326	-3.077916	-1.640822
41	1	2.018471	-1.988218	-2.603284
42	1	2.587376	-4.680741	1.307929
43	1	2.565514	-3.115330	2.128957
44	1	3.357868	-3.276163	0.557946
45	1	-0.383746	-5.161904	2.348543
46	1	-1.301777	-3.724433	2.830817
47	1	0.434007	-3.789708	3.122467
48	6	-2.834899	0.582628	-0.440252
49	6	-3.916623	0.164767	0.602901
50	6	-3.088210	2.059521	-0.869669
51	6	-3.027802	-0.294578	-1.702501
52	6	-5.342007	0.333652	0.020643

53	1	-3.741728	-0.879856	0.890073
54	1	-3.811878	0.767033	1.512729
55	6	-4.520319	2.224455	-1.440893
56	1	-2.954610	2.743273	-0.025949
57	1	-2.352785	2.344675	-1.632609
58	6	-4.451021	-0.142122	-2.292821
59	1	-2.272573	-0.014375	-2.448817
60	1	-2.850402	-1.336460	-1.433131
61	6	-5.499163	-0.560096	-1.232911
62	6	-5.562328	1.814942	-0.371770
63	1	-6.079553	0.038649	0.779520
64	6	-4.686827	1.332621	-2.693221
65	1	-4.670556	3.277578	-1.715461
66	1	-4.543756	-0.786166	-3.178565
67	1	-6.512651	-0.458977	-1.645521
68	1	-5.365202	-1.616949	-0.961567
69	1	-6.579087	1.954754	-0.764626
70	1	-5.467112	2.458127	0.514681
71	1	-5.693614	1.455029	-3.116271
72	1	-3.969353	1.633942	-3.469491
73	6	2.919459	0.747465	-0.354061
74	6	2.908373	1.108263	-1.869611
75	6	3.522216	1.953249	0.429314
76	6	3.860319	-0.461062	-0.131260
77	6	4.339759	1.421269	-2.371344
78	1	2.481209	0.267075	-2.431156
79	1	2.252709	1.973879	-2.031036
80	6	4.953668	2.271799	-0.072974
81	1	2.889867	2.839782	0.302372
82	1	3.547073	1.715917	1.501762
83	6	5.291268	-0.157812	-0.640245
84	1	3.879391	-0.701299	0.940039
85	1	3.457308	-1.328547	-0.655830
86	6	5.244797	0.184467	-2.150213
87	6	4.908578	2.623982	-1.579911
88	1	4.304521	1.666552	-3.441753
89	6	5.869191	1.044033	0.142758
90	1	5.344583	3.128039	0.493448
91	1	5.924791	-1.041574	-0.482117
92	1	6.259139	0.388380	-2.520574
93	1	4.858429	-0.671674	-2.721350
94	1	5.917467	2.870173	-1.939134
95	1	4.281625	3.512471	-1.741845
96	1	6.888821	1.267255	-0.200874
97	1	5.932224	0.802832	1.213013

7aAd (E = -1654.5977117 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.114194	1.019517	0.038242
2	7	1.893200	0.085804	0.115649
3	6	1.671367	0.636513	1.246698
4	7	-1.506788	-0.500960	0.418916
5	6	-0.451085	3.113168	1.456180
6	6	-1.661503	2.957015	0.713223
7	6	0.586368	3.474532	0.539746
8	17	0.045891	0.614709	-2.442611
9	6	-1.358420	3.167544	-0.661579
10	6	0.034840	3.499359	-0.761585
11	6	-1.038487	-1.071273	1.607747
12	6	-0.869283	-0.413545	2.789499
13	1	2.394465	0.629185	2.069017
14	6	-0.174597	-1.261028	3.767326
15	1	-1.234838	0.581224	3.001431

16	6	-0.428366	-2.460745	1.782084
17	6	0.079349	-2.466655	3.205173
18	1	-1.145153	-3.271746	1.613635
19	1	0.376851	-2.609276	1.054305
20	6	0.695400	-3.693323	3.820301
21	6	0.125430	-0.793913	5.168519
22	1	0.610159	-1.572124	5.765876
23	1	-0.795288	-0.495078	5.688099
24	1	0.786428	0.083434	5.158828
25	1	0.996695	-3.522052	4.858861
26	1	1.585930	-4.019238	3.264125
27	1	-0.008404	-4.538386	3.812858
28	6	-3.035720	2.780703	1.317034
29	6	-0.329348	3.179954	2.961091
30	6	1.986868	3.883346	0.928123
31	6	0.727562	3.960073	-2.019986
32	6	-2.334569	3.269693	-1.808154
33	1	-3.388019	3.731276	1.742176
34	1	-3.047869	2.035508	2.119322
35	1	-3.766721	2.464539	0.568533
36	1	-0.238711	4.225609	3.288533
37	1	0.550634	2.642097	3.330841
38	1	-1.210479	2.762684	3.458131
39	1	2.033862	4.966017	1.114187
40	1	2.714020	3.655851	0.141417
41	1	2.315376	3.380308	1.843481
42	1	0.484219	5.012681	-2.225476
43	1	0.422542	3.366567	-2.886420
44	1	1.816498	3.884185	-1.933302
45	1	-2.491051	4.323455	-2.079951
46	1	-3.310049	2.846466	-1.553773
47	1	-1.963962	2.748249	-2.696913
48	6	3.112229	-0.605935	-0.382526
49	6	3.770233	0.304280	-1.458760
50	6	4.139689	-0.893313	0.737033
51	6	2.683686	-1.939926	-1.048493
52	6	5.010539	-0.405071	-2.055483
53	1	3.034168	0.525556	-2.239285
54	1	4.062759	1.256487	-0.994033
55	6	5.378472	-1.608275	0.137758
56	1	4.451999	0.046520	1.213589
57	1	3.679706	-1.518846	1.515212
58	6	3.922037	-2.650285	-1.647433
59	1	2.207561	-2.584576	-0.296888
60	1	1.939114	-1.728792	-1.824193
61	6	4.574644	-1.737161	-2.714659
62	6	6.032785	-0.695950	-0.929600
63	1	5.466819	0.248764	-2.810495
64	6	4.942992	-2.941038	-0.520102
65	1	6.097879	-1.810496	0.942376
66	1	3.604636	-3.592986	-2.112316
67	1	5.445734	-2.239555	-3.157289
68	1	3.863678	-1.540479	-3.528368
69	1	6.923255	-1.186263	-1.346144
70	1	6.366471	0.244637	-0.469113
71	1	5.820355	-3.460286	-0.929398
72	1	4.495531	-3.605335	0.232802
73	6	-2.594395	-1.218090	-0.332700
74	6	-3.670000	-1.781576	0.640384
75	6	-3.300739	-0.206811	-1.273477
76	6	-2.033224	-2.380605	-1.204482
77	6	-4.807756	-2.478141	-0.148752
78	1	-3.219153	-2.497825	1.337991

79	1	-4.073218	-0.956244	1.243359
80	6	-4.440751	-0.888748	-2.069617
81	1	-3.709061	0.610278	-0.666064
82	1	-2.567103	0.220204	-1.964025
83	6	-3.177263	-3.071073	-1.989945
84	1	-1.284255	-1.972693	-1.893568
85	1	-1.530345	-3.118592	-0.568289
86	6	-4.219712	-3.635592	-0.993508
87	6	-5.491918	-1.454688	-1.085751
88	1	-5.543571	-2.878074	0.562556
89	6	-3.858400	-2.041415	-2.922637
90	1	-4.911403	-0.144897	-2.727204
91	1	-2.758153	-3.890987	-2.589397
92	1	-5.024652	-4.148185	-1.538651
93	1	-3.748870	-4.381258	-0.336445
94	1	-6.309896	-1.936737	-1.639355
95	1	-5.935524	-0.640278	-0.495360
96	1	-4.659032	-2.525104	-3.499880
97	1	-3.129320	-1.646576	-3.643086

TS(7a-7c)Ad (E = -1654.5779513 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.417371	0.091092	-0.007373
2	7	-0.240551	2.022532	-1.156590
3	6	0.917662	1.487042	-1.049138
4	7	0.933189	-1.635593	0.083351
5	6	-1.381787	0.482230	2.347408
6	6	-1.648080	-0.904208	2.106190
7	6	-2.198634	1.249702	1.463905
8	17	-1.392053	-0.807829	-2.115030
9	6	-2.609177	-0.984990	1.068395
10	6	-2.941210	0.344565	0.658016
11	6	1.971257	-0.886231	0.539267
12	6	1.824335	0.013917	1.583667
13	1	1.812245	1.932404	-1.497718
14	6	3.003565	0.894498	1.657857
15	1	1.130184	-0.119778	2.395037
16	6	3.324927	-0.599419	-0.115970
17	6	3.887395	0.546259	0.696306
18	1	4.000155	-1.462085	-0.111113
19	1	3.173912	-0.328596	-1.165054
20	6	5.260985	1.094150	0.419059
21	6	3.144575	1.962726	2.710939
22	1	4.120545	2.455719	2.667808
23	1	3.024674	1.539360	3.717567
24	1	2.372813	2.736243	2.595328
25	1	5.533944	1.889620	1.120181
26	1	5.334489	1.507412	-0.597530
27	1	6.024942	0.306266	0.494887
28	6	-1.105014	-2.046222	2.931426
29	6	-0.692172	1.050935	3.568186
30	6	-2.404675	2.739407	1.594180
31	6	-4.054718	0.675743	-0.304546
32	6	-3.306680	-2.218071	0.552104
33	1	-1.466940	-1.981831	3.966889
34	1	-0.009387	-2.057438	2.960581
35	1	-1.425718	-3.011095	2.529681
36	1	-1.445129	1.362220	4.306952
37	1	-0.078811	1.928939	3.338479
38	1	-0.050099	0.312407	4.058324
39	1	-3.052547	2.952686	2.457122
40	1	-2.884717	3.167142	0.711459
41	1	-1.463132	3.274930	1.756484

42	1	-5.021487	0.358413	0.111577
43	1	-3.921965	0.166538	-1.265096
44	1	-4.116817	1.749514	-0.499381
45	1	-4.347208	-2.238404	0.906969
46	1	-2.822509	-3.136515	0.893371
47	1	-3.330059	-2.236944	-0.542562
48	6	-0.558535	3.255574	-1.954825
49	6	-2.064143	3.259601	-2.304999
50	6	-0.214535	4.520075	-1.121255
51	6	0.259351	3.286016	-3.275444
52	6	-2.419900	4.533458	-3.110810
53	1	-2.305146	2.356626	-2.879072
54	1	-2.652129	3.224895	-1.382043
55	6	-0.567928	5.792940	-1.931887
56	1	-0.773250	4.503013	-0.177656
57	1	0.855935	4.510207	-0.872398
58	6	-0.092682	4.558311	-4.086729
59	1	1.334434	3.282407	-3.055768
60	1	0.037395	2.382802	-3.858799
61	6	-1.602864	4.557056	-4.425147
62	6	-2.080449	5.787820	-2.267486
63	1	-3.493088	4.523787	-3.342451
64	6	0.250162	5.813225	-3.246549
65	1	-0.324889	6.679106	-1.330570
66	1	0.495160	4.562695	-5.014111
67	1	-1.857650	5.449491	-5.013006
68	1	-1.851439	3.680976	-5.039623
69	1	-2.343150	6.697950	-2.823734
70	1	-2.673004	5.792714	-1.341679
71	1	0.019735	6.722720	-3.817837
72	1	1.325923	5.835651	-3.022252
73	6	1.173619	-2.963130	-0.569669
74	6	2.175865	-3.807641	0.275280
75	6	-0.167927	-3.745476	-0.593239
76	6	1.707564	-2.850672	-2.028094
77	6	2.376457	-5.211297	-0.349944
78	1	3.145440	-3.301357	0.342498
79	1	1.785989	-3.897653	1.298694
80	6	0.014252	-5.149612	-1.218753
81	1	-0.532100	-3.839998	0.437851
82	1	-0.910380	-3.177265	-1.158223
83	6	1.897093	-4.260609	-2.644429
84	1	0.998524	-2.262966	-2.621885
85	1	2.667806	-2.321602	-2.037937
86	6	2.913608	-5.062671	-1.795041
87	6	1.025930	-5.964665	-0.379706
88	1	3.100760	-5.772335	0.256831
89	6	0.541126	-5.005808	-2.667031
90	1	-0.956638	-5.664070	-1.229658
91	1	2.276688	-4.154905	-3.670138
92	1	3.076907	-6.055136	-2.238016
93	1	3.886130	-4.549063	-1.785834
94	1	1.160763	-6.966176	-0.812001
95	1	0.646764	-6.100802	0.643144
96	1	0.662832	-5.997797	-3.124762
97	1	-0.183194	-4.450927	-3.278607

7cAd (E = -1654.5819822 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	0.045422	-0.598637	0.126942
2	7	-1.902675	0.382818	-0.429674
3	6	-0.931683	1.155292	-0.740962
4	7	2.032945	0.431719	0.464425
5	6	-0.194942	-2.217288	2.157014
6	6	1.080548	-2.555922	1.610829
7	6	-1.194630	-2.576449	1.206896
8	17	0.625011	-0.991195	-2.288855
9	6	0.869995	-3.106055	0.320269
10	6	-0.537227	-3.102424	0.059509
11	6	1.387733	1.380272	1.144909
12	6	0.380007	0.996958	2.057159
13	1	-1.078486	2.099727	-1.271673
14	6	-0.357685	2.209864	2.475225
15	1	0.558098	0.189043	2.750924
16	6	1.303724	2.896655	0.962187
17	6	0.152477	3.298838	1.861856
18	1	2.231907	3.404890	1.249849
19	1	1.124604	3.147228	-0.086474
20	6	-0.238650	4.745456	2.002596
21	6	-1.470614	2.150691	3.487816
22	1	-1.880662	3.140455	3.711188
23	1	-1.114682	1.713026	4.431060
24	1	-2.292662	1.515636	3.131446
25	1	-1.061655	4.879565	2.712130
26	1	-0.555434	5.175137	1.040957
27	1	0.608179	5.352638	2.355721
28	6	2.387589	-2.448518	2.358257
29	6	-0.464565	-1.870794	3.603235
30	6	-2.665040	-2.693907	1.525074
31	6	-1.193929	-3.775379	-1.121695
32	6	1.890794	-3.758866	-0.577579
33	1	2.334374	-2.991358	3.311232
34	1	2.653688	-1.407184	2.577375
35	1	3.209919	-2.879139	1.780371
36	1	-0.731582	-2.778784	4.163429
37	1	-1.291092	-1.161308	3.717008
38	1	0.415660	-1.440153	4.091851
39	1	-2.860213	-3.661961	2.010053
40	1	-3.290455	-2.647059	0.630812
41	1	-3.000250	-1.913171	2.214465
42	1	-1.216096	-4.865566	-0.977378
43	1	-0.652770	-3.569506	-2.049839
44	1	-2.226456	-3.439763	-1.258765
45	1	1.748868	-4.848981	-0.577171
46	1	2.913267	-3.556792	-0.248322
47	1	1.796003	-3.411444	-1.611645
48	6	-3.352019	0.606206	-0.745464
49	6	-3.847597	-0.569791	-1.627913
50	6	-4.159107	0.640986	0.578336
51	6	-3.593126	1.933290	-1.507623
52	6	-5.357989	-0.406315	-1.928923
53	1	-3.268314	-0.590536	-2.560214
54	1	-3.665091	-1.518322	-1.111029
55	6	-5.669737	0.800667	0.273798
56	1	-3.980818	-0.280285	1.141618
57	1	-3.804909	1.479009	1.193666
58	6	-5.103681	2.103009	-1.813548
59	1	-3.238706	2.781260	-0.905534
60	1	-3.023318	1.934709	-2.446745
61	6	-5.590038	0.922084	-2.688475
62	6	-6.150559	-0.386185	-0.598036
63	1	-5.693380	-1.249849	-2.546613

64	6	-5.902279	2.127817	-0.487481
65	1	-6.226427	0.813363	1.220299
66	1	-5.252051	3.048096	-2.352417
67	1	-6.656654	1.042159	-2.922363
68	1	-5.047510	0.910486	-3.643808
69	1	-7.225536	-0.289336	-0.802629
70	1	-6.008691	-1.333432	-0.058919
71	1	-6.972518	2.261472	-0.695919
72	1	-5.583255	2.978781	0.130463
73	6	3.314706	0.687436	-0.265250
74	6	4.361100	1.307898	0.709211
75	6	3.876239	-0.680877	-0.736315
76	6	3.167451	1.612649	-1.509079
77	6	5.725777	1.495056	-0.000660
78	1	4.009154	2.277417	1.081187
79	1	4.470671	0.645350	1.578838
80	6	5.239952	-0.510134	-1.447525
81	1	3.989975	-1.330725	0.140064
82	1	3.156721	-1.152645	-1.410897
83	6	4.537885	1.787736	-2.213851
84	1	2.435139	1.174577	-2.195989
85	1	2.795032	2.598173	-1.208300
86	6	5.548280	2.423386	-1.227544
87	6	6.259346	0.120663	-0.469711
88	1	6.436266	1.947388	0.704991
89	6	5.066695	0.410477	-2.679392
90	1	5.600066	-1.496198	-1.771782
91	1	4.408576	2.446278	-3.083752
92	1	6.516316	2.576928	-1.724562
93	1	5.190407	3.412122	-0.904989
94	1	7.234270	0.242384	-0.962228
95	1	6.412864	-0.539872	0.395489
96	1	6.027334	0.530979	-3.199851
97	1	4.363648	-0.041379	-3.392141

TS(7c-8b)Ad (E = -1654.5558415 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	0.000047	-0.663498	0.123682
2	7	-1.600254	0.681780	-0.144302
3	6	-0.462990	1.386914	-0.199616
4	7	2.017494	0.415557	0.555247
5	6	-0.505859	-1.711638	2.350038
6	6	0.727991	-2.339637	1.978928
7	6	-1.538182	-2.245932	1.514382
8	17	0.222446	-1.465918	-2.179756
9	6	0.466302	-3.191351	0.873744
10	6	-0.933849	-3.124230	0.583098
11	6	1.763476	1.544892	1.193131
12	6	0.414497	1.873844	1.585709
13	1	-0.359620	2.330929	-0.729176
14	6	0.406242	3.288892	2.026488
15	1	-0.173402	1.176195	2.175419
16	6	2.619168	2.786892	1.426415
17	6	1.631513	3.835170	1.890022
18	1	3.357548	2.608688	2.217845
19	1	3.182673	3.092844	0.541477
20	6	2.093067	5.237963	2.178735
21	6	-0.848139	3.953003	2.529355
22	1	-0.658267	4.966301	2.896166
23	1	-1.293367	3.373929	3.350240
24	1	-1.605731	4.017802	1.737625
25	1	1.283842	5.862185	2.570941
26	1	2.481492	5.729090	1.274293

27	1	2.908564	5.244684	2.917278
28	6	1.987895	-2.260432	2.809351
29	6	-0.734866	-0.951136	3.638756
30	6	-3.013870	-2.126241	1.799847
31	6	-1.632609	-3.978702	-0.445550
32	6	1.407737	-4.159104	0.197825
33	1	1.796124	-2.660175	3.814855
34	1	2.350299	-1.233428	2.926608
35	1	2.797349	-2.852482	2.374120
36	1	-0.955877	-1.650144	4.459392
37	1	-1.581864	-0.260448	3.564360
38	1	0.145479	-0.370904	3.934185
39	1	-3.282032	-2.802443	2.625043
40	1	-3.624806	-2.407690	0.938365
41	1	-3.300119	-1.115896	2.101679
42	1	-1.710520	-5.018978	-0.097512
43	1	-1.088258	-3.985648	-1.395743
44	1	-2.646661	-3.620766	-0.648773
45	1	1.061176	-5.190330	0.351479
46	1	2.422637	-4.091352	0.598323
47	1	1.460305	-3.991855	-0.884612
48	6	-2.967424	1.151538	-0.495065
49	6	-2.913081	2.353436	-1.479657
50	6	-3.734531	-0.004136	-1.187030
51	6	-3.746736	1.599364	0.773636
52	6	-4.344484	2.805571	-1.863981
53	1	-2.378557	3.192797	-1.015791
54	1	-2.350934	2.061507	-2.377214
55	6	-5.170453	0.441096	-1.558123
56	1	-3.183373	-0.307173	-2.086748
57	1	-3.767876	-0.870219	-0.518499
58	6	-5.180958	2.048582	0.396015
59	1	-3.788301	0.770744	1.489975
60	1	-3.205395	2.422575	1.258013
61	6	-5.105790	3.241157	-0.588095
62	6	-5.098212	1.635098	-2.540119
63	1	-4.276369	3.652514	-2.560118
64	6	-5.928667	0.871081	-0.277520
65	1	-5.696370	-0.397573	-2.034100
66	1	-5.715553	2.353334	1.306171
67	1	-6.118193	3.578709	-0.849859
68	1	-4.593760	4.090586	-0.113957
69	1	-6.110521	1.953671	-2.825351
70	1	-4.580349	1.334351	-3.461375
71	1	-6.954282	1.173420	-0.531054
72	1	-6.004382	0.024302	0.419371
73	6	3.376909	0.114321	-0.035751
74	6	3.572293	0.951266	-1.337419
75	6	4.568746	0.364075	0.934802
76	6	3.424583	-1.385353	-0.431603
77	6	4.925325	0.603665	-2.007733
78	1	2.741212	0.737168	-2.020438
79	1	3.537573	2.022781	-1.111467
80	6	5.914085	0.011607	0.245648
81	1	4.613410	1.407523	1.249872
82	1	4.431840	-0.246580	1.837840
83	6	4.761077	-1.750274	-1.124360
84	1	3.303596	-1.993717	0.468216
85	1	2.597042	-1.614716	-1.109402
86	6	4.936495	-0.892766	-2.399683
87	6	6.084431	0.887398	-1.020827
88	1	5.045888	1.222830	-2.906832
89	6	5.932134	-1.480988	-0.152510

90	1	6.732375	0.218402	0.948821
91	1	4.738504	-2.814523	-1.395155
92	1	5.882310	-1.146946	-2.897912
93	1	4.126431	-1.102296	-3.111164
94	1	7.048484	0.668814	-1.500309
95	1	6.095297	1.951983	-0.745427
96	1	6.889033	-1.735025	-0.629015
97	1	5.837307	-2.112806	0.742073

8bAd (E = -1654.5740577 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.113751	-0.781584	-0.016673
2	7	-1.823097	0.302489	-0.053655
3	6	-0.793850	1.265586	-0.240308
4	7	1.805254	0.760780	0.241117
5	6	-0.231680	-1.809015	2.283640
6	6	1.028375	-2.285883	1.800010
7	6	-1.263634	-2.505060	1.580505
8	17	0.127359	-1.547094	-2.331135
9	6	0.772452	-3.200502	0.743724
10	6	-0.646735	-3.327935	0.604644
11	6	1.368052	1.855432	0.762024
12	6	-0.144721	2.046178	0.923776
13	1	-0.724996	1.790426	-1.197474
14	6	-0.274268	3.560366	1.064996
15	1	-0.491529	1.580170	1.859752
16	6	2.056679	3.153493	1.138912
17	6	0.922008	4.156796	1.172987
18	1	2.519453	3.054142	2.131797
19	1	2.857321	3.447065	0.458924
20	6	1.246003	5.616493	1.348554
21	6	-1.629100	4.208714	1.112061
22	1	-1.565054	5.296190	1.213185
23	1	-2.214521	3.823045	1.958468
24	1	-2.200573	3.983230	0.204059
25	1	0.348549	6.241232	1.367460
26	1	1.889774	5.976724	0.533306
27	1	1.795073	5.786934	2.286010
28	6	2.337161	-2.043381	2.516111
29	6	-0.431920	-0.988866	3.539610
30	6	-2.698527	-2.558209	2.041580
31	6	-1.327307	-4.293123	-0.335677
32	6	1.770371	-4.035381	-0.022749
33	1	2.301937	-2.505636	3.512934
34	1	2.549871	-0.978920	2.661810
35	1	3.184569	-2.485603	1.985662
36	1	-0.464891	-1.637362	4.428451
37	1	-1.371426	-0.426922	3.510072
38	1	0.381728	-0.270974	3.694187
39	1	-2.753924	-3.093189	3.001149
40	1	-3.335909	-3.095350	1.334363
41	1	-3.125343	-1.563215	2.196437
42	1	-1.226594	-5.326863	0.025919
43	1	-0.889560	-4.249540	-1.338910
44	1	-2.396073	-4.078228	-0.432638
45	1	1.621788	-5.103071	0.190867
46	1	2.801466	-3.788581	0.247054
47	1	1.666717	-3.901591	-1.106438
48	6	-3.248638	0.503121	-0.411691
49	6	-3.398652	1.508455	-1.591344
50	6	-3.871180	-0.842047	-0.870698
51	6	-4.062562	1.048076	0.798260
52	6	-4.888425	1.697357	-1.971424

53	1	-2.964573	2.475468	-1.309831
54	1	-2.830204	1.136365	-2.454887
55	6	-5.365502	-0.666108	-1.238782
56	1	-3.307694	-1.213216	-1.737110
57	1	-3.770128	-1.582261	-0.073553
58	6	-5.553806	1.232965	0.421787
59	1	-3.969064	0.348213	1.638867
60	1	-3.629527	2.003571	1.121909
61	6	-5.669553	2.239159	-0.749194
62	6	-5.491367	0.340444	-2.406698
63	1	-4.958804	2.415094	-2.800656
64	6	-6.145358	-0.131075	-0.011839
65	1	-5.779281	-1.637806	-1.542465
66	1	-6.106095	1.614461	1.292177
67	1	-6.725604	2.391181	-1.013688
68	1	-5.267818	3.217210	-0.447416
69	1	-6.546525	0.467529	-2.687581
70	1	-4.962568	-0.040978	-3.291332
71	1	-7.209761	-0.018276	-0.262247
72	1	-6.082928	-0.849118	0.818434
73	6	3.233061	0.615787	-0.256914
74	6	3.415223	1.528671	-1.509468
75	6	4.316848	0.940626	0.810446
76	6	3.452530	-0.846302	-0.727001
77	6	4.840152	1.358933	-2.094294
78	1	2.660433	1.252277	-2.256355
79	1	3.247484	2.580213	-1.255141
80	6	5.733482	0.767901	0.200108
81	1	4.217668	1.963053	1.181789
82	1	4.193491	0.267767	1.668761
83	6	4.868514	-1.037799	-1.325074
84	1	3.317197	-1.523154	0.119545
85	1	2.700574	-1.102145	-1.481389
86	6	5.042647	-0.105903	-2.546870
87	6	5.891077	1.716691	-1.014323
88	1	4.950384	2.032114	-2.954732
89	6	5.932748	-0.695395	-0.256838
90	1	6.478328	1.022718	0.965890
91	1	4.979038	-2.084132	-1.639026
92	1	6.044046	-0.233178	-2.980298
93	1	4.314422	-0.364440	-3.327339
94	1	6.902948	1.624568	-1.431581
95	1	5.768173	2.762245	-0.696563
96	1	6.941631	-0.828137	-0.670718
97	1	5.843178	-1.375109	0.602328

TS(8b-18)Ad (E = -1654.5458314 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.063521	-0.808867	-0.146452
2	7	-1.740675	0.336051	-0.087240
3	6	-0.843578	1.396219	-0.327802
4	7	1.757776	0.491769	0.196803
5	6	-0.569719	-2.100788	1.979169
6	6	0.797547	-2.442684	1.743669
7	6	-1.364267	-2.753553	0.988448
8	17	0.231186	-1.292418	-2.524515
9	6	0.854588	-3.234804	0.564461
10	6	-0.481229	-3.400391	0.084512
11	6	1.148785	1.682193	0.025626
12	6	-0.075330	2.139558	0.769572
13	1	-0.920439	1.955125	-1.257563
14	6	-0.086349	3.642187	0.708051
15	1	-0.222185	1.685413	1.752619

16	6	1.591330	2.910967	-0.793998
17	6	0.814419	4.066156	-0.190213
18	1	2.666196	3.081851	-0.723838
19	1	1.371983	2.788191	-1.860656
20	6	1.106140	5.468471	-0.650753
21	6	-1.060389	4.447382	1.523985
22	1	-0.981650	5.520918	1.326363
23	1	-0.892921	4.287966	2.598420
24	1	-2.093849	4.140034	1.314647
25	1	0.483862	6.209418	-0.139979
26	1	0.933594	5.570715	-1.731796
27	1	2.159134	5.729654	-0.471973
28	6	1.885365	-2.197086	2.764880
29	6	-1.081082	-1.441907	3.240457
30	6	-2.831659	-3.073705	1.136382
31	6	-0.872522	-4.308200	-1.055830
32	6	2.019827	-4.030922	0.024607
33	1	1.546929	-2.542067	3.750988
34	1	2.150903	-1.138024	2.862334
35	1	2.795720	-2.752462	2.523329
36	1	-1.183953	-2.180684	4.049925
37	1	-2.059249	-0.978388	3.087745
38	1	-0.398057	-0.662728	3.596897
39	1	-2.938108	-3.906473	1.848089
40	1	-3.283884	-3.397314	0.195132
41	1	-3.416321	-2.239137	1.526786
42	1	-0.867967	-5.359581	-0.732164
43	1	-0.179628	-4.214788	-1.897824
44	1	-1.874885	-4.080335	-1.431303
45	1	1.821970	-5.104612	0.151956
46	1	2.951747	-3.804355	0.547794
47	1	2.184300	-3.861138	-1.046188
48	6	-3.216739	0.577937	-0.233764
49	6	-3.516891	1.911298	-0.982621
50	6	-3.859847	-0.560461	-1.067959
51	6	-3.894184	0.660858	1.163484
52	6	-5.044433	2.135759	-1.122601
53	1	-3.068690	2.752677	-0.440128
54	1	-3.056344	1.884021	-1.979073
55	6	-5.391027	-0.357083	-1.192817
56	1	-3.394465	-0.567802	-2.062797
57	1	-3.647085	-1.524898	-0.606793
58	6	-5.423085	0.866976	1.024350
59	1	-3.687390	-0.256171	1.725098
60	1	-3.446322	1.491358	1.727565
61	6	-5.693618	2.196628	0.280832
62	6	-5.670976	0.973762	-1.929153
63	1	-5.215149	3.084943	-1.649014
64	6	-6.029986	-0.308516	0.217976
65	1	-5.820221	-1.192826	-1.762514
66	1	-5.878044	0.902300	2.024008
67	1	-6.775396	2.367025	0.188963
68	1	-5.280485	3.039425	0.853339
69	1	-6.753466	1.129631	-2.037895
70	1	-5.243564	0.941767	-2.940989
71	1	-7.118426	-0.182443	0.132532
72	1	-5.856407	-1.257260	0.745361
73	6	3.204786	0.329496	-0.235646
74	6	3.480422	0.639930	-1.742788
75	6	4.120135	1.200921	0.676953
76	6	3.617379	-1.144873	-0.023258
77	6	4.983319	0.432227	-2.072555
78	1	2.859829	-0.023304	-2.357185

79	1	3.213815	1.662698	-2.006752
80	6	5.612381	0.992827	0.316168
81	1	3.866086	2.263132	0.590372
82	1	3.938536	0.914206	1.721806
83	6	5.113001	-1.383491	-0.347867
84	1	3.420090	-1.421492	1.011788
85	1	3.005145	-1.779708	-0.669306
86	6	5.377611	-1.041370	-1.830743
87	6	5.844227	1.353354	-1.172382
88	1	5.148083	0.691355	-3.127245
89	6	5.993467	-0.487126	0.554013
90	1	6.228376	1.641596	0.953645
91	1	5.349673	-2.440466	-0.162005
92	1	6.437271	-1.198781	-2.075553
93	1	4.790421	-1.701238	-2.484220
94	1	6.907416	1.237437	-1.424421
95	1	5.584703	2.407084	-1.350944
96	1	7.055895	-0.648247	0.324677
97	1	5.846521	-0.748234	1.611604

TS(8b-19)Ad (E = -1654.5417965 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	72	-0.411074	-1.180146	0.714950
2	7	-1.830399	0.168867	0.084249
3	6	-0.633313	0.879508	-0.158231
4	7	2.287239	1.023637	-0.215069
5	6	-0.343974	-2.176623	3.031455
6	6	0.406792	-3.078898	2.214977
7	6	-1.708098	-2.239927	2.611302
8	17	0.549075	-2.086364	-1.350730
9	6	-0.489156	-3.700346	1.304229
10	6	-1.796116	-3.173373	1.530976
11	6	1.591313	1.775693	0.525736
12	6	0.211474	1.285415	0.944844
13	1	-0.224888	0.982311	-1.160382
14	6	-0.217702	2.217933	2.054006
15	1	0.589457	0.158061	1.681142
16	6	1.809446	3.127134	1.202714
17	6	0.654258	3.235441	2.169621
18	1	2.773199	3.189408	1.713638
19	1	1.793320	3.942128	0.467348
20	6	0.588923	4.422371	3.093184
21	6	-1.466288	2.001201	2.858647
22	1	-1.626475	2.804502	3.583211
23	1	-1.409308	1.056377	3.411962
24	1	-2.345357	1.934008	2.212308
25	1	-0.276506	4.391525	3.760609
26	1	0.538817	5.359404	2.520131
27	1	1.493772	4.479529	3.714938
28	6	1.880156	-3.382702	2.356819
29	6	0.184516	-1.474561	4.262037
30	6	-2.886475	-1.630536	3.334855
31	6	-3.064912	-3.751076	0.947468
32	6	-0.160784	-4.839561	0.373167
33	1	2.040212	-4.224934	3.045159
34	1	2.434198	-2.525619	2.754161
35	1	2.330630	-3.653312	1.396151
36	1	0.180969	-2.160444	5.121487
37	1	-0.423948	-0.607527	4.535019
38	1	1.212652	-1.124950	4.122721
39	1	-3.292957	-2.347849	4.062425
40	1	-3.694576	-1.361334	2.649189
41	1	-2.609149	-0.728681	3.887585

42	1	-3.286266	-4.721671	1.415136
43	1	-2.985021	-3.921138	-0.131745
44	1	-3.924690	-3.099585	1.120866
45	1	-0.330424	-5.800216	0.881012
46	1	0.882426	-4.810411	0.047206
47	1	-0.782889	-4.820995	-0.526375
48	6	-3.042924	0.472674	-0.710882
49	6	-2.747967	0.394121	-2.239535
50	6	-4.152167	-0.551485	-0.379917
51	6	-3.574459	1.897836	-0.385645
52	6	-4.027728	0.695235	-3.057933
53	1	-1.965293	1.115602	-2.506523
54	1	-2.364912	-0.606875	-2.477530
55	6	-5.437863	-0.250551	-1.189993
56	1	-3.789105	-1.558997	-0.613837
57	1	-4.366481	-0.515936	0.696666
58	6	-4.849897	2.206538	-1.208025
59	1	-3.802940	1.960321	0.686566
60	1	-2.787971	2.634427	-0.599105
61	6	-4.530587	2.119985	-2.720097
62	6	-5.123990	-0.338072	-2.703473
63	1	-3.792417	0.631177	-4.129050
64	6	-5.946409	1.172433	-0.852148
65	1	-6.208606	-0.988918	-0.929481
66	1	-5.202291	3.217699	-0.962071
67	1	-5.428898	2.353401	-3.308614
68	1	-3.765896	2.862898	-2.987731
69	1	-6.032902	-0.142036	-3.289343
70	1	-4.783922	-1.351010	-2.960879
71	1	-6.865831	1.387094	-1.414459
72	1	-6.196096	1.241021	0.216241
73	6	3.617022	1.266163	-0.799977
74	6	3.398535	1.400397	-2.337428
75	6	4.436151	2.490485	-0.303963
76	6	4.449334	-0.023470	-0.537048
77	6	4.757509	1.470728	-3.073618
78	1	2.811925	0.540242	-2.682011
79	1	2.806959	2.304855	-2.539044
80	6	5.798865	2.556974	-1.044480
81	1	3.881088	3.419126	-0.485032
82	1	4.612981	2.408869	0.776786
83	6	5.808955	0.042834	-1.271060
84	1	4.604541	-0.135500	0.545691
85	1	3.866232	-0.887942	-0.876647
86	6	5.563942	0.178319	-2.794317
87	6	5.555923	2.696345	-2.566985
88	1	4.576422	1.566608	-4.152656
89	6	6.608251	1.267853	-0.765308
90	1	6.358059	3.429496	-0.679563
91	1	6.373245	-0.877504	-1.068775
92	1	6.523576	0.210984	-3.328848
93	1	5.013555	-0.696575	-3.166272
94	1	6.516766	2.766889	-3.095442
95	1	5.001779	3.622084	-2.777925
96	1	7.582984	1.319627	-1.270011
97	1	6.805777	1.171683	0.311828

19Ad (E = -1654.5738258 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	72	-1.181385	-1.057586	-0.350355
2	7	-1.317835	0.880295	0.491914
3	6	0.067317	0.936363	0.547243
4	7	2.886639	0.558259	0.140313
5	6	-2.521057	-2.971856	0.660426
6	6	-1.992697	-3.476110	-0.563912
7	6	-3.471634	-1.952363	0.351684
8	17	-0.290348	-0.551144	-2.529872
9	6	-2.591752	-2.753362	-1.628994
10	6	-3.502464	-1.801862	-1.068718
11	6	2.301602	-0.061679	1.081739
12	6	0.836785	0.128141	1.348280
13	1	0.610331	1.556951	-0.166702
14	6	0.547644	-0.492540	2.656178
15	1	0.167210	-2.139367	0.225299
16	6	2.798626	-1.038530	2.149160
17	6	1.650641	-1.118385	3.124777
18	1	3.001315	-2.020098	1.702027
19	1	3.726557	-0.711581	2.627294
20	6	1.841893	-1.834545	4.431819
21	6	-0.747958	-0.296816	3.401916
22	1	-0.690962	-0.708576	4.413287
23	1	-1.595270	-0.763460	2.890165
24	1	-0.984122	0.771080	3.477298
25	1	0.938151	-1.842716	5.047371
26	1	2.647733	-1.370805	5.019091
27	1	2.140720	-2.878673	4.258297
28	6	-1.059660	-4.652948	-0.706005
29	6	-2.245656	-3.547698	2.029758
30	6	-4.424629	-1.336560	1.350568
31	6	-4.483680	-0.992902	-1.886533
32	6	-2.449770	-3.059456	-3.099514
33	1	-1.632487	-5.581062	-0.846562
34	1	-0.432709	-4.774543	0.181733
35	1	-0.393900	-4.541538	-1.567700
36	1	-2.759769	-4.511934	2.148892
37	1	-2.602468	-2.887653	2.825870
38	1	-1.176350	-3.721606	2.192156
39	1	-5.137445	-2.096264	1.699820
40	1	-5.001201	-0.520701	0.910095
41	1	-3.912876	-0.937801	2.233002
42	1	-5.207444	-1.662370	-2.371864
43	1	-3.991841	-0.418745	-2.679876
44	1	-5.051278	-0.292445	-1.268901
45	1	-3.210509	-3.791289	-3.407322
46	1	-1.467286	-3.479746	-3.333474
47	1	-2.576190	-2.163981	-3.714410
48	6	-2.021065	2.182146	0.262578
49	6	-1.741248	2.760102	-1.156012
50	6	-3.544650	1.977598	0.418389
51	6	-1.562966	3.222756	1.325431
52	6	-2.488006	4.104215	-1.347404
53	1	-0.664038	2.910857	-1.299357
54	1	-2.066673	2.034377	-1.912201
55	6	-4.302158	3.314720	0.222194
56	1	-3.888058	1.244042	-0.319271
57	1	-3.749924	1.567748	1.415184
58	6	-2.307888	4.565947	1.131523
59	1	-1.758883	2.819156	2.328450
60	1	-0.479074	3.379071	1.243643
61	6	-2.009036	5.121119	-0.282655
62	6	-4.010640	3.872757	-1.192200
63	1	-2.273821	4.493240	-2.351908

64	6	-3.830822	4.335897	1.285787
65	1	-5.380464	3.136438	0.334350
66	1	-1.963154	5.281710	1.889995
67	1	-2.519365	6.083823	-0.424667
68	1	-0.931529	5.305863	-0.395416
69	1	-4.554464	4.815391	-1.344279
70	1	-4.364271	3.167879	-1.958020
71	1	-4.371183	5.284687	1.163113
72	1	-4.055951	3.962331	2.294708
73	6	4.326317	0.489416	-0.188627
74	6	5.170646	1.277989	0.855776
75	6	4.895263	-0.952369	-0.325986
76	6	4.478353	1.199788	-1.564728
77	6	6.657356	1.319978	0.420050
78	1	4.768021	2.296081	0.943137
79	1	5.084999	0.806872	1.843581
80	6	6.381942	-0.900008	-0.764815
81	1	4.825625	-1.489006	0.625968
82	1	4.296512	-1.506419	-1.061630
83	6	5.957633	1.254715	-2.007084
84	1	3.870984	0.663763	-2.305873
85	1	4.061671	2.211781	-1.479121
86	6	6.779683	2.031699	-0.949637
87	6	7.201407	-0.125250	0.297579
88	1	7.236754	1.869369	1.174787
89	6	6.506102	-0.187245	-2.132318
90	1	6.764938	-1.926454	-0.847410
91	1	6.029633	1.763749	-2.977775
92	1	7.834893	2.083840	-1.252559
93	1	6.412728	3.064638	-0.871585
94	1	8.262233	-0.103751	0.011784
95	1	7.138985	-0.636406	1.269322
96	1	7.557324	-0.168027	-2.452622
97	1	5.943035	-0.739130	-2.897706

TS3bAr-20 (E = -1091.7995783 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.458872	-0.248124	-0.043970
2	6	-2.922191	-1.076224	-0.495165
3	6	-2.802809	-0.578702	0.831924
4	6	-1.906255	-2.060799	-0.691807
5	17	-0.900311	0.770155	-2.676573
6	6	-1.697842	-1.244547	1.457255
7	6	-1.159318	-2.176417	0.515153
8	6	1.127919	0.873932	0.631682
9	6	-1.217072	2.234576	0.583780
10	6	-0.310594	3.382150	0.717434
11	1	-1.254590	1.694198	1.545945
12	6	1.752016	2.070379	1.049354
13	6	1.017278	3.307742	1.104792
14	1	1.167051	1.026924	1.903944
15	1	2.833384	2.113434	1.196430
16	6	1.805617	4.547855	1.515603
17	6	-0.927917	4.748623	0.485836
18	1	-0.205954	5.487118	0.124665
19	1	-1.363692	5.139936	1.417882
20	1	-1.742236	4.672911	-0.242701
21	1	1.298719	5.115978	2.305942
22	1	1.968635	5.235566	0.675066
23	1	2.793073	4.264710	1.896786
24	6	-3.785284	0.332855	1.526396
25	6	-3.999935	-0.719075	-1.489747
26	6	-1.734373	-2.903777	-1.933728

27	6	-0.088165	-3.202920	0.796394
28	6	-1.338511	-1.155187	2.924079
29	1	-4.579330	-0.259915	2.001801
30	1	-4.265649	1.025341	0.828036
31	1	-3.311126	0.931544	2.310586
32	1	-4.827029	-1.441302	-1.437230
33	1	-3.619132	-0.721686	-2.515626
34	1	-4.417191	0.274335	-1.296680
35	1	-2.424716	-3.759090	-1.917320
36	1	-0.719313	-3.306156	-2.015312
37	1	-1.939976	-2.330640	-2.843481
38	1	-0.541043	-4.133532	1.166573
39	1	0.620740	-2.855580	1.552955
40	1	0.488258	-3.450256	-0.100226
41	1	-1.977807	-1.823916	3.517994
42	1	-1.471592	-0.142671	3.320577
43	1	-0.300207	-1.448988	3.107349
44	1	-2.230759	2.560646	0.336282
45	6	2.737929	-0.847742	-0.216080
46	6	3.158235	-1.219482	-1.522024
47	6	3.576863	-1.116065	0.900291
48	6	4.418869	-1.808847	-1.690140
49	6	4.833054	-1.706662	0.681700
50	6	5.261862	-2.046757	-0.601481
51	1	4.739916	-2.077277	-2.692459
52	1	5.468215	-1.913952	1.538395
53	1	6.235158	-2.502900	-0.751167
54	6	3.137915	-0.844345	2.322216
55	1	3.236680	0.212833	2.604484
56	1	2.090298	-1.124164	2.480225
57	1	3.748423	-1.420943	3.023838
58	6	2.280799	-0.976905	-2.725939
59	1	1.364131	-1.579654	-2.692640
60	1	1.961094	0.067084	-2.796832
61	1	2.812464	-1.236841	-3.646574
62	72	-0.642575	0.151574	-0.337798

20 (E = -1091.8746454 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.652216	0.104271	-0.024902
2	6	-2.678205	-0.781316	-0.511779
3	6	-2.380862	-0.728964	0.880532
4	6	-1.713820	-1.626038	-1.137453
5	17	-1.045644	1.355116	-2.502968
6	6	-1.222481	-1.529357	1.113161
7	6	-0.817948	-2.094909	-0.133907
8	6	1.785398	1.419668	0.371087
9	6	-1.004717	2.042529	1.211368
10	6	-0.433069	3.429147	0.933587
11	1	-0.660130	1.683515	2.197079
12	6	1.259001	2.397461	-0.429893
13	6	0.642938	3.614431	0.131601
14	1	2.099810	1.656234	1.387790
15	1	1.276441	2.255221	-1.506828
16	6	1.223577	4.938383	-0.322119
17	6	-1.208882	4.565590	1.571480
18	1	-0.780701	5.553767	1.384643
19	1	-1.259238	4.418364	2.659613
20	1	-2.246216	4.568568	1.207492
21	1	2.241002	5.077091	0.069880
22	1	0.624168	5.800885	-0.021510
23	1	1.304051	4.951795	-1.418435
24	6	-3.267062	-0.151213	1.955322

25	6	-3.884747	-0.170755	-1.182332
26	6	-1.734003	-2.071371	-2.579419
27	6	0.195862	-3.198894	-0.312962
28	6	-0.711030	-1.932664	2.475196
29	1	-3.940029	-0.930663	2.340199
30	1	-3.891817	0.663168	1.576864
31	1	-2.692721	0.236011	2.802478
32	1	-4.727465	-0.876320	-1.167733
33	1	-3.677367	0.085413	-2.224643
34	1	-4.211744	0.744212	-0.677687
35	1	-2.377825	-2.954862	-2.694529
36	1	-0.735629	-2.344663	-2.936308
37	1	-2.116897	-1.287015	-3.237620
38	1	-0.299763	-4.173706	-0.199112
39	1	0.999815	-3.146690	0.424049
40	1	0.654952	-3.182027	-1.305253
41	1	-1.324510	-2.753060	2.875002
42	1	-0.762013	-1.109984	3.195910
43	1	0.322476	-2.285218	2.435893
44	1	-2.089685	2.142797	1.330010
45	6	2.645970	-0.879744	0.293275
46	6	3.241698	-1.559435	-0.800914
47	6	3.041631	-1.176203	1.622038
48	6	4.198468	-2.552725	-0.547080
49	6	3.999656	-2.184945	1.829179
50	6	4.573604	-2.874102	0.760298
51	1	4.655264	-3.070122	-1.385558
52	1	4.294199	-2.423223	2.847356
53	1	5.311804	-3.648363	0.943074
54	6	2.494538	-0.440439	2.827277
55	1	3.080797	0.462672	3.046267
56	1	1.456386	-0.129179	2.688364
57	1	2.540601	-1.075517	3.717787
58	6	2.877791	-1.209572	-2.227081
59	1	1.832054	-1.445953	-2.458417
60	1	3.004058	-0.138602	-2.421900
61	1	3.508514	-1.762479	-2.929819
62	72	-0.435948	0.430340	-0.307646

21 (E = -1494.9384093 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.494464	0.166503	0.044993
2	6	-2.811298	-0.951763	0.562799
3	6	-1.774090	-1.329210	1.463862
4	6	-2.495870	-1.479162	-0.723616
5	17	-0.497320	0.299857	-2.778526
6	6	-0.818545	-2.101108	0.735216
7	6	-1.261392	-2.182019	-0.619249
8	6	1.509021	1.490233	0.345016
9	6	-1.061723	1.738915	1.602829
10	6	-0.686624	3.190224	1.346120
11	1	-0.460752	1.333732	2.433099
12	6	0.749296	2.381341	-0.395125
13	6	0.141044	3.519268	0.322359
14	1	1.946629	1.822337	1.289790
15	1	0.708154	2.288121	-1.475519
16	6	0.490793	4.913957	-0.155496
17	6	-1.346578	4.211143	2.253789
18	1	-1.068316	5.245614	2.031894
19	1	-1.080810	4.008451	3.301246
20	1	-2.442037	4.131464	2.193321
21	1	-0.134581	5.694667	0.286318
22	1	0.377569	4.970200	-1.247902

23	1	1.541318	5.156510	0.060382
24	6	-1.824400	-1.174352	2.964445
25	6	-4.107767	-0.291229	0.961151
26	6	-3.379925	-1.452306	-1.945597
27	6	-0.647411	-3.031867	-1.704433
28	6	0.273810	-2.943809	1.346797
29	1	-2.381500	-2.010536	3.411287
30	1	-2.323527	-0.248207	3.263227
31	1	-0.825619	-1.172070	3.411473
32	1	-4.783726	-1.028944	1.416391
33	1	-4.625093	0.137813	0.098339
34	1	-3.953963	0.507451	1.693677
35	1	-3.950004	-2.389204	-2.022110
36	1	-2.790367	-1.337199	-2.859196
37	1	-4.100849	-0.629412	-1.910175
38	1	-1.165154	-3.999974	-1.766807
39	1	0.409579	-3.235994	-1.509093
40	1	-0.718888	-2.545372	-2.681247
41	1	-0.132587	-3.930860	1.611534
42	1	0.676808	-2.498886	2.259415
43	1	1.110379	-3.102371	0.662258
44	1	-2.090257	1.713766	1.986561
45	6	2.580342	-0.683392	0.449293
46	6	3.276140	-1.360706	-0.585730
47	6	2.968524	-0.855073	1.802301
48	6	4.331227	-2.221830	-0.248441
49	6	4.034548	-1.725061	2.092719
50	6	4.711893	-2.409181	1.082925
51	1	4.862192	-2.737688	-1.043198
52	1	4.323735	-1.866940	3.130397
53	1	5.529377	-3.079216	1.329875
54	6	2.277433	-0.156674	2.954405
55	1	2.717137	0.828827	3.159808
56	1	1.213066	0.001757	2.762152
57	1	2.374582	-0.747138	3.871577
58	6	2.928076	-1.127213	-2.038296
59	1	1.872147	-1.313365	-2.251390
60	1	3.110049	-0.083622	-2.324849
61	1	3.535614	-1.767685	-2.685519
62	72	-0.666065	0.272082	-0.195725
63	6	-2.291522	1.812626	-0.969899
64	7	-3.053495	2.598123	-1.370050
65	6	-3.898597	3.553668	-1.935384
66	6	-3.622879	3.996073	-3.250960
67	6	-4.986033	4.039522	-1.173512
68	6	-4.486587	4.953113	-3.800719
69	6	-5.816219	4.996245	-1.772039
70	6	-5.571916	5.448322	-3.072263
71	1	-4.299997	5.309406	-4.808239
72	1	-6.658451	5.385953	-1.210146
73	1	-6.227754	6.188958	-3.517745
74	6	-5.245375	3.545885	0.228251
75	1	-5.479551	2.474512	0.241846
76	1	-4.371381	3.689985	0.874278
77	1	-6.088397	4.079725	0.673995
78	6	-2.437819	3.470521	-4.020624
79	1	-1.492622	3.774297	-3.552996
80	1	-2.422061	2.376052	-4.057774
81	1	-2.445149	3.852074	-5.044705

TS21-22 (E = -1494.9103469 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	7	1.368467	0.072728	-0.265580
2	6	-2.933535	-1.305824	-0.200897
3	6	-2.288498	-1.138626	1.068436
4	6	-2.115941	-2.154893	-0.997816
5	17	-0.644828	-0.190376	-3.069936
6	6	-1.079391	-1.893629	1.048309
7	6	-0.962794	-2.504429	-0.238469
8	6	1.349703	1.430264	-0.112711
9	6	-1.344200	2.174216	0.932814
10	6	-0.738485	3.477874	0.512479
11	1	-0.671617	1.531349	1.514270
12	6	0.692935	2.251303	-0.999325
13	6	0.178786	3.533600	-0.489438
14	1	1.707772	1.866840	0.821249
15	1	0.661698	2.003212	-2.056028
16	6	0.745593	4.796195	-1.111412
17	6	-1.291602	4.704794	1.215694
18	1	-0.923262	5.642130	0.791992
19	1	-1.011393	4.687789	2.278631
20	1	-2.387525	4.721387	1.172995
21	1	0.108727	5.673771	-0.969316
22	1	0.881868	4.649192	-2.191061
23	1	1.739202	5.029510	-0.701539
24	6	-2.900930	-0.514100	2.299560
25	6	-4.338646	-0.893848	-0.563373
26	6	-2.511049	-2.737298	-2.330009
27	6	0.080126	-3.520235	-0.636509
28	6	-0.243997	-2.245594	2.254388
29	1	-3.403143	-1.284603	2.901308
30	1	-3.648535	0.240584	2.043546
31	1	-2.153096	-0.035694	2.940349
32	1	-5.008066	-1.763612	-0.505735
33	1	-4.401465	-0.491177	-1.578984
34	1	-4.723976	-0.132906	0.117411
35	1	-3.103531	-3.650474	-2.174041
36	1	-1.639503	-2.998420	-2.935175
37	1	-3.114974	-2.038088	-2.914473
38	1	-0.236028	-4.525342	-0.322419
39	1	1.048664	-3.317974	-0.171426
40	1	0.225907	-3.546698	-1.720436
41	1	-0.591941	-3.203044	2.668574
42	1	-0.332532	-1.497788	3.046987
43	1	0.815063	-2.358500	2.011220
44	1	-2.239487	2.300521	1.538149
45	6	2.462501	-0.697146	0.260188
46	6	3.185024	-1.490378	-0.670409
47	6	2.844127	-0.676954	1.627128
48	6	4.247529	-2.283580	-0.212221
49	6	3.916779	-1.488442	2.040048
50	6	4.612473	-2.291759	1.136521
51	1	4.798192	-2.887277	-0.927534
52	1	4.200147	-1.483149	3.088837
53	1	5.435453	-2.911653	1.477618
54	6	2.158386	0.183016	2.668445
55	1	2.607038	1.183799	2.728171
56	1	1.093258	0.315525	2.461467
57	1	2.253621	-0.270745	3.660151
58	6	2.860035	-1.446464	-2.146432
59	1	1.824847	-1.729612	-2.356651
60	1	2.982309	-0.433145	-2.547729
61	1	3.522412	-2.116056	-2.703826
62	72	-0.766825	0.002318	-0.615914
63	6	-2.284707	1.578681	-0.811135

64	7	-3.146589	2.311544	-1.243194
65	6	-3.798183	3.550340	-1.136224
66	6	-3.465897	4.527900	-2.109140
67	6	-4.806784	3.787030	-0.171569
68	6	-4.108653	5.771331	-2.051287
69	6	-5.429007	5.045525	-0.162363
70	6	-5.080579	6.037559	-1.081966
71	1	-3.849789	6.528900	-2.784758
72	1	-6.200218	5.239232	0.577192
73	1	-5.573104	7.003999	-1.053653
74	6	-5.246356	2.721545	0.804032
75	1	-5.687395	1.862718	0.283174
76	1	-4.413795	2.342745	1.406481
77	1	-6.000735	3.117787	1.489714
78	6	-2.449553	4.221522	-3.180731
79	1	-1.466246	4.002736	-2.749422
80	1	-2.739956	3.336410	-3.760313
81	1	-2.343395	5.065563	-3.868238

22 (E = -1494.9611315 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.085761	0.311755	-0.075737
2	6	-3.089348	-1.225793	-0.183010
3	6	-2.246217	-1.341445	0.965076
4	6	-2.446529	-1.876941	-1.270890
5	17	-0.599754	0.145547	-3.099480
6	6	-1.098163	-2.110437	0.583902
7	6	-1.215342	-2.423568	-0.797781
8	6	1.265183	1.678723	0.040991
9	6	-1.205042	3.245910	1.191955
10	6	-0.302656	4.278067	0.487957
11	1	-0.755501	2.965571	2.152286
12	6	0.833327	2.580444	-0.878351
13	6	0.565683	3.981213	-0.505171
14	1	1.663378	2.055844	0.984894
15	1	0.656477	2.259734	-1.901779
16	6	1.313296	5.024101	-1.322234
17	6	-0.526847	5.676696	1.029958
18	1	0.215539	6.395176	0.676613
19	1	-0.479034	5.665515	2.128303
20	1	-1.525167	6.050500	0.760357
21	1	0.885736	6.027131	-1.246573
22	1	1.301132	4.732841	-2.380839
23	1	2.369583	5.074206	-1.023877
24	6	-2.614593	-1.002576	2.392005
25	6	-4.498821	-0.686683	-0.230160
26	6	-3.057097	-2.112316	-2.629741
27	6	-0.296795	-3.318315	-1.593974
28	6	-0.130102	-2.750458	1.546956
29	1	-3.019789	-1.888815	2.901315
30	1	-3.376275	-0.220316	2.443283
31	1	-1.750208	-0.660789	2.970135
32	1	-5.206366	-1.515855	-0.368343
33	1	-4.652342	0.016972	-1.054765
34	1	-4.768767	-0.176390	0.696104
35	1	-3.649272	-3.039046	-2.619760
36	1	-2.293100	-2.207138	-3.405224
37	1	-3.724408	-1.295592	-2.922615
38	1	-0.691001	-4.344369	-1.616769
39	1	0.705764	-3.360175	-1.158869
40	1	-0.201302	-2.977873	-2.629897
41	1	-0.548121	-3.708250	1.890652
42	1	0.043843	-2.133608	2.430902

43	1	0.840111	-2.956341	1.090442
44	1	-2.140068	3.762978	1.429294
45	6	2.116789	-0.498365	0.521084
46	6	2.969086	-1.231739	-0.343147
47	6	2.309099	-0.547225	1.924716
48	6	3.969862	-2.043049	0.214312
49	6	3.330437	-1.364172	2.440514
50	6	4.152121	-2.114982	1.598411
51	1	4.619758	-2.606961	-0.448686
52	1	3.469448	-1.413053	3.517146
53	1	4.931884	-2.744783	2.015148
54	6	1.444989	0.238521	2.888979
55	1	1.871065	1.228298	3.103660
56	1	0.439087	0.400236	2.490324
57	1	1.360796	-0.286339	3.846734
58	6	2.845741	-1.106576	-1.845339
59	1	1.848855	-1.371151	-2.208120
60	1	3.020855	-0.073107	-2.168618
61	1	3.578135	-1.748259	-2.345342
62	72	-0.975458	0.132761	-0.653340
63	6	-1.491145	2.002390	0.391185
64	7	-2.385500	1.897931	-0.536742
65	6	-3.418998	2.849592	-0.883857
66	6	-3.412893	3.464971	-2.161759
67	6	-4.463958	3.118083	0.037634
68	6	-4.463313	4.330626	-2.498839
69	6	-5.500602	3.985002	-0.352741
70	6	-5.508410	4.588580	-1.608237
71	1	-4.452771	4.806090	-3.474886
72	1	-6.306393	4.181394	0.349031
73	1	-6.316843	5.255039	-1.891074
74	6	-4.528651	2.530900	1.432872
75	1	-5.530262	2.136992	1.639957
76	1	-3.810136	1.725603	1.582211
77	1	-4.324325	3.297051	2.192966
78	6	-2.294230	3.239787	-3.148913
79	1	-1.326454	3.537992	-2.730010
80	1	-2.199873	2.188337	-3.433718
81	1	-2.463668	3.827200	-4.056346

***t*BuNC** (E = -250.6583893 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.737505	-0.430693	1.404646
2	6	0.263125	-0.000022	0.000011
3	1	0.375421	0.266012	2.166704
4	1	0.374586	-1.434410	1.645664
5	1	1.831820	-0.439411	1.431318
6	6	0.736938	-1.001115	-1.075554
7	6	0.737059	1.431851	-0.329658
8	1	0.373669	-0.707783	-2.065118
9	1	1.831264	-1.019829	-1.096823
10	1	0.374878	-2.009443	-0.853247
11	1	1.831374	1.459241	-0.336595
12	1	0.373986	1.743484	-1.313691
13	1	0.374919	2.142414	0.419470
14	7	-1.198682	-0.000043	0.000457
15	6	-2.367404	0.000005	0.000691

MeNC (E = -132.7370076 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	7	0.318638	0.000007	0.464006
2	6	1.486403	-0.000005	0.463974
3	6	-1.116184	0.000000	0.463782
4	1	-1.483851	0.930378	0.862416
5	1	-1.483826	-0.844873	-0.556668
6	1	-1.484098	-0.085526	1.085397

EtNC (E = -172.0442071 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	0.308823	0.020652	-0.009177
2	6	1.477067	0.032425	-0.014352
3	6	-1.134586	-0.016348	0.007225
4	1	-1.482227	0.839779	0.593959
5	1	-1.482143	0.120335	-1.021650
6	6	-1.662525	-1.332305	0.593204
7	1	-1.322787	-1.464168	1.624684
8	1	-2.756964	-1.318581	0.587035
9	1	-1.322701	-2.187143	0.001147

ArNC (E = -403.0543015 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	0.229094	-0.000343	-0.000107
2	6	1.401398	-0.000401	-0.000233
3	6	-1.167283	-0.000261	-0.000031
4	6	-1.843059	0.086721	1.237835
5	6	-1.843156	-0.087166	-1.237836
6	6	-3.244288	0.084845	1.210076
7	6	-3.244395	-0.085135	-1.209977
8	6	-3.939639	-0.000107	0.000074
9	1	-3.788608	0.150639	2.146375
10	1	-3.788803	-0.150867	-2.146231
11	1	-5.024663	-0.000046	0.000123
12	6	-1.078717	0.177807	2.535320
13	1	-0.430330	-0.694774	2.681748
14	1	-0.430153	1.062159	2.558308
15	1	-1.764396	0.237527	3.384370
16	6	-1.078890	-0.178339	-2.535364
17	1	-0.430390	0.694155	-2.681804
18	1	-0.430440	-1.062772	-2.558382
19	1	-1.764588	-0.237962	-3.384397

1-AdNC (E = -482.8664564 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	0.257579	-0.027219	-0.056585
2	6	1.424721	-0.039054	-0.123086
3	6	-1.188684	-0.011404	0.026632
4	6	-1.773992	-1.022005	-0.997342
5	6	-1.625317	-0.412173	1.462197
6	6	-1.706951	1.416857	-0.295807
7	6	-3.319755	-1.001584	-0.904722
8	1	-1.442956	-0.748718	-2.006900
9	1	-1.386537	-2.024985	-0.779391
10	6	-3.171607	-0.394231	1.546972
11	1	-1.236575	-1.411453	1.694036
12	1	-1.189981	0.290549	2.183433
13	6	-3.252986	1.429068	-0.205253
14	1	-1.271946	2.129810	0.415482
15	1	-1.375794	1.704792	-1.301260
16	6	-3.838432	0.422149	-1.226611
17	6	-3.757177	-1.401859	0.526360
18	1	-3.726547	-1.717205	-1.630480
19	6	-3.690577	1.029646	1.226000
20	1	-3.473143	-0.678343	2.563176

21	1	-3.612239	2.440429	-0.434192
22	1	-4.935556	0.439815	-1.183228
23	1	-3.549662	0.707826	-2.247358
24	1	-4.853169	-1.409952	0.594627
25	1	-3.410494	-2.418458	0.757217
26	1	-4.785667	1.055569	1.303764
27	1	-3.296664	1.749442	1.956541

Pyridine (E = -248.2546674 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.149804	-0.722726	-0.000195
2	6	-1.201845	0.675263	-0.000127
3	6	0.000234	1.389949	0.000097
4	6	1.202071	0.674860	0.000208
5	6	1.149561	-0.723113	0.000086
6	7	-0.000241	-1.427760	-0.000089
7	1	0.000410	2.474941	0.000168
8	1	-2.064633	-1.307919	-0.000368
9	1	-2.158930	1.184850	-0.000233
10	1	2.159332	1.184115	0.000383
11	1	2.064191	-1.308614	0.000202