Supplementary Data

Feasibility of Associative Mechanism in Enyne Metathesis Catalyzed by Grubbs Complexes

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Atomic Cartesian coordinates and computed energies (atomic units) for the stationary points calculated with basis set B_1 [B3LYP/6-31G(d) (C, H, N, O, P) LANL2DZ (Ru)]

Ethyne

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Zero-point correction=                           0.026655
(Hartree/Particle)
 Thermal correction to Energy=                    0.029583
 Thermal correction to Enthalpy=                  0.030527
 Thermal correction to Gibbs Free Energy=         0.007632
 Sum of electronic and zero-point Energies=           -77.297147
 Sum of electronic and thermal Energies=              -77.294219
 Sum of electronic and thermal Enthalpies=            -77.293275
 Sum of electronic and thermal Free Energies=         -77.316170
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000000	0.000000	0.602562
2	6	0	0.000000	0.000000	-0.602562
3	1	0	-0.000000	0.000000	1.669064
4	1	0	0.000000	0.000000	-1.669064

1-propyne

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Zero-point correction=                           0.055733
(Hartree/Particle)
 Thermal correction to Energy=                    0.059729
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 Thermal correction to Enthalpy=                  0.060673
 Thermal correction to Gibbs Free Energy=         0.031505
 Sum of electronic and zero-point Energies=           -116.594950
 Sum of electronic and thermal Energies=              -116.590954
 Sum of electronic and thermal Enthalpies=            -116.590010
 Sum of electronic and thermal Free Energies=         -116.619177

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.426249    0.000506   -0.001418
    2          6             0        0.218985   -0.000013    0.001406
    3          6             0       -1.241535   -0.000082   -0.000209
    4          1             0        2.492147   -0.002133    0.003103
    5          1             0       -1.637384   -0.873787   -0.531674
    6          1             0       -1.637598    0.896719   -0.491566
    7          1             0       -1.639361   -0.023263    1.021461
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3-methyl-1-butyne

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Zero-point correction=                           0.113315
(Hartree/Particle)
 Thermal correction to Energy=                    0.119607
 Thermal correction to Enthalpy=                  0.120552
 Thermal correction to Gibbs Free Energy=         0.084461
 Sum of electronic and zero-point Energies=           -195.163932
 Sum of electronic and thermal Energies=              -195.157639
 Sum of electronic and thermal Enthalpies=            -195.156695
 Sum of electronic and thermal Free Energies=         -195.192785

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        2.235116   -0.000570    0.117535
    2          6             0        1.050828   -0.001153   -0.121938
    3          6             0       -0.391342   -0.000053   -0.400734
    4          6             0       -1.060285    1.275260    0.152822
    5          6             0       -1.062523   -1.274113    0.153001
    6          1             0        3.279742   -0.000543    0.329927
    7          1             0       -0.520808   -0.000038   -1.493327
    8          1             0       -2.126833    1.282510   -0.099617
    9          1             0       -0.599180    2.175949   -0.264460
   10          1             0       -0.964630    1.318779    1.243378
   11          1             0       -2.129075   -1.279559   -0.099460
   12          1             0       -0.966984   -1.317637    1.243570
   13          1             0       -0.602995   -2.175685   -0.264124
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2-butyne

```
Zero-point correction=                           0.084674
(Hartree/Particle)
 Thermal correction to Energy=                    0.090421
 Thermal correction to Enthalpy=                  0.091365
 Thermal correction to Gibbs Free Energy=         0.055956
 Sum of electronic and zero-point Energies=           -155.890994
 Sum of electronic and thermal Energies=              -155.885248
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 Sum of electronic and thermal Enthalpies=           -155.884303
 Sum of electronic and thermal Free Energies=        -155.919713
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.604637	-0.000162	0.000316
2	6	0	-0.604643	-0.000725	0.000914
3	6	0	2.066248	0.000181	-0.000280
4	6	0	-2.066240	0.000257	-0.000357
5	1	0	2.466168	1.021196	-0.037474
6	1	0	2.466336	-0.542171	-0.866028
7	1	0	2.467073	-0.478069	0.902151
8	1	0	-2.466092	-0.515037	-0.882579
9	1	0	-2.465649	1.022103	-0.006318
10	1	0	-2.467846	-0.505333	0.886691

1

```
Zero-point correction=                           0.258172
(Hartree/Particle)
 Thermal correction to Energy=                    0.280477
 Thermal correction to Enthalpy=                  0.281421
 Thermal correction to Gibbs Free Energy=         0.204654
 Sum of electronic and zero-point Energies=          -1975.626592
 Sum of electronic and thermal Energies=             -1975.604288
 Sum of electronic and thermal Enthalpies=           -1975.603343
 Sum of electronic and thermal Free Energies=        -1975.680110
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.000015	-2.448191	0.024770
2	44	0	0.000000	0.001351	-0.209803
3	6	0	-0.000001	0.002396	-2.025252
4	17	0	-0.000014	2.450201	0.026175
5	15	0	-2.377367	-0.000342	0.167321
6	15	0	2.377367	-0.000330	0.167321
7	6	0	-3.330828	-1.450333	-0.444905
8	6	0	-3.332463	1.454761	-0.430041
9	6	0	-2.670491	-0.009930	1.989683
10	6	0	3.330841	-1.450290	-0.444961
11	6	0	2.670485	-0.009991	1.989684
12	6	0	3.332455	1.454802	-0.429980
13	1	0	-3.353110	1.447508	-1.524271
14	1	0	-2.823406	2.365773	-0.106348
15	1	0	-4.359955	1.434529	-0.049724
16	1	0	-2.211057	-0.903156	2.423882
17	1	0	-3.742756	-0.010841	2.215417
18	1	0	-2.210801	0.878358	2.433688
19	1	0	-2.820228	-2.363834	-0.130748
20	1	0	-3.352028	-1.431493	-1.538989
21	1	0	-4.358184	-1.435659	-0.063972
22	1	0	3.353104	1.447595	-1.524210
23	1	0	4.359946	1.434560	-0.049663

24	1	0	2.823393	2.365800	-0.106253
25	1	0	2.211057	-0.903240	2.423842
26	1	0	2.210785	0.878274	2.433726
27	1	0	3.742749	-0.010901	2.215421
28	1	0	3.352047	-1.431404	-1.539044
29	1	0	2.820245	-2.363806	-0.130843
30	1	0	4.358194	-1.435624	-0.064022
31	1	0	0.000015	-0.933507	-2.599417
32	1	0	-0.000001	0.939018	-2.598217

2

Zero-point correction= 0.143001
(Hartree/Particle)
Thermal correction to Energy= 0.156724
Thermal correction to Enthalpy= 0.157668
Thermal correction to Gibbs Free Energy= 0.102018
Sum of electronic and zero-point Energies= -1514.611307
Sum of electronic and thermal Energies= -1514.597584
Sum of electronic and thermal Enthalpies= -1514.596639
Sum of electronic and thermal Free Energies= -1514.652289

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.041271	-2.232370	-0.591665
2	44	0	-0.839238	0.000504	0.130873
3	6	0	-0.915808	0.000595	1.942875
4	17	0	-1.038317	2.233529	-0.591723
5	15	0	1.397773	-0.000814	-0.002681
6	6	0	2.220987	-1.459231	0.756273
7	6	0	2.222722	1.456563	0.756414
8	6	0	1.954347	-0.001082	-1.754636
9	1	0	-1.926249	0.001154	2.379796
10	1	0	-0.091973	0.000202	2.664808
11	1	0	1.817965	-2.367209	0.301209
12	1	0	2.007599	-1.489113	1.828679
13	1	0	3.305476	-1.411905	0.606451
14	1	0	2.010350	1.485824	1.829046
15	1	0	1.819920	2.365125	0.302326
16	1	0	3.307037	1.408547	0.605593
17	1	0	1.559587	-0.890061	-2.254769
18	1	0	3.048633	-0.001957	-1.814779
19	1	0	1.561041	0.888686	-2.254524

PMe_3

Zero-point correction= 0.113368
(Hartree/Particle)
Thermal correction to Energy= 0.120095
Thermal correction to Enthalpy= 0.121039
Thermal correction to Gibbs Free Energy= 0.083992
Sum of electronic and zero-point Energies= -460.980554
Sum of electronic and thermal Energies= -460.973827
Sum of electronic and thermal Enthalpies= -460.972883
Sum of electronic and thermal Free Energies= -461.009930

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.000202	-0.000526	-0.604976
2	6	0	0.325032	1.611150	0.280178
3	6	0	-1.558470	-0.523760	0.280795
4	6	0	1.233587	-1.086435	0.280828
5	1	0	1.305780	2.000315	-0.015001
6	1	0	0.302998	1.509328	1.372755
7	1	0	-0.425627	2.351762	-0.017209
8	1	0	-1.811513	-1.552125	-0.000149
9	1	0	-2.391023	0.116544	-0.031075
10	1	0	-1.466486	-0.471498	1.373143
11	1	0	1.081841	-2.130240	-0.015541
12	1	0	1.156438	-1.017332	1.373436
13	1	0	2.249727	-0.804590	-0.016516

3a

Zero-point correction= 0.172058
(Hartree/Particle)
Thermal correction to Energy= 0.189281
Thermal correction to Enthalpy= 0.190225
Thermal correction to Gibbs Free Energy= 0.127552
Sum of electronic and zero-point Energies= -1591.923944
Sum of electronic and thermal Energies= -1591.906721
Sum of electronic and thermal Enthalpies= -1591.905777
Sum of electronic and thermal Free Energies= -1591.968450

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.509794	2.295198	-0.636405
2	44	0	0.631038	-0.000264	0.090224
3	6	0	0.664383	-0.000790	1.910998
4	17	0	0.508613	-2.295243	-0.636603
5	15	0	-1.699440	0.000369	0.045203
6	6	0	-2.512479	1.447177	0.842792
7	6	0	-2.513243	-1.445896	0.843004
8	6	0	-2.343695	0.000239	-1.677126
9	1	0	-0.203803	-0.001003	2.580071
10	1	0	1.638929	-0.001044	2.413103
11	1	0	-3.600600	1.392437	0.727841
12	1	0	-2.132277	2.363645	0.386565
13	1	0	-2.267888	1.467556	1.909358
14	1	0	-2.271344	-1.464452	1.910222
15	1	0	-2.131114	-2.362664	0.388961
16	1	0	-3.601120	-1.392256	0.725331
17	1	0	-1.970484	0.888965	-2.194053
18	1	0	-3.439202	0.001483	-1.689594
19	1	0	-1.972461	-0.889927	-2.193009
20	6	0	3.027913	-0.609324	0.040309
21	6	0	3.028402	0.609272	0.040667
22	1	0	3.128634	-1.672700	0.011809
23	1	0	3.128057	1.672721	0.012731

3a’

Zero-point correction= 0.173149
(Hartree/Particle)
Thermal correction to Energy= 0.189678
Thermal correction to Enthalpy= 0.190622
Thermal correction to Gibbs Free Energy= 0.129619
Sum of electronic and zero-point Energies= -1591.920691
Sum of electronic and thermal Energies= -1591.904162
Sum of electronic and thermal Enthalpies= -1591.903218
Sum of electronic and thermal Free Energies= -1591.964221

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.603468	-0.707248	2.294877
2	44	0	-0.193628	-0.955487	-0.050873
3	6	0	-1.923712	-0.849576	0.510290
4	17	0	-0.958708	-0.734056	-2.394111
5	15	0	0.097667	1.441874	-0.061205
6	6	0	-0.575520	2.367678	1.376864
7	6	0	-0.518018	2.390418	-1.508767
8	6	0	1.908900	1.774909	-0.031912
9	1	0	-2.748439	-0.856298	-0.208548
10	1	0	-2.164303	-0.841435	1.577982
11	1	0	-0.225186	3.405559	1.360006
12	1	0	-0.256882	1.875993	2.297786
13	1	0	-1.668849	2.357114	1.327865
14	1	0	-1.602411	2.278747	-1.586978
15	1	0	-0.079597	1.994326	-2.426095
16	1	0	-0.261874	3.449323	-1.389763
17	1	0	2.333548	1.325107	0.869268
18	1	0	2.104600	2.853062	-0.037275
19	1	0	2.379721	1.323849	-0.911278
20	6	0	0.688836	-2.901564	0.318165
21	6	0	0.319380	-2.900390	-0.868964
22	1	0	1.091186	-3.189639	1.269455
23	1	0	0.103822	-3.182266	-1.880789

TS(3-4)a

Zero-point correction= 0.171685
(Hartree/Particle)
Thermal correction to Energy= 0.188207
Thermal correction to Enthalpy= 0.189151
Thermal correction to Gibbs Free Energy= 0.126897
Sum of electronic and zero-point Energies= -1591.896590
Sum of electronic and thermal Energies= -1591.880068
Sum of electronic and thermal Enthalpies= -1591.879124
Sum of electronic and thermal Free Energies= -1591.941378

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

1	17	0	0.386742	-2.435938	-0.175559
2	44	0	0.602624	0.003942	-0.029508
3	6	0	2.501755	-0.174975	-1.015030
4	17	0	0.718720	2.427540	-0.192213
5	15	0	-1.779624	0.075722	0.023918
6	6	0	-2.393856	-0.380721	-1.651052
7	6	0	-2.584600	1.681624	0.410355
8	6	0	-2.564926	-1.130714	1.166401
9	6	0	2.960850	-0.147958	0.147288
10	6	0	1.373538	-0.045178	1.654128
11	1	0	2.607864	-0.232326	-2.082482
12	1	0	-3.489264	-0.384861	-1.673793
13	1	0	-2.014166	-1.375126	-1.901488
14	1	0	-2.026375	0.339451	-2.388898
15	1	0	-2.182751	2.452352	-0.250756
16	1	0	-2.342488	1.969128	1.437473
17	1	0	-3.672170	1.606249	0.299072
18	1	0	-2.139852	-2.117995	0.971412
19	1	0	-3.651739	-1.144319	1.028042
20	1	0	-2.338729	-0.849987	2.199621
21	1	0	3.705259	-0.127033	0.918427
22	1	0	1.643829	0.876707	2.179736
23	1	0	1.530063	-0.991243	2.182824

4a

Zero-point correction= 0.176535
(Hartree/Particle)
Thermal correction to Energy= 0.192365
Thermal correction to Enthalpy= 0.193309
Thermal correction to Gibbs Free Energy= 0.132528
Sum of electronic and zero-point Energies= -1591.942432
Sum of electronic and thermal Energies= -1591.926602
Sum of electronic and thermal Enthalpies= -1591.925658
Sum of electronic and thermal Free Energies= -1591.986439

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.177404	-2.378185	-0.323944
2	44	0	0.695707	0.068328	-0.247196
3	6	0	2.410787	-0.726076	-0.513632
4	17	0	0.758658	2.416918	-0.336882
5	15	0	-1.757400	0.090207	0.099553
6	6	0	-2.728868	-0.582606	-1.315824
7	6	0	-2.510641	1.750551	0.379903
8	6	0	-2.335343	-0.884552	1.552380
9	6	0	2.690246	-0.147671	0.705995
10	6	0	1.575653	-0.197781	1.644053
11	1	0	2.961806	-1.183982	-1.326857
12	1	0	-3.802086	-0.572691	-1.094665
13	1	0	-2.401248	-1.605343	-1.516446
14	1	0	-2.543701	0.025989	-2.206810
15	1	0	-2.302319	2.395785	-0.476869
16	1	0	-2.057314	2.213934	1.260054
17	1	0	-3.593419	1.662694	0.525624
18	1	0	-1.979603	-1.912548	1.457011
19	1	0	-3.429118	-0.871216	1.616269

20	1	0	-1.918676	-0.451273	2.466848
21	1	0	3.514173	0.566163	0.816095
22	1	0	1.505733	0.617078	2.363198
23	1	0	1.271621	-1.173764	2.016672

3b

Zero-point correction= 0.200860
(Hartree/Particle)
Thermal correction to Energy= 0.219786
Thermal correction to Enthalpy= 0.220730
Thermal correction to Gibbs Free Energy= 0.153506
Sum of electronic and zero-point Energies= -1631.220940
Sum of electronic and thermal Energies= -1631.202013
Sum of electronic and thermal Enthalpies= -1631.201069
Sum of electronic and thermal Free Energies= -1631.268294

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.362811	2.427398	-0.562679
2	44	0	-0.371068	0.213314	0.044897
3	15	0	1.867607	-0.376706	0.094216
4	6	0	2.586512	-0.466555	-1.596408
5	6	0	2.242154	-2.015303	0.846898
6	6	0	2.976328	0.775858	1.006470
7	6	0	-0.507143	0.159599	1.859311
8	1	0	3.647343	-0.738668	-1.562938
9	1	0	2.474602	0.508751	-2.078562
10	1	0	2.034965	-1.212122	-2.176212
11	1	0	1.679951	-2.787586	0.317752
12	1	0	1.927549	-2.018794	1.895196
13	1	0	3.315239	-2.230179	0.797198
14	1	0	2.876116	1.776557	0.580852
15	1	0	4.018170	0.442650	0.945053
16	1	0	2.677520	0.819261	2.058311
17	1	0	0.284082	-0.108789	2.569454
18	1	0	-1.467630	0.429832	2.314164
19	6	0	-2.559544	1.371871	-0.172746
20	6	0	-3.091789	0.297644	0.049995
21	6	0	-3.827951	-0.937426	0.301975
22	1	0	-2.271802	2.381010	-0.375406
23	1	0	-4.889471	-0.787738	0.072255
24	1	0	-3.437845	-1.747742	-0.320294
25	1	0	-3.743084	-1.241688	1.351340
26	17	0	-0.817176	-1.976464	-0.822605

3b’

Zero-point correction= 0.201647
(Hartree/Particle)
Thermal correction to Energy= 0.219889
Thermal correction to Enthalpy= 0.220834
Thermal correction to Gibbs Free Energy= 0.155857
Sum of electronic and zero-point Energies= -1631.216395
Sum of electronic and thermal Energies= -1631.198153

Sum of electronic and thermal Enthalpies= -1631.197209
Sum of electronic and thermal Free Energies= -1631.262186

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.651729	-2.476369	-0.001808
2	44	0	-0.484193	-0.257772	-0.138120
3	6	0	-2.064656	-1.524006	0.547038
4	17	0	-1.093434	2.129615	-0.258032
5	15	0	1.784078	0.516227	0.218266
6	6	0	2.254905	0.070811	1.942666
7	6	0	2.137935	2.316766	0.105844
8	6	0	3.089743	-0.236512	-0.835228
9	6	0	-2.614678	-0.404297	0.518048
10	6	0	-0.329482	-0.287902	-1.953606
11	6	0	-3.675201	0.608496	0.623343
12	1	0	-1.931767	-2.580897	0.674452
13	1	0	3.283154	0.382260	2.157896
14	1	0	2.160999	-1.011690	2.060047
15	1	0	1.578896	0.565591	2.647458
16	1	0	1.504385	2.864944	0.805077
17	1	0	1.906111	2.676420	-0.899453
18	1	0	3.195396	2.498077	0.330080
19	1	0	2.971328	-1.321599	-0.827885
20	1	0	4.083911	0.038746	-0.466334
21	1	0	2.974100	0.128520	-1.860493
22	1	0	-0.638715	0.568649	-2.560234
23	1	0	0.017282	-1.189425	-2.468147
24	1	0	-4.594410	0.130149	0.981990
25	1	0	-3.387800	1.411201	1.306685
26	1	0	-3.861948	1.072305	-0.349221

TS(3-4)b

Zero-point correction= 0.201208
(Hartree/Particle)
Thermal correction to Energy= 0.219021
Thermal correction to Enthalpy= 0.219965
Thermal correction to Gibbs Free Energy= 0.154850
Sum of electronic and zero-point Energies= -1631.190949
Sum of electronic and thermal Energies= -1631.173136
Sum of electronic and thermal Enthalpies= -1631.172192
Sum of electronic and thermal Free Energies= -1631.237307

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.012316	-2.441257	-0.166865
2	44	0	0.369660	0.001409	-0.120984
3	6	0	2.101635	-0.490800	-1.223516
4	17	0	0.604825	2.405099	-0.293242
5	15	0	-2.008685	0.138035	0.114781
6	6	0	-2.803562	-0.437736	-1.443179
7	6	0	-2.722972	1.805626	0.417807
8	6	0	-2.726168	-0.922643	1.433379
9	6	0	2.748065	-0.267105	-0.163561
10	6	0	1.334378	-0.134508	1.456414

11	6	0	3.991651	0.067831	0.566982
12	1	0	2.105806	-0.764187	-2.263663
13	1	0	-3.895107	-0.405261	-1.353800
14	1	0	-2.475821	-1.461592	-1.641489
15	1	0	-2.496328	0.203513	-2.275465
16	1	0	-2.375046	2.491551	-0.357765
17	1	0	-2.363274	2.187077	1.377406
18	1	0	-3.818057	1.763257	0.427426
19	1	0	-2.356459	-1.941198	1.295440
20	1	0	-3.821032	-0.902648	1.392865
21	1	0	-2.396400	-0.557561	2.410763
22	1	0	1.673123	0.765302	1.979377
23	1	0	1.511075	-1.096767	1.946551
24	1	0	4.841242	-0.101134	-0.104385
25	1	0	3.991650	1.123054	0.860531
26	1	0	4.129039	-0.545234	1.463665

4b

Zero-point correction= 0.204441
(Hartree/Particle)
Thermal correction to Energy= 0.221901
Thermal correction to Enthalpy= 0.222846
Thermal correction to Gibbs Free Energy= 0.158437
Sum of electronic and zero-point Energies= -1631.236155
Sum of electronic and thermal Energies= -1631.218695
Sum of electronic and thermal Enthalpies= -1631.217751
Sum of electronic and thermal Free Energies= -1631.282159

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.334203	-2.411297	-0.349298
2	44	0	0.451045	-0.037834	-0.356988
3	6	0	2.053662	-1.053348	-0.607936
4	17	0	0.751741	2.290102	-0.556128
5	15	0	-1.930406	0.252828	0.205294
6	6	0	-3.107811	-0.333269	-1.087780
7	6	0	-2.476669	1.988362	0.512640
8	6	0	-2.465769	-0.628503	1.732201
9	6	0	2.495075	-0.434871	0.543159
10	6	0	1.393832	-0.292651	1.500251
11	6	0	3.797582	0.322405	0.649219
12	1	0	2.486085	-1.656600	-1.397956
13	1	0	-4.145656	-0.201332	-0.761485
14	1	0	-2.913966	-1.388985	-1.291188
15	1	0	-2.949613	0.236013	-2.009444
16	1	0	-2.282809	2.596375	-0.374111
17	1	0	-1.898820	2.413704	1.337238
18	1	0	-3.544615	2.017243	0.757848
19	1	0	-2.232748	-1.690540	1.631529
20	1	0	-3.540704	-0.495933	1.898757
21	1	0	-1.918777	-0.228043	2.591187
22	1	0	1.442877	0.562903	2.174991
23	1	0	1.007693	-1.205100	1.951910
24	1	0	4.430735	0.171533	-0.229530
25	1	0	3.589532	1.393957	0.746834

26	1	0	4.343358	-0.001380	1.543192

3c

Zero-point correction= 0.257914
(Hartree/Particle)
Thermal correction to Energy= 0.279525
Thermal correction to Enthalpy= 0.280469
Thermal correction to Gibbs Free Energy= 0.206506
Sum of electronic and zero-point Energies= -1709.790223
Sum of electronic and thermal Energies= -1709.768612
Sum of electronic and thermal Enthalpies= -1709.767668
Sum of electronic and thermal Free Energies= -1709.841631

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.138603	2.369394	-0.705600
2	44	0	0.146542	0.302541	0.031662
3	17	0	-0.579290	-1.862300	-0.698864
4	15	0	2.291618	-0.551280	0.136356
5	6	0	3.001105	-0.832424	-1.536786
6	6	0	2.458387	-2.176713	0.986158
7	6	0	3.530937	0.509996	0.989325
8	6	0	-0.000633	0.368640	1.844651
9	1	0	4.016230	-1.239557	-1.471485
10	1	0	3.021302	0.118860	-2.076148
11	1	0	2.359912	-1.532399	-2.080039
12	1	0	1.806433	-2.902686	0.495490
13	1	0	2.141798	-2.081297	2.029377
14	1	0	3.497222	-2.523825	0.958816
15	1	0	3.551356	1.489034	0.505808
16	1	0	4.525122	0.051026	0.954139
17	1	0	3.239989	0.650037	2.034941
18	1	0	0.750395	0.051148	2.577957
19	1	0	-0.928143	0.768653	2.270698
20	6	0	-1.899377	1.719508	-0.220617
21	6	0	-2.579653	0.721847	-0.046121
22	6	0	-3.511551	-0.393220	0.178171
23	6	0	-4.539626	-0.017855	1.266451
24	6	0	-4.195478	-0.803198	-1.142645
25	1	0	-1.465720	2.676870	-0.414201
26	1	0	-2.923108	-1.250539	0.525229
27	1	0	-5.151779	0.835038	0.953010
28	1	0	-4.046505	0.244045	2.208250
29	1	0	-5.206271	-0.867375	1.451810
30	1	0	-3.450284	-1.104569	-1.883398
31	1	0	-4.785538	0.024399	-1.552388
32	1	0	-4.867513	-1.649534	-0.962000

TS(3-4)c

Zero-point correction= 0.258096
(Hartree/Particle)
Thermal correction to Energy= 0.278706
Thermal correction to Enthalpy= 0.279651
Thermal correction to Gibbs Free Energy= 0.207620

```
 Sum of electronic and zero-point Energies=          -1709.760989
 Sum of electronic and thermal Energies=             -1709.740378
 Sum of electronic and thermal Enthalpies=           -1709.739434
 Sum of electronic and thermal Free Energies=        -1709.811464
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.559963	-2.469373	-0.060947
2	44	0	-0.097719	-0.039918	-0.135760
3	6	0	1.606926	-0.656724	-1.222571
4	17	0	0.191165	2.346994	-0.435166
5	15	0	-2.468015	0.182108	0.122528
6	6	0	-3.299555	-0.425936	-1.404105
7	6	0	-3.128156	1.880864	0.370904
8	6	0	-3.206070	-0.804061	1.487097
9	6	0	2.274258	-0.405132	-0.180627
10	6	0	0.874712	-0.132850	1.439238
11	6	0	3.573040	-0.111768	0.500832
12	6	0	4.677939	-0.929698	-0.199116
13	6	0	3.887980	1.397412	0.482324
14	1	0	1.581709	-0.995565	-2.242755
15	1	0	-4.388496	-0.357325	-1.304110
16	1	0	-3.005611	-1.466041	-1.568030
17	1	0	-2.983456	0.174540	-2.263094
18	1	0	-2.773577	2.526199	-0.435734
19	1	0	-2.741744	2.287419	1.309620
20	1	0	-4.223659	1.870767	0.399208
21	1	0	-2.876776	-1.840055	1.381086
22	1	0	-4.299883	-0.744047	1.459700
23	1	0	-2.849125	-0.417837	2.446661
24	1	0	1.241798	0.777486	1.923158
25	1	0	1.029112	-1.077526	1.969420
26	1	0	3.519634	-0.444025	1.545128
27	1	0	4.776510	-0.629535	-1.247930
28	1	0	4.463941	-2.002150	-0.163931
29	1	0	5.636791	-0.749532	0.299722
30	1	0	3.079633	1.988038	0.921042
31	1	0	4.025530	1.745020	-0.546525
32	1	0	4.810648	1.586734	1.042951

4c

```
Zero-point correction=                           0.262138
(Hartree/Particle)
 Thermal correction to Energy=                    0.282068
 Thermal correction to Enthalpy=                  0.283012
 Thermal correction to Gibbs Free Energy=         0.212567
 Sum of electronic and zero-point Energies=          -1709.802564
 Sum of electronic and thermal Energies=             -1709.782634
 Sum of electronic and thermal Enthalpies=           -1709.781690
 Sum of electronic and thermal Free Energies=        -1709.852134
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.890294	-2.431562	-0.209008
2	44	0	0.003270	-0.096694	-0.394950

3	6	0	1.521063	-1.266974	-0.566597
4	17	0	0.360803	2.190130	-0.823637
5	15	0	-2.324498	0.323807	0.223750
6	6	0	-3.584601	-0.302031	-0.968589
7	6	0	-2.785365	2.099801	0.420012
8	6	0	-2.823287	-0.412010	1.837219
9	6	0	2.050008	-0.634982	0.533307
10	6	0	0.955185	-0.296467	1.460106
11	6	0	3.493456	-0.155044	0.660153
12	6	0	4.353952	-0.554611	-0.546247
13	6	0	3.591214	1.356881	0.938543
14	1	0	1.861707	-1.962435	-1.322907
15	1	0	-4.599212	-0.099239	-0.607449
16	1	0	-3.445622	-1.377249	-1.101498
17	1	0	-3.445737	0.191587	-1.935812
18	1	0	-2.623303	2.627855	-0.522407
19	1	0	-2.144007	2.564198	1.173335
20	1	0	-3.835152	2.189595	0.722103
21	1	0	-2.648505	-1.489372	1.808624
22	1	0	-3.880494	-0.209799	2.042974
23	1	0	-2.214022	0.022898	2.635322
24	1	0	1.076961	0.594864	2.075275
25	1	0	0.500471	-1.136385	1.985239
26	1	0	3.881153	-0.682287	1.547387
27	1	0	4.002653	-0.059049	-1.459204
28	1	0	4.340679	-1.637248	-0.715137
29	1	0	5.395040	-0.256559	-0.382844
30	1	0	3.052770	1.643279	1.846895
31	1	0	3.177204	1.933971	0.106922
32	1	0	4.642649	1.635751	1.072226

3d

Zero-point correction= 0.229940
(Hartree/Particle)
Thermal correction to Energy= 0.250513
Thermal correction to Enthalpy= 0.251457
Thermal correction to Gibbs Free Energy= 0.179950
Sum of electronic and zero-point Energies= -1670.512019
Sum of electronic and thermal Energies= -1670.491446
Sum of electronic and thermal Enthalpies= -1670.490502
Sum of electronic and thermal Free Energies= -1670.562009

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.127617	-2.154128	-0.963285
2	44	0	0.259835	0.010510	0.063580
3	15	0	-2.058540	-0.025193	0.084949
4	6	0	-2.769911	0.146310	-1.601875
5	6	0	-2.876038	1.300492	1.068874
6	6	0	-2.816540	-1.567290	0.748924
7	6	0	0.349051	-0.150932	1.875104
8	1	0	-3.864696	0.110453	-1.575369
9	1	0	-2.390587	-0.667414	-2.226245
10	1	0	-2.443790	1.099506	-2.027323
11	1	0	-2.538819	2.273520	0.705849

12	1	0	-2.590935	1.207884	2.121489
13	1	0	-3.966136	1.225247	0.988262
14	1	0	-2.455544	-2.419843	0.169938
15	1	0	-3.909650	-1.513350	0.698413
16	1	0	-2.514388	-1.706662	1.791519
17	1	0	-0.496993	-0.222475	2.569307
18	1	0	1.338760	-0.164680	2.346757
19	6	0	2.808071	-0.627525	0.152942
20	6	0	2.835498	0.578241	-0.046650
21	6	0	3.081052	-2.045225	0.410642
22	6	0	3.207831	1.979205	-0.268631
23	1	0	4.156015	-2.179776	0.583314
24	1	0	2.775419	-2.665022	-0.435373
25	1	0	2.541044	-2.404051	1.293037
26	1	0	2.823773	2.349687	-1.222640
27	1	0	4.301814	2.060930	-0.270777
28	1	0	2.806424	2.629733	0.513408
29	17	0	0.046477	2.343665	-0.456202

3d’

Zero-point correction= 0.230794
(Hartree/Particle)
Thermal correction to Energy= 0.250579
Thermal correction to Enthalpy= 0.251523
Thermal correction to Gibbs Free Energy= 0.183197
Sum of electronic and zero-point Energies= -1670.508507
Sum of electronic and thermal Energies= -1670.488722
Sum of electronic and thermal Enthalpies= -1670.487778
Sum of electronic and thermal Free Energies= -1670.556104

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.220207	2.481200	-0.191638
2	44	0	0.398531	0.015376	-0.190551
3	6	0	2.418426	0.519311	0.404978
4	17	0	-0.095258	-2.426607	-0.200060
5	15	0	-1.998419	0.065722	0.275168
6	6	0	-2.266796	-0.630923	1.960023
7	6	0	-3.081014	-0.936311	-0.824448
8	6	0	-2.863910	1.687839	0.332500
9	6	0	2.343673	-0.735015	0.378320
10	6	0	0.195962	0.044412	-2.003610
11	6	0	3.137185	1.797400	0.571853
12	6	0	2.908707	-2.094116	0.494543
13	1	0	-3.333108	-0.633797	2.212186
14	1	0	-1.729230	-0.025106	2.696688
15	1	0	-1.875196	-1.650634	1.984435
16	1	0	-2.656098	-1.935869	-0.929060
17	1	0	-3.124497	-0.460626	-1.809163
18	1	0	-4.093571	-0.996104	-0.410236
19	1	0	-2.384190	2.341409	1.062932
20	1	0	-3.916020	1.531151	0.597558
21	1	0	-2.795728	2.177711	-0.641561
22	1	0	0.108434	-0.887389	-2.570699
23	1	0	0.221815	0.986777	-2.558271

24	1	0	4.165443	1.589215	0.893271
25	1	0	2.647749	2.439619	1.307804
26	1	0	3.159429	2.355317	-0.368534
27	1	0	2.358955	-2.694939	1.222855
28	1	0	3.959494	-2.019245	0.801210
29	1	0	2.849681	-2.623494	-0.460762

TS (3-4)d

Zero-point correction= 0.229852
(Hartree/Particle)
Thermal correction to Energy= 0.249393
Thermal correction to Enthalpy= 0.250337
Thermal correction to Gibbs Free Energy= 0.181502
Sum of electronic and zero-point Energies= -1670.488452
Sum of electronic and thermal Energies= -1670.468910
Sum of electronic and thermal Enthalpies= -1670.467966
Sum of electronic and thermal Free Energies= -1670.536802

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.002644	-2.387540	-0.332787
2	44	0	-0.258176	0.058064	-0.039116
3	6	0	-2.164811	-0.492397	0.779159
4	17	0	-0.414055	2.411577	0.513858
5	15	0	2.132435	0.092348	-0.012215
6	6	0	2.748118	-0.740125	1.511915
7	6	0	2.944247	1.743131	0.000610
8	6	0	2.943973	-0.807190	-1.395610
9	6	0	-2.622291	-0.035419	-0.304081
10	6	0	-1.012793	0.224434	-1.720643
11	6	0	-2.316414	-1.104457	2.113473
12	6	0	-3.726328	0.567137	-1.088859
13	1	0	3.843582	-0.752670	1.532743
14	1	0	2.365086	-1.763944	1.527342
15	1	0	2.382554	-0.208853	2.396483
16	1	0	2.548464	2.332425	0.830855
17	1	0	2.699592	2.274448	-0.923365
18	1	0	4.031954	1.641611	0.087709
19	1	0	2.513304	-1.809229	-1.454879
20	1	0	4.027252	-0.863751	-1.240220
21	1	0	2.743337	-0.282468	-2.334708
22	1	0	-1.238614	1.210953	-2.138695
23	1	0	-1.184162	-0.640839	-2.369045
24	1	0	-3.378223	-1.233110	2.356591
25	1	0	-1.855789	-0.478375	2.886075
26	1	0	-1.827837	-2.084369	2.122974
27	1	0	-3.589607	1.650826	-1.173369
28	1	0	-4.668499	0.382296	-0.559785
29	1	0	-3.807408	0.145687	-2.096378

4d

Zero-point correction= 0.233071
(Hartree/Particle)

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 Thermal correction to Energy=                  0.252232
 Thermal correction to Enthalpy=                0.253176
 Thermal correction to Gibbs Free Energy=       0.185290
 Sum of electronic and zero-point Energies=         -1670.536782
 Sum of electronic and thermal Energies=            -1670.517622
 Sum of electronic and thermal Enthalpies=          -1670.516678
 Sum of electronic and thermal Free Energies=       -1670.584564
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.172157	-2.381939	0.102993
2	44	0	0.343859	0.036071	-0.201133
3	6	0	2.115506	-0.678863	-0.323109
4	17	0	0.357552	2.356400	-0.677243
5	15	0	-2.141017	0.105937	0.057773
6	6	0	-3.070447	-0.843158	-1.223310
7	6	0	-2.937577	1.769399	-0.004155
8	6	0	-2.751401	-0.590408	1.652197
9	6	0	2.324648	0.096153	0.813748
10	6	0	1.187164	0.059879	1.724896
11	6	0	2.915316	-1.472346	-1.271750
12	6	0	3.401365	1.156425	0.889121
13	1	0	-4.147850	-0.822321	-1.023977
14	1	0	-2.713310	-1.875665	-1.225675
15	1	0	-2.882905	-0.404963	-2.209008
16	1	0	-2.714699	2.244410	-0.962678
17	1	0	-2.521760	2.404514	0.782269
18	1	0	-4.022620	1.684287	0.125046
19	1	0	-2.366323	-1.606485	1.762285
20	1	0	-3.846941	-0.599734	1.682407
21	1	0	-2.375786	0.019167	2.479964
22	1	0	1.040702	0.941601	2.349349
23	1	0	0.932457	-0.885319	2.199847
24	1	0	3.987615	-1.259181	-1.174478
25	1	0	2.594870	-1.319018	-2.306975
26	1	0	2.757511	-2.533887	-1.032655
27	1	0	2.941110	2.149594	0.926173
28	1	0	4.072252	1.123164	0.025789
29	1	0	3.991965	1.015347	1.802016

5b

```
Zero-point correction=                           0.200666
(Hartree/Particle)
 Thermal correction to Energy=                  0.219595
 Thermal correction to Enthalpy=                0.220539
 Thermal correction to Gibbs Free Energy=       0.153316
 Sum of electronic and zero-point Energies=         -1631.221133
 Sum of electronic and thermal Energies=            -1631.202205
 Sum of electronic and thermal Enthalpies=          -1631.201261
 Sum of electronic and thermal Free Energies=       -1631.268483
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.817728	-1.976480	-0.822072

2	44	0	0.370797	0.213328	0.044873
3	6	0	3.092520	0.297976	0.049728
4	17	0	-0.363174	2.427570	-0.562117
5	15	0	-1.867740	-0.376830	0.094053
6	6	0	-2.586138	-0.467263	-1.596739
7	6	0	-2.976926	0.775614	1.005890
8	6	0	-2.241930	-2.015420	0.846944
9	6	0	2.559643	1.371751	-0.173733
10	6	0	0.506846	0.159928	1.859289
11	6	0	3.828821	-0.936886	0.302260
12	1	0	-3.646956	-0.739448	-1.563497
13	1	0	-2.034354	-1.213033	-2.176063
14	1	0	-2.474150	0.507845	-2.079277
15	1	0	-2.876632	1.776348	0.580392
16	1	0	-2.678578	0.818923	2.057857
17	1	0	-4.018709	0.442307	0.944011
18	1	0	-1.679014	-2.787502	0.318273
19	1	0	-3.314872	-2.230898	0.796765
20	1	0	-1.927841	-2.018432	1.895398
21	1	0	2.271569	2.380567	-0.377526
22	1	0	-0.284371	-0.108001	2.569593
23	1	0	1.467498	0.430032	2.313848
24	1	0	4.890045	-0.787691	0.070950
25	1	0	3.437756	-1.747805	-0.318659
26	1	0	3.745202	-1.239922	1.352085

ET (5-6)b

Zero-point correction= 0.200522
(Hartree/Particle)
Thermal correction to Energy= 0.218704
Thermal correction to Enthalpy= 0.219648
Thermal correction to Gibbs Free Energy= 0.153243
Sum of electronic and zero-point Energies= -1631.195305
Sum of electronic and thermal Energies= -1631.177123
Sum of electronic and thermal Enthalpies= -1631.176179
Sum of electronic and thermal Free Energies= -1631.242584

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.399234	-2.383861	-0.154580
2	44	0	-0.431440	0.077001	-0.188066
3	6	0	-2.515648	-0.110755	0.433921
4	17	0	-0.441707	2.483578	0.141352
5	15	0	1.922270	-0.026670	0.159660
6	6	0	2.231391	-0.580287	1.890132
7	6	0	2.872515	1.537342	-0.015054
8	6	0	2.829970	-1.238339	-0.883581
9	6	0	-2.705614	0.121683	-0.781618
10	6	0	-0.896929	0.151940	-1.977825
11	6	0	-2.872842	-0.395048	1.833817
12	1	0	3.306078	-0.669901	2.084015
13	1	0	1.748871	-1.550700	2.036480
14	1	0	1.803030	0.142510	2.591629
15	1	0	2.413138	2.306441	0.609648
16	1	0	2.817195	1.879111	-1.052722
17	1	0	3.921801	1.389261	0.263749
18	1	0	2.335377	-2.208686	-0.799282

19	1	0	3.876934	-1.312099	-0.568699
20	1	0	2.791743	-0.917151	-1.928943
21	1	0	-3.299775	0.392081	-1.632521
22	1	0	-0.997083	1.111330	-2.497302
23	1	0	-1.036066	-0.754795	-2.575964
24	1	0	-3.962744	-0.424659	1.948446
25	1	0	-2.471971	0.379032	2.497220
26	1	0	-2.458244	-1.364190	2.130391

6b

Zero-point correction= 0.204439
(Hartree/Particle)
Thermal correction to Energy= 0.222101
Thermal correction to Enthalpy= 0.223045
Thermal correction to Gibbs Free Energy= 0.157791
Sum of electronic and zero-point Energies= -1631.245221
Sum of electronic and thermal Energies= -1631.227559
Sum of electronic and thermal Enthalpies= -1631.226615
Sum of electronic and thermal Free Energies= -1631.291869

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.334028	-2.299508	0.036122
2	44	0	0.521165	0.182246	-0.063029
3	6	0	2.375156	-0.234807	-0.211588
4	17	0	0.250252	2.516817	-0.322450
5	15	0	-1.975130	-0.113153	-0.062899
6	6	0	-2.609929	-1.052449	-1.518558
7	6	0	-2.994623	1.425098	-0.079205
8	6	0	-2.635367	-1.040503	1.386654
9	6	0	2.404220	0.421967	1.014706
10	6	0	1.297345	0.129835	1.902256
11	6	0	3.320043	-0.740732	-1.218206
12	1	0	-3.693551	-1.199696	-1.449493
13	1	0	-2.106077	-2.021174	-1.559335
14	1	0	-2.384101	-0.500626	-2.436788
15	1	0	-2.741120	2.022417	-0.958549
16	1	0	-2.763671	2.026339	0.804134
17	1	0	-4.063581	1.182918	-0.090070
18	1	0	-2.119291	-2.000628	1.455155
19	1	0	-3.715053	-1.201154	1.289873
20	1	0	-2.438042	-0.470127	2.299500
21	1	0	2.974801	1.352993	1.109188
22	1	0	1.008075	0.919198	2.593842
23	1	0	1.167292	-0.885496	2.268710
24	1	0	4.304035	-0.264871	-1.113568
25	1	0	2.942956	-0.606864	-2.236332
26	1	0	3.449208	-1.819483	-1.048303

5c

Zero-point correction= 0.258167
(Hartree/Particle)
Thermal correction to Energy= 0.279645

```
 Thermal correction to Enthalpy=                  0.280589
 Thermal correction to Gibbs Free Energy=         0.207420
 Sum of electronic and zero-point Energies=          -1709.790076
 Sum of electronic and thermal Energies=             -1709.768598
 Sum of electronic and thermal Enthalpies=           -1709.767654
 Sum of electronic and thermal Free Energies=        -1709.840823

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1         17             0        1.115498    2.449299   -0.396073
    2         44             0        0.126854    0.297397    0.047296
    3         17             0       -0.551209   -1.767221   -0.966176
    4         15             0        2.285665   -0.543216    0.050994
    5          6             0        3.011088   -0.558840   -1.639448
    6          6             0        2.473791   -2.275368    0.648925
    7          6             0        3.504760    0.392907    1.065234
    8          6             0       -0.030744    0.129643    1.852772
    9          1             0        4.033913   -0.951675   -1.628723
   10          1             0        3.015812    0.462546   -2.030467
   11          1             0        2.386960   -1.181501   -2.286851
   12          1             0        1.841672   -2.930853    0.046090
   13          1             0        2.143920   -2.343626    1.690132
   14          1             0        3.519209   -2.596640    0.584630
   15          1             0        3.514848    1.434548    0.737141
   16          1             0        4.505302   -0.042513    0.967100
   17          1             0        3.207562    0.366310    2.118136
   18          1             0       -0.963841    0.464232    2.320290
   19          1             0        0.720607   -0.269552    2.544600
   20          6             0       -2.581036    0.719271   -0.053548
   21          6             0       -1.899923    1.730764    0.003253
   22          6             0       -3.532863   -0.397706   -0.127535
   23          6             0       -4.879041    0.112957   -0.687095
   24          6             0       -3.709342   -1.090197    1.238235
   25          1             0       -1.476085    2.711595    0.024035
   26          1             0       -3.117495   -1.131831   -0.827783
   27          1             0       -4.749264    0.577554   -1.669348
   28          1             0       -5.330704    0.850814   -0.014747
   29          1             0       -5.574265   -0.727414   -0.790810
   30          1             0       -4.095967   -0.389870    1.987658
   31          1             0       -2.759649   -1.498824    1.594961
   32          1             0       -4.422145   -1.916411    1.141502
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5c’

```
 Zero-point correction=                           0.259180
(Hartree/Particle)
 Thermal correction to Energy=                    0.280054
 Thermal correction to Enthalpy=                  0.280999
 Thermal correction to Gibbs Free Energy=         0.209786
 Sum of electronic and zero-point Energies=          -1709.785231
 Sum of electronic and thermal Energies=             -1709.764356
 Sum of electronic and thermal Enthalpies=           -1709.763412
 Sum of electronic and thermal Free Energies=        -1709.834625

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

1	17	0	-0.589359	-1.976988	-0.646632
2	44	0	0.005817	0.393928	-0.200970
3	17	0	1.119224	2.556143	0.288114
4	15	0	2.157020	-0.622189	0.257552
5	6	0	2.004985	-1.559614	1.836935
6	6	0	3.608084	0.473147	0.525097
7	6	0	2.786842	-1.852401	-0.956595
8	6	0	0.367759	0.642836	-1.969966
9	1	0	2.954974	-2.040403	2.095909
10	1	0	1.225226	-2.316828	1.722056
11	1	0	1.721531	-0.875823	2.643542
12	1	0	3.397071	1.182855	1.326413
13	1	0	3.805667	1.049614	-0.382024
14	1	0	4.484636	-0.135348	0.775185
15	1	0	2.003870	-2.581713	-1.170337
16	1	0	3.675668	-2.355651	-0.560192
17	1	0	3.052299	-1.334220	-1.883366
18	1	0	0.127470	-0.132384	-2.704614
19	1	0	0.772469	1.592381	-2.332551
20	6	0	-2.186828	0.523937	0.219765
21	6	0	-1.621223	1.603471	0.493377
22	6	0	-3.319727	-0.421994	0.072628
23	6	0	-4.590361	0.359630	-0.318721
24	6	0	-3.520337	-1.226784	1.372490
25	1	0	-1.472925	2.622561	0.793234
26	1	0	-3.072066	-1.131952	-0.722158
27	1	0	-4.444220	0.917912	-1.249113
28	1	0	-4.873627	1.070083	0.466013
29	1	0	-5.422423	-0.338740	-0.464611
30	1	0	-3.741380	-0.562248	2.215715
31	1	0	-2.626424	-1.811293	1.605024
32	1	0	-4.361937	-1.917779	1.250022

TS(5-6)c

Zero-point correction= 0.257805
(Hartree/Particle)
Thermal correction to Energy= 0.278656
Thermal correction to Enthalpy= 0.279601
Thermal correction to Gibbs Free Energy= 0.206377
Sum of electronic and zero-point Energies= -1709.765063
Sum of electronic and thermal Energies= -1709.744211
Sum of electronic and thermal Enthalpies= -1709.743267
Sum of electronic and thermal Free Energies= -1709.816491

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.096464	-2.432504	-0.197890
2	44	0	0.037827	0.010430	-0.421186
3	6	0	-2.117828	-0.064931	-0.287986
4	17	0	-0.078014	2.445701	-0.306498
5	15	0	2.225767	0.035639	0.518531
6	6	0	2.112999	-0.441746	2.295106
7	6	0	3.160284	1.618689	0.519451
8	6	0	3.385189	-1.186388	-0.218874
9	6	0	-2.016872	-0.093363	-1.539362

10	6	0	-0.006710	-0.022113	-2.274677
11	6	0	-2.860342	-0.052514	1.002165
12	6	0	-3.838703	-1.242639	1.054800
13	6	0	-3.562050	1.307010	1.191783
14	1	0	3.107856	-0.467541	2.753781
15	1	0	1.649061	-1.429625	2.363060
16	1	0	1.493283	0.282584	2.833156
17	1	0	2.547195	2.397829	0.977318
18	1	0	3.362446	1.921738	-0.511781
19	1	0	4.106942	1.506433	1.059910
20	1	0	2.899103	-2.164812	-0.222910
21	1	0	4.321200	-1.224394	0.349552
22	1	0	3.604454	-0.900269	-1.252068
23	1	0	-2.404894	-0.149206	-2.537785
24	1	0	-0.025195	0.901914	-2.861813
25	1	0	0.049550	-0.964262	-2.830142
26	1	0	-2.136026	-0.178298	1.817493
27	1	0	-3.307997	-2.190145	0.924812
28	1	0	-4.595538	-1.156121	0.267273
29	1	0	-4.351158	-1.255682	2.023477
30	1	0	-4.329107	1.454452	0.423604
31	1	0	-2.843989	2.129028	1.123540
32	1	0	-4.047541	1.336517	2.173921

6c

Zero-point correction= 0.262720
(Hartree/Particle)
Thermal correction to Energy= 0.283124
Thermal correction to Enthalpy= 0.284068
Thermal correction to Gibbs Free Energy= 0.213193
Sum of electronic and zero-point Energies= -1709.844816
Sum of electronic and thermal Energies= -1709.824412
Sum of electronic and thermal Enthalpies= -1709.823468
Sum of electronic and thermal Free Energies= -1709.894343

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.621032	-0.606954	2.527114
2	44	0	0.085507	-0.722598	0.211292
3	6	0	-1.492500	0.187115	0.032294
4	17	0	0.459949	-1.794026	-1.889629
5	15	0	1.682577	0.816530	-0.257049
6	6	0	1.756384	2.292064	0.843080
7	6	0	1.671806	1.518398	-1.959312
8	6	0	3.359136	0.067786	-0.099345
9	6	0	-2.437156	-0.828589	0.521224
10	6	0	-2.528206	-2.079495	0.018415
11	6	0	-1.909184	1.585867	-0.332969
12	6	0	-2.642597	2.279102	0.836473
13	6	0	-2.784873	1.558626	-1.605379
14	1	0	2.615408	2.922317	0.586051
15	1	0	1.836554	1.953228	1.878691
16	1	0	0.840348	2.881642	0.743488
17	1	0	0.739591	2.062977	-2.134772
18	1	0	1.728307	0.696795	-2.677141
19	1	0	2.517570	2.201010	-2.099588
20	1	0	3.485222	-0.309380	0.919700

21	1	0	4.142607	0.802290	-0.317160
22	1	0	3.440455	-0.770233	-0.797739
23	1	0	-2.994210	-0.580653	1.428041
24	1	0	-2.024715	-2.367892	-0.899408
25	1	0	-3.139414	-2.829607	0.513258
26	1	0	-1.007872	2.167455	-0.556396
27	1	0	-2.033877	2.281202	1.746731
28	1	0	-3.592918	1.782008	1.060239
29	1	0	-2.866653	3.317905	0.568523
30	1	0	-3.706221	0.991713	-1.432718
31	1	0	-2.253688	1.094956	-2.442983
32	1	0	-3.061010	2.580060	-1.892029

TS(1-7)a

Zero-point correction= 0.286666
(Hartree/Particle)
Thermal correction to Energy= 0.311857
Thermal correction to Enthalpy= 0.312802
Thermal correction to Gibbs Free Energy= 0.232185
Sum of electronic and zero-point Energies= -2052.911880
Sum of electronic and thermal Energies= -2052.886689
Sum of electronic and thermal Enthalpies= -2052.885745
Sum of electronic and thermal Free Energies= -2052.966362

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000345	3.131983	-0.347303
2	6	0	-0.000320	3.437662	-1.517240
3	1	0	-0.000097	2.834860	0.686020
4	1	0	-0.001546	3.718852	-2.546470
5	6	0	0.000038	-0.106070	-2.142784
6	17	0	0.000078	-2.432681	-0.308202
7	44	0	0.000037	-0.026571	-0.302222
8	17	0	-0.000012	0.845777	2.179393
9	15	0	2.385957	-0.156239	0.061628
10	6	0	3.350251	-0.925246	-1.309509
11	6	0	3.245727	1.443766	0.377659
12	6	0	2.817849	-1.188351	1.519103
13	15	0	-2.385892	-0.156412	0.061667
14	6	0	-2.817702	-1.188613	1.519108
15	6	0	-3.245734	1.443536	0.377797
16	6	0	-3.350213	-0.925403	-1.309465
17	1	0	0.000002	-1.024592	-2.745303
18	1	0	0.000101	0.822488	-2.734680
19	1	0	3.289299	-0.297111	-2.203640
20	1	0	4.402220	-1.057445	-1.032712
21	1	0	2.907767	-1.899442	-1.536841
22	1	0	2.789686	1.911361	1.254779
23	1	0	4.314342	1.285897	0.562719
24	1	0	3.120664	2.112595	-0.478926
25	1	0	3.905084	-1.239802	1.648296
26	1	0	2.350921	-0.751680	2.405019
27	1	0	2.409540	-2.190824	1.368180
28	1	0	-2.409377	-2.191068	1.368118
29	1	0	-2.350751	-0.751980	2.405027
30	1	0	-3.904931	-1.240100	1.648341

31	1	0	-2.789695	1.911097	1.254936
32	1	0	-3.120708	2.112422	-0.478748
33	1	0	-4.314340	1.285610	0.562863
34	1	0	-3.289320	-0.297235	-2.203576
35	1	0	-2.907721	-1.899579	-1.536853
36	1	0	-4.402166	-1.057646	-1.032627

TS(1-7)b

Zero-point correction= 0.315421
(Hartree/Particle)
Thermal correction to Energy= 0.342408
Thermal correction to Enthalpy= 0.343352
Thermal correction to Gibbs Free Energy= 0.256823
Sum of electronic and zero-point Energies= -2092.209940
Sum of electronic and thermal Energies= -2092.182953
Sum of electronic and thermal Enthalpies= -2092.182009
Sum of electronic and thermal Free Energies= -2092.268538

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000835	2.920359	0.898625
2	6	0	-0.001352	3.756373	0.022324
3	6	0	-0.001949	4.770552	-1.028621
4	1	0	-0.000467	2.192811	1.688190
5	1	0	0.882408	5.414904	-0.958183
6	1	0	0.000192	4.311388	-2.025252
7	1	0	-0.888913	5.411555	-0.960438
8	6	0	-0.000149	0.588833	-1.912067
9	17	0	0.000791	-2.306204	-1.286821
10	44	0	0.000078	-0.144247	-0.225146
11	15	0	2.383042	-0.412115	0.055716
12	6	0	3.348418	-0.579420	-1.506210
13	6	0	3.242541	0.928452	0.983168
14	6	0	2.797698	-1.941574	0.986084
15	15	0	-2.382744	-0.413432	0.055742
16	6	0	-2.796537	-1.943258	0.985887
17	6	0	-3.242824	0.926589	0.983439
18	6	0	-3.348142	-0.580976	-1.506144
19	1	0	0.000126	0.033567	-2.860103
20	1	0	-0.000609	1.684566	-2.021909
21	1	0	3.295890	0.354079	-2.075103
22	1	0	4.398086	-0.819911	-1.303608
23	1	0	2.898867	-1.377561	-2.103714
24	1	0	2.793531	0.997401	1.977754
25	1	0	4.314256	0.719342	1.077592
26	1	0	3.101507	1.885293	0.471820
27	1	0	3.883141	-2.052346	1.090476
28	1	0	2.326067	-1.886968	1.970177
29	1	0	2.384065	-2.798254	0.447575
30	1	0	-2.382396	-2.799613	0.447251
31	1	0	-2.324944	-1.888531	1.969990
32	1	0	-3.881915	-2.054685	1.090254
33	1	0	-2.793677	0.995713	1.977952
34	1	0	-3.102376	1.883540	0.472135
35	1	0	-4.314413	0.716907	1.078020
36	1	0	-3.296075	0.352632	-2.074902

37	1	0	-2.898278	-1.378826	-2.103802
38	1	0	-4.397686	-0.821970	-1.303504
39	17	0	0.000061	-0.247945	2.394289

TS(1-9)b

Zero-point correction= 0.315305
(Hartree/Particle)
Thermal correction to Energy= 0.342216
Thermal correction to Enthalpy= 0.343160
Thermal correction to Gibbs Free Energy= 0.257303
Sum of electronic and zero-point Energies= -2092.208368
Sum of electronic and thermal Energies= -2092.181457
Sum of electronic and thermal Enthalpies= -2092.180512
Sum of electronic and thermal Free Energies= -2092.266370

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000003	2.904534	-1.967195
2	6	0	0.000157	3.475633	-0.899588
3	6	0	0.000345	4.157699	0.390185
4	1	0	-0.000145	2.477907	-2.943498
5	1	0	-0.885798	4.794814	0.496207
6	1	0	0.000301	3.419694	1.202062
7	1	0	0.886678	4.794573	0.496078
8	6	0	-0.000019	-0.643426	-2.112220
9	17	0	-0.000113	-2.677404	0.030928
10	44	0	-0.000019	-0.295440	-0.300033
11	15	0	2.387093	-0.344007	0.057054
12	6	0	3.357443	-1.291761	-1.192567
13	6	0	3.197878	1.309784	0.110925
14	6	0	2.851575	-1.135306	1.648406
15	15	0	-2.387133	-0.343832	0.057072
16	6	0	-2.851671	-1.135075	1.648436
17	6	0	-3.197806	1.310013	0.110928
18	6	0	-3.357542	-1.291538	-1.192540
19	1	0	-0.000068	-1.644112	-2.566432
20	1	0	0.000047	0.174742	-2.849490
21	1	0	3.265958	-0.813428	-2.172659
22	1	0	4.416451	-1.350753	-0.917144
23	1	0	2.940516	-2.301000	-1.257599
24	1	0	2.743239	1.881326	0.924654
25	1	0	4.277138	1.221279	0.279888
26	1	0	3.016993	1.841856	-0.827787
27	1	0	3.939476	-1.138006	1.780914
28	1	0	2.370826	-0.586382	2.461351
29	1	0	2.472348	-2.160629	1.649903
30	1	0	-2.472542	-2.160434	1.649938
31	1	0	-2.370860	-0.586186	2.461368
32	1	0	-3.939570	-1.137673	1.780958
33	1	0	-2.743173	1.881510	0.924692
34	1	0	-3.016835	1.842092	-0.827762
35	1	0	-4.277082	1.221577	0.279833
36	1	0	-3.266026	-0.813221	-2.172637
37	1	0	-2.940674	-2.300802	-1.257560
38	1	0	-4.416554	-1.350463	-0.917116
39	17	0	0.000033	0.921246	2.001000

TS(1-7)c

Zero-point correction= 0.373075
(Hartree/Particle)
Thermal correction to Energy= 0.402338
Thermal correction to Enthalpy= 0.403282
Thermal correction to Gibbs Free Energy= 0.311518
Sum of electronic and zero-point Energies= -2170.779050
Sum of electronic and thermal Energies= -2170.749787
Sum of electronic and thermal Enthalpies= -2170.748842
Sum of electronic and thermal Free Energies= -2170.840606

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.333964	-0.293425	1.263892
2	6	0	3.244527	-0.345248	0.465461
3	6	0	4.365791	-0.405852	-0.481546
4	6	0	5.482495	-1.329776	0.048911
5	6	0	4.905008	1.004423	-0.799103
6	1	0	1.534912	-0.246036	1.979069
7	1	0	3.989363	-0.840981	-1.420250
8	1	0	5.101851	-2.336587	0.246717
9	1	0	5.898897	-0.934446	0.981764
10	1	0	6.291950	-1.402424	-0.686167
11	1	0	5.297647	1.480072	0.106152
12	1	0	4.117628	1.646593	-1.207049
13	1	0	5.714968	0.942608	-1.534618
14	6	0	0.377251	-0.026491	-1.793243
15	17	0	-2.555923	0.261407	-1.521739
16	44	0	-0.552296	0.025257	-0.206217
17	15	0	-1.089213	-2.320342	-0.022212
18	6	0	-1.144985	-3.253031	-1.612309
19	6	0	0.029904	-3.316229	1.051095
20	6	0	-2.760297	-2.587537	0.692696
21	15	0	-0.619093	2.417790	0.105352
22	6	0	-2.203683	2.974627	0.850758
23	6	0	0.672357	3.121525	1.215665
24	6	0	-0.493969	3.418765	-1.438437
25	1	0	-0.056518	0.039171	-2.800576
26	1	0	1.472717	-0.133836	-1.771567
27	1	0	-0.144492	-3.290911	-2.054313
28	1	0	-1.512187	-4.274595	-1.462330
29	1	0	-1.810327	-2.723027	-2.299895
30	1	0	0.011542	-2.884320	2.055445
31	1	0	-0.290500	-4.363435	1.094510
32	1	0	1.054033	-3.263619	0.669780
33	1	0	-2.984094	-3.657457	0.772159
34	1	0	-2.793019	-2.118619	1.679022
35	1	0	-3.495302	-2.097658	0.048695
36	1	0	-3.023939	2.658044	0.201269
37	1	0	-2.319604	2.488775	1.822440
38	1	0	-2.216986	4.064281	0.967832
39	1	0	0.568000	2.652357	2.197919
40	1	0	1.667475	2.889134	0.825092
41	1	0	0.561999	4.207589	1.313072
42	1	0	0.493390	3.280757	-1.889875
43	1	0	-1.251777	3.061287	-2.141437

44	1	0	-0.653509	4.484272	-1.238315
45	17	0	-0.982236	-0.006733	2.379909

TS(1-9)c

Zero-point correction= 0.372664
(Hartree/Particle)
Thermal correction to Energy= 0.402130
Thermal correction to Enthalpy= 0.403074
Thermal correction to Gibbs Free Energy= 0.311463
Sum of electronic and zero-point Energies= -2170.777064
Sum of electronic and thermal Energies= -2170.747598
Sum of electronic and thermal Enthalpies= -2170.746654
Sum of electronic and thermal Free Energies= -2170.838265

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.332252	-0.000105	-2.114552
2	6	0	3.003271	-0.000281	-1.105546
3	6	0	3.830646	-0.000050	0.106383
4	6	0	4.697471	1.274102	0.182096
5	6	0	4.698207	-1.273694	0.182160
6	1	0	1.816884	-0.000043	-3.046957
7	1	0	3.137278	-0.000178	0.958838
8	1	0	4.078274	2.176283	0.158688
9	1	0	5.402103	1.320953	-0.656139
10	1	0	5.272333	1.277164	1.114795
11	1	0	5.403054	-1.320020	-0.655923
12	1	0	4.079633	-2.176279	0.158514
13	1	0	5.272859	-1.276489	1.114987
14	6	0	-1.180235	0.000008	-2.086965
15	17	0	-3.065181	0.000017	0.182622
16	44	0	-0.707943	-0.000007	-0.302122
17	15	0	-0.744314	-2.386723	0.060867
18	6	0	-1.768021	-3.351845	-1.131653
19	6	0	0.902816	-3.211276	0.024049
20	6	0	-1.445318	-2.845259	1.696209
21	15	0	-0.744318	2.386702	0.060849
22	6	0	-1.445397	2.845153	1.696187
23	6	0	0.902799	3.211296	0.024105
24	6	0	-1.767975	3.351871	-1.131675
25	17	0	0.656133	-0.000025	1.913755
26	1	0	-2.210776	0.000219	-2.468322
27	1	0	-0.419009	-0.000198	-2.882851
28	1	0	-1.343763	-3.266259	-2.136908
29	1	0	-1.821430	-4.409704	-0.850771
30	1	0	-2.775322	-2.925502	-1.141638
31	1	0	1.521916	-2.757877	0.802971
32	1	0	0.814862	-4.289038	0.202252
33	1	0	1.382347	-3.038235	-0.943852
34	1	0	-1.441702	-3.932859	1.831345
35	1	0	-0.849918	-2.363774	2.475434
36	1	0	-2.468360	-2.464808	1.755533
37	1	0	-2.468430	2.464665	1.755446
38	1	0	-0.850023	2.363642	2.475424
39	1	0	-1.441820	3.932747	1.831375
40	1	0	1.521869	2.757923	0.803067
41	1	0	1.382389	3.038257	-0.943782
42	1	0	0.814817	4.289060	0.202280
43	1	0	-1.343664	3.266339	-2.136912

44	1	0	-2.775276	2.925529	-1.141737
45	1	0	-1.821399	4.409717	-0.850742

TS(1-7)d

Zero-point correction= 0.345039
(Hartree/Particle)
Thermal correction to Energy= 0.373139
Thermal correction to Enthalpy= 0.374084
Thermal correction to Gibbs Free Energy= 0.286667
Sum of electronic and zero-point Energies= -2131.500183
Sum of electronic and thermal Energies= -2131.472083
Sum of electronic and thermal Enthalpies= -2131.471139
Sum of electronic and thermal Free Energies= -2131.558555

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.885500	2.853223	-0.883028
2	6	0	0.365364	3.029739	0.201277
3	6	0	-0.188179	3.382542	1.507797
4	6	0	1.571369	2.873624	-2.177588
5	1	0	-1.188862	3.819262	1.407129
6	1	0	-0.254582	2.496710	2.150111
7	1	0	0.452652	4.125522	1.998660
8	1	0	2.190419	1.983253	-2.332560
9	1	0	2.225293	3.752090	-2.242165
10	1	0	0.862559	2.932855	-3.012194
11	6	0	-0.004638	-0.128449	-2.129711
12	17	0	-0.340836	-2.596863	-0.544355
13	44	0	-0.052231	-0.214644	-0.282228
14	15	0	2.276346	-0.675593	0.212582
15	6	0	3.303788	-1.197497	-1.231591
16	6	0	3.241368	0.697822	0.976019
17	6	0	2.500350	-2.057402	1.403330
18	15	0	-2.464899	-0.105501	-0.114807
19	6	0	-3.162637	-1.283331	1.110442
20	6	0	-3.178044	1.520707	0.383083
21	6	0	-3.376786	-0.526948	-1.663515
22	1	0	-0.077830	-1.006912	-2.785730
23	1	0	0.055884	0.820149	-2.682022
24	1	0	3.363795	-0.385307	-1.963117
25	1	0	4.317424	-1.477950	-0.923429
26	1	0	2.818985	-2.055552	-1.706517
27	1	0	2.738443	0.986131	1.903195
28	1	0	4.266265	0.378576	1.197120
29	1	0	3.264214	1.566161	0.312428
30	1	0	3.565194	-2.220608	1.605785
31	1	0	1.971409	-1.804259	2.325032
32	1	0	2.051721	-2.961332	0.985400
33	1	0	-2.864001	-2.295097	0.825505
34	1	0	-2.733319	-1.062284	2.090106
35	1	0	-4.255500	-1.205484	1.141582
36	1	0	-2.793877	1.775944	1.374129
37	1	0	-2.869225	2.295998	-0.324704
38	1	0	-4.272535	1.476634	0.418458
39	1	0	-3.150070	0.208322	-2.441990
40	1	0	-3.039038	-1.510165	-2.003686
41	1	0	-4.459541	-0.552847	-1.496218
42	17	0	-0.177056	0.014321	2.318002

7a

Zero-point correction= 0.289447
(Hartree/Particle)
Thermal correction to Energy= 0.313764
Thermal correction to Enthalpy= 0.314708
Thermal correction to Gibbs Free Energy= 0.237096
Sum of electronic and zero-point Energies= -2052.921631
Sum of electronic and thermal Energies= -2052.897314
Sum of electronic and thermal Enthalpies= -2052.896370
Sum of electronic and thermal Free Energies= -2052.973982

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.004480	-0.092027	-0.449339
2	15	0	-2.371070	0.115151	0.099480
3	6	0	-3.338749	1.177768	-1.058414
4	6	0	-3.348193	-1.447013	0.196816
5	6	0	-2.674899	0.878690	1.742123
6	17	0	0.070611	2.254492	0.404184
7	6	0	0.487648	-2.131267	-1.199938
8	6	0	-0.681417	-1.919488	-1.552730
9	6	0	0.106978	0.687067	-2.134164
10	1	0	-3.342483	0.736098	-2.059786
11	1	0	-4.372252	1.298331	-0.714589
12	1	0	-2.856972	2.158279	-1.109608
13	1	0	-2.792661	-2.155734	0.817254
14	1	0	-4.326496	-1.251181	0.648807
15	1	0	-3.507705	-1.881875	-0.794039
16	1	0	-3.753114	0.918952	1.935062
17	1	0	-2.171624	0.271868	2.497866
18	1	0	-2.246412	1.881660	1.756327
19	1	0	1.389592	-2.685295	-1.046388
20	1	0	-1.639134	-2.098881	-1.994013
21	1	0	0.105980	0.100898	-3.064593
22	1	0	0.200284	1.769009	-2.287453
23	17	0	-0.077832	-1.395170	1.848346
24	15	0	2.382196	0.061219	0.095677
25	6	0	3.291214	1.282883	-0.944792
26	6	0	2.699059	0.623799	1.815178
27	6	0	3.437021	-1.451029	-0.017428
28	1	0	2.762977	2.238035	-0.883533
29	1	0	4.322082	1.410409	-0.595929
30	1	0	3.301132	0.949570	-1.987407
31	1	0	2.242235	-0.091425	2.502476
32	1	0	3.779207	0.693208	1.988520
33	1	0	2.225773	1.596125	1.960508
34	1	0	4.450012	-1.226410	0.333682
35	1	0	3.010465	-2.234196	0.616787
36	1	0	3.500128	-1.810744	-1.049303

TS(7-8)a

Zero-point correction= 0.287648
(Hartree/Particle)

Thermal correction to Energy= 0.311766
Thermal correction to Enthalpy= 0.312711
Thermal correction to Gibbs Free Energy= 0.235303
Sum of electronic and zero-point Energies= -2052.906384
Sum of electronic and thermal Energies= -2052.882265
Sum of electronic and thermal Enthalpies= -2052.881321
Sum of electronic and thermal Free Energies= -2052.958728

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.007595	0.218287	-0.157763
2	15	0	2.422865	0.032561	-0.044106
3	6	0	3.272044	-0.110146	-1.679566
4	6	0	3.359327	1.399093	0.782480
5	6	0	3.003514	-1.463497	0.852001
6	17	0	0.132749	-2.016063	-1.129091
7	6	0	0.017289	1.946283	1.154167
8	6	0	-0.063184	2.577585	0.076610
9	6	0	0.059901	1.279432	-1.740724
10	1	0	3.154994	0.811094	-2.259900
11	1	0	4.342020	-0.311101	-1.556303
12	1	0	2.807290	-0.931537	-2.232266
13	1	0	3.041059	1.475111	1.826898
14	1	0	4.438419	1.211677	0.755462
15	1	0	3.151167	2.354940	0.291730
16	1	0	4.098382	-1.505782	0.874485
17	1	0	2.597122	-1.447666	1.865910
18	1	0	2.599995	-2.344298	0.347047
19	1	0	0.054318	1.864864	2.223709
20	1	0	-0.188993	3.424170	-0.569932
21	1	0	0.970112	1.689562	-2.197727
22	1	0	-0.831216	1.599721	-2.295852
23	17	0	-0.175130	-0.918619	2.182116
24	15	0	-2.412498	0.010636	-0.124200
25	6	0	-3.364950	0.561113	-1.616339
26	6	0	-3.012880	-1.708835	0.123945
27	6	0	-3.239260	0.938175	1.242073
28	1	0	-3.018811	0.008612	-2.495725
29	1	0	-4.437755	0.380442	-1.486634
30	1	0	-3.215320	1.631250	-1.797235
31	1	0	-2.546820	-2.101322	1.031051
32	1	0	-4.104885	-1.727449	0.214710
33	1	0	-2.691525	-2.328476	-0.715934
34	1	0	-4.318595	0.749788	1.255833
35	1	0	-2.796629	0.605381	2.185411
36	1	0	-3.064327	2.012822	1.132133

8a

Zero-point correction= 0.292445
(Hartree/Particle)
Thermal correction to Energy= 0.316455
Thermal correction to Enthalpy= 0.317399
Thermal correction to Gibbs Free Energy= 0.238803
Sum of electronic and zero-point Energies= -2052.969908
Sum of electronic and thermal Energies= -2052.945898
Sum of electronic and thermal Enthalpies= -2052.944954

Sum of electronic and thermal Free Energies= -2053.023550

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.007227	0.303838	-0.217342
2	15	0	-2.358874	-0.159395	0.066655
3	6	0	-3.283954	0.824656	1.324000
4	6	0	-3.354404	0.024399	-1.477244
5	6	0	-2.685851	-1.893761	0.576638
6	6	0	0.038755	1.392144	-1.715108
7	6	0	0.411811	2.464577	-0.825558
8	6	0	-0.348829	2.706764	0.306289
9	15	0	2.342586	-0.185265	0.121422
10	6	0	3.178330	0.896792	1.355986
11	6	0	2.689614	-1.892843	0.694256
12	6	0	3.366879	-0.025360	-1.405634
13	1	0	-3.372709	1.871529	1.017975
14	1	0	-4.290870	0.416439	1.465538
15	1	0	-2.730419	0.773645	2.265573
16	1	0	-2.880271	-0.575147	-2.259658
17	1	0	-4.385768	-0.315931	-1.330543
18	1	0	-3.363283	1.071554	-1.795832
19	1	0	-3.765357	-2.060488	0.668057
20	1	0	-2.258684	-2.566465	-0.169755
21	1	0	-2.190326	-2.071249	1.533462
22	1	0	0.067567	1.327492	-2.804179
23	1	0	1.422404	2.881339	-0.882421
24	1	0	-1.426070	2.626391	0.288929
25	1	0	0.086070	3.222161	1.157388
26	1	0	2.642511	0.800359	2.304148
27	1	0	4.226843	0.607639	1.489970
28	1	0	3.136208	1.941590	1.031856
29	1	0	2.295995	-2.593637	-0.045308
30	1	0	3.768651	-2.036890	0.820609
31	1	0	2.168340	-2.051112	1.640493
32	1	0	4.405934	-0.320159	-1.220230
33	1	0	2.933542	-0.673887	-2.172301
34	1	0	3.349659	1.007331	-1.768467
35	17	0	-0.022750	-0.492554	2.284285
36	17	0	0.023471	-1.770135	-1.548705

7b

Zero-point correction= 0.317099
(Hartree/Particle)
Thermal correction to Energy= 0.343649
Thermal correction to Enthalpy= 0.344593
Thermal correction to Gibbs Free Energy= 0.261789
Sum of electronic and zero-point Energies= -2092.215574
Sum of electronic and thermal Energies= -2092.189024
Sum of electronic and thermal Enthalpies= -2092.188080
Sum of electronic and thermal Free Energies= -2092.270884

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.037641	0.166376	-0.214909

2	15	0	2.469795	0.055323	0.017861
3	6	0	3.375650	0.032866	-1.589594
4	6	0	3.326105	1.399845	0.953556
5	6	0	3.063675	-1.471077	0.848539
6	17	0	0.343902	-2.065989	-1.248035
7	6	0	0.172852	0.812826	-1.959203
8	15	0	-2.306921	-0.444338	0.014799
9	6	0	-3.345302	-0.243126	-1.502596
10	6	0	-2.578151	-2.207168	0.454960
11	6	0	-3.242218	0.452901	1.327171
12	1	0	3.240525	0.986102	-2.110462
13	1	0	4.446116	-0.145508	-1.437574
14	1	0	2.955932	-0.768975	-2.203397
15	1	0	3.007803	1.375831	2.000121
16	1	0	4.412000	1.258909	0.916864
17	1	0	3.076845	2.378316	0.532045
18	1	0	4.158515	-1.470679	0.901944
19	1	0	2.627373	-1.523339	1.848069
20	1	0	2.709934	-2.332055	0.277388
21	1	0	0.163283	1.870238	-2.258897
22	1	0	0.340141	0.132289	-2.802858
23	1	0	-2.897278	-0.833174	-2.307696
24	1	0	-4.370697	-0.589878	-1.330616
25	1	0	-3.370699	0.804917	-1.816001
26	1	0	-2.053011	-2.411721	1.390241
27	1	0	-3.650886	-2.403597	0.566030
28	1	0	-2.151998	-2.840664	-0.325054
29	1	0	-4.254338	0.045280	1.427365
30	1	0	-2.695432	0.322603	2.264872
31	1	0	-3.308861	1.521588	1.107611
32	6	0	0.132114	2.021403	1.083377
33	6	0	-0.650262	2.424322	0.219095
34	6	0	-1.564426	3.245941	-0.583337
35	1	0	0.690989	1.967695	1.993387
36	1	0	-1.637450	4.248040	-0.143880
37	1	0	-1.217105	3.359197	-1.615514
38	1	0	-2.572000	2.817685	-0.619038
39	17	0	0.015555	-0.761470	2.259761

TS(7-8)b

Zero-point correction= 0.317056
(Hartree/Particle)
Thermal correction to Energy= 0.342554
Thermal correction to Enthalpy= 0.343498
Thermal correction to Gibbs Free Energy= 0.262915
Sum of electronic and zero-point Energies= -2092.198752
Sum of electronic and thermal Energies= -2092.173253
Sum of electronic and thermal Enthalpies= -2092.172309
Sum of electronic and thermal Free Energies= -2092.252893

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.031054	0.069606	-0.114363
2	15	0	2.457109	-0.012900	-0.046155
3	6	0	3.266416	0.013622	-1.706009
4	6	0	3.359114	1.322818	0.865124

5	6	0	3.111161	-1.550020	0.720943
6	17	0	0.269107	-2.022981	-1.347822
7	6	0	0.076690	1.602377	1.347926
8	6	0	-0.211873	2.388801	0.398118
9	6	0	0.052262	1.407979	-1.480236
10	15	0	-2.368147	-0.280753	-0.129402
11	6	0	-3.327814	0.324139	-1.595560
12	6	0	-2.881286	-2.042162	-0.018750
13	6	0	-3.253217	0.501187	1.290666
14	6	0	-0.782700	3.675955	-0.075665
15	1	0	3.085003	0.971527	-2.204069
16	1	0	4.347857	-0.142057	-1.624498
17	1	0	2.823906	-0.782107	-2.311307
18	1	0	3.082083	1.291897	1.923444
19	1	0	4.443998	1.195150	0.780723
20	1	0	3.083958	2.305595	0.469558
21	1	0	4.207212	-1.554804	0.720810
22	1	0	2.724551	-1.627858	1.740013
23	1	0	2.728391	-2.403416	0.156240
24	1	0	0.218765	1.460578	2.404153
25	1	0	0.941555	1.962383	-1.805581
26	1	0	-0.832820	1.730348	-2.041815
27	1	0	-2.926754	-0.137720	-2.503328
28	1	0	-4.389250	0.067115	-1.506261
29	1	0	-3.243290	1.411736	-1.695517
30	1	0	-2.401459	-2.478276	0.860526
31	1	0	-3.971737	-2.121736	0.058389
32	1	0	-2.524677	-2.578179	-0.900968
33	1	0	-4.326322	0.281365	1.265285
34	1	0	-2.817390	0.103656	2.211736
35	1	0	-3.108608	1.586226	1.278467
36	1	0	-0.830866	4.362596	0.777815
37	1	0	-0.181531	4.143893	-0.861978
38	1	0	-1.799999	3.545373	-0.463487
39	17	0	-0.121217	-1.336979	2.080623

8b

Zero-point correction= 0.320516
(Hartree/Particle)
Thermal correction to Energy= 0.346354
Thermal correction to Enthalpy= 0.347298
Thermal correction to Gibbs Free Energy= 0.264508
Sum of electronic and zero-point Energies= -2092.287960
Sum of electronic and thermal Energies= -2092.262122
Sum of electronic and thermal Enthalpies= -2092.261177
Sum of electronic and thermal Free Energies= -2092.343968

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.154675	-0.206715	0.040428
2	15	0	-2.179260	-0.865233	0.102409
3	6	0	-3.291858	-0.290679	1.458273
4	6	0	-3.162930	-0.552304	-1.427150
5	6	0	-2.253829	-2.703389	0.282333
6	17	0	0.158073	0.027321	2.455910
7	6	0	-0.065305	1.498846	-0.640938

8	6	0	-1.088239	2.521971	-0.410343
9	6	0	-1.627297	2.725486	0.809055
10	15	0	2.550743	-0.000488	0.040306
11	6	0	3.304847	1.194646	1.225713
12	6	0	3.331793	-1.609604	0.493620
13	6	0	3.354618	0.425874	-1.565261
14	6	0	-1.421316	3.408674	-1.596685
15	1	0	-3.482850	0.780692	1.352467
16	1	0	-4.246082	-0.828911	1.434045
17	1	0	-2.795330	-0.457132	2.418035
18	1	0	-2.608393	-0.947702	-2.282697
19	1	0	-4.150823	-1.023752	-1.375527
20	1	0	-3.289998	0.526359	-1.562017
21	1	0	-3.287728	-3.066943	0.266958
22	1	0	-1.690880	-3.161983	-0.535409
23	1	0	-1.789616	-2.990464	1.231539
24	1	0	0.673272	1.810474	-1.396960
25	1	0	-1.342306	2.108821	1.655476
26	1	0	-2.322953	3.543148	0.984919
27	1	0	2.916277	0.990237	2.226716
28	1	0	4.398361	1.124315	1.225919
29	1	0	3.011298	2.212837	0.950540
30	1	0	3.014444	-2.371884	-0.224233
31	1	0	4.425516	-1.540376	0.492471
32	1	0	2.990950	-1.903302	1.491304
33	1	0	4.446544	0.377638	-1.488833
34	1	0	3.002314	-0.270344	-2.330929
35	1	0	3.068179	1.439777	-1.864095
36	1	0	-0.527463	3.929426	-1.963379
37	1	0	-1.811283	2.819306	-2.436079
38	1	0	-2.169628	4.161915	-1.331194
39	17	0	0.354123	-1.491909	-2.022399

7c

Zero-point correction= 0.374620
(Hartree/Particle)
Thermal correction to Energy= 0.403644
Thermal correction to Enthalpy= 0.404588
Thermal correction to Gibbs Free Energy= 0.316328
Sum of electronic and zero-point Energies= -2170.783447
Sum of electronic and thermal Energies= -2170.754423
Sum of electronic and thermal Enthalpies= -2170.753479
Sum of electronic and thermal Free Energies= -2170.841739

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.168840	-0.154421	-0.174926
2	15	0	2.449043	0.664639	0.093784
3	6	0	3.276466	1.063330	-1.506365
4	6	0	2.703216	2.202811	1.086800
5	6	0	3.599396	-0.541576	0.864052
6	6	0	-0.037022	0.633762	-1.857356
7	15	0	-1.846118	-1.514583	-0.102267
8	6	0	-2.982368	-1.356005	-1.553926
9	6	0	-1.527987	-3.321496	-0.026271
10	6	0	-2.951620	-1.218363	1.342722
11	1	0	2.772188	1.907538	-1.987432

12	1	0	4.333023	1.311696	-1.356305
13	1	0	3.193224	0.186459	-2.154366
14	1	0	2.386721	2.029674	2.119430
15	1	0	3.759229	2.495356	1.086184
16	1	0	2.102901	3.019756	0.675512
17	1	0	4.618201	-0.137330	0.883846
18	1	0	3.256720	-0.774452	1.874001
19	1	0	3.565247	-1.462700	0.277634
20	1	0	-0.558670	1.564255	-2.113415
21	1	0	0.401242	0.145294	-2.735870
22	1	0	-2.431477	-1.615405	-2.463084
23	1	0	-3.848937	-2.020077	-1.457370
24	1	0	-3.334335	-0.323492	-1.645228
25	1	0	-0.916926	-3.520529	0.856881
26	1	0	-2.473650	-3.873159	0.027851
27	1	0	-0.959101	-3.622795	-0.908132
28	1	0	-3.803919	-1.906593	1.325169
29	1	0	-2.362444	-1.380159	2.249183
30	1	0	-3.316462	-0.188053	1.342550
31	17	0	1.277685	-1.985098	-1.411816
32	6	0	-0.508413	1.303307	1.459168
33	6	0	-1.151429	1.782637	0.523229
34	6	0	-2.038052	2.655764	-0.275439
35	6	0	-1.304439	3.945213	-0.701668
36	6	0	-3.312961	2.990270	0.528554
37	1	0	-0.121635	1.062160	2.427769
38	1	0	-2.344067	2.120690	-1.184121
39	1	0	-0.403863	3.722816	-1.282343
40	1	0	-1.005324	4.523353	0.179461
41	1	0	-1.964421	4.569198	-1.314945
42	1	0	-3.061219	3.531376	1.446874
43	1	0	-3.859907	2.084356	0.807265
44	1	0	-3.977614	3.622028	-0.071613
45	17	0	0.563122	-1.448166	2.095205

TS(7-8)c

Zero-point correction= 0.374224
(Hartree/Particle)
Thermal correction to Energy= 0.402322
Thermal correction to Enthalpy= 0.403266
Thermal correction to Gibbs Free Energy= 0.316934
Sum of electronic and zero-point Energies= -2170.767275
Sum of electronic and thermal Energies= -2170.739176
Sum of electronic and thermal Enthalpies= -2170.738232
Sum of electronic and thermal Free Energies= -2170.824564

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.204765	-0.220197	-0.126875
2	15	0	2.419192	0.773316	0.017266
3	6	0	3.222208	1.086807	-1.616245
4	6	0	2.607332	2.406774	0.870610
5	6	0	3.637691	-0.288919	0.892090
6	17	0	1.409586	-2.022755	-1.251097
7	6	0	-0.465790	1.228923	1.278297
8	6	0	-1.075560	1.775091	0.313270

9	6	0	-0.287763	0.945155	-1.554965
10	15	0	-1.787746	-1.595372	-0.203818
11	6	0	-2.861857	-1.491102	-1.711098
12	6	0	-1.462197	-3.399748	-0.073731
13	6	0	-2.983003	-1.293409	1.170982
14	6	0	-2.210587	2.628534	-0.169568
15	6	0	-1.750446	3.850029	-0.987578
16	6	0	-3.041680	3.071645	1.053160
17	1	0	2.676231	1.857869	-2.169454
18	1	0	4.260628	1.412669	-1.490544
19	1	0	3.192810	0.158151	-2.192194
20	1	0	2.316460	2.307179	1.920898
21	1	0	3.644511	2.757093	0.823998
22	1	0	1.957322	3.155198	0.406315
23	1	0	4.621908	0.191855	0.930679
24	1	0	3.268738	-0.494157	1.899919
25	1	0	3.702279	-1.242598	0.362987
26	1	0	-0.282223	1.174994	2.335959
27	1	0	0.296327	1.813590	-1.881216
28	1	0	-1.200550	0.841074	-2.154229
29	1	0	-2.264712	-1.733920	-2.595706
30	1	0	-3.701666	-2.191891	-1.647141
31	1	0	-3.264576	-0.479690	-1.832500
32	1	0	-0.880464	-3.572382	0.834820
33	1	0	-2.403918	-3.959698	-0.040227
34	1	0	-0.860762	-3.720459	-0.926904
35	1	0	-3.815148	-2.005473	1.138703
36	1	0	-2.437558	-1.404715	2.112230
37	1	0	-3.380517	-0.275465	1.113970
38	1	0	-2.852504	2.009484	-0.810874
39	1	0	-1.207674	3.556981	-1.890361
40	1	0	-1.096365	4.491915	-0.386809
41	1	0	-2.620233	4.442079	-1.292951
42	1	0	-2.437795	3.685077	1.730601
43	1	0	-3.414764	2.210136	1.614961
44	1	0	-3.898229	3.670579	0.724129
45	17	0	0.568708	-1.492224	2.130530

8c

Zero-point correction= 0.378238
(Hartree/Particle)
Thermal correction to Energy= 0.406415
Thermal correction to Enthalpy= 0.407359
Thermal correction to Gibbs Free Energy= 0.319659
Sum of electronic and zero-point Energies= -2170.854654
Sum of electronic and thermal Energies= -2170.826478
Sum of electronic and thermal Enthalpies= -2170.825534
Sum of electronic and thermal Free Energies= -2170.913233

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.518544	0.307301	0.012094
2	15	0	1.141102	2.078139	-0.019864
3	6	0	2.208250	2.408715	1.449487
4	6	0	2.327840	2.118974	-1.431201
5	6	0	0.216501	3.667823	-0.210118

6	6	0	0.581690	-1.177401	-0.126293
7	6	0	1.873212	-1.527726	0.473695
8	6	0	2.214468	-1.078676	1.699995
9	15	0	-2.500529	-1.050273	-0.013557
10	6	0	-2.811479	-2.145065	1.437664
11	6	0	-3.996876	0.028313	-0.068826
12	6	0	-2.730885	-2.175130	-1.457715
13	6	0	2.725877	-2.510057	-0.338340
14	6	0	3.906663	-3.110502	0.434129
15	6	0	3.208749	-1.857437	-1.649931
16	1	0	2.939136	1.603383	1.564535
17	1	0	2.739076	3.361154	1.340153
18	1	0	1.579822	2.434635	2.343801
19	1	0	1.763065	2.019758	-2.362100
20	1	0	2.903908	3.051139	-1.442564
21	1	0	3.016787	1.272867	-1.353869
22	1	0	0.898376	4.523488	-0.274743
23	1	0	-0.391069	3.616407	-1.118407
24	1	0	-0.446955	3.802907	0.650092
25	1	0	0.218948	-1.959778	-0.812261
26	1	0	1.549505	-0.421154	2.249916
27	1	0	3.127168	-1.397654	2.193966
28	1	0	-2.722638	-1.550686	2.350667
29	1	0	-3.803428	-2.607731	1.385680
30	1	0	-2.050358	-2.931322	1.469860
31	1	0	-3.941362	0.663854	-0.957693
32	1	0	-4.918847	-0.563408	-0.100076
33	1	0	-4.008955	0.667191	0.819751
34	1	0	-3.716531	-2.653023	-1.436105
35	1	0	-2.616514	-1.594195	-2.376568
36	1	0	-1.961682	-2.954580	-1.445738
37	1	0	2.058867	-3.340270	-0.618350
38	1	0	3.579065	-3.615003	1.349577
39	1	0	4.637301	-2.341009	0.711839
40	1	0	4.427108	-3.845776	-0.189659
41	1	0	3.909758	-1.040635	-1.437070
42	1	0	2.376420	-1.443428	-2.229321
43	1	0	3.728849	-2.590193	-2.277951
44	17	0	-0.842363	0.692391	2.389825
45	17	0	-0.923021	0.780719	-2.348851

7d

Zero-point correction= 0.345890
(Hartree/Particle)
Thermal correction to Energy= 0.374229
Thermal correction to Enthalpy= 0.375173
Thermal correction to Gibbs Free Energy= 0.286913
Sum of electronic and zero-point Energies= -2131.505016
Sum of electronic and thermal Energies= -2131.476678
Sum of electronic and thermal Enthalpies= -2131.475733
Sum of electronic and thermal Free Energies= -2131.563994

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.011247	-0.039579	-0.267237
2	15	0	2.447549	-0.171377	-0.118614

3	6	0	3.211540	-1.142656	-1.488345
4	6	0	3.444443	1.388781	-0.172420
5	6	0	3.050681	-1.030470	1.388266
6	17	0	0.169554	-2.511655	-0.425100
7	6	0	0.136521	2.200034	0.451443
8	6	0	-0.384648	2.219816	-0.671751
9	6	0	0.097612	-0.080538	-2.137480
10	15	0	-2.386215	-0.338025	0.035089
11	6	0	-3.367576	-0.512910	-1.524467
12	6	0	-2.876945	-1.840586	0.970913
13	6	0	-3.240091	1.027076	0.933175
14	6	0	-0.996501	2.838926	-1.863208
15	6	0	0.617729	2.706519	1.747442
16	1	0	3.092142	-0.604358	-2.434350
17	1	0	4.278521	-1.308462	-1.301880
18	1	0	2.692402	-2.101503	-1.559800
19	1	0	3.236062	2.012621	0.699994
20	1	0	4.515357	1.156996	-0.189337
21	1	0	3.188987	1.959888	-1.070247
22	1	0	4.143215	-1.117372	1.373518
23	1	0	2.718628	-0.491651	2.277883
24	1	0	2.590296	-2.021390	1.414788
25	1	0	0.057747	0.757943	-2.843026
26	1	0	0.216844	-1.047175	-2.641363
27	1	0	-2.985692	-1.375760	-2.078533
28	1	0	-4.431481	-0.666842	-1.311074
29	1	0	-3.256574	0.376659	-2.151871
30	1	0	-2.409370	-1.802234	1.956609
31	1	0	-3.968406	-1.887358	1.061864
32	1	0	-2.499087	-2.722168	0.449004
33	1	0	-4.306457	0.807393	1.056514
34	1	0	-2.769222	1.125524	1.914747
35	1	0	-3.125072	1.970597	0.392590
36	1	0	-1.298552	3.866305	-1.627147
37	1	0	-0.295766	2.889851	-2.704524
38	1	0	-1.881508	2.292453	-2.206331
39	1	0	1.530016	2.206881	2.079090
40	1	0	-0.127060	2.526686	2.526356
41	1	0	0.806786	3.785061	1.663191
42	17	0	-0.127449	-0.303052	2.334701

ET(7-8)d

Zero-point correction= 0.345834
(Hartree/Particle)
Thermal correction to Energy= 0.372960
Thermal correction to Enthalpy= 0.373904
Thermal correction to Gibbs Free Energy= 0.290042
Sum of electronic and zero-point Energies= -2131.492133
Sum of electronic and thermal Energies= -2131.465007
Sum of electronic and thermal Enthalpies= -2131.464063
Sum of electronic and thermal Free Energies= -2131.547924

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.016237	-0.046197	-0.197574
2	15	0	2.437092	-0.157503	-0.121120
3	6	0	3.236841	-0.599308	-1.728296

4	6	0	3.386281	1.355670	0.373360
5	6	0	3.084918	-1.445840	1.019771
6	17	0	0.201503	-2.391543	-0.918649
7	6	0	0.016804	1.889795	0.819291
8	6	0	-0.156409	2.329999	-0.351960
9	6	0	0.046360	0.772615	-1.911836
10	15	0	-2.391381	-0.324026	-0.130871
11	6	0	-3.353846	0.045711	-1.672709
12	6	0	-2.950502	-2.023276	0.290855
13	6	0	-3.252398	0.713386	1.131816
14	6	0	-0.501574	3.431265	-1.284240
15	6	0	0.135364	2.236124	2.253108
16	1	0	3.078364	0.190837	-2.469585
17	1	0	4.314802	-0.750181	-1.603263
18	1	0	2.775530	-1.519755	-2.096034
19	1	0	3.122645	1.641787	1.395767
20	1	0	4.466358	1.177097	0.326114
21	1	0	3.135405	2.189896	-0.289556
22	1	0	4.180590	-1.471985	1.000503
23	1	0	2.721783	-1.246747	2.030517
24	1	0	2.677505	-2.410769	0.708057
25	1	0	0.945053	1.143738	-2.421309
26	1	0	-0.844459	0.941358	-2.529333
27	1	0	-2.989753	-0.586329	-2.489087
28	1	0	-4.422213	-0.148114	-1.526834
29	1	0	-3.229661	1.094409	-1.964434
30	1	0	-2.481192	-2.305636	1.236348
31	1	0	-4.042512	-2.062319	0.376957
32	1	0	-2.604267	-2.718337	-0.476941
33	1	0	-4.328425	0.507364	1.154601
34	1	0	-2.814691	0.479001	2.106185
35	1	0	-3.094724	1.775775	0.921269
36	1	0	-0.533367	4.363017	-0.705400
37	1	0	0.230279	3.557072	-2.089622
38	1	0	-1.485737	3.288651	-1.745810
39	1	0	1.039838	1.799903	2.685521
40	1	0	-0.698243	1.809016	2.815814
41	1	0	0.153709	3.325562	2.384316
42	17	0	-0.132311	-0.964077	2.218851

8d

Zero-point correction= 0.349218
(Hartree/Particle)
Thermal correction to Energy= 0.376226
Thermal correction to Enthalpy= 0.377170
Thermal correction to Gibbs Free Energy= 0.293630
Sum of electronic and zero-point Energies= -2131.556469
Sum of electronic and thermal Energies= -2131.529462
Sum of electronic and thermal Enthalpies= -2131.528518
Sum of electronic and thermal Free Energies= -2131.612058

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.026885	0.140822	-0.072507
2	15	0	2.431135	-0.202620	-0.057100
3	6	0	3.321262	-0.196802	-1.675161

4	6	0	3.382290	1.003321	0.968973
5	6	0	2.913414	-1.824988	0.659553
6	17	0	0.206903	-2.075870	-1.469019
7	6	0	-0.023337	1.959263	0.364942
8	6	0	-0.501764	2.149258	-0.986344
9	6	0	0.228794	1.516637	-1.999081
10	15	0	-2.235363	-0.700671	0.126932
11	6	0	-3.211335	-0.769005	-1.435677
12	6	0	-2.328431	-2.417746	0.773404
13	6	0	-3.308323	0.229477	1.308738
14	6	0	-1.849918	2.784328	-1.265464
15	6	0	0.065000	2.896792	1.511510
16	1	0	3.338288	0.804289	-2.116950
17	1	0	4.354801	-0.534475	-1.540334
18	1	0	2.797756	-0.878128	-2.351362
19	1	0	2.952608	1.007923	1.974700
20	1	0	4.441685	0.729238	1.027637
21	1	0	3.297059	2.009213	0.545088
22	1	0	4.004642	-1.928410	0.647343
23	1	0	2.536247	-1.886169	1.682085
24	1	0	2.448294	-2.614703	0.065916
25	1	0	1.307464	1.548036	-2.024323
26	1	0	-0.255523	1.299475	-2.948339
27	1	0	-2.639135	-1.355605	-2.159775
28	1	0	-4.188440	-1.236862	-1.270724
29	1	0	-3.361017	0.237916	-1.835680
30	1	0	-1.835867	-2.447692	1.747714
31	1	0	-3.376082	-2.727177	0.864904
32	1	0	-1.792313	-3.076829	0.088086
33	1	0	-4.274818	-0.270177	1.439739
34	1	0	-2.786671	0.273155	2.268930
35	1	0	-3.483735	1.249817	0.956060
36	1	0	-2.533069	2.725109	-0.413578
37	1	0	-1.700562	3.847454	-1.496558
38	1	0	-2.327365	2.327539	-2.138328
39	1	0	0.169826	2.354403	2.453755
40	1	0	-0.824612	3.542664	1.553877
41	1	0	0.927466	3.567964	1.384541
42	17	0	0.178840	-0.582835	2.315257

9b

Zero-point correction= 0.317651
(Hartree/Particle)
Thermal correction to Energy= 0.343890
Thermal correction to Enthalpy= 0.344835
Thermal correction to Gibbs Free Energy= 0.263114
Sum of electronic and zero-point Energies= -2092.214734
Sum of electronic and thermal Energies= -2092.188494
Sum of electronic and thermal Enthalpies= -2092.187550
Sum of electronic and thermal Free Energies= -2092.269271

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.023611	-0.089762	-0.356357
2	15	0	2.392744	-0.237643	-0.020387
3	6	0	3.172365	-1.624138	-0.955692

4	6	0	3.480696	1.190043	-0.472924
5	6	0	2.872240	-0.590659	1.717253
6	6	0	0.095869	-0.890195	-2.042200
7	15	0	-2.434098	-0.138616	-0.027006
8	6	0	-3.406761	-0.872976	-1.417920
9	6	0	-2.992493	-1.114289	1.424999
10	6	0	-3.225096	1.506946	0.226191
11	1	0	3.119549	-1.424840	-2.030790
12	1	0	4.221148	-1.750912	-0.664466
13	1	0	2.616075	-2.538719	-0.735920
14	1	0	3.291901	2.026752	0.204207
15	1	0	4.536279	0.907246	-0.390989
16	1	0	3.275941	1.513709	-1.497953
17	1	0	3.958742	-0.712109	1.796608
18	1	0	2.526319	0.220675	2.360662
19	1	0	2.362899	-1.505332	2.029749
20	1	0	0.046707	-0.392548	-3.022347
21	1	0	0.238937	-1.973903	-2.127706
22	1	0	-3.069593	-1.901513	-1.577689
23	1	0	-4.480113	-0.877579	-1.196703
24	1	0	-3.236091	-0.305505	-2.338354
25	1	0	-2.525000	-0.697123	2.319553
26	1	0	-4.084614	-1.075997	1.509302
27	1	0	-2.654245	-2.146302	1.312798
28	1	0	-4.293693	1.395693	0.441281
29	1	0	-2.726610	1.992026	1.069525
30	1	0	-3.098070	2.130758	-0.662756
31	17	0	0.027795	-2.404927	0.517032
32	6	0	0.153327	2.372898	-0.777227
33	6	0	-0.405029	1.716629	-1.660064
34	6	0	0.705333	3.387147	0.120244
35	1	0	-0.894313	1.585284	-2.605274
36	1	0	0.129257	4.314738	0.010852
37	1	0	0.632458	3.049303	1.159242
38	1	0	1.750596	3.609243	-0.121051
39	17	0	-0.185911	0.855629	2.081374

TS(9-10)b

Zero-point correction= 0.316129
(Hartree/Particle)
Thermal correction to Energy= 0.342245
Thermal correction to Enthalpy= 0.343189
Thermal correction to Gibbs Free Energy= 0.261351
Sum of electronic and zero-point Energies= -2092.201113
Sum of electronic and thermal Energies= -2092.174997
Sum of electronic and thermal Enthalpies= -2092.174053
Sum of electronic and thermal Free Energies= -2092.255891

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.001312	-0.072957	-0.274457
2	15	0	2.412143	-0.181798	-0.084156
3	6	0	3.210950	-1.472195	-1.140205
4	6	0	3.415583	1.323253	-0.489421
5	6	0	2.997637	-0.627132	1.600945
6	17	0	0.075525	-2.404193	0.505361
7	6	0	0.068367	2.237320	-0.578018

8	6	0	-0.096549	1.824535	-1.737993
9	6	0	0.047095	-0.534236	-2.105284
10	15	0	-2.417123	-0.184348	-0.119056
11	6	0	-3.351777	-0.819929	-1.588490
12	6	0	-3.045730	-1.252512	1.239254
13	6	0	-3.258714	1.427061	0.215007
14	6	0	0.227705	3.260446	0.468355
15	1	0	3.106008	-1.225308	-2.201861
16	1	0	4.277547	-1.566972	-0.908120
17	1	0	2.707251	-2.424255	-0.950991
18	1	0	3.166781	2.131929	0.204222
19	1	0	4.488489	1.114546	-0.411310
20	1	0	3.191655	1.663957	-1.505213
21	1	0	4.091314	-0.691761	1.632775
22	1	0	2.634259	0.115630	2.314673
23	1	0	2.553146	-1.588347	1.870682
24	1	0	-0.266689	1.844609	-2.794549
25	1	0	0.950053	-0.559264	-2.731261
26	1	0	-0.842161	-0.777316	-2.702829
27	1	0	-3.006574	-1.830907	-1.827788
28	1	0	-4.427502	-0.855469	-1.384687
29	1	0	-3.185753	-0.179756	-2.461887
30	1	0	-2.602288	-0.905257	2.175524
31	1	0	-4.139484	-1.207855	1.293553
32	1	0	-2.715711	-2.279878	1.071616
33	1	0	-4.345243	1.302780	0.284381
34	1	0	-2.878775	1.815916	1.164032
35	1	0	-3.029692	2.146371	-0.577254
36	1	0	0.376608	4.243263	0.004865
37	1	0	-0.656832	3.284540	1.109072
38	1	0	1.067481	3.023771	1.125344
39	17	0	-0.173692	0.634056	2.202075

10b

Zero-point correction= 0.321282
(Hartree/Particle)
Thermal correction to Energy= 0.346594
Thermal correction to Enthalpy= 0.347538
Thermal correction to Gibbs Free Energy= 0.267507
Sum of electronic and zero-point Energies= -2092.268924
Sum of electronic and thermal Energies= -2092.243612
Sum of electronic and thermal Enthalpies= -2092.242668
Sum of electronic and thermal Free Energies= -2092.322699

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.012076	0.169175	-0.199543
2	15	0	2.363678	-0.273729	0.083915
3	6	0	3.298186	-0.949619	-1.357192
4	6	0	3.363471	1.185468	0.616697
5	6	0	2.696746	-1.509189	1.402871
6	17	0	-0.008438	-2.428178	-0.511024
7	6	0	0.009839	2.007977	-0.529500
8	6	0	-0.421297	1.587097	-1.843986
9	6	0	0.306817	0.599184	-2.510349
10	15	0	-2.356073	-0.296908	0.098710

11	6	0	-3.212366	-0.923501	-1.407522
12	6	0	-2.726930	-1.547423	1.388676
13	6	0	-3.354759	1.166101	0.621687
14	6	0	0.095920	3.338321	0.115009
15	1	0	3.392091	-0.203137	-2.151921
16	1	0	4.303078	-1.260860	-1.051276
17	1	0	2.748313	-1.813232	-1.741597
18	1	0	2.898494	1.607167	1.512440
19	1	0	4.397201	0.901325	0.843828
20	1	0	3.367533	1.947836	-0.169000
21	1	0	3.777143	-1.650994	1.521245
22	1	0	2.253624	-1.154510	2.335577
23	1	0	2.215639	-2.448930	1.123715
24	1	0	-1.442723	1.811335	-2.167630
25	1	0	1.387220	0.614295	-2.535155
26	1	0	-0.177413	0.001568	-3.277163
27	1	0	-2.684253	-1.820464	-1.742560
28	1	0	-4.260054	-1.166498	-1.197509
29	1	0	-3.174970	-0.173763	-2.204536
30	1	0	-2.306163	-1.202288	2.335737
31	1	0	-3.809836	-1.689208	1.479502
32	1	0	-2.239074	-2.483773	1.110321
33	1	0	-4.400928	0.892567	0.799303
34	1	0	-2.919355	1.560043	1.544508
35	1	0	-3.319293	1.947023	-0.145039
36	1	0	0.956759	3.895010	-0.283867
37	1	0	-0.794957	3.938987	-0.123072
38	1	0	0.196978	3.243831	1.198550
39	17	0	-0.008124	0.433827	2.278541

9c

Zero-point correction= 0.375008
(Hartree/Particle)
Thermal correction to Energy= 0.403791
Thermal correction to Enthalpy= 0.404735
Thermal correction to Gibbs Free Energy= 0.318005
Sum of electronic and zero-point Energies= -2170.782636
Sum of electronic and thermal Energies= -2170.753853
Sum of electronic and thermal Enthalpies= -2170.752909
Sum of electronic and thermal Free Energies= -2170.839639

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.187299	-0.363804	-0.351867
2	15	0	2.041926	-1.290594	0.050228
3	6	0	2.333068	-2.881813	-0.837952
4	6	0	3.554957	-0.331720	-0.412773
5	6	0	2.341103	-1.731750	1.808297
6	17	0	-0.894265	-2.575905	0.513040
7	6	0	-0.247844	-1.169360	-2.038721
8	15	0	-2.514343	0.301868	-0.099467
9	6	0	-3.611717	-0.188147	-1.504908
10	6	0	-3.368286	-0.415214	1.359494
11	6	0	-2.830242	2.110154	0.073881
12	1	0	2.370063	-2.702032	-1.917330
13	1	0	3.275747	-3.339669	-0.517782
14	1	0	1.501673	-3.556035	-0.618632

15	1	0	3.638014	0.568507	0.200548
16	1	0	4.453116	-0.941073	-0.261123
17	1	0	3.499467	-0.033727	-1.464141
18	1	0	3.325895	-2.199208	1.923781
19	1	0	2.264088	-0.834751	2.426120
20	1	0	1.553594	-2.420948	2.122493
21	1	0	-0.102453	-0.679136	-3.012953
22	1	0	-0.428735	-2.246837	-2.131953
23	1	0	-3.566064	-1.274950	-1.621919
24	1	0	-4.650458	0.110940	-1.324424
25	1	0	-3.264593	0.275573	-2.433798
26	1	0	-2.808274	-0.136695	2.254763
27	1	0	-4.396718	-0.040407	1.417172
28	1	0	-3.362773	-1.503632	1.277407
29	1	0	-3.901180	2.302929	0.203175
30	1	0	-2.284999	2.468196	0.950673
31	1	0	-2.469393	2.650805	-0.805074
32	6	0	0.760518	1.870327	-0.742941
33	6	0	0.015260	1.480719	-1.647838
34	6	0	1.642321	2.701923	0.104582
35	6	0	0.829274	3.812280	0.803378
36	6	0	2.774652	3.306582	-0.754369
37	1	0	-0.505334	1.527820	-2.583464
38	1	0	2.067588	2.071747	0.891736
39	1	0	0.079344	3.369765	1.461441
40	1	0	0.335737	4.457664	0.067411
41	1	0	1.502959	4.432271	1.406197
42	1	0	2.364381	3.973662	-1.520758
43	1	0	3.364600	2.535379	-1.258348
44	1	0	3.446716	3.894124	-0.118472
45	17	0	-0.113557	0.618499	2.072090

TS(9-10)c

Zero-point correction= 0.373636
(Hartree/Particle)
Thermal correction to Energy= 0.402103
Thermal correction to Enthalpy= 0.403047
Thermal correction to Gibbs Free Energy= 0.316441
Sum of electronic and zero-point Energies= -2170.769097
Sum of electronic and thermal Energies= -2170.740630
Sum of electronic and thermal Enthalpies= -2170.739686
Sum of electronic and thermal Free Energies= -2170.826292

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.091444	-0.360104	-0.263437
2	15	0	2.248221	-0.979850	-0.049704
3	6	0	2.726642	-2.441008	-1.077202
4	6	0	3.571811	0.244569	-0.476823
5	6	0	2.723673	-1.512295	1.645492
6	17	0	-0.531305	-2.616015	0.615647
7	6	0	-0.107382	-0.851663	-2.090510
8	15	0	-2.499375	-0.094474	-0.158567
9	6	0	-3.452361	-1.190046	-1.306411
10	6	0	-3.238615	-0.505905	1.474053
11	6	0	-3.221658	1.570802	-0.524276
12	1	0	2.670561	-2.199975	-2.143720

13	1	0	3.746167	-2.769613	-0.847242
14	1	0	2.023037	-3.250934	-0.864842
15	1	0	3.512271	1.098712	0.204071
16	1	0	4.567647	-0.204238	-0.389011
17	1	0	3.435931	0.609624	-1.499853
18	1	0	3.773044	-1.827683	1.675643
19	1	0	2.549054	-0.687928	2.340267
20	1	0	2.072061	-2.338040	1.941382
21	1	0	0.787621	-0.992936	-2.711550
22	1	0	-1.016276	-0.983799	-2.693810
23	1	0	-3.131203	-2.223275	-1.145091
24	1	0	-4.529005	-1.111459	-1.119455
25	1	0	-3.262668	-0.922976	-2.351466
26	1	0	-2.808879	0.151294	2.232751
27	1	0	-4.329104	-0.399765	1.441661
28	1	0	-2.965356	-1.532631	1.728548
29	1	0	-4.313836	1.553822	-0.436663
30	1	0	-2.819103	2.302905	0.181063
31	1	0	-2.951520	1.889352	-1.536047
32	6	0	0.477702	1.844668	-0.678460
33	6	0	0.114758	1.441791	-1.801859
34	6	0	0.972773	2.910427	0.235018
35	6	0	-0.202058	3.726772	0.810116
36	6	0	1.969780	3.818210	-0.513377
37	1	0	-0.183201	1.503487	-2.829215
38	1	0	1.468058	2.426431	1.082601
39	1	0	-0.851731	3.082478	1.406081
40	1	0	-0.782341	4.201028	0.009815
41	1	0	0.190792	4.515177	1.462160
42	1	0	1.477532	4.343698	-1.339891
43	1	0	2.808642	3.247968	-0.924538
44	1	0	2.372016	4.570421	0.174949
45	17	0	-0.041034	0.473095	2.178007

10c

Zero-point correction= 0.378620
(Hartree/Particle)
Thermal correction to Energy= 0.406696
Thermal correction to Enthalpy= 0.407640
Thermal correction to Gibbs Free Energy= 0.321319
Sum of electronic and zero-point Energies= -2170.836427
Sum of electronic and thermal Energies= -2170.808352
Sum of electronic and thermal Enthalpies= -2170.807407
Sum of electronic and thermal Free Energies= -2170.893729

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.042365	-0.125518	-0.168632
2	15	0	2.246229	-0.906624	0.113027
3	6	0	3.096745	-1.622343	-1.361229
4	6	0	3.460216	0.333629	0.747642
5	6	0	2.378100	-2.251307	1.359940
6	6	0	0.333800	0.363723	-2.450534
7	15	0	-2.441191	-0.327842	0.028336
8	6	0	-3.289764	-0.807926	-1.536175
9	6	0	-3.003686	-1.575800	1.251307
10	6	0	-3.332855	1.198786	0.564826

11	1	0	3.314736	-0.848054	-2.103460
12	1	0	4.039463	-2.095861	-1.065377
13	1	0	2.436168	-2.370672	-1.807558
14	1	0	3.061775	0.767069	1.669567
15	1	0	4.426527	-0.137369	0.960555
16	1	0	3.608755	1.133547	0.016097
17	1	0	3.427422	-2.543280	1.484540
18	1	0	1.967159	-1.890316	2.304985
19	1	0	1.781792	-3.101004	1.022445
20	1	0	1.402686	0.210572	-2.491490
21	1	0	-0.244309	-0.111371	-3.237733
22	1	0	-2.849575	-1.747471	-1.880589
23	1	0	-4.366339	-0.937492	-1.378210
24	1	0	-3.133599	-0.042283	-2.303047
25	1	0	-2.591497	-1.313713	2.228309
26	1	0	-4.098833	-1.599342	1.291128
27	1	0	-2.609559	-2.550175	0.956549
28	1	0	-4.409383	1.013440	0.651791
29	1	0	-2.938961	1.501671	1.539090
30	1	0	-3.170174	2.011699	-0.149041
31	17	0	-0.362386	-2.679008	-0.632927
32	6	0	0.296739	1.701263	-0.402531
33	6	0	-0.223661	1.420349	-1.725514
34	6	0	0.694279	2.969342	0.273570
35	6	0	-0.554676	3.851292	0.512343
36	6	0	1.752457	3.737882	-0.544231
37	1	0	-1.199966	1.816186	-2.020245
38	1	0	1.103682	2.707377	1.255051
39	1	0	-1.272099	3.343939	1.161829
40	1	0	-1.050194	4.109539	-0.431467
41	1	0	-0.251908	4.785859	0.997952
42	1	0	1.347878	4.048938	-1.514445
43	1	0	2.643655	3.129281	-0.730016
44	1	0	2.066846	4.636022	-0.000404
45	17	0	-0.067015	-0.015127	2.323285

11

Zero-point correction= 0.296561
(Hartree/Particle)
Thermal correction to Energy= 0.319201
Thermal correction to Enthalpy= 0.320145
Thermal correction to Gibbs Free Energy= 0.244156
Sum of electronic and zero-point Energies= -1820.507054
Sum of electronic and thermal Energies= -1820.484415
Sum of electronic and thermal Enthalpies= -1820.483471
Sum of electronic and thermal Free Energies= -1820.559459

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.360932	-2.241255	-1.039947
2	6	0	0.263070	-0.721582	-1.795373
3	17	0	0.122488	-1.745188	1.527198
4	44	0	0.235932	0.007821	-0.125082
5	15	0	2.667260	-0.101162	0.042837
6	6	0	3.408648	-1.793089	0.041228
7	6	0	3.660252	0.787010	-1.236300
8	6	0	3.281186	0.622875	1.626686

9	6	0	-1.886250	0.051428	-0.085845
10	6	0	-4.093691	0.671951	0.456017
11	7	0	-2.668856	1.028694	0.427825
12	7	0	-2.709251	-0.928109	-0.530326
13	6	0	-4.132946	-0.584026	-0.418985
14	6	0	-2.247796	2.128300	1.277287
15	1	0	-2.995914	-2.989511	-0.550103
16	1	0	-1.323386	-2.465768	-0.802258
17	1	0	-2.523823	-2.312049	-2.124546
18	1	0	1.163309	-1.133007	-2.270218
19	1	0	-0.626712	-0.741572	-2.434405
20	1	0	3.222586	-2.274118	-0.924917
21	1	0	4.489485	-1.762741	0.218635
22	1	0	2.919728	-2.388912	0.816579
23	1	0	3.334911	1.829889	-1.270408
24	1	0	4.733665	0.735852	-1.022193
25	1	0	3.472921	0.343049	-2.219635
26	1	0	4.372143	0.556712	1.708818
27	1	0	2.978171	1.673306	1.677337
28	1	0	2.821751	0.086724	2.462730
29	1	0	-4.706359	1.490805	0.064892
30	1	0	-4.409590	0.473577	1.490655
31	1	0	-4.558042	-0.390676	-1.413782
32	1	0	-4.693938	-1.408087	0.035010
33	1	0	-1.188797	2.327317	1.133155
34	1	0	-2.804973	3.033354	1.009444
35	1	0	-2.449846	1.893564	2.332848
36	17	0	0.505764	2.354706	-0.661766

12

Zero-point correction= 0.181056
(Hartree/Particle)
Thermal correction to Energy= 0.195533
Thermal correction to Enthalpy= 0.196477
Thermal correction to Gibbs Free Energy= 0.138402
Sum of electronic and zero-point Energies= -1359.493552
Sum of electronic and thermal Energies= -1359.479075
Sum of electronic and thermal Enthalpies= -1359.478131
Sum of electronic and thermal Free Energies= -1359.536206

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.720657	-1.849829	1.642099
2	44	0	1.045916	-0.225472	-0.038248
3	6	0	1.118417	-1.058002	-1.644296
4	6	0	-0.885071	0.177475	-0.102847
5	6	0	-2.924427	1.251635	0.312011
6	7	0	-1.459130	1.336063	0.310027
7	7	0	-1.868732	-0.652383	-0.528088
8	6	0	-3.181271	0.003627	-0.537404
9	17	0	2.065848	1.840866	-0.583077
10	6	0	-0.849653	2.372913	1.128469
11	6	0	-1.778828	-2.035779	-0.962027
12	1	0	0.324305	-1.098836	-2.395245
13	1	0	2.070663	-1.531154	-1.927926
14	1	0	-3.363788	2.159896	-0.111407
15	1	0	-3.291640	1.138168	1.342511

16	1	0	-3.476535	0.251236	-1.566587
17	1	0	-3.943152	-0.656955	-0.111908
18	1	0	-1.059309	2.197082	2.193334
19	1	0	0.224783	2.403983	0.960070
20	1	0	-1.268919	3.343579	0.843833
21	1	0	-0.836070	-2.466783	-0.631775
22	1	0	-2.597392	-2.599162	-0.499698
23	1	0	-1.873824	-2.124891	-2.052673

13a

Zero-point correction= 0.210979
(Hartree/Particle)
Thermal correction to Energy= 0.228383
Thermal correction to Enthalpy= 0.229328
Thermal correction to Gibbs Free Energy= 0.165605
Sum of electronic and zero-point Energies= -1436.807106
Sum of electronic and thermal Energies= -1436.789701
Sum of electronic and thermal Enthalpies= -1436.788757
Sum of electronic and thermal Free Energies= -1436.852480

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.532217	2.262202	-1.025470
2	44	0	0.956026	0.077918	0.072170
3	6	0	1.184953	0.925347	1.662749
4	6	0	-1.120245	-0.057760	-0.024217
5	6	0	-3.115923	-0.951768	-0.831292
6	7	0	-1.660183	-0.830383	-0.982924
7	7	0	-2.104422	0.510688	0.688417
8	6	0	-3.425828	0.221997	0.104727
9	6	0	-0.933225	-1.775586	-1.814107
10	6	0	-1.987664	1.621269	1.612723
11	17	0	0.738199	-2.083855	1.278928
12	1	0	1.321493	0.350510	2.583557
13	1	0	1.291702	2.013661	1.704024
14	1	0	-3.365533	-1.921476	-0.378198
15	1	0	-3.618132	-0.877510	-1.800270
16	1	0	-4.149349	-0.026783	0.886255
17	1	0	-3.788058	1.104089	-0.441552
18	1	0	-0.819149	-2.744552	-1.314838
19	1	0	0.059117	-1.382369	-2.048046
20	1	0	-1.473491	-1.901685	-2.757661
21	1	0	-2.119316	2.579391	1.094473
22	1	0	-1.001272	1.604341	2.072985
23	1	0	-2.749374	1.518324	2.392349
24	6	0	2.755903	0.243006	-1.104130
25	6	0	2.802435	-0.862155	-0.528843
26	1	0	3.007857	1.097099	-1.702775
27	1	0	3.131063	-1.821592	-0.178667

TS(13-14)a

Zero-point correction= 0.209240
(Hartree/Particle)
Thermal correction to Energy= 0.226748
Thermal correction to Enthalpy= 0.227692
Thermal correction to Gibbs Free Energy= 0.162426
Sum of electronic and zero-point Energies= -1436.787501

Sum of electronic and thermal Energies= -1436.769993
Sum of electronic and thermal Enthalpies= -1436.769048
Sum of electronic and thermal Free Energies= -1436.834315

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.871503	-2.113582	-1.222278
2	44	0	-0.825290	-0.005062	0.003777
3	6	0	-1.533772	-0.767052	1.519956
4	6	0	1.206433	-0.052779	-0.004150
5	6	0	3.316240	0.618045	-0.734070
6	7	0	1.880712	0.516628	-1.022735
7	7	0	2.088637	-0.538889	0.885157
8	6	0	3.471429	-0.405682	0.398369
9	6	0	-3.268209	0.021579	0.104874
10	6	0	-2.757408	0.605386	-0.860206
11	6	0	1.257167	1.348052	-2.037727
12	6	0	1.811087	-1.438625	1.985960
13	17	0	-0.670706	2.221555	1.014472
14	1	0	-1.734139	-0.167678	2.415288
15	1	0	-1.783477	-1.833651	1.556008
16	1	0	3.566940	1.636854	-0.405969
17	1	0	3.912852	0.376689	-1.618747
18	1	0	4.134085	-0.065266	1.199487
19	1	0	3.833470	-1.376976	0.032306
20	1	0	-3.950402	-0.416516	0.801591
21	1	0	-2.752990	1.176768	-1.768064
22	1	0	1.089502	2.370998	-1.679863
23	1	0	0.300663	0.903451	-2.332362
24	1	0	1.895003	1.364292	-2.926772
25	1	0	2.034462	-2.478400	1.711165
26	1	0	0.759182	-1.362629	2.256420
27	1	0	2.421915	-1.158458	2.851041

14a

Zero-point correction= 0.214905
(Hartree/Particle)
Thermal correction to Energy= 0.231906
Thermal correction to Enthalpy= 0.232851
Thermal correction to Gibbs Free Energy= 0.168345
Sum of electronic and zero-point Energies= -1436.867412
Sum of electronic and thermal Energies= -1436.850410
Sum of electronic and thermal Enthalpies= -1436.849466
Sum of electronic and thermal Free Energies= -1436.913972

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.705930	2.590674	-0.545495
2	44	0	0.690173	0.344508	0.227374
3	6	0	3.690812	-0.885576	-0.434154
4	6	0	-1.181325	-0.166834	-0.105800
5	6	0	-3.088979	-1.415579	-0.661972
6	7	0	-1.621738	-1.336739	-0.647483
7	7	0	-2.261326	0.596994	0.178544
8	6	0	-3.506325	0.021757	-0.336501
9	6	0	2.810430	-0.655621	-1.430004

10	6	0	1.376635	-0.501477	-1.250446
11	6	0	-0.901738	-2.599553	-0.735623
12	6	0	-2.298249	1.943785	0.721277
13	17	0	0.912262	-1.172364	2.032231
14	1	0	3.363357	-1.018528	0.593858
15	1	0	4.753306	-0.982290	-0.638360
16	1	0	-3.426369	-2.129735	0.102805
17	1	0	-3.454530	-1.760023	-1.634765
18	1	0	-4.301782	0.080497	0.413666
19	1	0	-3.833951	0.575722	-1.227532
20	1	0	3.175973	-0.590200	-2.457724
21	1	0	0.739137	-0.792138	-2.093456
22	1	0	-1.407062	-3.347907	-0.111059
23	1	0	0.114093	-2.482019	-0.366791
24	1	0	-0.887041	-2.964634	-1.769766
25	1	0	-2.543650	2.676501	-0.056844
26	1	0	-1.332346	2.212798	1.141982
27	1	0	-3.062142	1.985123	1.506902

13b

Zero-point correction= 0.239592
(Hartree/Particle)
Thermal correction to Energy= 0.258742
Thermal correction to Enthalpy= 0.259686
Thermal correction to Gibbs Free Energy= 0.191825
Sum of electronic and zero-point Energies= -1476.103115
Sum of electronic and thermal Energies= -1476.083964
Sum of electronic and thermal Enthalpies= -1476.083020
Sum of electronic and thermal Free Energies= -1476.150881

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.740563	-2.237913	0.461145
2	44	0	-0.753679	0.134416	-0.262965
3	6	0	-2.473015	1.278718	0.256403
4	17	0	-0.036410	2.385459	-1.051808
5	6	0	-2.768503	0.124262	0.638023
6	6	0	-0.876149	-0.411885	-1.991811
7	6	0	-3.578396	-0.971596	1.193057
8	1	0	-2.570945	2.325230	0.038454
9	1	0	-0.811751	0.312659	-2.808882
10	1	0	-1.116514	-1.452032	-2.232512
11	1	0	-4.512602	-0.569754	1.603044
12	1	0	-3.812444	-1.702433	0.412706
13	1	0	-3.032201	-1.509563	1.971787
14	6	0	1.284494	-0.067401	0.114125
15	6	0	3.526819	-0.673391	0.224150
16	7	0	2.279962	-0.661361	-0.560079
17	7	0	1.774986	0.457444	1.252143
18	6	0	3.241164	0.382621	1.297398
19	6	0	2.156175	-1.577020	-1.677469
20	6	0	1.068859	1.385510	2.119955
21	1	0	4.385334	-0.428669	-0.407768
22	1	0	3.681623	-1.671877	0.656675
23	1	0	3.673956	1.360576	1.043152
24	1	0	3.588485	0.093018	2.293461
25	1	0	2.039920	-2.610899	-1.329510

26	1	0	1.284859	-1.305751	-2.271684
27	1	0	3.052575	-1.497608	-2.300864
28	1	0	0.008705	1.123944	2.164569
29	1	0	1.478579	1.302295	3.131530
30	1	0	1.159516	2.416788	1.760107

TS(13-14)b

Zero-point correction= 0.238492
(Hartree/Particle)
Thermal correction to Energy= 0.257535
Thermal correction to Enthalpy= 0.258479
Thermal correction to Gibbs Free Energy= 0.189217
Sum of electronic and zero-point Energies= -1476.082863
Sum of electronic and thermal Energies= -1476.063820
Sum of electronic and thermal Enthalpies= -1476.062876
Sum of electronic and thermal Free Energies= -1476.132138

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.407838	-1.987162	-1.362616
2	44	0	0.594076	0.079716	-0.061305
3	6	0	2.325397	0.693419	-1.137601
4	17	0	0.645035	2.231672	1.112408
5	6	0	3.027547	0.070273	-0.308002
6	6	0	1.592328	-0.734087	1.258786
7	6	0	4.255552	-0.498810	0.277467
8	1	0	2.256188	1.303164	-2.020083
9	1	0	1.931088	-0.175102	2.136712
10	1	0	1.824868	-1.802868	1.211145
11	1	0	5.107053	-0.172620	-0.331470
12	1	0	4.417480	-0.157212	1.305115
13	1	0	4.231491	-1.593589	0.272285
14	6	0	-1.441771	0.027692	0.113924
15	6	0	-3.608647	-0.740834	0.480984
16	7	0	-2.194661	-0.774523	0.888500
17	7	0	-2.243733	0.768997	-0.666282
18	6	0	-3.666777	0.507311	-0.413715
19	6	0	-1.709701	-1.908465	1.655983
20	6	0	-1.831627	1.865381	-1.524912
21	1	0	-4.264762	-0.674933	1.354359
22	1	0	-3.856831	-1.656765	-0.072968
23	1	0	-4.116792	1.370312	0.095987
24	1	0	-4.208482	0.336999	-1.349622
25	1	0	-1.610318	-2.801355	1.026573
26	1	0	-0.735483	-1.667262	2.080205
27	1	0	-2.411094	-2.106815	2.472697
28	1	0	-0.813668	2.168409	-1.269408
29	1	0	-1.891214	1.582905	-2.583066
30	1	0	-2.482756	2.729972	-1.350502

14b

Zero-point correction= 0.243337
(Hartree/Particle)
Thermal correction to Energy= 0.261669

```
 Thermal correction to Enthalpy=                  0.262613
 Thermal correction to Gibbs Free Energy=         0.195350
 Sum of electronic and zero-point Energies=          -1476.156200
 Sum of electronic and thermal Energies=             -1476.137868
 Sum of electronic and thermal Enthalpies=           -1476.136924
 Sum of electronic and thermal Free Energies=        -1476.204187

 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1         17             0        0.295799   -0.752077    2.419911
    2         44             0        0.439107    0.449454    0.384614
    3          6             0        1.416265   -0.552498   -0.801260
    4         17             0        0.609191    2.571136   -0.678045
    5          6             0        2.879311   -0.570351   -0.762128
    6          6             0        3.597138    0.547684   -0.523290
    7          6             0        3.537831   -1.912888   -1.016206
    8          1             0        0.944005   -1.218402   -1.532611
    9          1             0        3.122215    1.516052   -0.400182
   10          1             0        4.683525    0.517802   -0.496065
   11          1             0        3.231408   -2.322336   -1.987633
   12          1             0        4.628477   -1.825274   -1.011291
   13          1             0        3.251998   -2.644417   -0.250477
   14          6             0       -1.330219   -0.200423   -0.203122
   15          6             0       -3.635210   -0.239470   -0.631033
   16          7             0       -2.438591    0.567718   -0.367856
   17          7             0       -1.667621   -1.484385   -0.485878
   18          6             0       -3.037177   -1.600040   -0.998602
   19          6             0       -2.645555    1.923084    0.117273
   20          6             0       -0.877152   -2.693388   -0.337974
   21          1             0       -4.229750    0.202595   -1.436393
   22          1             0       -4.260795   -0.288502    0.272483
   23          1             0       -3.025593   -1.772590   -2.084000
   24          1             0       -3.555162   -2.439646   -0.524221
   25          1             0       -3.140929    1.909369    1.099025
   26          1             0       -1.695649    2.448625    0.185929
   27          1             0       -3.284884    2.462258   -0.589837
   28          1             0       -0.018429   -2.497090    0.300463
   29          1             0       -1.496092   -3.458529    0.145006
   30          1             0       -0.547789   -3.083483   -1.310765
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15b

```
Zero-point correction=                           0.239350
(Hartree/Particle)
 Thermal correction to Energy=                    0.258766
 Thermal correction to Enthalpy=                  0.259710
 Thermal correction to Gibbs Free Energy=         0.190836
 Sum of electronic and zero-point Energies=          -1476.102244
 Sum of electronic and thermal Energies=             -1476.082828
 Sum of electronic and thermal Enthalpies=           -1476.081884
 Sum of electronic and thermal Free Energies=        -1476.150758

 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1         17             0       -0.147141    2.379679   -1.026350
    2         44             0        0.725182    0.323287    0.070850
```

3	6	0	0.771671	1.200138	1.659842
4	6	0	-1.282325	-0.232592	-0.023711
5	6	0	-3.125501	-1.300387	-0.979191
6	7	0	-1.664480	-1.183902	-0.894268
7	7	0	-2.361085	0.231929	0.617099
8	6	0	-3.577398	-0.518100	0.263371
9	6	0	2.416261	0.878597	-1.116708
10	6	0	2.812808	-0.150476	-0.529717
11	17	0	0.927672	-1.821449	1.304384
12	1	0	1.007142	0.666458	2.585468
13	1	0	0.658674	2.287538	1.701593
14	1	0	-3.431254	-2.351020	-0.959998
15	1	0	-3.488436	-0.847603	-1.912499
16	1	0	-3.866156	-1.181253	1.089901
17	1	0	-4.406657	0.165495	0.059337
18	1	0	2.422484	1.757972	-1.731791
19	6	0	-0.813902	-1.824286	-1.879169
20	1	0	-0.827281	-1.286215	-2.836481
21	1	0	0.207033	-1.878407	-1.495352
22	1	0	-1.162102	-2.849545	-2.041764
23	6	0	-2.386230	1.239506	1.662437
24	1	0	-1.727338	2.062825	1.385403
25	1	0	-3.407260	1.623763	1.742798
26	1	0	-2.088310	0.825154	2.633398
27	6	0	3.724187	-1.219260	-0.092384
28	1	0	3.282551	-2.205971	-0.251988
29	1	0	4.670470	-1.143524	-0.641180
30	1	0	3.920935	-1.135246	0.980725

TS(15-16)b

Zero-point correction= 0.238248
(Hartree/Particle)
Thermal correction to Energy= 0.257363
Thermal correction to Enthalpy= 0.258308
Thermal correction to Gibbs Free Energy= 0.189350
Sum of electronic and zero-point Energies= -1476.085589
Sum of electronic and thermal Energies= -1476.066474
Sum of electronic and thermal Enthalpies= -1476.065530
Sum of electronic and thermal Free Energies= -1476.134487

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.515517	-1.877534	1.591085
2	44	0	0.657205	-0.170136	-0.152939
3	6	0	1.097673	-1.377255	-1.467998
4	6	0	-1.359521	0.102687	0.012295
5	6	0	-3.364291	1.043090	0.748265
6	7	0	-1.917531	1.203874	0.555103
7	7	0	-2.339179	-0.748072	-0.338610
8	6	0	-3.669917	-0.145228	-0.173609
9	6	0	3.010073	-0.605920	-0.433236
10	6	0	2.764602	0.247227	0.435127
11	17	0	0.800179	1.715901	-1.713286
12	1	0	1.285936	-1.050883	-2.496612
13	1	0	1.185808	-2.449083	-1.256706
14	1	0	-3.896708	1.956124	0.465535

15	1	0	-3.587228	0.818967	1.801473
16	1	0	-4.067682	0.177448	-1.146249
17	1	0	-4.367704	-0.862905	0.267520
18	1	0	3.562559	-1.272831	-1.060885
19	6	0	-1.194100	2.274814	1.215089
20	1	0	-1.029658	2.059539	2.280351
21	1	0	-0.241445	2.428583	0.702611
22	1	0	-1.771088	3.201064	1.128884
23	6	0	-2.171598	-2.018612	-1.019558
24	1	0	-1.295274	-2.526613	-0.616408
25	1	0	-3.052592	-2.636729	-0.821915
26	1	0	-2.068010	-1.890697	-2.105636
27	6	0	2.998612	1.244258	1.493096
28	1	0	2.469006	0.961090	2.408974
29	1	0	4.069896	1.310219	1.715852
30	1	0	2.648091	2.229471	1.167682

16b

Zero-point correction= 0.243028
(Hartree/Particle)
Thermal correction to Energy= 0.261603
Thermal correction to Enthalpy= 0.262547
Thermal correction to Gibbs Free Energy= 0.195233
Sum of electronic and zero-point Energies= -1476.156757
Sum of electronic and thermal Energies= -1476.138181
Sum of electronic and thermal Enthalpies= -1476.137237
Sum of electronic and thermal Free Energies= -1476.204551

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.383276	-1.223331	2.257031
2	44	0	-0.670508	0.194378	0.371093
3	6	0	-3.726345	0.049663	-0.210978
4	6	0	1.251465	0.003581	-0.077627
5	6	0	3.328950	-0.946017	-0.621040
6	7	0	1.869965	-1.111275	-0.565052
7	7	0	2.193851	0.957939	0.093133
8	6	0	3.497710	0.565042	-0.447971
9	6	0	-2.886936	-0.938916	-0.572825
10	6	0	-1.486055	-0.740911	-0.978156
11	17	0	-1.034291	2.362413	-0.587787
12	1	0	-3.443727	1.095314	-0.293013
13	1	0	-4.727264	-0.176317	0.146468
14	1	0	3.732035	-1.320034	-1.567544
15	1	0	3.795645	-1.511491	0.198670
16	1	0	3.678764	1.079073	-1.402719
17	1	0	4.302947	0.833691	0.243260
18	1	0	-3.224424	-1.977984	-0.516848
19	6	0	1.377929	-2.478594	-0.490699
20	1	0	1.927541	-3.030554	0.283092
21	1	0	0.325529	-2.482409	-0.221745
22	1	0	1.522826	-2.984545	-1.452674
23	6	0	2.024855	2.320425	0.568432
24	1	0	1.078163	2.425271	1.092778
25	1	0	2.846329	2.551110	1.256918
26	1	0	2.035257	3.037103	-0.260638
27	6	0	-1.028255	-1.227125	-2.315950

28	1	0	0.047794	-1.124877	-2.460028
29	1	0	-1.325302	-2.273315	-2.482580
30	1	0	-1.537723	-0.626594	-3.084320

13c

Zero-point correction= 0.296946
(Hartree/Particle)
Thermal correction to Energy= 0.318668
Thermal correction to Enthalpy= 0.319612
Thermal correction to Gibbs Free Energy= 0.245825
Sum of electronic and zero-point Energies= -1554.672513
Sum of electronic and thermal Energies= -1554.650791
Sum of electronic and thermal Enthalpies= -1554.649847
Sum of electronic and thermal Free Energies= -1554.723633

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.575957	-2.086645	-0.465412
2	44	0	0.267188	0.375169	-0.383727
3	6	0	0.147727	0.406216	-2.197023
4	6	0	-1.655771	-0.204292	0.166885
5	6	0	-3.434113	-0.380371	1.662754
6	7	0	-2.006071	-0.102516	1.462380
7	7	0	-2.686652	-0.708468	-0.527469
8	6	0	-3.789032	-1.110134	0.362759
9	6	0	2.401026	0.374651	0.199705
10	6	0	1.938490	1.537715	0.246765
11	6	0	-1.255199	0.607434	2.484751
12	6	0	-2.661017	-1.238528	-1.876270
13	17	0	-0.768096	2.640188	-0.315942
14	6	0	3.437597	-0.684375	0.273093
15	6	0	3.451199	-1.330749	1.672715
16	6	0	4.812048	-0.093726	-0.099046
17	1	0	-0.119581	1.328847	-2.720546
18	1	0	0.444560	-0.464159	-2.790516
19	1	0	-3.986732	0.563541	1.771995
20	1	0	-3.594106	-0.987069	2.558848
21	1	0	-4.754198	-0.808370	-0.053964
22	1	0	-3.784954	-2.202404	0.485426
23	1	0	1.892434	2.603067	0.368342
24	1	0	-1.500390	1.675637	2.492952
25	1	0	-0.182890	0.497453	2.305990
26	1	0	-1.481218	0.162388	3.458974
27	1	0	-2.453000	-2.315749	-1.870187
28	1	0	-1.883027	-0.734464	-2.447191
29	1	0	-3.630844	-1.054731	-2.350332
30	1	0	3.169964	-1.465079	-0.446184
31	1	0	2.483487	-1.789484	1.892461
32	1	0	3.680612	-0.588701	2.446810
33	1	0	4.218921	-2.111827	1.709308
34	1	0	5.116617	0.678298	0.616755
35	1	0	4.795686	0.354340	-1.097990
36	1	0	5.570069	-0.885348	-0.090872

TS(13-14)c

Zero-point correction= 0.296019
(Hartree/Particle)
Thermal correction to Energy= 0.317458
Thermal correction to Enthalpy= 0.318402
Thermal correction to Gibbs Free Energy= 0.244106
Sum of electronic and zero-point Energies= -1554.652296
Sum of electronic and thermal Energies= -1554.630857
Sum of electronic and thermal Enthalpies= -1554.629913
Sum of electronic and thermal Free Energies= -1554.704209

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.333153	-1.995439	-1.285482
2	44	0	-0.135022	0.104699	-0.062537
3	6	0	-1.118027	-0.520149	1.367591
4	6	0	1.889996	-0.122532	0.014855
5	6	0	4.096912	0.369318	-0.541003
6	7	0	2.680425	0.434003	-0.922925
7	7	0	2.657752	-0.754229	0.917283
8	6	0	4.075310	-0.736611	0.522841
9	6	0	-2.559103	0.418480	-0.109727
10	6	0	-1.844899	1.032316	-0.939543
11	6	0	2.211842	1.394121	-1.908226
12	6	0	2.209365	-1.685759	1.932936
13	17	0	0.245624	2.279604	1.028977
14	6	0	-3.841581	-0.105024	0.436982
15	6	0	-4.147657	-1.516606	-0.104175
16	6	0	-4.962220	0.892866	0.075613
17	1	0	-1.324118	0.113203	2.236211
18	1	0	-1.478275	-1.553166	1.396326
19	1	0	4.421866	1.333913	-0.125597
20	1	0	4.725670	0.127516	-1.402945
21	1	0	4.715967	-0.520643	1.382982
22	1	0	4.360378	-1.714862	0.109928
23	1	0	-1.757748	1.729239	-1.752921
24	1	0	2.121731	2.400789	-1.482930
25	1	0	1.236308	1.076214	-2.289924
26	1	0	2.907494	1.404798	-2.752939
27	1	0	2.361996	-2.723761	1.608228
28	1	0	1.148543	-1.526539	2.119673
29	1	0	2.766568	-1.514738	2.860597
30	1	0	-3.776720	-0.155714	1.530930
31	1	0	-3.329385	-2.214103	0.092609
32	1	0	-4.296543	-1.484013	-1.188229
33	1	0	-5.061826	-1.900209	0.363271
34	1	0	-5.070003	0.977034	-1.011246
35	1	0	-4.755740	1.887626	0.481718
36	1	0	-5.914074	0.538916	0.487107

14c

Zero-point correction= 0.299920
(Hartree/Particle)
Thermal correction to Energy= 0.320848
Thermal correction to Enthalpy= 0.321792
Thermal correction to Gibbs Free Energy= 0.248405
Sum of electronic and zero-point Energies= -1554.691178

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 Sum of electronic and thermal Energies=            -1554.670250
 Sum of electronic and thermal Enthalpies=          -1554.669306
 Sum of electronic and thermal Free Energies=       -1554.742693
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.384714	2.052049	-1.170468
2	44	0	0.231417	-0.047758	-0.094869
3	6	0	1.516912	0.136956	1.523270
4	6	0	-1.857732	0.092630	-0.060944
5	6	0	-4.076697	-0.313520	-0.627596
6	7	0	-2.657484	-0.479776	-0.974521
7	7	0	-2.598772	0.806244	0.794075
8	6	0	-4.017996	0.820684	0.408120
9	6	0	2.423948	-0.474045	0.516233
10	6	0	1.729020	-1.223217	-0.389119
11	6	0	-2.249355	-1.515224	-1.906869
12	6	0	-2.096756	1.719793	1.802399
13	17	0	-0.525107	-2.113295	1.128077
14	6	0	3.882385	-0.035197	0.348563
15	6	0	3.998755	1.455848	-0.021973
16	6	0	4.647230	-0.911992	-0.651801
17	1	0	1.182947	-0.512743	2.330018
18	1	0	1.775928	1.147664	1.844159
19	1	0	-4.466984	-1.246946	-0.198027
20	1	0	-4.669468	-0.060779	-1.511665
21	1	0	-4.660292	0.645247	1.276465
22	1	0	-4.276874	1.796339	-0.026273
23	1	0	2.032819	-1.884335	-1.192410
24	1	0	-2.443913	-2.514111	-1.496761
25	1	0	-1.179898	-1.424747	-2.103945
26	1	0	-2.792489	-1.390345	-2.849622
27	1	0	-2.212344	2.762054	1.477943
28	1	0	-1.038730	1.514899	1.964988
29	1	0	-2.644082	1.571636	2.740043
30	1	0	4.342880	-0.170840	1.339015
31	1	0	3.499548	2.101575	0.706337
32	1	0	3.547090	1.650955	-0.999406
33	1	0	5.055615	1.745848	-0.059620
34	1	0	4.263765	-0.778457	-1.670690
35	1	0	4.576646	-1.974954	-0.394970
36	1	0	5.707691	-0.636994	-0.659260

15c

```
Zero-point correction=                           0.296649
(Hartree/Particle)
 Thermal correction to Energy=                    0.318595
 Thermal correction to Enthalpy=                  0.319540
 Thermal correction to Gibbs Free Energy=         0.245046
 Sum of electronic and zero-point Energies=          -1554.671978
 Sum of electronic and thermal Energies=             -1554.650032
 Sum of electronic and thermal Enthalpies=           -1554.649087
 Sum of electronic and thermal Free Energies=        -1554.723581
```

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	17	0	0.738076	2.363264	-1.237094
2	44	0	-0.263173	0.238509	-0.400868
3	6	0	-0.210136	-0.393821	-2.102330
4	6	0	1.691754	-0.131551	0.221925
5	6	0	3.896025	-0.844156	0.485910
6	7	0	2.623689	-0.972661	-0.242713
7	7	0	2.175222	0.505643	1.302561
8	6	0	3.488033	-0.010005	1.710030
9	6	0	2.528953	-1.817908	-1.419800
10	6	0	1.434624	1.405246	2.166425
11	17	0	-0.588191	-2.076564	0.438267
12	1	0	-0.519164	-1.418830	-2.329611
13	1	0	0.040467	0.267986	-2.936131
14	1	0	4.639338	-0.330814	-0.138768
15	1	0	4.288014	-1.830182	0.752535
16	1	0	4.178030	0.813874	1.917170
17	1	0	3.390805	-0.620266	2.618701
18	1	0	2.702641	-1.249744	-2.341974
19	1	0	1.547504	-2.291621	-1.447968
20	1	0	3.289775	-2.600010	-1.340991
21	1	0	0.975796	0.870860	3.009147
22	1	0	0.667381	1.916984	1.582207
23	1	0	2.116114	2.167433	2.558228
24	6	0	-1.914750	1.575828	-0.172802
25	6	0	-2.378936	0.487990	0.235362
26	6	0	-3.407931	-0.456385	0.732308
27	6	0	-4.452895	0.309489	1.567884
28	6	0	-4.055752	-1.207656	-0.447554
29	1	0	-1.860055	2.607298	-0.463803
30	1	0	-2.910776	-1.199590	1.364014
31	1	0	-4.979787	1.050716	0.956296
32	1	0	-3.985744	0.831512	2.409684
33	1	0	-5.193544	-0.391977	1.968940
34	1	0	-3.303056	-1.773397	-1.002839
35	1	0	-4.553401	-0.510216	-1.131395
36	1	0	-4.805100	-1.911572	-0.068271

TS(15-16)c

Zero-point correction= 0.295509
(Hartree/Particle)
Thermal correction to Energy= 0.317290
Thermal correction to Enthalpy= 0.318234
Thermal correction to Gibbs Free Energy= 0.242462
Sum of electronic and zero-point Energies= -1554.655121
Sum of electronic and thermal Energies= -1554.633340
Sum of electronic and thermal Enthalpies= -1554.632396
Sum of electronic and thermal Free Energies= -1554.708168

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.110569	-1.811602	-1.728412
2	44	0	-0.185776	-0.425331	0.283167
3	6	0	-0.163224	-1.875370	1.413552
4	6	0	1.687557	0.246003	-0.150616
5	6	0	3.303985	1.781361	-0.837235

6	7	0	1.886613	1.398695	-0.822239
7	7	0	2.884861	-0.296622	0.141400
8	6	0	3.982145	0.451219	-0.493246
9	6	0	-2.349614	-1.323459	0.873154
10	6	0	-2.404745	-0.329969	0.128127
11	6	0	0.859406	2.394901	-1.071895
12	6	0	3.131647	-1.657710	0.577572
13	6	0	-3.060343	0.727296	-0.688789
14	17	0	-0.262787	1.187493	2.131212
15	6	0	-4.137794	0.089983	-1.588460
16	6	0	-3.626408	1.829343	0.228394
17	1	0	-0.192754	-1.749052	2.501740
18	1	0	-0.130112	-2.900636	1.027256
19	1	0	3.495490	2.551249	-0.075836
20	1	0	3.594683	2.175332	-1.815596
21	1	0	4.827354	0.560879	0.192551
22	1	0	4.325826	-0.081561	-1.391600
23	1	0	-2.646076	-2.163938	1.463963
24	1	0	0.705710	3.046941	-0.204061
25	1	0	-0.084620	1.898206	-1.309774
26	1	0	1.148652	2.991645	-1.942752
27	1	0	3.271796	-2.330872	-0.278478
28	1	0	2.285702	-2.008357	1.166343
29	1	0	4.030492	-1.675483	1.202703
30	1	0	-2.307390	1.180259	-1.346373
31	1	0	-4.925185	-0.368945	-0.980383
32	1	0	-3.702729	-0.679022	-2.233189
33	1	0	-4.595591	0.860700	-2.219040
34	1	0	-2.846531	2.235863	0.878584
35	1	0	-4.424651	1.427418	0.861750
36	1	0	-4.044864	2.637712	-0.382231

16c

Zero-point correction= 0.300625
(Hartree/Particle)
Thermal correction to Energy= 0.321819
Thermal correction to Enthalpy= 0.322763
Thermal correction to Gibbs Free Energy= 0.249940
Sum of electronic and zero-point Energies= -1554.725532
Sum of electronic and thermal Energies= -1554.704338
Sum of electronic and thermal Enthalpies= -1554.703394
Sum of electronic and thermal Free Energies= -1554.776217

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.291177	-1.887449	-1.885621
2	44	0	-0.264909	-0.805881	0.253650
3	6	0	-3.142343	-0.985813	1.325758
4	6	0	1.386390	0.253947	-0.016495
5	6	0	2.983618	1.968656	0.120170
6	7	0	1.582726	1.565672	0.302763
7	7	0	2.546960	-0.230059	-0.513435
8	6	0	3.556169	0.814365	-0.706697
9	6	0	-2.876581	-0.332119	0.176393
10	6	0	-1.624544	0.374683	-0.128549
11	6	0	0.803528	2.343877	1.252991
12	6	0	2.838004	-1.571964	-0.988103

13	6	0	-1.659169	1.658641	-0.927571
14	6	0	-2.125995	1.370375	-2.375273
15	6	0	-2.556704	2.722953	-0.262695
16	1	0	-2.469159	-0.949738	2.177239
17	1	0	-4.062517	-1.553472	1.436280
18	1	0	3.472647	2.057792	1.101210
19	1	0	3.051850	2.937040	-0.385545
20	1	0	4.537024	0.477406	-0.356001
21	1	0	3.640007	1.063709	-1.773981
22	1	0	-3.610100	-0.374689	-0.632161
23	1	0	1.363504	2.455905	2.190938
24	1	0	-0.127008	1.829997	1.476340
25	1	0	0.596064	3.340399	0.845762
26	1	0	2.856585	-1.613584	-2.083065
27	1	0	2.083865	-2.272236	-0.636994
28	1	0	3.817574	-1.872987	-0.597844
29	1	0	-0.637987	2.045234	-0.991024
30	1	0	-3.177714	1.064247	-2.405143
31	1	0	-1.525243	0.580419	-2.834683
32	1	0	-2.029299	2.283314	-2.974504
33	1	0	-2.226359	2.958991	0.754542
34	1	0	-3.596583	2.382149	-0.204880
35	1	0	-2.538535	3.648722	-0.849768
36	17	0	0.163843	-0.823418	2.605493

13d

Zero-point correction= 0.268411
(Hartree/Particle)
Thermal correction to Energy= 0.289201
Thermal correction to Enthalpy= 0.290145
Thermal correction to Gibbs Free Energy= 0.218660
Sum of electronic and zero-point Energies= -1515.396429
Sum of electronic and thermal Energies= -1515.375640
Sum of electronic and thermal Enthalpies= -1515.374695
Sum of electronic and thermal Free Energies= -1515.446180

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.278000	-2.224748	-1.061815
2	44	0	0.621385	0.107885	-0.267608
3	6	0	0.649991	0.655344	-2.002636
4	6	0	-1.422551	-0.086430	0.121400
5	6	0	-3.254582	-0.877749	1.325485
6	7	0	-1.801584	-0.670862	1.272891
7	7	0	-2.514232	0.288691	-0.560342
8	6	0	-3.739684	0.075673	0.227641
9	17	0	0.097661	2.439405	0.419075
10	6	0	-0.930110	-1.426393	2.156064
11	6	0	-2.570417	1.184621	-1.698244
12	1	0	0.692896	1.720143	-2.250732
13	1	0	0.728422	-0.072915	-2.815066
14	1	0	-3.650060	-0.634908	2.316184
15	1	0	-3.491954	-1.926834	1.098436
16	1	0	-4.086439	1.035465	0.635703
17	1	0	-4.533380	-0.347786	-0.394452
18	1	0	-0.848940	-2.472675	1.838233

19	1	0	0.069375	-0.984738	2.162539
20	1	0	-1.327949	-1.375073	3.174672
21	1	0	-1.634605	1.119965	-2.250801
22	1	0	-3.396548	0.882430	-2.350397
23	1	0	-2.718447	2.222049	-1.373275
24	6	0	2.563354	-0.649528	0.274731
25	6	0	2.519775	0.553600	0.643806
26	6	0	3.225469	-1.951204	0.058294
27	6	0	3.089385	1.792873	1.208833
28	1	0	4.210992	-1.946496	0.540654
29	1	0	3.351686	-2.143310	-1.011657
30	1	0	2.627568	-2.775860	0.454032
31	1	0	2.459077	2.194878	2.005853
32	1	0	4.094057	1.590314	1.600651
33	1	0	3.154011	2.569616	0.440631

TS(13-14)d

Zero-point correction= 0.267515
(Hartree/Particle)
Thermal correction to Energy= 0.288053
Thermal correction to Enthalpy= 0.288998
Thermal correction to Gibbs Free Energy= 0.216787
Sum of electronic and zero-point Energies= -1515.379221
Sum of electronic and thermal Energies= -1515.358683
Sum of electronic and thermal Enthalpies= -1515.357739
Sum of electronic and thermal Free Energies= -1515.429949

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.428796	-1.671139	1.784249
2	44	0	0.480697	-0.061079	-0.052679
3	6	0	1.256754	-1.254363	-1.220952
4	6	0	-1.565217	-0.012382	-0.031735
5	6	0	-3.715747	0.724139	0.494813
6	7	0	-2.287455	1.046347	0.385372
7	7	0	-2.408731	-1.001410	-0.374296
8	6	0	-3.809918	-0.557796	-0.343737
9	17	0	0.474310	1.702788	-1.768320
10	6	0	-1.748878	2.246177	0.997896
11	6	0	-2.044318	-2.277973	-0.959643
12	1	0	1.503839	-0.967049	-2.248120
13	1	0	1.454931	-2.290637	-0.927156
14	1	0	-4.328543	1.541720	0.103326
15	1	0	-3.989670	0.553362	1.546027
16	1	0	-4.171024	-0.359981	-1.363050
17	1	0	-4.447727	-1.322486	0.109353
18	1	0	-1.670868	2.146438	2.089816
19	1	0	-0.770574	2.458895	0.561825
20	1	0	-2.406136	3.091176	0.768333
21	1	0	-1.102493	-2.612387	-0.524642
22	1	0	-2.820085	-3.009520	-0.712616
23	1	0	-1.953657	-2.214489	-2.052687
24	6	0	2.900625	-0.188088	-0.096630
25	6	0	2.390563	0.747678	0.563174
26	6	0	4.002490	-1.065778	-0.541566
27	6	0	2.456402	1.952876	1.414923
28	1	0	4.946402	-0.652186	-0.166611

29	1	0	4.067580	-1.131986	-1.632895
30	1	0	3.891289	-2.077826	-0.137551
31	1	0	1.880084	1.814058	2.336328
32	1	0	3.496820	2.166226	1.688346
33	1	0	2.053149	2.814608	0.872281

14d

Zero-point correction= 0.271352
(Hartree/Particle)
Thermal correction to Energy= 0.291414
Thermal correction to Enthalpy= 0.292358
Thermal correction to Gibbs Free Energy= 0.221783
Sum of electronic and zero-point Energies= -1515.446870
Sum of electronic and thermal Energies= -1515.426808
Sum of electronic and thermal Enthalpies= -1515.425864
Sum of electronic and thermal Free Energies= -1515.496440

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.481920	-1.050138	2.251435
2	44	0	-0.442369	0.414578	0.370545
3	6	0	-3.382384	0.970918	-0.152390
4	6	0	1.402924	-0.175371	-0.068894
5	6	0	3.242261	-1.512578	-0.654449
6	7	0	1.780144	-1.374082	-0.599825
7	7	0	2.520600	0.553429	0.143670
8	6	0	3.721333	-0.079329	-0.408405
9	17	0	-0.258279	2.567066	-0.688169
10	6	0	1.012531	-2.609248	-0.571558
11	6	0	2.630995	1.896055	0.687210
12	1	0	-2.872739	1.894685	-0.407789
13	1	0	-4.362492	1.048795	0.312927
14	1	0	3.564106	-1.915369	-1.620067
15	1	0	3.577031	-2.202465	0.133884
16	1	0	4.020303	0.428597	-1.336173
17	1	0	4.554535	-0.018015	0.299192
18	1	0	1.452769	-3.302724	0.157335
19	1	0	-0.008983	-2.403331	-0.264297
20	1	0	1.021208	-3.087137	-1.558396
21	1	0	1.703828	2.185043	1.177010
22	1	0	3.445911	1.908944	1.420967
23	1	0	2.840526	2.628500	-0.100446
24	6	0	-2.848670	-0.238316	-0.427693
25	6	0	-1.462536	-0.339524	-0.943837
26	6	0	-3.560904	-1.537954	-0.112743
27	6	0	-1.163270	-0.859291	-2.310594
28	1	0	-2.997725	-2.110362	0.633690
29	1	0	-3.662760	-2.163433	-1.008801
30	1	0	-4.562104	-1.345822	0.284419
31	1	0	-0.092407	-0.950594	-2.496861
32	1	0	-1.652794	-1.826331	-2.494934
33	1	0	-1.579474	-0.145783	-3.037954

TS(11-17)a

Zero-point correction= 0.324159
(Hartree/Particle)
Thermal correction to Energy= 0.350183
Thermal correction to Enthalpy= 0.351127
Thermal correction to Gibbs Free Energy= 0.267772
Sum of electronic and zero-point Energies= -1897.783089
Sum of electronic and thermal Energies= -1897.757065
Sum of electronic and thermal Enthalpies= -1897.756121
Sum of electronic and thermal Free Energies= -1897.839476

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.306969	2.883077	1.358146
2	6	0	0.045365	2.823035	2.512874
3	1	0	-0.603482	2.913467	0.325744
4	1	0	0.348524	2.779293	3.534729
5	6	0	-0.201832	-0.787273	1.844736
6	17	0	-0.336583	-2.295568	-0.839378
7	44	0	-0.190321	-0.114909	0.134239
8	15	0	-2.632100	-0.202434	0.046594
9	6	0	-3.414754	-1.441950	1.173403
10	6	0	-3.518170	1.359576	0.476400
11	6	0	-3.335691	-0.658400	-1.590641
12	6	0	1.982702	-0.094829	-0.036881
13	6	0	4.207460	0.591915	-0.376165
14	7	0	2.774782	0.877262	-0.539381
15	7	0	2.794305	-1.101025	0.370841
16	6	0	4.198260	-0.889219	-0.008622
17	6	0	2.414335	2.242488	-0.880105
18	6	0	2.451679	-2.422646	0.860441
19	1	0	-0.657151	-1.736713	2.161414
20	1	0	0.202231	-0.193541	2.679500
21	1	0	-3.232501	-1.170572	2.218147
22	1	0	-4.495825	-1.500759	1.005746
23	1	0	-2.967787	-2.422475	0.983235
24	1	0	-3.229719	2.127846	-0.245768
25	1	0	-4.604319	1.217406	0.441724
26	1	0	-3.229587	1.692774	1.478003
27	1	0	-4.430710	-0.670927	-1.545363
28	1	0	-2.994441	0.067297	-2.331308
29	1	0	-2.961320	-1.645589	-1.871158
30	1	0	4.623333	1.222284	0.423907
31	1	0	4.752470	0.810355	-1.299597
32	1	0	4.867311	-1.138086	0.821650
33	1	0	4.454880	-1.535276	-0.860459
34	1	0	2.620952	2.919273	-0.038848
35	1	0	1.363880	2.290537	-1.159063
36	1	0	3.015163	2.560157	-1.739574
37	1	0	1.411616	-2.453076	1.169946
38	1	0	3.102323	-2.663464	1.710974
39	1	0	2.596002	-3.178611	0.078689
40	17	0	-0.734837	1.573958	-1.829411

TS(11-17)b

Zero-point correction= 0.353948
(Hartree/Particle)

Thermal correction to Energy=	0.381159
Thermal correction to Enthalpy=	0.382103
Thermal correction to Gibbs Free Energy=	0.296006
Sum of electronic and zero-point Energies=	-1937.088771
Sum of electronic and thermal Energies=	-1937.061560
Sum of electronic and thermal Enthalpies=	-1937.060616
Sum of electronic and thermal Free Energies=	-1937.146713

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.442392	2.305662	1.476176
2	6	0	-0.812280	3.234441	0.789016
3	6	0	-1.251999	4.354070	-0.037997
4	1	0	-0.171858	1.491334	2.127524
5	1	0	-0.467583	5.113616	-0.136816
6	1	0	-1.520984	4.016282	-1.046986
7	1	0	-2.135267	4.838386	0.394988
8	6	0	-0.354560	0.938456	-1.812830
9	17	0	-0.068658	-1.976835	-1.683395
10	44	0	-0.156059	-0.027359	-0.257065
11	15	0	-2.525306	-0.549076	-0.020149
12	6	0	-2.826663	-2.291993	0.481999
13	6	0	-3.462656	0.425631	1.234113
14	6	0	-3.545933	-0.386116	-1.551788
15	1	0	-0.442741	0.497815	-2.814582
16	1	0	-0.446587	2.035800	-1.805334
17	1	0	-2.373012	-2.951802	-0.261428
18	1	0	-2.341116	-2.463048	1.445286
19	1	0	-3.902079	-2.490445	0.556306
20	1	0	-2.967335	0.298296	2.200516
21	1	0	-3.448880	1.487822	0.974648
22	1	0	-4.500407	0.080060	1.303449
23	1	0	-3.577186	0.660941	-1.869639
24	1	0	-3.075981	-0.976410	-2.343875
25	1	0	-4.569605	-0.743255	-1.391566
26	17	0	-0.169893	-0.901053	2.269789
27	6	0	1.959464	-0.056153	-0.057079
28	6	0	4.206553	0.606237	-0.201492
29	7	0	2.792796	1.006385	-0.215800
30	7	0	2.711779	-1.123309	0.254781
31	6	0	4.127820	-0.777346	0.441948
32	6	0	2.450206	2.281229	-0.812248
33	6	0	2.285210	-2.442516	0.696082
34	1	0	4.810218	1.318694	0.368983
35	1	0	4.598491	0.564340	-1.229170
36	1	0	4.363893	-0.754029	1.515507
37	1	0	4.774152	-1.519049	-0.037095
38	1	0	2.468725	2.237195	-1.911505
39	1	0	1.463269	2.592701	-0.476625
40	1	0	3.180151	3.028075	-0.481767
41	1	0	1.234922	-2.589322	0.471112
42	1	0	2.880716	-3.196405	0.167720
43	1	0	2.439014	-2.544712	1.776498

TS(11-19)b

Zero-point correction=	0.353118
(Hartree/Particle)	

Thermal correction to Energy=	0.380798
Thermal correction to Enthalpy=	0.381742
Thermal correction to Gibbs Free Energy=	0.293951
Sum of electronic and zero-point Energies=	-1937.080153
Sum of electronic and thermal Energies=	-1937.052474
Sum of electronic and thermal Enthalpies=	-1937.051529
Sum of electronic and thermal Free Energies=	-1937.139320

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.490622	3.254266	1.343580
2	6	0	0.059505	2.543302	2.223305
3	6	0	1.004042	4.096872	0.268667
4	1	0	-0.315282	1.975354	3.042985
5	1	0	1.090254	3.510745	-0.655412
6	1	0	1.992820	4.497887	0.521174
7	1	0	0.335470	4.945525	0.081118
8	6	0	-2.654601	-2.404769	0.917890
9	6	0	0.037086	-0.950670	1.824822
10	17	0	0.243303	-2.560288	-0.797373
11	44	0	0.134378	-0.335649	0.089913
12	15	0	2.566474	-0.521019	0.095565
13	6	0	3.268629	-1.735542	1.299887
14	6	0	3.472815	1.035399	0.500863
15	6	0	3.323242	-1.054996	-1.493791
16	6	0	-2.030116	-0.167535	-0.070953
17	6	0	-4.195787	0.675984	-0.456611
18	7	0	-2.746511	0.917892	-0.429467
19	7	0	-2.915404	-1.143199	0.250012
20	6	0	-4.309828	-0.679637	0.239587
21	6	0	-2.280715	2.197579	-0.928730
22	1	0	-3.353128	-3.157890	0.535701
23	1	0	-1.641870	-2.737523	0.708647
24	1	0	-2.811084	-2.311267	2.003963
25	1	0	0.495413	-1.876311	2.200955
26	1	0	-0.467987	-0.374163	2.616561
27	1	0	3.044125	-1.423612	2.324816
28	1	0	4.354647	-1.823707	1.186127
29	1	0	2.808464	-2.712401	1.122908
30	1	0	3.221592	1.780929	-0.257948
31	1	0	4.556719	0.873092	0.509544
32	1	0	3.153315	1.411445	1.477482
33	1	0	4.414015	-1.109102	-1.401682
34	1	0	3.042439	-0.340260	-2.269848
35	1	0	2.921285	-2.034690	-1.762503
36	1	0	-4.731894	1.478841	0.060687
37	1	0	-4.545815	0.648471	-1.497782
38	1	0	-4.683806	-0.593351	1.270921
39	1	0	-4.950530	-1.389534	-0.293361
40	1	0	-1.196764	2.199554	-0.996116
41	1	0	-2.628240	3.001621	-0.267289
42	1	0	-2.684307	2.371209	-1.934885
43	17	0	0.738723	1.177263	-1.936235

TS(11-17)c

Zero-point correction= (Hartree/Particle)	0.411489

Thermal correction to Energy=	0.441021
Thermal correction to Enthalpy=	0.441965
Thermal correction to Gibbs Free Energy=	0.350711
Sum of electronic and zero-point Energies=	-2015.657578
Sum of electronic and thermal Energies=	-2015.628047
Sum of electronic and thermal Enthalpies=	-2015.627102
Sum of electronic and thermal Free Energies=	-2015.718357

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.149395	1.392173	1.441607
2	6	0	-2.005770	1.889434	0.736052
3	6	0	-3.050876	2.514652	-0.085357
4	6	0	-2.808655	4.029744	-0.252492
5	6	0	-4.452207	2.237018	0.500348
6	1	0	-0.479143	0.926966	2.143140
7	1	0	-3.005838	2.052308	-1.083253
8	1	0	-1.832779	4.232247	-0.704466
9	1	0	-2.845789	4.535949	0.718116
10	1	0	-3.582075	4.463139	-0.896120
11	1	0	-4.547135	2.673813	1.500167
12	1	0	-4.646969	1.163206	0.578939
13	1	0	-5.220054	2.680413	-0.143191
14	6	0	-0.436035	0.409213	-1.857223
15	17	0	1.305254	-1.939003	-1.654402
16	44	0	0.152876	-0.317537	-0.267218
17	15	0	-1.594047	-2.013687	-0.075983
18	6	0	-0.948215	-3.688899	0.321223
19	6	0	-2.866250	-1.738121	1.230033
20	6	0	-2.592478	-2.317146	-1.601885
21	6	0	1.971672	0.767928	-0.020395
22	6	0	3.543088	2.510212	-0.140395
23	7	0	2.129266	2.112085	-0.174542
24	7	0	3.167178	0.255635	0.312890
25	6	0	4.187984	1.292952	0.517542
26	6	0	1.192007	3.014087	-0.810277
27	6	0	3.505926	-1.094332	0.738843
28	1	0	-0.207208	-0.014334	-2.843945
29	1	0	-1.086367	1.296632	-1.907090
30	1	0	-0.248462	-3.990845	-0.461189
31	1	0	-0.409100	-3.632635	1.269446
32	1	0	-1.771275	-4.409426	0.392136
33	1	0	-2.345309	-1.627661	2.184901
34	1	0	-3.421896	-0.818465	1.029433
35	1	0	-3.563818	-2.581706	1.282940
36	1	0	-3.140047	-1.409810	-1.876192
37	1	0	-1.907523	-2.568032	-2.417289
38	1	0	-3.303778	-3.138938	-1.461271
39	1	0	3.676823	3.436094	0.427329
40	1	0	3.914160	2.674328	-1.163750
41	1	0	4.356540	1.438552	1.594242
42	1	0	5.136002	0.998449	0.057372
43	1	0	1.271070	2.981401	-1.907451
44	1	0	0.178431	2.760352	-0.510627
45	1	0	1.408455	4.034987	-0.476973
46	1	0	2.702947	-1.778350	0.490414
47	1	0	4.421403	-1.400737	0.218808
48	1	0	3.675063	-1.114457	1.821470
49	17	0	0.599920	-1.212412	2.228938

TS(11-19)c

Zero-point correction= 0.411247
(Hartree/Particle)
Thermal correction to Energy= 0.441046
Thermal correction to Enthalpy= 0.441990
Thermal correction to Gibbs Free Energy= 0.350477
Sum of electronic and zero-point Energies= -2015.656938
Sum of electronic and thermal Energies= -2015.627139
Sum of electronic and thermal Enthalpies= -2015.626195
Sum of electronic and thermal Free Energies= -2015.717708

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.057798	2.772914	-0.712458
2	6	0	0.349717	2.523545	-1.664686
3	6	0	1.897634	3.103991	0.443551
4	6	0	1.826200	4.614040	0.751868
5	6	0	3.351044	2.633045	0.235271
6	1	0	-0.259310	2.380475	-2.526927
7	1	0	1.475637	2.549437	1.293217
8	1	0	0.793993	4.931798	0.929328
9	1	0	2.230241	5.207169	-0.076774
10	1	0	2.412201	4.836247	1.650600
11	1	0	3.812097	3.135578	-0.623278
12	1	0	3.389585	1.551937	0.068975
13	1	0	3.945162	2.863797	1.126604
14	6	0	-0.738307	-0.630767	-2.185031
15	17	0	-1.619407	-2.553121	-0.172107
16	44	0	-0.511768	-0.415721	-0.366602
17	15	0	-2.713356	0.548637	0.031475
18	6	0	-3.502581	-0.105815	1.558757
19	6	0	-2.781535	2.376591	0.266148
20	6	0	-3.994154	0.223287	-1.259750
21	6	0	1.381316	-1.328510	-0.091379
22	6	0	3.565071	-2.069343	-0.520898
23	7	0	2.483820	-1.133866	-0.863990
24	7	0	1.709894	-2.191068	0.883070
25	6	0	3.139738	-2.529861	0.872861
26	6	0	2.505876	-0.502967	-2.169847
27	6	0	0.941370	-2.548607	2.065786
28	1	0	-1.288702	-1.458671	-2.651771
29	1	0	-0.355788	0.101218	-2.913480
30	1	0	-3.589491	-1.191551	1.470029
31	1	0	-2.856564	0.127285	2.408240
32	1	0	-4.493835	0.339326	1.702666
33	1	0	-2.094510	2.636307	1.075754
34	1	0	-2.454467	2.889815	-0.642540
35	1	0	-3.796926	2.700682	0.521383
36	1	0	-3.708986	0.707594	-2.199074
37	1	0	-4.048569	-0.856313	-1.427597
38	1	0	-4.978125	0.593304	-0.950048
39	1	0	4.537698	-1.568579	-0.537117
40	1	0	3.590273	-2.900616	-1.241748
41	1	0	3.657193	-1.978078	1.671020
42	1	0	3.285891	-3.600805	1.042556
43	1	0	2.149909	-1.181086	-2.959114

44	1	0	1.893449	0.397634	-2.158252
45	1	0	3.537036	-0.213884	-2.398111
46	1	0	-0.104882	-2.304188	1.914693
47	1	0	1.041845	-3.627092	2.234207
48	1	0	1.316762	-2.003627	2.939593
49	17	0	-0.096582	0.616788	2.009791

17a

Zero-point correction= 0.327049
(Hartree/Particle)
Thermal correction to Energy= 0.352157
Thermal correction to Enthalpy= 0.353101
Thermal correction to Gibbs Free Energy= 0.273574
Sum of electronic and zero-point Energies= -1897.796038
Sum of electronic and thermal Energies= -1897.770930
Sum of electronic and thermal Enthalpies= -1897.769986
Sum of electronic and thermal Free Energies= -1897.849512

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.193389	-0.039683	0.384018
2	15	0	-2.630663	-0.137832	-0.071212
3	6	0	-3.466922	-1.635046	0.622806
4	6	0	-3.691464	1.236490	0.562436
5	6	0	-3.116710	-0.211091	-1.843562
6	17	0	-0.201426	-1.797161	-1.361362
7	6	0	-0.368423	-1.365911	1.667186
8	6	0	1.948333	-0.019777	0.095145
9	6	0	4.094266	-0.834746	-0.388610
10	7	0	2.758206	-1.102405	0.162788
11	7	0	2.705925	1.036599	-0.263726
12	6	0	4.124825	0.690910	-0.428567
13	6	0	2.421567	-2.494222	0.391087
14	6	0	2.389717	2.454560	-0.214536
15	1	0	-3.388889	-1.644407	1.714755
16	1	0	-4.525012	-1.661888	0.339692
17	1	0	-2.968924	-2.524607	0.226256
18	1	0	-3.307613	2.181798	0.167755
19	1	0	-4.724406	1.102664	0.223810
20	1	0	-3.686734	1.263856	1.656857
21	1	0	-4.207398	-0.295824	-1.916887
22	1	0	-2.765130	0.694954	-2.339184
23	1	0	-2.634863	-1.071710	-2.309305
24	1	0	-0.635093	-2.400698	1.414701
25	1	0	-0.326173	-1.177658	2.750691
26	1	0	4.175813	-1.281223	-1.389356
27	1	0	4.871350	-1.271559	0.246909
28	1	0	4.512511	1.095248	-1.368579
29	1	0	4.709406	1.124396	0.396532
30	1	0	1.493505	-2.564074	0.951045
31	1	0	3.231384	-2.951996	0.972403
32	1	0	2.294551	-3.034218	-0.552792
33	1	0	2.927073	2.923598	0.623601
34	1	0	1.317947	2.601752	-0.122437
35	1	0	2.716503	2.928481	-1.146277
36	6	0	-0.702226	1.614409	1.801704

37	6	0	0.452687	1.274852	2.090802
38	1	0	-1.607542	2.183191	1.810888
39	1	0	1.411821	1.246578	2.564182
40	17	0	-0.603153	1.946865	-1.354675

TS(17-18)a

Zero-point correction= 0.325690
(Hartree/Particle)
Thermal correction to Energy= 0.350481
Thermal correction to Enthalpy= 0.351425
Thermal correction to Gibbs Free Energy= 0.272509
Sum of electronic and zero-point Energies= -1897.782748
Sum of electronic and thermal Energies= -1897.757957
Sum of electronic and thermal Enthalpies= -1897.757013
Sum of electronic and thermal Free Energies= -1897.835929

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.185801	-0.066828	0.202724
2	15	0	-2.649727	-0.192567	0.138568
3	6	0	-3.467742	-1.519871	1.146108
4	6	0	-3.558492	1.318914	0.697077
5	6	0	-3.371491	-0.481606	-1.529852
6	17	0	-0.183922	-1.567076	-1.694544
7	6	0	-0.310044	1.789728	1.452978
8	6	0	-0.120796	1.010415	2.396403
9	6	0	-0.046776	-1.250714	1.669315
10	6	0	1.939707	-0.030226	0.071037
11	6	0	4.163723	-0.802703	-0.044983
12	7	0	2.748162	-1.117462	0.196601
13	7	0	2.743926	1.041433	-0.098677
14	6	0	4.171429	0.722623	0.029139
15	6	0	2.393841	-2.525616	0.128562
16	6	0	2.368036	2.441417	-0.178049
17	1	0	-3.267598	-1.375140	2.213522
18	1	0	-4.552996	-1.518303	0.995414
19	1	0	-3.073261	-2.497174	0.849056
20	1	0	-3.235602	2.155968	0.071293
21	1	0	-4.642305	1.190017	0.599864
22	1	0	-3.318946	1.546206	1.740680
23	1	0	-4.466235	-0.444377	-1.488613
24	1	0	-2.987907	0.289775	-2.201815
25	1	0	-3.040382	-1.451600	-1.906446
26	1	0	-0.499823	2.699860	0.920670
27	1	0	0.050289	0.600766	3.369368
28	1	0	-0.905332	-1.734120	2.153661
29	1	0	0.889359	-1.478202	2.197179
30	1	0	4.461286	-1.174876	-1.036033
31	1	0	4.804401	-1.279381	0.704437
32	1	0	4.747300	1.194361	-0.773297
33	1	0	4.556509	1.095331	0.990081
34	1	0	1.315218	-2.649062	0.145577
35	1	0	2.856756	-3.064180	0.966095
36	1	0	2.762461	-2.958190	-0.810665
37	1	0	2.438511	2.931451	0.803938
38	1	0	1.361607	2.527746	-0.587693
39	1	0	3.058215	2.946741	-0.862881

40	17	0	-0.686864	1.847863	-1.585670

18a

Zero-point correction= 0.330956
(Hartree/Particle)
Thermal correction to Energy= 0.355291
Thermal correction to Enthalpy= 0.356235
Thermal correction to Gibbs Free Energy= 0.277769
Sum of electronic and zero-point Energies= -1897.844175
Sum of electronic and thermal Energies= -1897.819841
Sum of electronic and thermal Enthalpies= -1897.818897
Sum of electronic and thermal Free Energies= -1897.897362

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.211414	-0.114298	0.278755
2	15	0	2.615044	0.068523	-0.100025
3	6	0	3.333811	1.646561	0.528067
4	6	0	3.616851	-1.238285	0.746057
5	6	0	3.217731	-0.038669	-1.830329
6	17	0	0.399568	1.767561	-1.516846
7	6	0	0.259857	-1.227485	1.760066
8	6	0	0.562284	-0.037727	2.514114
9	6	0	-0.241805	1.085947	2.392414
10	6	0	-1.924327	0.006238	0.019106
11	6	0	-4.058873	0.852584	-0.452379
12	7	0	-2.677258	1.126546	-0.032515
13	7	0	-2.748219	-1.050859	-0.150962
14	6	0	-4.161013	-0.656919	-0.239972
15	6	0	-2.260294	2.517122	0.014966
16	6	0	-2.468120	-2.447933	0.128195
17	1	0	3.183842	1.729252	1.609501
18	1	0	4.406581	1.707568	0.313291
19	1	0	2.809417	2.468872	0.034203
20	1	0	3.285365	-2.213501	0.377026
21	1	0	4.685827	-1.118521	0.537618
22	1	0	3.463723	-1.203983	1.829530
23	1	0	4.307395	0.079114	-1.851001
24	1	0	2.929857	-1.007562	-2.242579
25	1	0	2.732818	0.744475	-2.414986
26	1	0	0.387584	-2.276794	2.031973
27	1	0	1.565566	0.079887	2.935769
28	1	0	0.155602	2.060732	2.660774
29	1	0	-1.316553	1.003870	2.306896
30	1	0	-4.187248	1.137379	-1.505792
31	1	0	-4.769664	1.428521	0.148928
32	1	0	-4.658257	-1.179833	-1.062444
33	1	0	-4.680811	-0.915227	0.695152
34	1	0	-1.242668	2.590508	0.385595
35	1	0	-2.950612	3.062877	0.671972
36	1	0	-2.280641	2.963916	-0.984673
37	1	0	-2.795671	-2.710264	1.146172
38	1	0	-1.407140	-2.644533	0.000322
39	1	0	-3.021578	-3.069230	-0.584017
40	17	0	0.399909	-1.886071	-1.424422

17b

Zero-point correction= 0.355672
(Hartree/Particle)
Thermal correction to Energy= 0.382554
Thermal correction to Enthalpy= 0.383498
Thermal correction to Gibbs Free Energy= 0.299600
Sum of electronic and zero-point Energies= -1937.090832
Sum of electronic and thermal Energies= -1937.063950
Sum of electronic and thermal Enthalpies= -1937.063006
Sum of electronic and thermal Free Energies= -1937.146904

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.243802	0.014541	0.277745
2	15	0	2.708917	0.104603	-0.004934
3	6	0	3.585646	1.242671	1.162442
4	6	0	3.662151	-1.465935	0.195329
5	6	0	3.296953	0.710420	-1.639014
6	17	0	0.365423	2.169906	-0.932990
7	6	0	0.427514	0.957248	1.863898
8	6	0	-1.874831	0.119490	-0.089415
9	6	0	-3.967663	1.109500	-0.473991
10	7	0	-2.672663	1.170079	0.219072
11	7	0	-2.624080	-0.775911	-0.765397
12	6	0	-4.019360	-0.346525	-0.932029
13	6	0	-2.327279	2.437923	0.833686
14	6	0	-2.333743	-2.166779	-1.067594
15	1	0	3.447787	0.909983	2.196284
16	1	0	4.658043	1.285147	0.941262
17	1	0	3.161655	2.245625	1.057013
18	1	0	3.277892	-2.198991	-0.520008
19	1	0	4.723750	-1.290631	-0.009582
20	1	0	3.562186	-1.857373	1.212569
21	1	0	4.393202	0.706976	-1.657903
22	1	0	2.894377	0.058284	-2.415702
23	1	0	2.915085	1.719232	-1.802167
24	1	0	0.698255	2.021177	1.879711
25	1	0	0.410367	0.503209	2.867290
26	1	0	-3.967070	1.812937	-1.318094
27	1	0	-4.784014	1.384832	0.201806
28	1	0	-4.336516	-0.465729	-1.972610
29	1	0	-4.676391	-0.965365	-0.302575
30	1	0	-2.095766	3.197972	0.080726
31	1	0	-1.456734	2.315785	1.472938
32	1	0	-3.179208	2.765683	1.442151
33	1	0	-2.971078	-2.816685	-0.448247
34	1	0	-1.283431	-2.378435	-0.898042
35	1	0	-2.551427	-2.365600	-2.122094
36	6	0	0.586665	-2.038986	1.119302
37	6	0	-0.447563	-1.714158	1.713128
38	6	0	-1.632827	-1.689785	2.579068
39	1	0	1.381279	-2.665263	0.773643
40	1	0	-1.660949	-0.785433	3.195909
41	1	0	-1.626738	-2.559941	3.246600
42	1	0	-2.555452	-1.716537	1.989051
43	17	0	0.670053	-1.391047	-1.949438

TS(17-18)b

Zero-point correction= 0.355215
(Hartree/Particle)
Thermal correction to Energy= 0.381287
Thermal correction to Enthalpy= 0.382231
Thermal correction to Gibbs Free Energy= 0.299918
Sum of electronic and zero-point Energies= -1937.075507
Sum of electronic and thermal Energies= -1937.049435
Sum of electronic and thermal Enthalpies= -1937.048491
Sum of electronic and thermal Free Energies= -1937.130804

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.172195	0.003390	-0.093496
2	15	0	2.628097	-0.186856	-0.185387
3	6	0	3.462966	0.207592	-1.797718
4	6	0	3.557101	0.886979	0.998945
5	6	0	3.294583	-1.861382	0.184666
6	17	0	0.039269	-2.339139	-0.671010
7	6	0	0.211663	1.818689	1.032066
8	6	0	0.284808	2.430935	-0.066222
9	6	0	0.038233	0.998774	-1.709802
10	6	0	-1.958137	-0.042675	-0.023362
11	6	0	-4.180821	-0.378883	-0.731534
12	7	0	-2.759011	-0.291068	-1.095162
13	7	0	-2.768212	0.187625	1.030825
14	6	0	-4.191880	0.220508	0.673469
15	6	0	-2.396366	-0.873759	-2.376769
16	6	0	-2.397881	0.576803	2.379431
17	1	0	3.289504	1.251780	-2.081025
18	1	0	4.544711	0.043502	-1.736852
19	1	0	3.054291	-0.434489	-2.584896
20	1	0	3.211016	0.645891	2.007927
21	1	0	4.637737	0.718768	0.929611
22	1	0	3.345389	1.942432	0.800359
23	1	0	4.390529	-1.848903	0.192460
24	1	0	2.907990	-2.169373	1.158824
25	1	0	2.930468	-2.569870	-0.562553
26	1	0	0.892252	1.247327	-2.351281
27	1	0	-0.894708	1.421516	-2.101718
28	1	0	-4.500100	-1.431117	-0.739406
29	1	0	-4.802857	0.171323	-1.445476
30	1	0	-4.784721	-0.358447	1.388648
31	1	0	-4.559063	1.257447	0.686162
32	1	0	-2.795914	-1.893804	-2.448078
33	1	0	-1.316644	-0.934400	-2.475145
34	1	0	-2.823377	-0.273957	-3.191473
35	1	0	-2.471644	1.665897	2.514849
36	1	0	-1.390710	0.222562	2.600694
37	1	0	-3.090594	0.098091	3.080830
38	6	0	0.520995	3.633250	-0.897917
39	1	0	1.460550	3.564409	-1.458127
40	1	0	0.586997	4.499428	-0.228153
41	1	0	-0.286203	3.815375	-1.615027
42	1	0	0.234587	1.857922	2.104679
43	17	0	0.693170	-0.886302	2.371458

18b

Zero-point correction= 0.358731
(Hartree/Particle)
Thermal correction to Energy= 0.384898
Thermal correction to Enthalpy= 0.385842
Thermal correction to Gibbs Free Energy= 0.302578
Sum of electronic and zero-point Energies= -1937.130737
Sum of electronic and thermal Energies= -1937.104571
Sum of electronic and thermal Enthalpies= -1937.103626
Sum of electronic and thermal Free Energies= -1937.186891

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.163093	0.193748	0.042359
2	15	0	2.530959	-0.461950	0.065571
3	6	0	3.323869	-0.547248	-1.600559
4	6	0	3.646971	0.656095	1.032961
5	6	0	2.935531	-2.097274	0.800642
6	17	0	0.164508	-2.188390	-1.031624
7	6	0	0.152744	1.982193	0.539663
8	6	0	0.526140	2.320355	-0.805957
9	6	0	-0.191041	1.712855	-1.836737
10	6	0	-1.979428	0.002676	-0.008608
11	6	0	-4.132542	-0.643076	-0.672178
12	7	0	-2.735367	-0.396265	-1.055944
13	7	0	-2.811734	0.239357	1.030746
14	6	0	-4.226535	0.087547	0.664485
15	6	0	-2.325766	-0.864556	-2.369124
16	6	0	-2.525505	0.994733	2.238132
17	6	0	1.802686	3.091933	-1.087147
18	1	0	3.335844	0.437036	-2.078648
19	1	0	4.353243	-0.916453	-1.527505
20	1	0	2.731698	-1.232240	-2.213459
21	1	0	3.245122	0.741577	2.046746
22	1	0	4.662031	0.245910	1.081031
23	1	0	3.691375	1.651537	0.583938
24	1	0	4.016831	-2.265969	0.736547
25	1	0	2.607909	-2.105668	1.841484
26	1	0	2.390062	-2.870302	0.258193
27	1	0	0.182751	2.599587	1.439574
28	1	0	0.257737	1.652017	-2.826161
29	1	0	-1.266508	1.622650	-1.795081
30	1	0	-4.299891	-1.724415	-0.571033
31	1	0	-4.819082	-0.257431	-1.432556
32	1	0	-4.768041	-0.473386	1.431899
33	1	0	-4.695011	1.078962	0.567611
34	1	0	-2.403723	-1.954813	-2.432225
35	1	0	-1.290887	-0.599134	-2.557711
36	1	0	-2.985171	-0.406546	-3.118499
37	1	0	-2.751490	2.062207	2.089986
38	1	0	-1.486907	0.852914	2.525870
39	1	0	-3.161044	0.616990	3.046011
40	1	0	2.397545	2.614019	-1.872930
41	1	0	2.423567	3.211747	-0.196232
42	1	0	1.534529	4.094186	-1.444565
43	17	0	0.291020	-0.714534	2.347700

19b

Zero-point correction= 0.355858
(Hartree/Particle)
Thermal correction to Energy= 0.382593
Thermal correction to Enthalpy= 0.383538
Thermal correction to Gibbs Free Energy= 0.300678
Sum of electronic and zero-point Energies= -1937.087120
Sum of electronic and thermal Energies= -1937.060385
Sum of electronic and thermal Enthalpies= -1937.059440
Sum of electronic and thermal Free Energies= -1937.142301

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.156421	-0.099985	-0.291098
2	15	0	2.606999	-0.359732	0.019515
3	6	0	3.258380	-1.937901	-0.690870
4	6	0	3.787929	0.870282	-0.705663
5	6	0	3.173956	-0.462737	1.765794
6	6	0	0.326388	-1.185204	-1.796641
7	6	0	-1.992154	-0.062598	-0.081714
8	6	0	-4.193426	-0.862484	0.101575
9	7	0	-2.817575	-1.102222	-0.357056
10	7	0	-2.760436	0.957257	0.355230
11	6	0	-4.196015	0.646931	0.322107
12	6	0	-2.491427	-2.470017	-0.712803
13	6	0	-2.404183	2.350395	0.559795
14	1	0	3.180034	-1.924694	-1.782724
15	1	0	4.307748	-2.084443	-0.412033
16	1	0	2.659243	-2.764392	-0.299757
17	1	0	3.698524	1.822619	-0.177987
18	1	0	4.818839	0.512298	-0.605875
19	1	0	3.567806	1.030705	-1.765793
20	1	0	4.245488	-0.692471	1.796248
21	1	0	2.965252	0.481174	2.270921
22	1	0	2.600860	-1.246224	2.265778
23	1	0	0.608302	-2.242102	-1.704542
24	1	0	0.249924	-0.862913	-2.846497
25	1	0	-4.376633	-1.421267	1.030283
26	1	0	-4.917342	-1.196981	-0.648456
27	1	0	-4.676985	0.951352	1.256672
28	1	0	-4.676720	1.193120	-0.503581
29	1	0	-2.498165	-3.120794	0.168524
30	1	0	-1.501949	-2.516601	-1.156689
31	1	0	-3.236511	-2.825881	-1.435456
32	1	0	-2.696486	2.953526	-0.312072
33	1	0	-1.339681	2.434203	0.756018
34	1	0	-2.943240	2.722038	1.438175
35	17	0	0.172745	-2.142405	1.103170
36	6	0	0.461086	2.096293	-1.291266
37	6	0	-0.369778	1.408786	-1.890781
38	6	0	1.280004	3.208310	-0.797047
39	1	0	-1.103148	1.153057	-2.627896
40	1	0	2.267307	3.221956	-1.269597
41	1	0	1.394076	3.137060	0.289519
42	1	0	0.780047	4.155328	-1.036619
43	17	0	0.405928	1.338879	1.905469

TS(19-20)b

Zero-point correction= 0.354702
(Hartree/Particle)
Thermal correction to Energy= 0.381007
Thermal correction to Enthalpy= 0.381951
Thermal correction to Gibbs Free Energy= 0.299837
Sum of electronic and zero-point Energies= -1937.075119
Sum of electronic and thermal Energies= -1937.048815
Sum of electronic and thermal Enthalpies= -1937.047871
Sum of electronic and thermal Free Energies= -1937.129984

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.163991	-0.093863	-0.176859
2	15	0	2.606578	-0.378596	-0.125160
3	6	0	3.152538	-2.014617	-0.797544
4	6	0	3.712887	0.785284	-1.057645
5	6	0	3.358887	-0.373184	1.554063
6	17	0	0.222455	-2.048021	1.283378
7	6	0	0.489092	2.050796	-1.105178
8	6	0	-0.086537	1.406230	-2.001189
9	6	0	0.081468	-0.859330	-1.904725
10	6	0	-1.964270	-0.103849	-0.076623
11	6	0	-4.178754	-0.905907	-0.091722
12	7	0	-2.760748	-1.162033	-0.383441
13	7	0	-2.781072	0.923498	0.246510
14	6	0	-4.203980	0.612570	0.063296
15	6	0	-2.394594	-2.555069	-0.578342
16	6	0	-2.422018	2.309714	0.482936
17	6	0	1.091477	3.241279	-0.480275
18	1	0	2.922273	-2.088013	-1.865576
19	1	0	4.229853	-2.161381	-0.660535
20	1	0	2.604212	-2.798985	-0.268917
21	1	0	3.671371	1.777863	-0.599955
22	1	0	4.752588	0.439384	-1.042976
23	1	0	3.383457	0.871702	-2.098479
24	1	0	4.433225	-0.584651	1.504672
25	1	0	3.179024	0.595843	2.024430
26	1	0	2.850451	-1.130054	2.156028
27	1	0	-0.661120	1.284621	-2.898183
28	1	0	0.948026	-1.023815	-2.560014
29	1	0	-0.851503	-1.102055	-2.432966
30	1	0	-4.465098	-1.425171	0.834281
31	1	0	-4.817689	-1.274313	-0.901185
32	1	0	-4.789518	0.953015	0.923131
33	1	0	-4.588764	1.121056	-0.833883
34	1	0	-2.679666	-3.149009	0.299330
35	1	0	-1.321737	-2.655192	-0.708160
36	1	0	-2.925530	-2.947291	-1.455879
37	1	0	-2.509351	2.905558	-0.437405
38	1	0	-1.412459	2.357078	0.886475
39	1	0	-3.108469	2.723604	1.229924
40	1	0	2.045166	3.475086	-0.967732
41	1	0	1.247179	3.080386	0.590088
42	1	0	0.426876	4.103776	-0.613915
43	17	0	0.371574	1.257792	2.038551

20b

Zero-point correction= 0.359298
(Hartree/Particle)
Thermal correction to Energy= 0.385202
Thermal correction to Enthalpy= 0.386146
Thermal correction to Gibbs Free Energy= 0.304426
Sum of electronic and zero-point Energies= -1937.143047
Sum of electronic and thermal Energies= -1937.117143
Sum of electronic and thermal Enthalpies= -1937.116199
Sum of electronic and thermal Free Energies= -1937.197919

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.174979	0.071489	0.167213
2	15	0	-2.603019	-0.275468	-0.076925
3	6	0	-3.271636	-1.790657	0.742877
4	6	0	-3.713621	1.053634	0.584252
5	6	0	-3.201636	-0.453246	-1.805444
6	17	0	-0.319245	-2.202970	-1.065791
7	6	0	-0.334040	1.608301	1.214825
8	6	0	0.199305	0.740789	2.232894
9	6	0	-0.405887	-0.500740	2.460212
10	6	0	1.951396	-0.107244	-0.012493
11	6	0	4.082865	-1.083294	-0.041381
12	7	0	2.675081	-1.181498	0.367495
13	7	0	2.811011	0.818778	-0.490072
14	6	0	4.215459	0.404143	-0.368984
15	6	0	2.209295	-2.466371	0.858130
16	6	0	2.548438	2.219548	-0.762060
17	6	0	-0.635059	3.056335	1.166830
18	1	0	-3.209468	-1.711021	1.832357
19	1	0	-4.319701	-1.945082	0.463074
20	1	0	-2.669354	-2.640678	0.413070
21	1	0	-3.482476	1.996746	0.079798
22	1	0	-4.768445	0.810957	0.412759
23	1	0	-3.553757	1.184963	1.659792
24	1	0	-4.273680	-0.682331	-1.804175
25	1	0	-3.007879	0.471381	-2.351323
26	1	0	-2.637787	-1.257530	-2.281775
27	1	0	1.224670	0.904904	2.578341
28	1	0	-1.480802	-0.598098	2.530250
29	1	0	0.166000	-1.282456	2.952088
30	1	0	4.258019	-1.723299	-0.917323
31	1	0	4.746062	-1.414689	0.764165
32	1	0	4.757833	0.597763	-1.299415
33	1	0	4.705721	0.970894	0.437129
34	1	0	2.306093	-3.234188	0.082750
35	1	0	1.160728	-2.398640	1.128903
36	1	0	2.816259	-2.750790	1.728006
37	1	0	2.856702	2.843317	0.091743
38	1	0	1.493099	2.355267	-0.987201
39	1	0	3.128674	2.527449	-1.638732
40	1	0	-1.516779	3.282533	1.783857
41	1	0	-0.814318	3.388772	0.141519
42	1	0	0.198153	3.629645	1.600415
43	17	0	-0.363762	1.268414	-2.014412

17c

Zero-point correction= 0.412784
(Hartree/Particle)
Thermal correction to Energy= 0.442326
Thermal correction to Enthalpy= 0.443270
Thermal correction to Gibbs Free Energy= 0.353758
Sum of electronic and zero-point Energies= -2015.658417
Sum of electronic and thermal Energies= -2015.628875
Sum of electronic and thermal Enthalpies= -2015.627931
Sum of electronic and thermal Free Energies= -2015.717443

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.373760	-0.095211	-0.145376
2	15	0	2.829780	0.235981	-0.041309
3	6	0	3.630232	0.731171	-1.635649
4	6	0	3.461438	1.523552	1.125060
5	6	0	3.812401	-1.243017	0.437302
6	17	0	1.003020	-2.295109	-1.084226
7	6	0	0.232073	1.804783	1.088170
8	6	0	-0.664750	2.021360	0.267823
9	6	0	0.397385	0.556777	-1.886173
10	6	0	-1.648634	-0.807971	0.010901
11	6	0	-3.724439	-1.701087	-0.638240
12	7	0	-2.335080	-1.389326	-1.000177
13	7	0	-2.459238	-0.793308	1.093399
14	6	0	-3.688883	-1.571931	0.881638
15	6	0	-1.970537	-1.453606	-2.404709
16	6	0	-2.168487	-0.392133	2.459707
17	6	0	-1.759688	2.661673	-0.497812
18	6	0	-1.311221	4.045183	-1.015552
19	6	0	-3.032805	2.781708	0.365519
20	1	0	3.232940	1.692871	-1.976028
21	1	0	4.717413	0.812387	-1.525504
22	1	0	3.405763	-0.026819	-2.392156
23	1	0	3.143584	1.259053	2.137846
24	1	0	4.555897	1.561216	1.093776
25	1	0	3.065410	2.510507	0.866681
26	1	0	4.877784	-0.985735	0.465907
27	1	0	3.470235	-1.583459	1.416162
28	1	0	3.630895	-2.039632	-0.286049
29	1	0	0.868750	1.879857	1.943847
30	1	0	0.773636	-0.058688	-2.712988
31	1	0	0.163836	1.584951	-2.200176
32	1	0	-3.998504	-2.702723	-0.982287
33	1	0	-4.410712	-0.977877	-1.104957
34	1	0	-3.600611	-2.545724	1.383478
35	1	0	-4.555451	-1.048226	1.297445
36	1	0	-2.542946	-2.263447	-2.868138
37	1	0	-0.911561	-1.683517	-2.498862
38	1	0	-2.212533	-0.516510	-2.928245
39	1	0	-3.038902	0.149195	2.852268
40	1	0	-1.288395	0.239385	2.488041
41	1	0	-1.973581	-1.268356	3.087898
42	1	0	-1.993958	2.033574	-1.365701
43	1	0	-0.426860	3.964703	-1.655602
44	1	0	-1.064692	4.709237	-0.179875

45	1	0	-2.117081	4.508633	-1.596469
46	1	0	-2.848323	3.411458	1.242689
47	1	0	-3.365628	1.799684	0.712141
48	1	0	-3.839427	3.237922	-0.220042
49	17	0	0.971486	-0.967519	2.291323

TS(17-18)c

Zero-point correction= 0.412650
(Hartree/Particle)
Thermal correction to Energy= 0.441234
Thermal correction to Enthalpy= 0.442178
Thermal correction to Gibbs Free Energy= 0.354500
Sum of electronic and zero-point Energies= -2015.644020
Sum of electronic and thermal Energies= -2015.615436
Sum of electronic and thermal Enthalpies= -2015.614492
Sum of electronic and thermal Free Energies= -2015.702170

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.097160	-0.329587	-0.083824
2	15	0	2.520777	-0.788290	-0.127254
3	6	0	3.446410	-0.392935	-1.687727
4	6	0	3.523148	0.090431	1.154272
5	6	0	2.983186	-2.548554	0.147275
6	17	0	-0.236192	-2.580654	-0.894291
7	6	0	0.338290	1.346341	1.214298
8	6	0	0.407070	2.073903	0.186048
9	6	0	0.131943	0.829671	-1.594126
10	6	0	-2.025254	-0.156157	-0.065673
11	6	0	-4.248957	-0.233946	-0.838301
12	7	0	-2.816810	-0.240506	-1.170218
13	7	0	-2.838585	0.073176	0.986520
14	6	0	-4.241647	0.272993	0.601675
15	6	0	-2.476825	-0.759352	-2.485251
16	6	0	-2.466908	0.341685	2.364164
17	6	0	0.584336	3.412924	-0.461335
18	6	0	2.030766	3.651265	-0.936103
19	6	0	0.153129	4.493867	0.552646
20	1	0	3.406444	0.680168	-1.903007
21	1	0	4.498542	-0.689720	-1.612861
22	1	0	2.987737	-0.930112	-2.524338
23	1	0	3.122529	-0.184913	2.134099
24	1	0	4.581423	-0.188073	1.098984
25	1	0	3.430987	1.174111	1.031370
26	1	0	4.072482	-2.659392	0.199494
27	1	0	2.518576	-2.876603	1.079961
28	1	0	2.580842	-3.159753	-0.663385
29	1	0	0.385139	1.260686	2.283572
30	1	0	1.032118	1.063682	-2.173639
31	1	0	-0.745912	1.358500	-1.983261
32	1	0	-4.651461	-1.254280	-0.918719
33	1	0	-4.808401	0.409231	-1.525612
34	1	0	-4.909368	-0.286729	1.263983
35	1	0	-4.503899	1.339228	0.673701
36	1	0	-2.912412	-1.757757	-2.620152
37	1	0	-1.400386	-0.850924	-2.592917
38	1	0	-2.881727	-0.091952	-3.257313

39	1	0	-2.414935	1.422577	2.560724
40	1	0	-1.516061	-0.142734	2.588205
41	1	0	-3.232811	-0.088712	3.018948
42	1	0	-0.077883	3.486672	-1.332144
43	1	0	2.347297	2.903029	-1.668521
44	1	0	2.725466	3.617717	-0.089747
45	1	0	2.111061	4.638114	-1.405759
46	1	0	0.785848	4.463354	1.446249
47	1	0	-0.886501	4.353358	0.863208
48	1	0	0.249886	5.486660	0.098734
49	17	0	0.399386	-1.509392	2.300288

18c

Zero-point correction= 0.415783
(Hartree/Particle)
Thermal correction to Energy= 0.444652
Thermal correction to Enthalpy= 0.445597
Thermal correction to Gibbs Free Energy= 0.355596
Sum of electronic and zero-point Energies= -2015.697079
Sum of electronic and thermal Energies= -2015.668209
Sum of electronic and thermal Enthalpies= -2015.667265
Sum of electronic and thermal Free Energies= -2015.757266

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.105307	-0.426058	0.004040
2	15	0	-2.433043	-1.244467	0.166686
3	6	0	-3.211818	-1.318312	1.840993
4	6	0	-3.728469	-0.420197	-0.858493
5	6	0	-2.516349	-3.006697	-0.380987
6	6	0	-0.966185	1.281323	1.044165
7	6	0	2.002586	-0.335035	-0.050029
8	6	0	4.259032	0.201176	0.302177
9	7	0	2.850680	0.458272	0.629169
10	7	0	2.744327	-1.217293	-0.764292
11	6	0	4.172215	-1.144470	-0.421468
12	6	0	2.518413	1.550979	1.520035
13	6	0	2.260762	-2.456257	-1.351668
14	1	0	-3.372303	-0.308523	2.230304
15	1	0	-4.174892	-1.839682	1.801958
16	1	0	-2.533781	-1.837926	2.522606
17	1	0	-3.408614	-0.431325	-1.903079
18	1	0	-4.694857	-0.927062	-0.758322
19	1	0	-3.839195	0.622264	-0.543263
20	1	0	-3.539170	-3.395162	-0.320278
21	1	0	-2.157459	-3.070762	-1.411482
22	1	0	-1.865627	-3.611947	0.258355
23	1	0	-0.549940	1.283747	2.055273
24	1	0	-2.056763	1.230282	1.103620
25	1	0	4.868297	0.165777	1.210858
26	1	0	4.650739	0.999352	-0.344658
27	1	0	4.441979	-1.985754	0.233993
28	1	0	4.792129	-1.195658	-1.321812
29	1	0	3.222456	1.541641	2.360033
30	1	0	1.515547	1.406861	1.910290
31	1	0	2.582876	2.522976	1.015405
32	1	0	2.877875	-2.703996	-2.222061

33	1	0	1.233919	-2.331436	-1.692075
34	1	0	2.321955	-3.282368	-0.628272
35	17	0	0.323240	-1.351643	2.221325
36	6	0	0.226094	1.479304	-0.771650
37	6	0	-0.426543	2.272236	0.069072
38	6	0	-0.633252	3.773453	0.089944
39	6	0	-2.130657	4.133126	0.015937
40	6	0	0.154757	4.478644	-1.021861
41	1	0	0.787365	1.664737	-1.681436
42	1	0	-0.260814	4.143626	1.060370
43	1	0	-2.699454	3.660051	0.824412
44	1	0	-2.559255	3.803932	-0.938487
45	1	0	-2.274331	5.217466	0.097240
46	1	0	-0.186294	4.148581	-2.010373
47	1	0	1.227395	4.264778	-0.949914
48	1	0	0.020603	5.565070	-0.964499
49	17	0	-0.575582	-0.738266	-2.390965

19c

Zero-point correction= 0.412550
(Hartree/Particle)
Thermal correction to Energy= 0.442236
Thermal correction to Enthalpy= 0.443180
Thermal correction to Gibbs Free Energy= 0.353060
Sum of electronic and zero-point Energies= -2015.664464
Sum of electronic and thermal Energies= -2015.634778
Sum of electronic and thermal Enthalpies= -2015.633834
Sum of electronic and thermal Free Energies= -2015.723954

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.368003	-0.272893	-0.363382
2	15	0	-2.797448	0.056143	-0.162013
3	6	0	-3.592464	-0.859956	1.218971
4	6	0	-3.373910	1.788693	0.104259
5	6	0	-3.791471	-0.492585	-1.624436
6	6	0	-0.412302	-0.867045	-2.125195
7	6	0	1.695010	-0.746336	-0.039130
8	6	0	3.672715	-1.563594	0.917205
9	7	0	2.218608	-1.373485	1.022999
10	7	0	2.708765	-0.522140	-0.926342
11	6	0	3.936396	-1.239813	-0.552123
12	6	0	1.585069	-1.788704	2.266007
13	6	0	2.564445	-0.133216	-2.315843
14	1	0	-3.149607	-0.520782	2.157500
15	1	0	-4.673434	-0.677108	1.217195
16	1	0	-3.384773	-1.925391	1.101873
17	1	0	-3.131473	2.416754	-0.757685
18	1	0	-4.456901	1.811566	0.268808
19	1	0	-2.857211	2.182587	0.982941
20	1	0	-4.865391	-0.354484	-1.454589
21	1	0	-3.497510	0.072643	-2.515104
22	1	0	-3.590713	-1.552933	-1.805293
23	1	0	-0.402608	-0.229164	-3.022213
24	1	0	-0.518176	-1.933156	-2.359250
25	1	0	3.945897	-2.586638	1.193275
26	1	0	4.187748	-0.874458	1.601157

27	1	0	4.044415	-2.147243	-1.165021
28	1	0	4.820184	-0.613388	-0.708399
29	1	0	1.725893	-2.868157	2.392199
30	1	0	0.526780	-1.555361	2.245378
31	1	0	2.054165	-1.261131	3.106172
32	1	0	3.514073	0.292355	-2.658607
33	1	0	1.789982	0.624139	-2.413089
34	1	0	2.320448	-0.993388	-2.957277
35	17	0	-0.859315	-2.640413	0.188816
36	6	0	-0.397516	1.762323	-1.356236
37	6	0	0.450467	1.991868	-0.486605
38	6	0	1.428246	2.656202	0.405344
39	6	0	0.750383	3.855217	1.102106
40	6	0	2.682477	3.096919	-0.376572
41	1	0	-1.036034	1.957907	-2.193642
42	1	0	1.716858	1.945472	1.184685
43	1	0	-0.103265	3.511391	1.689972
44	1	0	0.410662	4.595221	0.367925
45	1	0	1.467016	4.342311	1.773852
46	1	0	2.423023	3.803569	-1.173134
47	1	0	3.194681	2.241347	-0.826036
48	1	0	3.382423	3.595777	0.303597
49	17	0	-0.633637	0.662438	2.125226

TS(19-20)c

Zero-point correction= 0.411948
(Hartree/Particle)
Thermal correction to Energy= 0.440961
Thermal correction to Enthalpy= 0.441905
Thermal correction to Gibbs Free Energy= 0.354012
Sum of electronic and zero-point Energies= -2015.640529
Sum of electronic and thermal Energies= -2015.611516
Sum of electronic and thermal Enthalpies= -2015.610572
Sum of electronic and thermal Free Energies= -2015.698464

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.033300	-0.376242	-0.140963
2	15	0	2.388379	-1.130531	-0.173650
3	6	0	2.545215	-2.875120	-0.776994
4	6	0	3.654002	-0.298599	-1.249549
5	6	0	3.227213	-1.219811	1.463235
6	17	0	-0.280480	-2.383540	1.204040
7	6	0	0.602061	1.873663	-0.865976
8	6	0	0.178359	1.306005	-1.882558
9	6	0	-0.177995	-1.058443	-1.886596
10	6	0	-2.077294	-0.073774	-0.055553
11	6	0	-4.381970	-0.540974	-0.247233
12	7	0	-3.000234	-0.960745	-0.522788
13	7	0	-2.762698	1.000037	0.393330
14	6	0	-4.203939	0.927741	0.127397
15	6	0	-2.831870	-2.364109	-0.862913
16	6	0	-2.228619	2.252268	0.889665
17	6	0	1.100918	3.036137	-0.086939

18	6	0	0.684496	4.336898	-0.805432
19	6	0	2.621996	2.986639	0.138566
20	17	0	0.530136	0.741757	2.165170
21	1	0	2.250476	-2.946547	-1.829220
22	1	0	3.576900	-3.230975	-0.679941
23	1	0	1.877621	-3.506260	-0.185660
24	1	0	3.834537	0.722339	-0.907080
25	1	0	4.602228	-0.847956	-1.236036
26	1	0	3.291327	-0.251011	-2.282199
27	1	0	4.225861	-1.662562	1.371853
28	1	0	3.290841	-0.221619	1.901470
29	1	0	2.604550	-1.826123	2.126047
30	1	0	-0.155980	1.188141	-2.891726
31	1	0	0.626078	-1.499411	-2.492720
32	1	0	-1.104036	-0.981624	-2.473893
33	1	0	-4.791016	-1.137427	0.581189
34	1	0	-5.019769	-0.694261	-1.124258
35	1	0	-4.777301	1.224829	1.011338
36	1	0	-4.469747	1.607807	-0.695849
37	1	0	-3.318133	-2.992053	-0.104924
38	1	0	-1.779851	-2.631022	-0.882942
39	1	0	-3.299809	-2.566585	-1.835638
40	1	0	-2.184081	3.011035	0.095045
41	1	0	-1.244987	2.073053	1.320731
42	1	0	-2.888633	2.623397	1.682035
43	1	0	0.638828	2.995356	0.902763
44	1	0	-0.400469	4.391283	-0.941069
45	1	0	1.155880	4.411720	-1.792235
46	1	0	0.999183	5.202249	-0.210968
47	1	0	3.168583	2.972347	-0.811422
48	1	0	2.890338	2.110367	0.731852
49	1	0	2.930640	3.878256	0.695494

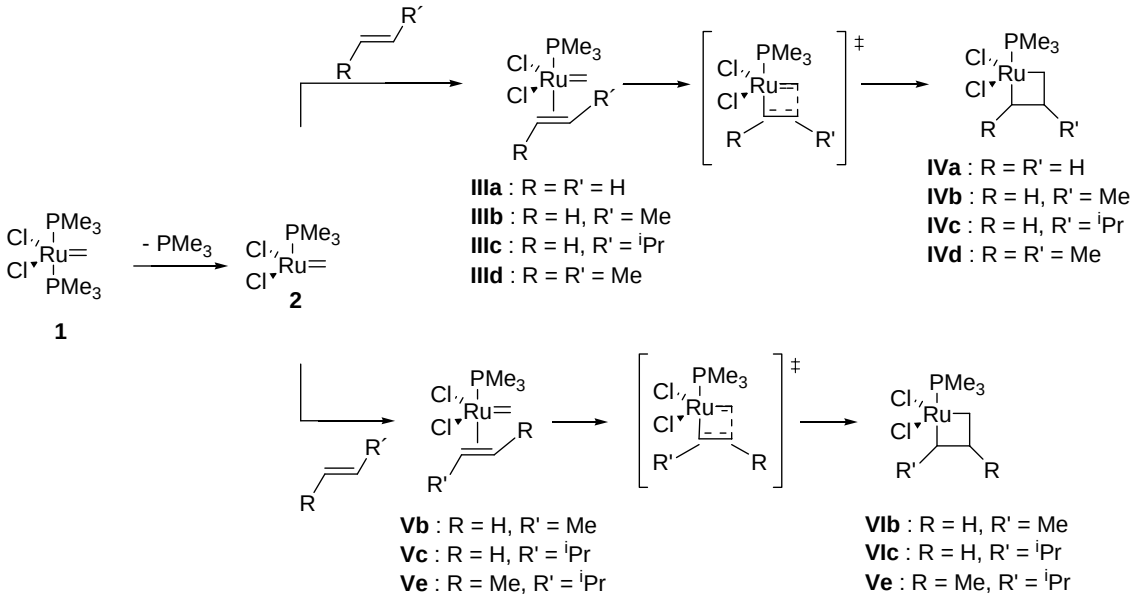
20c

Zero-point correction= 0.417032
(Hartree/Particle)
Thermal correction to Energy= 0.445595
Thermal correction to Enthalpy= 0.446540
Thermal correction to Gibbs Free Energy= 0.358618
Sum of electronic and zero-point Energies= -2015.709015
Sum of electronic and thermal Energies= -2015.680451
Sum of electronic and thermal Enthalpies= -2015.679507
Sum of electronic and thermal Free Energies= -2015.767429

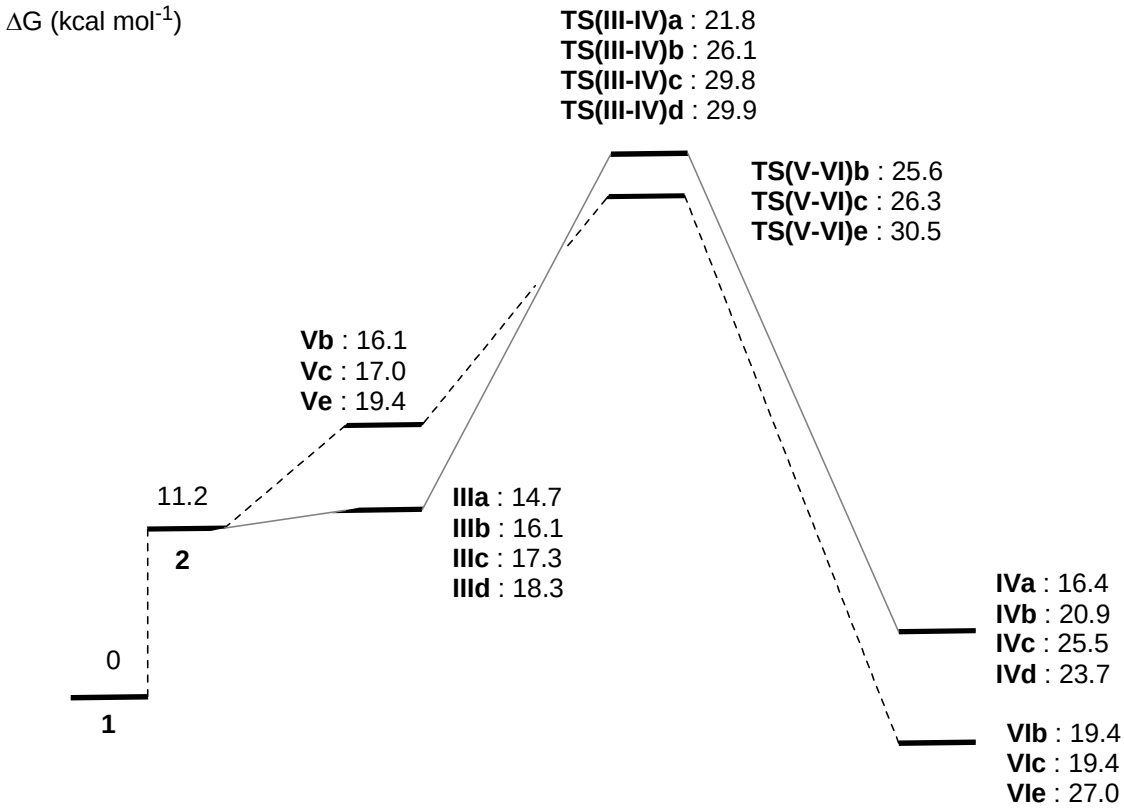
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.169530	-0.127893	-0.092153
2	15	0	2.537180	-0.796078	0.100269
3	6	0	3.114436	-2.030443	-1.149266
4	6	0	3.812186	0.540870	-0.052673
5	6	0	3.015185	-1.593555	1.686543
6	6	0	0.330001	1.666964	-0.602792
7	6	0	-0.110074	1.146743	-1.877302
8	6	0	0.580275	0.079404	-2.451765
9	6	0	-1.969320	-0.291229	-0.008330
10	6	0	-4.087169	-1.210779	-0.431020
11	7	0	-2.685399	-1.075081	-0.847695

12	7	0	-2.837653	0.293035	0.842571
13	6	0	-4.236319	-0.063990	0.567240
14	6	0	-2.203286	-2.027630	-1.831861
15	6	0	-2.615100	1.385089	1.770703
16	6	0	0.495783	3.064552	-0.110269
17	6	0	-0.747736	3.915467	-0.454327
18	6	0	1.757514	3.712864	-0.724078
19	1	0	3.072816	-1.618935	-2.161911
20	1	0	4.145352	-2.333719	-0.934386
21	1	0	2.453809	-2.898940	-1.092399
22	1	0	3.641939	1.281304	0.734459
23	1	0	4.824587	0.134772	0.053994
24	1	0	3.731662	1.038587	-1.024401
25	1	0	4.054968	-1.935898	1.627829
26	1	0	2.892550	-0.879215	2.501797
27	1	0	2.343832	-2.436191	1.862801
28	1	0	-1.121087	1.372481	-2.226254
29	1	0	1.661638	0.050516	-2.448101
30	1	0	0.097758	-0.518593	-3.219405
31	1	0	-4.235397	-2.194529	0.035749
32	1	0	-4.760263	-1.132641	-1.291054
33	1	0	-4.748721	-0.353789	1.490039
34	1	0	-4.763954	0.802501	0.141699
35	1	0	-2.371197	-3.052236	-1.481821
36	1	0	-1.136270	-1.900296	-1.978706
37	1	0	-2.745757	-1.872971	-2.774318
38	1	0	-3.115325	2.294107	1.403946
39	1	0	-1.549338	1.549912	1.904778
40	1	0	-3.043980	1.127632	2.746003
41	1	0	0.614028	3.023330	0.978018
42	1	0	-1.661678	3.485842	-0.034009
43	1	0	-0.875042	4.006717	-1.539616
44	1	0	-0.628009	4.924255	-0.043303
45	1	0	1.687168	3.751164	-1.817697
46	1	0	2.663872	3.164139	-0.455816
47	1	0	1.860770	4.739121	-0.353265
48	17	0	0.027051	-2.690259	0.357596
49	17	0	0.404440	0.317224	2.348116

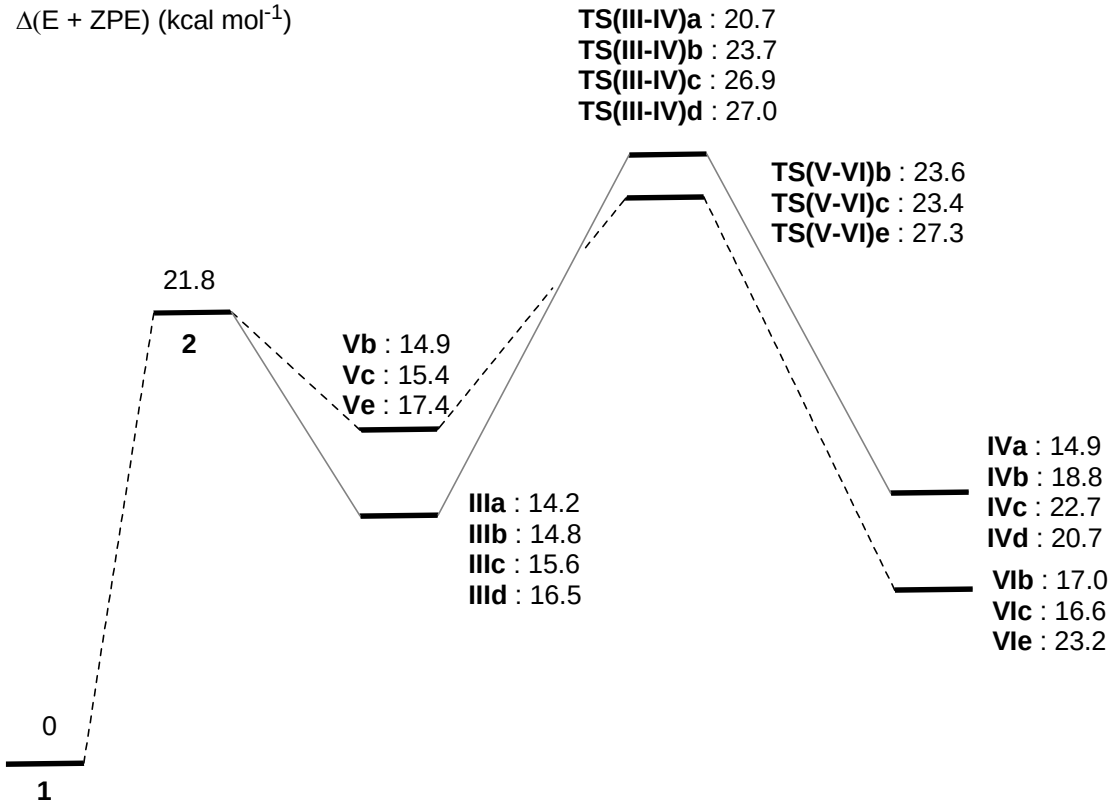
Alkene metathesis-First generation Grubbs catalyst



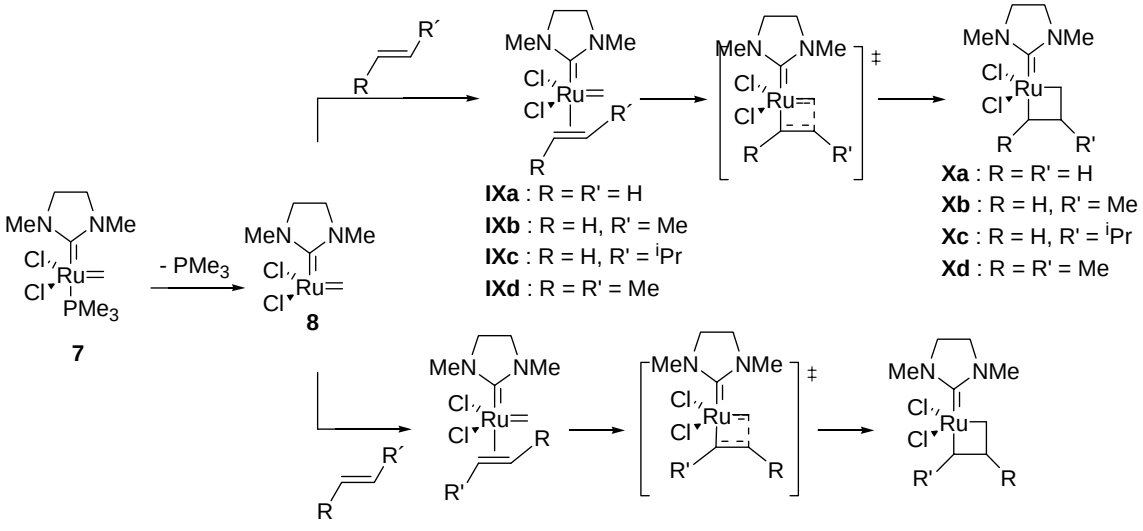
Relative energies for the stationary points involved in dissociative pathways



Relative energies for the stationary points involved in dissociative pathways



Alkene metathesis-Second generation Grubbs catalyst



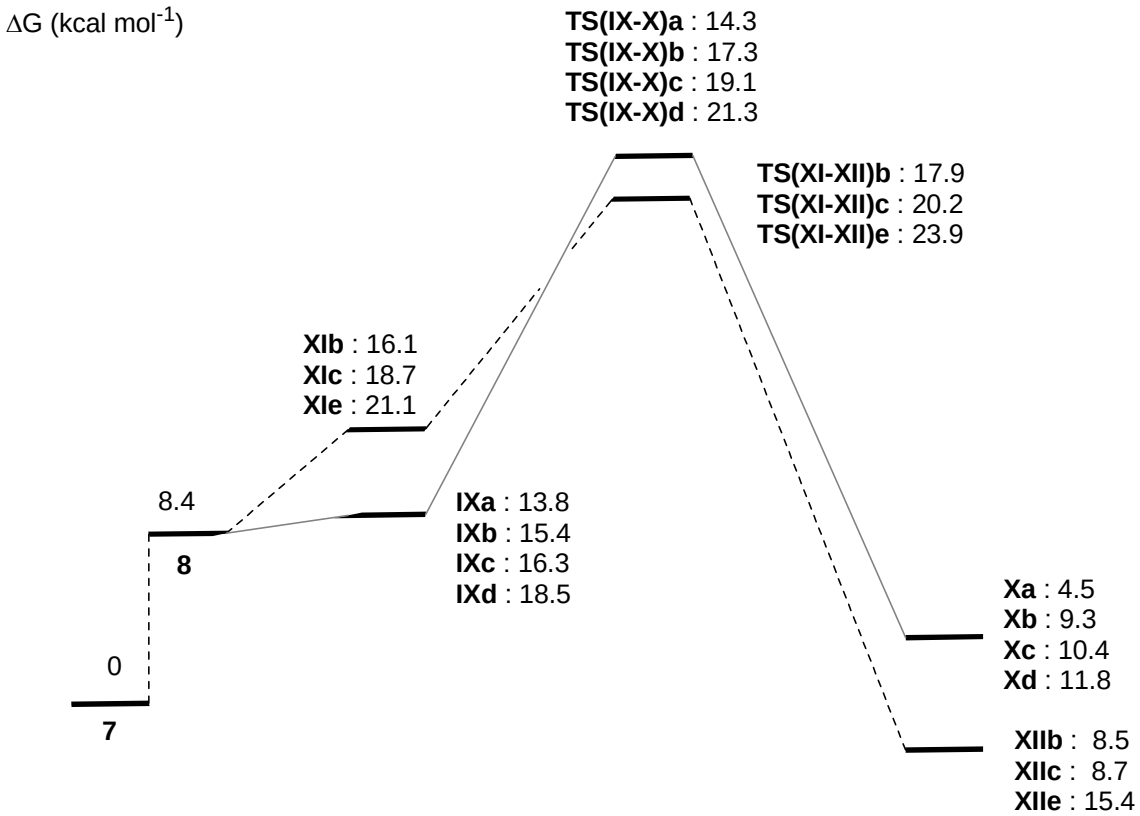
IXa : R = R' = H
IXb : R = H, R' = Me
IXc : R = H, R' = ^{i}Pr
IXd : R = R' = Me

Xa : R = R' = H
Xb : R = H, R' = Me
Xc : R = H, R' = ^{i}Pr
Xd : R = R' = Me

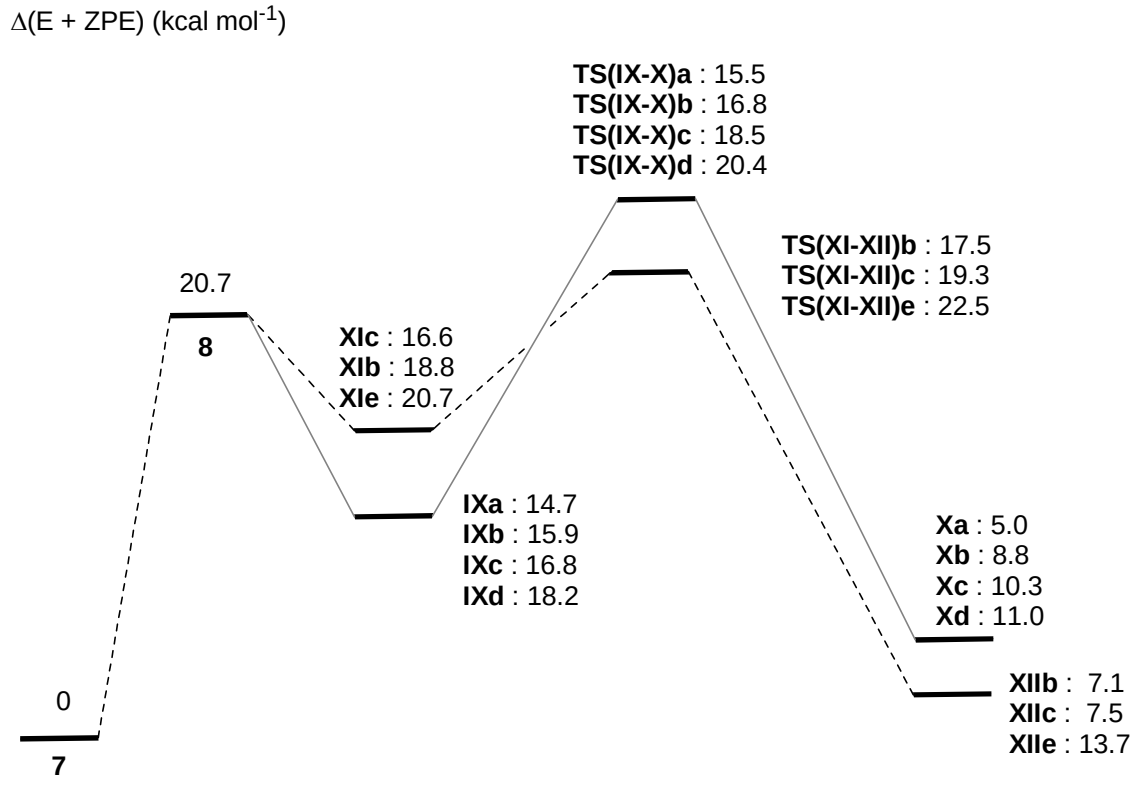
XIb : R = H, R' = Me
XIc : R = H, R' = ^{i}Pr
XIe : R = Me, R' = ^{i}Pr

XIIb : R = H, R' = Me
XIIc : R = H, R' = ^{i}Pr
XIIe : R = Me, R' = ^{i}Pr

Relative energies for the stationary points involved in dissociative pathways



Relative energies for the stationary points involved in dissociative pathways



Ethene

Zero-point correction= 0.051236
(Hartree/Particle)
Thermal correction to Energy= 0.054278
Thermal correction to Enthalpy= 0.055222
Thermal correction to Gibbs Free Energy= 0.029052
Sum of electronic and zero-point Energies= -78.534588
Sum of electronic and thermal Energies= -78.531546
Sum of electronic and thermal Enthalpies= -78.530602
Sum of electronic and thermal Free Energies= -78.556773

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.665624	-0.000000	-0.000296
2	6	0	-0.665624	0.000000	-0.000296
3	1	0	1.239931	0.923524	0.000897
4	1	0	1.239929	-0.923526	0.000880
5	1	0	-1.239932	-0.923524	0.000897
6	1	0	-1.239929	0.923526	0.000880

1-propene

Zero-point correction= 0.080096
(Hartree/Particle)
Thermal correction to Energy= 0.084172
Thermal correction to Enthalpy= 0.085116
Thermal correction to Gibbs Free Energy= 0.055095
Sum of electronic and zero-point Energies= -117.825117
Sum of electronic and thermal Energies= -117.821042
Sum of electronic and thermal Enthalpies= -117.820097
Sum of electronic and thermal Free Energies= -117.850118

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.283228	0.220541	-0.000088
2	6	0	-0.133820	-0.455881	-0.000213
3	6	0	1.235103	0.162992	0.000044
4	1	0	-2.245576	-0.284532	0.000723
5	1	0	-1.305246	1.308809	0.000071
6	1	0	-0.163921	-1.546608	0.000302
7	1	0	1.811749	-0.148580	0.881705
8	1	0	1.181217	1.256954	-0.002016
9	1	0	1.813445	-0.151958	-0.879243

3-methyl-1-butene

Zero-point correction= 0.137322
(Hartree/Particle)
Thermal correction to Energy= 0.143842
Thermal correction to Enthalpy= 0.144787
Thermal correction to Gibbs Free Energy= 0.107910
Sum of electronic and zero-point Energies= -196.394462
Sum of electronic and thermal Energies= -196.387942
Sum of electronic and thermal Enthalpies= -196.386998

Sum of electronic and thermal Free Energies= -196.423874

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.153959	0.000007	-0.161975
2	6	0	0.951908	-0.000005	0.415537
3	6	0	-0.371777	-0.000008	-0.309485
4	6	0	-1.178669	1.268190	0.028209
5	6	0	-1.178724	-1.268149	0.028159
6	1	0	3.071314	-0.000162	0.421127
7	1	0	2.267682	0.000093	-1.244620
8	1	0	0.886368	-0.000221	1.506479
9	1	0	-0.167896	0.000031	-1.389594
10	1	0	-2.138278	1.274390	-0.502766
11	1	0	-0.627700	2.173545	-0.248724
12	1	0	-1.392724	1.321516	1.103544
13	1	0	-2.138230	-1.274423	-0.503004
14	1	0	-1.393015	-1.321435	1.103450
15	1	0	-0.627699	-2.173539	-0.248558

2-butene

Zero-point correction= 0.108557
(Hartree/Particle)
Thermal correction to Energy= 0.114011
Thermal correction to Enthalpy= 0.114955
Thermal correction to Gibbs Free Energy= 0.081180
Sum of electronic and zero-point Energies= -157.115314
Sum of electronic and thermal Energies= -157.109860
Sum of electronic and thermal Enthalpies= -157.108916
Sum of electronic and thermal Free Energies= -157.142690

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.538159	0.395571	-0.000033
2	6	0	0.538153	-0.395530	0.000025
3	6	0	1.963799	0.079239	0.000004
4	6	0	-1.963794	-0.079266	0.000011
5	1	0	-0.392426	1.477906	0.000019
6	1	0	0.392390	-1.477862	-0.000079
7	1	0	2.508205	-0.289037	0.880508
8	1	0	2.022922	1.173232	-0.000037
9	1	0	2.508177	-0.289122	-0.880477
10	1	0	-2.508232	0.289059	0.880474
11	1	0	-2.022846	-1.173262	0.000057
12	1	0	-2.508183	0.289003	-0.880502

4-methyl-2-pentene

Zero-point correction= 0.165600
(Hartree/Particle)

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 Thermal correction to Energy=                  0.173614
 Thermal correction to Enthalpy=                0.174558
 Thermal correction to Gibbs Free Energy=       0.133946
 Sum of electronic and zero-point Energies=          -235.684795
 Sum of electronic and thermal Energies=             -235.676781
 Sum of electronic and thermal Enthalpies=           -235.675837
 Sum of electronic and thermal Free Energies=        -235.716449

 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.373811   -0.000381    0.271949
    2          6             0       -1.515133    0.000411   -0.421997
    3          6             0        1.015100    0.000022   -0.318710
    4          6             0        1.787776    1.267512    0.094522
    5          6             0        1.788094   -1.267334    0.094036
    6          6             0       -2.894666   -0.000164    0.174398
    7          1             0       -0.420147   -0.001415    1.364762
    8          1             0       -1.464811    0.001360   -1.512986
    9          1             0        0.919605    0.000319   -1.413937
   10          1             0        1.897653    1.320596    1.185483
   11          1             0        1.266301    2.173413   -0.233274
   12          1             0        2.794177    1.273681   -0.341723
   13          1             0        1.266850   -2.173365   -0.233812
   14          1             0        1.898233   -1.320624    1.184970
   15          1             0        2.794437   -1.273303   -0.342373
   16          1             0       -2.858993   -0.000845    1.269337
   17          1             0       -3.468493   -0.880564   -0.146416
   18          1             0       -3.468973    0.880349   -0.145219
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IIIa

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Zero-point correction=                           0.196986
(Hartree/Particle)
 Thermal correction to Energy=                  0.214483
 Thermal correction to Enthalpy=                0.215427
 Thermal correction to Gibbs Free Energy=       0.151443
 Sum of electronic and zero-point Energies=         -1593.158024
 Sum of electronic and thermal Energies=            -1593.140527
 Sum of electronic and thermal Enthalpies=          -1593.139583
 Sum of electronic and thermal Free Energies=       -1593.203567

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 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1         17             0        0.626081   -2.275166   -0.553060
    2         44             0        0.553657    0.016194    0.130212
    3          6             0        2.930480    0.119289   -0.747073
    4         17             0        0.510034    2.321291   -0.517793
    5         15             0       -1.764140   -0.030469   -0.009677
    6          6             0       -2.298099   -0.032836   -1.770515
    7          6             0       -2.652472    1.396278    0.741191
    8          6             0       -2.585766   -1.505110    0.724237
    9          6             0        3.069137   -0.100056    0.579375
   10          6             0        0.465952    0.013899    1.958460
   11          1             0        2.868550   -0.709254   -1.446962
   12          1             0        2.952799    1.123795   -1.156958
   13          1             0       -3.390428   -0.060594   -1.852516
```

14	1	0	-1.873049	-0.908690	-2.269375
15	1	0	-1.918797	0.870000	-2.257925
16	1	0	-2.267729	2.320111	0.302814
17	1	0	-2.462327	1.424807	1.818567
18	1	0	-3.732077	1.319379	0.572184
19	1	0	-2.150880	-2.405589	0.284200
20	1	0	-3.666198	-1.481699	0.544944
21	1	0	-2.404794	-1.530314	1.803271
22	1	0	3.220364	0.726372	1.268111
23	1	0	3.126383	-1.107063	0.981590
24	1	0	1.372618	0.017932	2.572068
25	1	0	-0.462582	0.012390	2.542257

IIIb

Zero-point correction= 0.225666
(Hartree/Particle)
Thermal correction to Energy= 0.244545
Thermal correction to Enthalpy= 0.245489
Thermal correction to Gibbs Free Energy= 0.178699
Sum of electronic and zero-point Energies= -1632.447607
Sum of electronic and thermal Energies= -1632.428728
Sum of electronic and thermal Enthalpies= -1632.427784
Sum of electronic and thermal Free Energies= -1632.494575

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.025428	2.428512	-0.451300
2	44	0	-0.335928	0.107538	0.023939
3	6	0	-2.598634	0.503361	-1.089371
4	17	0	-0.592706	-2.121847	-0.809274
5	15	0	1.951141	-0.203008	0.109840
6	6	0	2.662284	-0.147428	-1.585689
7	6	0	2.534153	-1.807847	0.800286
8	6	0	2.909569	1.056580	1.051064
9	6	0	-3.017632	0.489510	0.197021
10	6	0	-0.450329	0.001441	1.843022
11	6	0	-3.682889	-0.681115	0.861817
12	1	0	-2.271583	1.424444	-1.560880
13	1	0	-2.687498	-0.380735	-1.714762
14	1	0	3.748672	-0.287796	-1.562743
15	1	0	2.427545	0.821704	-2.035354
16	1	0	2.204737	-0.937107	-2.188705
17	1	0	2.055791	-2.622738	0.251885
18	1	0	2.243562	-1.886471	1.852533
19	1	0	3.624004	-1.891428	0.724722
20	1	0	2.675960	2.047243	0.654130
21	1	0	3.985384	0.864232	0.974757
22	1	0	2.618145	1.032810	2.105755
23	1	0	-2.970609	1.420120	0.762637
24	1	0	-1.420016	0.089977	2.344230
25	1	0	0.391398	-0.147436	2.530369
26	1	0	-3.293858	-0.858091	1.871701
27	1	0	-3.555776	-1.596459	0.277812
28	1	0	-4.757530	-0.479154	0.971848

IIIc

Zero-point correction= 0.282788
(Hartree/Particle)
Thermal correction to Energy= 0.304257
Thermal correction to Enthalpy= 0.305201
Thermal correction to Gibbs Free Energy= 0.232050
Sum of electronic and zero-point Energies= -1711.015678
Sum of electronic and thermal Energies= -1710.994209
Sum of electronic and thermal Enthalpies= -1710.993264
Sum of electronic and thermal Free Energies= -1711.066415

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.438890	2.393583	-0.617985
2	44	0	0.139889	0.083023	-0.063038
3	6	0	-2.023225	0.238002	-1.430485
4	17	0	0.098560	-2.193167	-0.817409
5	15	0	2.411479	-0.120578	0.267360
6	6	0	3.293459	-0.165023	-1.346667
7	6	0	2.971288	-1.642500	1.138758
8	6	0	3.223550	1.245751	1.196902
9	6	0	-2.569815	0.706938	-0.285545
10	6	0	-0.162986	0.015913	1.732803
11	6	0	-3.528368	-0.028523	0.621610
12	6	0	-3.725165	-1.509190	0.275988
13	6	0	-4.874971	0.729889	0.635396
14	1	0	-1.497524	0.911429	-2.102322
15	1	0	-2.192720	-0.774060	-1.780775
16	1	0	4.375006	-0.266225	-1.202721
17	1	0	3.083933	0.759417	-1.892686
18	1	0	2.920942	-1.012239	-1.929581
19	1	0	2.584724	-2.514551	0.606343
20	1	0	2.568585	-1.656074	2.156238
21	1	0	4.064820	-1.684104	1.188499
22	1	0	3.003620	2.192348	0.697929
23	1	0	4.306735	1.090008	1.250056
24	1	0	2.820094	1.293681	2.212999
25	1	0	-2.394290	1.751978	-0.030875
26	1	0	-1.189142	0.081538	2.111927
27	1	0	0.596404	-0.096910	2.516263
28	1	0	-3.130510	0.033289	1.647470
29	1	0	-2.774561	-2.051839	0.258505
30	1	0	-4.199473	-1.625207	-0.706041
31	1	0	-4.379575	-1.984395	1.015415
32	1	0	-5.344840	0.703599	-0.354704
33	1	0	-4.743940	1.780510	0.919106
34	1	0	-5.564857	0.268881	1.351373

IIId

Zero-point correction= 0.253870
(Hartree/Particle)
Thermal correction to Energy= 0.274287
Thermal correction to Enthalpy= 0.275231
Thermal correction to Gibbs Free Energy= 0.205161
Sum of electronic and zero-point Energies= -1671.735023

Sum of electronic and thermal Energies= -1671.714606
Sum of electronic and thermal Enthalpies= -1671.713662
Sum of electronic and thermal Free Energies= -1671.783732

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.264061	-2.205362	0.768443
2	44	0	-0.210395	0.010871	-0.153069
3	17	0	-0.066560	2.379089	0.253657
4	15	0	2.094786	-0.064824	-0.037033
5	6	0	2.677427	0.094419	1.700669
6	6	0	2.998648	1.256303	-0.947164
7	6	0	2.875061	-1.618683	-0.643176
8	6	0	-0.162590	-0.145990	-1.966174
9	1	0	3.771041	0.052914	1.755460
10	1	0	2.250732	-0.720253	2.292852
11	1	0	2.328306	1.048251	2.106589
12	1	0	2.639995	2.230010	-0.606411
13	1	0	2.794823	1.172171	-2.019113
14	1	0	4.078489	1.172006	-0.782449
15	1	0	2.451603	-2.465214	-0.098324
16	1	0	3.961645	-1.587368	-0.506967
17	1	0	2.653210	-1.750614	-1.706613
18	1	0	-1.100960	-0.161656	-2.529679
19	1	0	0.737755	-0.214546	-2.589372
20	6	0	-2.685961	0.546105	0.575362
21	6	0	-2.930728	-0.478195	-0.277167
22	6	0	-3.474374	-0.317395	-1.668503
23	6	0	-2.491236	0.400466	2.063110
24	1	0	-2.789734	1.565630	0.207101
25	1	0	-2.871812	-1.496476	0.102734
26	1	0	-3.002804	-1.006209	-2.379230
27	1	0	-3.364620	0.707812	-2.038048
28	1	0	-4.546232	-0.560333	-1.670286
29	1	0	-1.684960	1.046811	2.427579
30	1	0	-2.279994	-0.634174	2.347415
31	1	0	-3.407799	0.719750	2.579839

TS(III-IV)a

Zero-point correction= 0.198069
(Hartree/Particle)
Thermal correction to Energy= 0.214360
Thermal correction to Enthalpy= 0.215304
Thermal correction to Gibbs Free Energy= 0.153487
Sum of electronic and zero-point Energies= -1593.147655
Sum of electronic and thermal Energies= -1593.131364
Sum of electronic and thermal Enthalpies= -1593.130420
Sum of electronic and thermal Free Energies= -1593.192238

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.423164	-2.438917	-0.156019
2	44	0	0.560660	0.002321	-0.022544
3	6	0	2.479457	-0.101851	-1.084565
4	17	0	0.685619	2.432926	-0.162587
5	15	0	-1.822675	0.063366	0.009557

6	6	0	-2.421589	-0.358365	-1.681571
7	6	0	-2.637044	1.658527	0.420921
8	6	0	-2.624708	-1.172211	1.109509
9	6	0	2.925956	-0.126363	0.246892
10	6	0	1.234891	-0.024757	1.695386
11	1	0	2.432516	-1.035055	-1.639234
12	1	0	2.536955	0.830005	-1.640260
13	1	0	-3.516672	-0.361970	-1.717293
14	1	0	-2.041330	-1.348081	-1.950046
15	1	0	-2.045282	0.375101	-2.401678
16	1	0	-2.229503	2.443488	-0.219980
17	1	0	-2.405499	1.924818	1.456284
18	1	0	-3.723311	1.585723	0.296752
19	1	0	-2.201302	-2.156079	0.893447
20	1	0	-3.709997	-1.180311	0.959195
21	1	0	-2.409175	-0.922001	2.152776
22	1	0	3.329828	0.782727	0.681826
23	1	0	3.222929	-1.074966	0.683452
24	1	0	1.470297	0.901154	2.230236
25	1	0	1.369543	-0.965204	2.240001

TS(III-IV)b

Zero-point correction= 0.227121
(Hartree/Particle)
Thermal correction to Energy= 0.244503
Thermal correction to Enthalpy= 0.245447
Thermal correction to Gibbs Free Energy= 0.181816
Sum of electronic and zero-point Energies= -1632.433353
Sum of electronic and thermal Energies= -1632.415971
Sum of electronic and thermal Enthalpies= -1632.415026
Sum of electronic and thermal Free Energies= -1632.478658

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.107620	-2.493899	-0.131345
2	44	0	0.347839	-0.082933	-0.073804
3	6	0	2.088667	-0.461933	-1.265220
4	17	0	0.719768	2.318741	-0.260455
5	15	0	-2.020784	0.249893	0.073026
6	6	0	-2.788673	-0.240886	-1.528217
7	6	0	-2.644212	1.948616	0.396952
8	6	0	-2.848795	-0.801109	1.334162
9	6	0	2.699587	-0.550071	0.022987
10	6	0	1.239712	-0.234312	1.543204
11	6	0	3.721430	0.486554	0.447492
12	1	0	1.867530	-1.385585	-1.793539
13	1	0	2.285472	0.426814	-1.862171
14	1	0	-3.878549	-0.136273	-1.485719
15	1	0	-2.524783	-1.281209	-1.737504
16	1	0	-2.402354	0.392735	-2.332884
17	1	0	-2.236839	2.631286	-0.352010
18	1	0	-2.288096	2.284213	1.374857
19	1	0	-3.739645	1.970418	0.377964
20	1	0	-2.539718	-1.837242	1.177676
21	1	0	-3.938262	-0.710908	1.259908
22	1	0	-2.530121	-0.487734	2.332935
23	1	0	2.835753	-1.565589	0.390495

24	1	0	1.629747	0.651457	2.051941
25	1	0	1.280399	-1.182677	2.087505
26	1	0	3.987838	0.399323	1.504487
27	1	0	3.350260	1.496105	0.250941
28	1	0	4.635406	0.332019	-0.140441

TS(III-IV)c

Zero-point correction= 0.284099
(Hartree/Particle)
Thermal correction to Energy= 0.304199
Thermal correction to Enthalpy= 0.305143
Thermal correction to Gibbs Free Energy= 0.235129
Sum of electronic and zero-point Energies= -1710.997563
Sum of electronic and thermal Energies= -1710.977463
Sum of electronic and thermal Enthalpies= -1710.976518
Sum of electronic and thermal Free Energies= -1711.046533

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.408991	2.573217	-0.131882
2	44	0	0.102143	0.152901	-0.084340
3	6	0	-1.644648	0.347094	-1.302085
4	17	0	-0.031295	-2.290916	-0.304564
5	15	0	2.471993	-0.186920	0.098507
6	6	0	3.116552	-0.787868	-1.519012
7	6	0	2.969557	-1.474579	1.313250
8	6	0	3.517759	1.267515	0.511454
9	6	0	-2.234949	0.654490	-0.030198
10	6	0	-0.872442	0.235484	1.491966
11	6	0	-3.466498	-0.089463	0.514191
12	6	0	-3.526438	-1.592256	0.219955
13	6	0	-4.705354	0.631659	-0.063178
14	1	0	-1.400546	1.184411	-1.952635
15	1	0	-1.879234	-0.599574	-1.781072
16	1	0	4.191328	-0.991722	-1.456115
17	1	0	2.943681	-0.030966	-2.290695
18	1	0	2.579759	-1.701194	-1.789269
19	1	0	2.402265	-2.384535	1.105028
20	1	0	2.726875	-1.132467	2.323902
21	1	0	4.045706	-1.671065	1.249370
22	1	0	3.316958	2.070729	-0.200766
23	1	0	4.579579	0.997017	0.493841
24	1	0	3.250362	1.636001	1.505701
25	1	0	-2.236652	1.719639	0.195794
26	1	0	-1.249576	-0.676199	1.963009
27	1	0	-0.955704	1.162458	2.066992
28	1	0	-3.496996	0.052106	1.601949
29	1	0	-2.633917	-2.120767	0.562959
30	1	0	-3.627341	-1.785546	-0.853921
31	1	0	-4.403749	-2.024623	0.714677
32	1	0	-4.748190	0.522013	-1.153153
33	1	0	-4.701963	1.702222	0.171291
34	1	0	-5.618906	0.196650	0.357989

TS(III-IV)d

Zero-point correction= 0.255149
(Hartree/Particle)
Thermal correction to Energy= 0.274083
Thermal correction to Enthalpy= 0.275027
Thermal correction to Gibbs Free Energy= 0.208317
Sum of electronic and zero-point Energies= -1671.718353
Sum of electronic and thermal Energies= -1671.699419
Sum of electronic and thermal Enthalpies= -1671.698475
Sum of electronic and thermal Free Energies= -1671.765185

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.044386	-2.404435	-0.419875
2	44	0	-0.250426	0.013318	-0.042319
3	6	0	-2.169720	-0.195674	0.978632
4	17	0	-0.409640	2.402561	0.446414
5	15	0	2.142589	0.139974	0.033332
6	6	0	2.772893	-0.787054	1.496325
7	6	0	2.933995	1.794870	0.153038
8	6	0	2.960086	-0.659048	-1.408173
9	6	0	-2.614096	-0.210446	-0.378047
10	6	0	-0.980022	0.199620	-1.731405
11	6	0	-3.506749	0.912483	-0.879576
12	6	0	-2.204749	-1.418188	1.868698
13	1	0	-2.304122	0.755873	1.494576
14	1	0	3.868418	-0.786006	1.517411
15	1	0	2.402898	-1.814376	1.440690
16	1	0	2.400747	-0.324591	2.416226
17	1	0	2.558942	2.314420	1.037638
18	1	0	2.654930	2.392866	-0.718462
19	1	0	4.024598	1.699432	0.203300
20	1	0	2.549177	-1.664748	-1.523783
21	1	0	4.045199	-0.703667	-1.261878
22	1	0	2.744218	-0.083259	-2.313243
23	1	0	-2.781055	-1.200038	-0.801665
24	1	0	-1.242840	1.183192	-2.130192
25	1	0	-1.060250	-0.652748	-2.413554
26	1	0	-3.632958	0.895173	-1.965814
27	1	0	-3.113052	1.887220	-0.578003
28	1	0	-4.500309	0.788693	-0.428487
29	1	0	-1.435161	-1.367870	2.647692
30	1	0	-2.063229	-2.342444	1.307277
31	1	0	-3.176736	-1.450249	2.384235

IVa

Zero-point correction= 0.200707
(Hartree/Particle)
Thermal correction to Energy= 0.216726
Thermal correction to Enthalpy= 0.217670
Thermal correction to Gibbs Free Energy= 0.156847
Sum of electronic and zero-point Energies= -1593.156941
Sum of electronic and thermal Energies= -1593.140922
Sum of electronic and thermal Enthalpies= -1593.139978
Sum of electronic and thermal Free Energies= -1593.200801

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.340934	-2.431387	0.000288
2	44	0	-0.551040	0.006573	0.000189
3	6	0	-1.983940	-0.089461	1.352575
4	17	0	-0.690853	2.430666	0.000198
5	15	0	1.832013	0.086135	-0.000262
6	6	0	2.502094	-0.792493	1.468189
7	6	0	2.649976	1.729764	-0.001821
8	6	0	2.502878	-0.795950	-1.466156
9	6	0	-2.807793	-0.157536	-0.000990
10	6	0	-1.982799	-0.089371	-1.353489
11	1	0	-2.021475	-1.015112	1.925712
12	1	0	-2.155835	0.826929	1.915571
13	1	0	3.596945	-0.819901	1.433783
14	1	0	2.095756	-1.806757	1.478382
15	1	0	2.187051	-0.275680	2.379920
16	1	0	2.332276	2.293844	0.878333
17	1	0	2.331234	2.292803	-0.882253
18	1	0	3.739885	1.615396	-0.002374
19	1	0	2.095054	-1.809641	-1.475004
20	1	0	3.597620	-0.825082	-1.429739
21	1	0	2.190173	-0.280419	-2.379395
22	1	0	-3.468004	0.710821	-0.001122
23	1	0	-3.323594	-1.118369	-0.001119
24	1	0	-2.154122	0.827280	-1.916187
25	1	0	-2.019532	-1.014802	-1.926994

IVb

Zero-point correction= 0.228962
(Hartree/Particle)
Thermal correction to Energy= 0.246457
Thermal correction to Enthalpy= 0.247401
Thermal correction to Gibbs Free Energy= 0.183169
Sum of electronic and zero-point Energies= -1632.441222
Sum of electronic and thermal Energies= -1632.423728
Sum of electronic and thermal Enthalpies= -1632.422783
Sum of electronic and thermal Free Energies= -1632.487015

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.118746	-2.478772	-0.000908
2	44	0	0.331488	-0.073187	-0.001128
3	6	0	1.754088	-0.335671	-1.342950
4	17	0	0.686357	2.331244	-0.001463
5	15	0	-2.030657	0.244208	0.000285
6	6	0	-2.789836	-0.566817	-1.463622
7	6	0	-2.688649	1.958406	-0.001504
8	6	0	-2.783690	-0.561775	1.470151
9	6	0	2.584492	-0.521459	0.001382
10	6	0	1.751344	-0.335204	1.343662
11	6	0	3.786465	0.436600	0.002384
12	1	0	1.679820	-1.251376	-1.928804
13	1	0	2.035306	0.558380	-1.900494
14	1	0	-3.881208	-0.473754	-1.430033

15	1	0	-2.496276	-1.619254	-1.467024
16	1	0	-2.420284	-0.092883	-2.378205
17	1	0	-2.321135	2.487894	-0.883711
18	1	0	-2.317463	2.491198	0.877146
19	1	0	-3.784496	1.945277	0.000707
20	1	0	-2.490687	-1.614364	1.475457
21	1	0	-3.875148	-0.468205	1.441189
22	1	0	-2.409707	-0.085201	2.381549
23	1	0	2.859985	-1.578987	0.001742
24	1	0	2.031302	0.559082	1.901469
25	1	0	1.675747	-1.250692	1.929707
26	1	0	4.404582	0.269213	0.890632
27	1	0	3.443121	1.475113	0.002048
28	1	0	4.406237	0.269169	-0.884702

IVc

Zero-point correction= 0.286027
(Hartree/Particle)
Thermal correction to Energy= 0.306219
Thermal correction to Enthalpy= 0.307164
Thermal correction to Gibbs Free Energy= 0.236912
Sum of electronic and zero-point Energies= -1711.004301
Sum of electronic and thermal Energies= -1710.984108
Sum of electronic and thermal Enthalpies= -1710.983164
Sum of electronic and thermal Free Energies= -1711.053416

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.469237	2.592029	-0.087517
2	44	0	-0.115868	0.201332	-0.046705
3	6	0	1.429931	0.358447	1.187455
4	17	0	0.074225	-2.257393	0.014229
5	15	0	-2.459559	-0.243362	0.085800
6	6	0	-2.875609	-1.202715	1.596184
7	6	0	-3.018112	-1.260079	-1.338707
8	6	0	-3.592548	1.202996	0.112868
9	6	0	2.136340	0.642365	-0.197767
10	6	0	1.246166	0.291144	-1.471365
11	6	0	3.537598	-0.055063	-0.307464
12	6	0	3.547448	-1.584322	-0.202467
13	6	0	4.498538	0.573760	0.715344
14	1	0	1.403715	1.236626	1.832367
15	1	0	1.731112	-0.567163	1.675594
16	1	0	-3.943034	-1.450260	1.610150
17	1	0	-2.635899	-0.609127	2.483879
18	1	0	-2.270726	-2.112132	1.602972
19	1	0	-2.423318	-2.175897	-1.363117
20	1	0	-2.857236	-0.706204	-2.268805
21	1	0	-4.083944	-1.496352	-1.243975
22	1	0	-3.350280	1.839414	0.967367
23	1	0	-4.635087	0.870792	0.176253
24	1	0	-3.444555	1.799229	-0.790708
25	1	0	2.261436	1.726635	-0.238535
26	1	0	1.500690	-0.655503	-1.946429
27	1	0	1.152616	1.141055	-2.147909
28	1	0	3.901520	0.213859	-1.308937
29	1	0	2.876130	-2.061038	-0.920347

30	1	0	3.250071	-1.928719	0.792955
31	1	0	4.564844	-1.948074	-0.390264
32	1	0	4.210431	0.318319	1.741912
33	1	0	4.522911	1.666493	0.631878
34	1	0	5.516848	0.201873	0.553149

IVd

Zero-point correction= 0.257303
(Hartree/Particle)
Thermal correction to Energy= 0.276274
Thermal correction to Enthalpy= 0.277218
Thermal correction to Gibbs Free Energy= 0.210472
Sum of electronic and zero-point Energies= -1671.728323
Sum of electronic and thermal Energies= -1671.709352
Sum of electronic and thermal Enthalpies= -1671.708408
Sum of electronic and thermal Free Energies= -1671.775153

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.095115	-2.386324	-0.537480
2	44	0	-0.233354	0.008229	-0.109846
3	6	0	-1.814310	-0.179700	1.073420
4	17	0	-0.390438	2.428847	0.179480
5	15	0	2.137668	0.155190	0.097991
6	6	0	2.789687	-1.023834	1.349346
7	6	0	2.899012	1.770008	0.528541
8	6	0	2.911811	-0.335849	-1.495966
9	6	0	-2.495090	-0.204376	-0.389790
10	6	0	-1.532916	0.092580	-1.601808
11	6	0	-3.641444	0.824027	-0.386265
12	6	0	-2.056041	-1.389918	1.945952
13	1	0	-2.043781	0.765035	1.572307
14	1	0	3.885295	-1.002796	1.361987
15	1	0	2.429516	-2.025162	1.102058
16	1	0	2.417919	-0.749519	2.341614
17	1	0	2.524820	2.101431	1.500324
18	1	0	2.602336	2.519284	-0.208532
19	1	0	3.990696	1.678824	0.561240
20	1	0	2.549401	-1.331107	-1.765053
21	1	0	4.003843	-0.341011	-1.405461
22	1	0	2.621645	0.372612	-2.277846
23	1	0	-2.834772	-1.234899	-0.518052
24	1	0	-1.676149	1.078505	-2.044580
25	1	0	-1.460700	-0.732122	-2.310445
26	1	0	-4.188831	0.779902	-1.333809
27	1	0	-3.241937	1.833622	-0.255560
28	1	0	-4.343948	0.613457	0.427242
29	1	0	-1.454566	-1.318147	2.859784
30	1	0	-1.810997	-2.324792	1.439936
31	1	0	-3.110999	-1.413546	2.261608

Vb

Zero-point correction= 0.225656
(Hartree/Particle)
Thermal correction to Energy= 0.244581
Thermal correction to Enthalpy= 0.245525
Thermal correction to Gibbs Free Energy= 0.178386
Sum of electronic and zero-point Energies= -1632.447347
Sum of electronic and thermal Energies= -1632.428422
Sum of electronic and thermal Enthalpies= -1632.427478
Sum of electronic and thermal Free Energies= -1632.494616

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.361932	2.325220	0.329466
2	44	0	0.355736	0.007917	-0.312476
3	6	0	2.935312	0.434440	0.042110
4	17	0	0.474429	-2.263932	0.444494
5	15	0	-1.913635	-0.025773	0.172554
6	6	0	-2.194076	0.002247	1.990565
7	6	0	-2.838104	-1.507076	-0.412187
8	6	0	-2.907423	1.387933	-0.464259
9	6	0	2.806898	-0.429038	-0.992643
10	6	0	0.009980	-0.004128	-2.104700
11	6	0	3.150296	0.043600	1.477509
12	1	0	2.976028	1.499872	-0.171499
13	1	0	-3.264067	-0.017866	2.225117
14	1	0	-1.746221	0.910896	2.403125
15	1	0	-1.705140	-0.868238	2.437306
16	1	0	-2.356573	-2.403743	-0.015530
17	1	0	-2.805329	-1.555267	-1.505064
18	1	0	-3.883902	-1.465571	-0.088307
19	1	0	-2.467664	2.320057	-0.102458
20	1	0	-3.949298	1.309233	-0.134770
21	1	0	-2.880778	1.398530	-1.558313
22	1	0	2.831071	-1.504761	-0.848774
23	1	0	2.808085	-0.065509	-2.015801
24	1	0	0.830679	-0.016179	-2.829566
25	1	0	-0.987523	0.009430	-2.561149
26	1	0	4.182523	0.284463	1.768515
27	1	0	2.494313	0.617115	2.142977
28	1	0	2.980525	-1.023996	1.639146

Vc

Zero-point correction= 0.282422
(Hartree/Particle)
Thermal correction to Energy= 0.304118
Thermal correction to Enthalpy= 0.305062
Thermal correction to Gibbs Free Energy= 0.231393
Sum of electronic and zero-point Energies= -1711.015944
Sum of electronic and thermal Energies= -1710.994249
Sum of electronic and thermal Enthalpies= -1710.993305
Sum of electronic and thermal Free Energies= -1711.066973

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	17	0	-0.094339	2.348744	0.328107
2	44	0	-0.151349	0.093555	-0.486867
3	6	0	2.565418	0.528169	-0.492297
4	17	0	0.261203	-2.232236	-0.098184
5	15	0	-2.258033	-0.142539	0.428202
6	6	0	-2.157949	-0.279783	2.260596
7	6	0	-3.206558	-1.633298	-0.090065
8	6	0	-3.430930	1.247398	0.139395
9	6	0	2.127821	0.138757	-1.711347
10	6	0	-0.856339	0.195003	-2.167477
11	6	0	3.239837	-0.356532	0.527088
12	6	0	4.762990	-0.106366	0.457224
13	6	0	2.715479	-0.101059	1.950088
14	1	0	2.526158	1.588864	-0.246070
15	1	0	-3.154573	-0.387610	2.703117
16	1	0	-1.677862	0.619588	2.656978
17	1	0	-1.548754	-1.150650	2.519819
18	1	0	-2.609231	-2.523379	0.120667
19	1	0	-3.394735	-1.595564	-1.167538
20	1	0	-4.165025	-1.688422	0.437721
21	1	0	-2.971382	2.175102	0.488303
22	1	0	-4.376550	1.074127	0.664728
23	1	0	-3.631754	1.346446	-0.931912
24	1	0	2.189704	-0.896579	-2.035784
25	1	0	1.828440	0.878690	-2.447400
26	1	0	-0.201705	0.308017	-3.038629
27	1	0	-1.923855	0.154050	-2.416163
28	1	0	3.045242	-1.402022	0.262572
29	1	0	5.004969	0.937481	0.693393
30	1	0	5.158468	-0.328023	-0.539788
31	1	0	5.283564	-0.742777	1.182372
32	1	0	1.654417	-0.357876	2.035936
33	1	0	2.834553	0.951535	2.234272
34	1	0	3.264457	-0.713718	2.674600

Ve

Zero-point correction= 0.310743
(Hartree/Particle)
Thermal correction to Energy= 0.334002
Thermal correction to Enthalpy= 0.334946
Thermal correction to Gibbs Free Energy= 0.257807
Sum of electronic and zero-point Energies= -1750.302772
Sum of electronic and thermal Energies= -1750.279513
Sum of electronic and thermal Enthalpies= -1750.278569
Sum of electronic and thermal Free Energies= -1750.355708

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.412307	2.328472	-0.735558
2	44	0	-0.259654	-0.037879	-0.393226
3	17	0	0.234942	-1.861485	1.077101
4	15	0	-2.426563	-0.040692	0.382929
5	6	0	-2.504099	0.647297	2.087486
6	6	0	-3.232555	-1.690686	0.519374

7	6	0	-3.639012	0.961415	-0.573948
8	6	0	-0.781719	-0.790062	-1.970325
9	1	0	-3.530184	0.634044	2.471803
10	1	0	-2.132331	1.675972	2.073317
11	1	0	-1.862328	0.047561	2.739328
12	1	0	-2.609541	-2.337725	1.141019
13	1	0	-3.315423	-2.145056	-0.472802
14	1	0	-4.233718	-1.599106	0.954818
15	1	0	-3.268570	1.986141	-0.651424
16	1	0	-4.621571	0.950706	-0.089442
17	1	0	-3.736875	0.555519	-1.585641
18	1	0	-0.039413	-1.004748	-2.747588
19	1	0	-1.807163	-1.064042	-2.247553
20	6	0	2.424014	0.560120	-0.393396
21	6	0	2.212562	-0.232808	-1.473574
22	6	0	3.131938	0.193750	0.891426
23	6	0	4.637617	0.505553	0.736599
24	6	0	2.545326	0.951081	2.093734
25	6	0	2.622828	-1.672007	-1.631690
26	1	0	2.177460	1.615276	-0.502325
27	1	0	1.839953	0.259611	-2.371543
28	1	0	3.018979	-0.879824	1.075151
29	1	0	4.800967	1.571356	0.533690
30	1	0	5.083371	-0.065313	-0.085222
31	1	0	5.175060	0.254048	1.658778
32	1	0	1.498526	0.677136	2.260906
33	1	0	2.596455	2.036477	1.940742
34	1	0	3.101656	0.712327	3.007642
35	1	0	2.782299	-2.167148	-0.671854
36	1	0	3.553537	-1.733096	-2.213693
37	1	0	1.865890	-2.243748	-2.180460

TS(V-VI)b

Zero-point correction= 0.226624
(Hartree/Particle)
Thermal correction to Energy= 0.244276
Thermal correction to Enthalpy= 0.245220
Thermal correction to Gibbs Free Energy= 0.180691
Sum of electronic and zero-point Energies= -1632.433618
Sum of electronic and thermal Energies= -1632.415966
Sum of electronic and thermal Enthalpies= -1632.415022
Sum of electronic and thermal Free Energies= -1632.479552

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.015872	-2.481794	0.106226
2	44	0	-0.415584	-0.070246	-0.141485
3	6	0	-2.428811	-0.531661	0.661250
4	17	0	-0.743513	2.349043	-0.244817
5	15	0	1.941181	0.211138	0.154079
6	6	0	2.405302	-0.281646	1.868553
7	6	0	2.653544	1.893859	-0.050792
8	6	0	2.971873	-0.859565	-0.929001
9	6	0	-2.686721	-0.353583	-0.717238
10	6	0	-0.867924	-0.259612	-1.923910
11	6	0	-2.828357	0.476702	1.712916

12	1	0	-2.335789	-1.561856	0.999879
13	1	0	3.488579	-0.204385	2.014606
14	1	0	2.079291	-1.312082	2.033886
15	1	0	1.903627	0.370440	2.590786
16	1	0	2.133557	2.591166	0.609817
17	1	0	2.492335	2.234315	-1.077163
18	1	0	3.726576	1.887471	0.171819
19	1	0	2.607221	-1.885964	-0.845413
20	1	0	4.027303	-0.804253	-0.639818
21	1	0	2.867494	-0.531676	-1.967778
22	1	0	-3.088960	0.595412	-1.060236
23	1	0	-2.910625	-1.236147	-1.310499
24	1	0	-1.102061	0.610095	-2.546130
25	1	0	-0.844305	-1.234818	-2.420717
26	1	0	-3.813458	0.195741	2.113987
27	1	0	-2.130699	0.469143	2.558703
28	1	0	-2.875665	1.490953	1.313818

TS(V-VI)c

Zero-point correction= 0.283463
(Hartree/Particle)
Thermal correction to Energy= 0.303797
Thermal correction to Enthalpy= 0.304741
Thermal correction to Gibbs Free Energy= 0.234546
Sum of electronic and zero-point Energies= -1711.003277
Sum of electronic and thermal Energies= -1710.982943
Sum of electronic and thermal Enthalpies= -1710.981999
Sum of electronic and thermal Free Energies= -1711.052194

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.430053	2.475734	0.349318
2	44	0	0.007898	0.164664	-0.373974
3	6	0	2.154054	0.637711	-0.025857
4	17	0	0.391991	-2.178372	-0.958799
5	15	0	-2.194264	-0.329218	0.415720
6	6	0	-2.283979	-0.063014	2.237637
7	6	0	-2.849087	-2.029503	0.166385
8	6	0	-3.495187	0.774296	-0.271707
9	6	0	2.049401	0.731456	-1.430311
10	6	0	-0.026348	0.647357	-2.156505
11	6	0	2.889541	-0.487630	0.683621
12	6	0	4.370836	-0.082801	0.840915
13	6	0	2.263238	-0.794607	2.053569
14	1	0	2.103570	1.579093	0.521921
15	1	0	-3.297184	-0.254003	2.608964
16	1	0	-1.996461	0.969897	2.451314
17	1	0	-1.587561	-0.736441	2.747350
18	1	0	-2.159938	-2.751594	0.610345
19	1	0	-2.902406	-2.246452	-0.903699
20	1	0	-3.843735	-2.130177	0.615124
21	1	0	-3.178506	1.810239	-0.128876
22	1	0	-4.456395	0.598408	0.223935
23	1	0	-3.604270	0.583122	-1.343595
24	1	0	2.389176	-0.101016	-2.040401
25	1	0	2.058994	1.719568	-1.882101

26	1	0	0.080112	-0.099737	-2.949705
27	1	0	-0.216167	1.679662	-2.467761
28	1	0	2.828964	-1.388515	0.065341
29	1	0	4.472665	0.826488	1.446619
30	1	0	4.840592	0.104279	-0.131185
31	1	0	4.929565	-0.882974	1.340576
32	1	0	1.247454	-1.192675	1.941613
33	1	0	2.219206	0.103144	2.683270
34	1	0	2.851012	-1.552003	2.584722

TS(V-VI)e

Zero-point correction= 0.311999
(Hartree/Particle)
Thermal correction to Energy= 0.333791
Thermal correction to Enthalpy= 0.334735
Thermal correction to Gibbs Free Energy= 0.261258
Sum of electronic and zero-point Energies= -1750.287320
Sum of electronic and thermal Energies= -1750.265528
Sum of electronic and thermal Enthalpies= -1750.264584
Sum of electronic and thermal Free Energies= -1750.338061

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.585310	2.506200	0.221830
2	44	0	-0.098882	0.146079	-0.289704
3	17	0	0.287425	-2.246505	-0.613532
4	15	0	-2.383262	-0.290798	0.289858
5	6	0	-2.593148	-0.133843	2.113834
6	6	0	-3.088870	-1.939244	-0.120880
7	6	0	-3.589585	0.900353	-0.423365
8	6	0	0.181818	0.541771	-2.081872
9	1	0	-3.640399	-0.284772	2.398549
10	1	0	-2.267466	0.864281	2.419387
11	1	0	-1.975880	-0.881200	2.622231
12	1	0	-2.465164	-2.722921	0.313886
13	1	0	-3.079273	-2.075301	-1.206052
14	1	0	-4.117768	-2.019072	0.248127
15	1	0	-3.242052	1.914186	-0.213394
16	1	0	-4.587775	0.739009	-0.001092
17	1	0	-3.633354	0.763975	-1.508347
18	1	0	0.362009	-0.253978	-2.809789
19	1	0	0.009756	1.545465	-2.481691
20	6	0	1.951042	0.629693	0.267174
21	6	0	2.043990	0.712575	-1.169134
22	6	0	2.684662	-0.401173	1.112031
23	6	0	4.120494	0.104306	1.378478
24	6	0	1.954688	-0.641046	2.443969
25	6	0	2.862301	-0.280546	-1.973695
26	1	0	1.826668	1.592598	0.763560
27	1	0	2.050748	1.740556	-1.529279
28	1	0	2.734056	-1.351154	0.572819
29	1	0	4.107866	1.055296	1.925482
30	1	0	4.681646	0.259478	0.450582
31	1	0	4.670686	-0.624509	1.985333
32	1	0	0.974007	-1.100932	2.278343
33	1	0	1.812746	0.299138	2.992444
34	1	0	2.532078	-1.319281	3.082909

35	1	0	2.548247	-1.308148	-1.775383
36	1	0	3.920953	-0.182201	-1.703006
37	1	0	2.777095	-0.087893	-3.046835

VIb

Zero-point correction= 0.229150
(Hartree/Particle)
Thermal correction to Energy= 0.246687
Thermal correction to Enthalpy= 0.247632
Thermal correction to Gibbs Free Energy= 0.183845
Sum of electronic and zero-point Energies= -1632.444097
Sum of electronic and thermal Energies= -1632.426560
Sum of electronic and thermal Enthalpies= -1632.425616
Sum of electronic and thermal Free Energies= -1632.489402

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.074758	-2.476957	0.019404
2	44	0	-0.417519	-0.069077	-0.160344
3	6	0	-2.011028	-0.402249	0.975373
4	17	0	-0.725175	2.321361	-0.472405
5	15	0	1.935164	0.223460	0.151084
6	6	0	2.522771	-0.557440	1.708118
7	6	0	2.594105	1.938043	0.203954
8	6	0	2.859969	-0.603674	-1.204663
9	6	0	-2.609612	-0.452430	-0.515641
10	6	0	-1.589430	-0.453109	-1.710352
11	6	0	-2.592368	0.644753	1.896776
12	1	0	-1.987732	-1.404152	1.407851
13	1	0	3.614334	-0.493979	1.780475
14	1	0	2.199626	-1.600951	1.713680
15	1	0	2.079593	-0.043943	2.567102
16	1	0	2.123082	2.484213	1.025132
17	1	0	2.334724	2.455320	-0.722515
18	1	0	3.681592	1.926258	0.338984
19	1	0	2.556347	-1.652739	-1.238316
20	1	0	3.939972	-0.522771	-1.038082
21	1	0	2.608909	-0.130388	-2.158915
22	1	0	-3.274242	0.404675	-0.624042
23	1	0	-3.117865	-1.418420	-0.557297
24	1	0	-1.726054	0.383366	-2.394909
25	1	0	-1.448976	-1.426754	-2.177123
26	1	0	-3.614478	0.356882	2.187597
27	1	0	-2.003081	0.697687	2.819780
28	1	0	-2.611724	1.634954	1.439113

VIc

Zero-point correction= 0.285875
(Hartree/Particle)
Thermal correction to Energy= 0.306244
Thermal correction to Enthalpy= 0.307189
Thermal correction to Gibbs Free Energy= 0.236833
Sum of electronic and zero-point Energies= -1711.014094
Sum of electronic and thermal Energies= -1710.993724

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 Sum of electronic and thermal Enthalpies=          -1710.992780
 Sum of electronic and thermal Free Energies=       -1711.063136
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.558757	2.413205	0.685078
2	44	0	0.004756	0.268178	-0.383675
3	6	0	1.834382	0.453127	0.366362
4	17	0	0.368333	-1.842010	-1.532189
5	15	0	-2.141295	-0.458310	0.380091
6	6	0	-2.365706	-0.207763	2.187217
7	6	0	-2.623389	-2.206162	0.080767
8	6	0	-3.451331	0.547968	-0.426584
9	6	0	1.980422	1.080767	-1.105199
10	6	0	0.673418	1.258781	-1.961054
11	6	0	2.734728	-0.724722	0.705891
12	6	0	4.179821	-0.230206	0.925170
13	6	0	2.212923	-1.443332	1.961639
14	1	0	1.870110	1.244321	1.120613
15	1	0	-3.388647	-0.464412	2.484539
16	1	0	-2.149405	0.837668	2.418749
17	1	0	-1.664818	-0.843576	2.736917
18	1	0	-1.919353	-2.870197	0.588939
19	1	0	-2.561502	-2.421685	-0.988262
20	1	0	-3.639110	-2.393321	0.447415
21	1	0	-3.257957	1.601679	-0.211429
22	1	0	-4.440807	0.259521	-0.054449
23	1	0	-3.417786	0.394078	-1.509474
24	1	0	2.663601	0.435394	-1.658173
25	1	0	2.362989	2.088202	-0.930021
26	1	0	0.680608	0.685091	-2.887263
27	1	0	0.337228	2.290874	-2.046824
28	1	0	2.720031	-1.434751	-0.126689
29	1	0	4.231260	0.488540	1.752890
30	1	0	4.583515	0.257086	0.030011
31	1	0	4.836214	-1.073167	1.170946
32	1	0	1.227952	-1.883700	1.773064
33	1	0	2.128184	-0.752469	2.810631
34	1	0	2.893482	-2.251415	2.253822

VIe

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Zero-point correction=                           0.314358
(Hartree/Particle)
 Thermal correction to Energy=                    0.335991
 Thermal correction to Enthalpy=                  0.336935
 Thermal correction to Gibbs Free Energy=         0.264715
 Sum of electronic and zero-point Energies=          -1750.293900
 Sum of electronic and thermal Energies=             -1750.272267
 Sum of electronic and thermal Enthalpies=           -1750.271323
 Sum of electronic and thermal Free Energies=        -1750.343543
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.667232	2.289647	1.009719
2	44	0	-0.073929	0.274570	-0.291927

3	17	0	0.292848	-1.712999	-1.635168
4	15	0	-2.315987	-0.405285	0.189431
5	6	0	-2.659393	-0.446794	1.994687
6	6	0	-2.867393	-2.047652	-0.426916
7	6	0	-3.518795	0.790212	-0.519531
8	6	0	0.721362	1.471912	-1.633869
9	1	0	-3.707432	-0.709009	2.178230
10	1	0	-2.431966	0.536319	2.412735
11	1	0	-2.016392	-1.191669	2.473462
12	1	0	-2.239402	-2.830620	0.005617
13	1	0	-2.741197	-2.089868	-1.511112
14	1	0	-3.916014	-2.223224	-0.160911
15	1	0	-3.289193	1.784323	-0.129042
16	1	0	-4.543047	0.503228	-0.255885
17	1	0	-3.420942	0.804663	-1.609384
18	1	0	0.785708	1.054134	-2.639796
19	1	0	0.424807	2.518604	-1.583325
20	6	0	1.696162	0.343870	0.627994
21	6	0	2.003638	1.129108	-0.747059
22	6	0	2.469270	-0.916358	0.994715
23	6	0	3.799762	-0.537774	1.680766
24	6	0	1.630523	-1.795276	1.942926
25	6	0	3.075189	0.476360	-1.628149
26	1	0	1.663642	1.056713	1.455728
27	1	0	2.296919	2.113657	-0.370718
28	1	0	2.672078	-1.500956	0.093186
29	1	0	3.612714	0.006569	2.615064
30	1	0	4.431627	0.095437	1.049070
31	1	0	4.370575	-1.440873	1.927118
32	1	0	0.742479	-2.178035	1.429852
33	1	0	1.312745	-1.231820	2.829741
34	1	0	2.218634	-2.655070	2.285168
35	1	0	2.711311	-0.465194	-2.047942
36	1	0	3.994564	0.282328	-1.068955
37	1	0	3.323015	1.149907	-2.455349

IXa

Zero-point correction= 0.235559
(Hartree/Particle)
Thermal correction to Energy= 0.253631
Thermal correction to Enthalpy= 0.254575
Thermal correction to Gibbs Free Energy= 0.188998
Sum of electronic and zero-point Energies= -1438.037696
Sum of electronic and thermal Energies= -1438.019623
Sum of electronic and thermal Enthalpies= -1438.018679
Sum of electronic and thermal Free Energies= -1438.084257

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.565054	-1.823525	1.524965
2	44	0	0.793442	-0.062725	-0.090223
3	6	0	0.784516	-0.812616	-1.753186
4	17	0	1.166350	2.212380	-0.823507
5	6	0	-1.239003	0.088682	-0.091822
6	6	0	-3.376420	0.857339	0.502813
7	7	0	-1.931373	1.112139	0.462035
8	7	0	-2.134586	-0.810418	-0.563622

9	6	0	-3.522366	-0.348539	-0.430710
10	6	0	-1.897516	-2.148486	-1.075942
11	6	0	-1.411015	2.135085	1.353762
12	1	0	1.666292	-1.299411	-2.183904
13	1	0	-0.081043	-0.761735	-2.421428
14	1	0	-3.933098	1.735996	0.162199
15	1	0	-3.688013	0.630773	1.532846
16	1	0	-3.928084	-0.071777	-1.413335
17	1	0	-4.151659	-1.141085	-0.012700
18	1	0	-2.049879	-2.200693	-2.162401
19	1	0	-0.888901	-2.467991	-0.821443
20	1	0	-2.604796	-2.836268	-0.597542
21	1	0	-0.354626	2.302303	1.156472
22	1	0	-1.561863	1.842313	2.402915
23	1	0	-1.940707	3.076314	1.171810
24	6	0	3.297647	-0.601299	-0.240619
25	6	0	3.131390	0.177744	0.850715
26	1	0	3.568524	-0.167548	-1.198818
27	1	0	3.254751	-1.684149	-0.170641
28	1	0	2.949049	-0.261498	1.827415
29	1	0	3.257059	1.254336	0.794629

IXb

Zero-point correction= 0.263416
(Hartree/Particle)
Thermal correction to Energy= 0.283174
Thermal correction to Enthalpy= 0.284118
Thermal correction to Gibbs Free Energy= 0.214527
Sum of electronic and zero-point Energies= -1477.326287
Sum of electronic and thermal Energies= -1477.306529
Sum of electronic and thermal Enthalpies= -1477.305585
Sum of electronic and thermal Free Energies= -1477.375176

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.693007	-1.944219	-1.306998
2	44	0	-0.568395	0.123347	-0.001362
3	6	0	-1.095330	-0.680432	1.542573
4	17	0	-0.477652	2.308997	1.112847
5	6	0	1.463245	-0.050822	0.038041
6	6	0	3.653196	0.333063	-0.675490
7	7	0	2.259960	0.795277	-0.649396
8	7	0	2.235423	-0.977272	0.632320
9	6	0	3.666675	-0.679305	0.476984
10	6	0	1.784480	-2.046771	1.502742
11	6	0	1.806712	1.807220	-1.587113
12	1	0	-1.418490	-1.728196	1.559800
13	1	0	-1.152781	-0.122240	2.485016
14	1	0	4.341868	1.169414	-0.523251
15	1	0	3.880991	-0.136753	-1.643409
16	1	0	4.070280	-0.246283	1.403187
17	1	0	4.228778	-1.588162	0.243814
18	1	0	1.612477	-1.696517	2.529501
19	1	0	0.870739	-2.479198	1.094587
20	1	0	2.555672	-2.822644	1.524328
21	1	0	0.861291	2.226192	-1.235031

22	1	0	1.693179	1.398328	-2.601059
23	1	0	2.539071	2.620363	-1.615947
24	6	0	-3.166959	0.354333	0.053965
25	6	0	-2.530839	0.841860	-1.058842
26	6	0	-3.936712	-0.937992	0.075166
27	1	0	-3.271827	1.023235	0.905985
28	1	0	-2.530179	0.267077	-1.982097
29	1	0	-2.248547	1.890675	-1.098368
30	1	0	-3.975551	-1.379694	1.075041
31	1	0	-3.507806	-1.663866	-0.621104
32	1	0	-4.973095	-0.733175	-0.229130

IXc

Zero-point correction= 0.320249
(Hartree/Particle)
Thermal correction to Energy= 0.342718
Thermal correction to Enthalpy= 0.343662
Thermal correction to Gibbs Free Energy= 0.267010
Sum of electronic and zero-point Energies= -1555.894156
Sum of electronic and thermal Energies= -1555.871687
Sum of electronic and thermal Enthalpies= -1555.870743
Sum of electronic and thermal Free Energies= -1555.947395

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.371242	1.820201	-1.376012
2	44	0	-0.106362	-0.061412	0.176075
3	6	0	-0.653147	-1.275653	-1.060909
4	17	0	0.164535	-1.764797	1.910448
5	6	0	1.895841	0.004755	-0.118651
6	6	0	3.988292	1.010948	0.130022
7	7	0	2.607313	0.892390	0.609618
8	7	0	2.739445	-0.648437	-0.941345
9	6	0	4.140827	-0.287375	-0.669932
10	6	0	2.467878	-1.862567	-1.682660
11	6	0	2.005261	1.937843	1.420027
12	6	0	-2.708954	-0.166373	0.670179
13	6	0	-1.968248	0.757184	1.356986
14	6	0	-3.657843	0.186430	-0.454086
15	6	0	-4.034225	-1.023062	-1.320709
16	6	0	-4.932914	0.810637	0.163917
17	1	0	-0.907377	-0.966567	-2.082155
18	1	0	-0.778314	-2.335786	-0.807306
19	1	0	4.689713	1.088717	0.965968
20	1	0	4.095998	1.901851	-0.505460
21	1	0	4.624231	-1.080423	-0.081314
22	1	0	4.696310	-0.157175	-1.603199
23	1	0	2.710074	-2.755760	-1.090949
24	1	0	1.414212	-1.895001	-1.956640
25	1	0	3.068222	-1.865463	-2.598382
26	1	0	1.149785	1.528233	1.968134
27	1	0	1.673038	2.786814	0.810810
28	1	0	2.734119	2.274273	2.163671
29	1	0	-2.755326	-1.178451	1.072096
30	1	0	-1.996636	1.805256	1.068066
31	1	0	-1.550298	0.496531	2.326441
32	1	0	-3.172982	0.948291	-1.076848

33	1	0	-4.501147	-1.811561	-0.716237
34	1	0	-3.160361	-1.454972	-1.818693
35	1	0	-4.750301	-0.731331	-2.096737
36	1	0	-4.697112	1.711957	0.738292
37	1	0	-5.437157	0.102889	0.833707
38	1	0	-5.638661	1.083678	-0.628969

IXd

Zero-point correction= 0.291852
(Hartree/Particle)
Thermal correction to Energy= 0.313041
Thermal correction to Enthalpy= 0.313985
Thermal correction to Gibbs Free Energy= 0.241932
Sum of electronic and zero-point Energies= -1516.612817
Sum of electronic and thermal Energies= -1516.591628
Sum of electronic and thermal Enthalpies= -1516.590684
Sum of electronic and thermal Free Energies= -1516.662736

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.349899	-1.965657	1.481601
2	44	0	0.487653	-0.074123	-0.087626
3	6	0	0.720843	-1.155543	-1.525690
4	17	0	0.611555	1.887304	-1.575828
5	6	0	-1.557090	0.045571	-0.054546
6	6	0	-3.650176	0.881535	0.566167
7	7	0	-2.208168	1.124505	0.433236
8	7	0	-2.471711	-0.871880	-0.418487
9	6	0	-3.843173	-0.352652	-0.321976
10	6	0	-2.211066	-2.155158	-1.044564
11	6	0	-1.605965	2.261988	1.104784
12	1	0	0.832778	-2.240389	-1.407651
13	1	0	0.818042	-0.749046	-2.539072
14	1	0	-4.221089	1.751183	0.227320
15	1	0	-3.907470	0.682326	1.616680
16	1	0	-4.223544	-0.090125	-1.319422
17	1	0	-4.510192	-1.099154	0.118703
18	1	0	-2.019496	-2.054182	-2.121696
19	1	0	-1.363435	-2.631112	-0.551044
20	1	0	-3.092522	-2.788715	-0.907674
21	1	0	-0.630537	2.467254	0.660629
22	1	0	-1.512822	2.089642	2.186848
23	1	0	-2.237135	3.142236	0.945330
24	6	0	3.040063	-0.396148	0.177659
25	6	0	2.597462	0.771372	0.734036
26	6	0	2.192939	0.939243	2.179182
27	6	0	3.807396	-0.450159	-1.118964
28	1	0	2.992476	-1.306858	0.771875
29	1	0	2.723945	1.688161	0.160871
30	1	0	2.069668	-0.020186	2.685548
31	1	0	1.258147	1.508717	2.283288
32	1	0	2.962701	1.528404	2.697924
33	1	0	4.884321	-0.418248	-0.898842
34	1	0	3.565363	0.401376	-1.761464
35	1	0	3.621096	-1.376564	-1.670530

TS(IX-X)a

Zero-point correction= 0.234485
(Hartree/Particle)
Thermal correction to Energy= 0.252245
Thermal correction to Enthalpy= 0.253189
Thermal correction to Gibbs Free Energy= 0.187363
Sum of electronic and zero-point Energies= -1438.036329
Sum of electronic and thermal Energies= -1438.018569
Sum of electronic and thermal Enthalpies= -1438.017625
Sum of electronic and thermal Free Energies= -1438.083451

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.681602	-2.021782	1.367584
2	44	0	0.790916	-0.039469	-0.036812
3	6	0	1.019757	-0.880508	-1.634746
4	17	0	0.949603	2.179946	-1.067457
5	6	0	-1.246838	0.058405	-0.044230
6	6	0	-3.357169	0.727731	0.710174
7	7	0	-1.916473	1.003569	0.650477
8	7	0	-2.147676	-0.771078	-0.606432
9	6	0	-3.527250	-0.304000	-0.411557
10	6	0	-1.881759	-1.920432	-1.447993
11	6	0	-1.327817	1.949079	1.583426
12	1	0	1.529082	-1.849833	-1.710788
13	1	0	0.681774	-0.435880	-2.579136
14	1	0	-3.933765	1.642881	0.545374
15	1	0	-3.625106	0.319345	1.695400
16	1	0	-3.911629	0.147846	-1.336846
17	1	0	-4.181478	-1.136334	-0.135191
18	1	0	-1.867828	-1.655462	-2.514278
19	1	0	-0.930723	-2.366610	-1.157929
20	1	0	-2.670786	-2.662359	-1.286354
21	1	0	-0.340617	2.244272	1.223843
22	1	0	-1.260696	1.526069	2.595674
23	1	0	-1.951285	2.848196	1.618708
24	6	0	3.322455	-0.272014	-0.142983
25	6	0	2.934003	0.397103	0.975207
26	1	0	3.599900	0.263456	-1.045540
27	1	0	3.470428	-1.347322	-0.123967
28	1	0	2.786877	-0.133615	1.911654
29	1	0	2.911796	1.483555	0.984851

TS(IX-X)b

Zero-point correction= 0.264215
(Hartree/Particle)
Thermal correction to Energy= 0.282723
Thermal correction to Enthalpy= 0.283667
Thermal correction to Gibbs Free Energy= 0.216909
Sum of electronic and zero-point Energies= -1477.324812
Sum of electronic and thermal Energies= -1477.306304
Sum of electronic and thermal Enthalpies= -1477.305360
Sum of electronic and thermal Free Energies= -1477.372118

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.705601	-1.964762	-1.267121
2	44	0	-0.575175	0.129473	-0.004812
3	6	0	-1.394971	-0.579981	1.477605
4	17	0	-0.408678	2.317941	1.094380
5	6	0	1.465777	-0.067114	0.027468
6	6	0	3.668534	0.249100	-0.673916
7	7	0	2.279951	0.726692	-0.695186
8	7	0	2.212650	-0.970892	0.682228
9	6	0	3.650604	-0.703564	0.529865
10	6	0	1.734781	-1.957511	1.631946
11	6	0	1.845118	1.705253	-1.675532
12	1	0	-1.724701	-1.623770	1.499841
13	1	0	-1.549825	0.017061	2.382569
14	1	0	4.364318	1.084646	-0.552438
15	1	0	3.906906	-0.272109	-1.612234
16	1	0	4.049100	-0.230596	1.438528
17	1	0	4.199835	-1.632643	0.351527
18	1	0	1.686833	-1.551940	2.651719
19	1	0	0.749147	-2.301330	1.319647
20	1	0	2.419553	-2.811448	1.624845
21	1	0	0.894517	2.137017	-1.353097
22	1	0	1.744140	1.261152	-2.675555
23	1	0	2.578733	2.516520	-1.722092
24	6	0	-3.048622	0.334458	0.089138
25	6	0	-2.388550	0.879676	-1.020635
26	6	0	-3.903880	-0.905137	-0.023361
27	1	0	-3.250283	1.016627	0.912308
28	1	0	-2.432989	0.345755	-1.968008
29	1	0	-2.198323	1.949090	-1.042665
30	1	0	-4.131398	-1.344855	0.951712
31	1	0	-3.417649	-1.655527	-0.652991
32	1	0	-4.858448	-0.626165	-0.490060

TS(IX-X)c

Zero-point correction= 0.321102
(Hartree/Particle)
Thermal correction to Energy= 0.342374
Thermal correction to Enthalpy= 0.343318
Thermal correction to Gibbs Free Energy= 0.269561
Sum of electronic and zero-point Energies= -1555.891484
Sum of electronic and thermal Energies= -1555.870212
Sum of electronic and thermal Enthalpies= -1555.869268
Sum of electronic and thermal Free Energies= -1555.943025

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.369255	1.934129	-1.190728
2	44	0	-0.114252	-0.081199	0.182883
3	6	0	-1.032049	-1.138726	-1.009754
4	17	0	0.219239	-1.970611	1.703098
5	6	0	1.904434	0.028271	-0.114105
6	6	0	4.029845	0.952691	0.134599

7	7	0	2.663039	0.830495	0.656887
8	7	0	2.688804	-0.572748	-1.023964
9	6	0	4.110104	-0.263991	-0.797411
10	6	0	2.332137	-1.698074	-1.864847
11	6	0	2.121746	1.814130	1.579423
12	6	0	-2.556014	-0.304140	0.514679
13	6	0	-1.823410	0.527127	1.387423
14	6	0	-3.595455	0.258389	-0.450949
15	6	0	-4.231540	-0.822964	-1.338068
16	6	0	-4.701878	0.963591	0.367699
17	1	0	-1.392335	-0.718628	-1.952841
18	1	0	-1.177289	-2.210563	-0.840579
19	1	0	4.764402	0.925043	0.944842
20	1	0	4.143352	1.899686	-0.412187
21	1	0	4.605377	-1.120647	-0.318435
22	1	0	4.618135	-0.050905	-1.742591
23	1	0	2.704969	-2.639467	-1.439208
24	1	0	1.247941	-1.752920	-1.946779
25	1	0	2.761638	-1.562039	-2.863435
26	1	0	1.240083	1.399726	2.078160
27	1	0	1.841550	2.742096	1.066649
28	1	0	2.866840	2.026824	2.352297
29	1	0	-2.704868	-1.328536	0.854496
30	1	0	-1.914285	1.605729	1.278904
31	1	0	-1.553532	0.136787	2.365598
32	1	0	-3.104997	1.013407	-1.076876
33	1	0	-4.706772	-1.600841	-0.726254
34	1	0	-3.503848	-1.311981	-1.992708
35	1	0	-5.007205	-0.384649	-1.975335
36	1	0	-4.300362	1.791678	0.959328
37	1	0	-5.195820	0.263533	1.053391
38	1	0	-5.466056	1.367560	-0.306142

TS(IX-X)d

Zero-point correction= 0.292480
(Hartree/Particle)
Thermal correction to Energy= 0.312502
Thermal correction to Enthalpy= 0.313446
Thermal correction to Gibbs Free Energy= 0.243474
Sum of electronic and zero-point Energies= -1516.609265
Sum of electronic and thermal Energies= -1516.589242
Sum of electronic and thermal Enthalpies= -1516.588298
Sum of electronic and thermal Free Energies= -1516.658271

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.285999	2.155976	1.222229
2	44	0	-0.473671	0.063010	-0.056304
3	6	0	-1.170214	0.994902	-1.477847
4	17	0	-0.562030	-2.051638	-1.310991
5	6	0	1.575654	-0.060373	-0.043140
6	6	0	3.689746	-0.762252	0.655428
7	7	0	2.243215	-1.014724	0.635398
8	7	0	2.466755	0.753423	-0.632110
9	6	0	3.842647	0.256661	-0.482646
10	6	0	2.168568	1.845685	-1.539430

11	6	0	1.642454	-1.975974	1.541248
12	1	0	-1.311450	2.080311	-1.436807
13	1	0	-1.425162	0.489861	-2.414008
14	1	0	4.247460	-1.687800	0.483490
15	1	0	3.992090	-0.346998	1.627635
16	1	0	4.181744	-0.213407	-1.416681
17	1	0	4.525089	1.076004	-0.238094
18	1	0	2.087475	1.499327	-2.578861
19	1	0	1.239116	2.322037	-1.229244
20	1	0	2.974632	2.583463	-1.475643
21	1	0	0.650160	-2.243450	1.170145
22	1	0	1.576554	-1.584752	2.566301
23	1	0	2.249211	-2.887149	1.550907
24	6	0	-2.910198	0.340905	-0.100363
25	6	0	-2.409216	-0.562359	0.857242
26	6	0	-2.359626	-0.268271	2.340987
27	6	0	-3.754445	-0.152916	-1.257757
28	1	0	-3.068591	1.365384	0.232531
29	1	0	-2.491407	-1.616668	0.591012
30	1	0	-2.261810	0.798602	2.545979
31	1	0	-1.525966	-0.787386	2.829139
32	1	0	-3.283024	-0.646280	2.805228
33	1	0	-4.762700	-0.372835	-0.880390
34	1	0	-3.340051	-1.073178	-1.679428
35	1	0	-3.857342	0.591798	-2.052213

Xa

Zero-point correction= 0.238769
(Hartree/Particle)
Thermal correction to Energy= 0.255770
Thermal correction to Enthalpy= 0.256714
Thermal correction to Gibbs Free Energy= 0.192775
Sum of electronic and zero-point Energies= -1438.053069
Sum of electronic and thermal Energies= -1438.036069
Sum of electronic and thermal Enthalpies= -1438.035124
Sum of electronic and thermal Free Energies= -1438.099064

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.733690	2.146940	1.155060
2	44	0	-0.769905	0.000067	-0.000092
3	6	0	-2.216107	0.644235	-1.181734
4	17	0	-0.735283	-2.146840	-1.155088
5	6	0	1.256169	-0.000224	-0.000199
6	6	0	3.448063	-0.415287	0.647997
7	7	0	2.027675	-0.771381	0.778892
8	7	0	2.028153	0.770549	-0.779151
9	6	0	3.448419	0.414241	-0.647590
10	6	0	1.558616	1.638676	-1.843639
11	6	0	1.557264	-1.638962	1.843491
12	6	0	-3.050380	0.000342	0.000110
13	6	0	-2.216023	-0.642971	1.182241
14	1	0	-2.324484	1.726713	-1.240483
15	1	0	-2.317751	0.106406	-2.123692
16	1	0	4.066826	-1.315052	0.582126
17	1	0	3.774048	0.172279	1.517444
18	1	0	3.774683	-0.173340	-1.516923

19	1	0	4.067297	1.313909	-0.581434
20	1	0	1.577149	1.129387	-2.816273
21	1	0	0.542236	1.963590	-1.614657
22	1	0	2.198362	2.525699	-1.892617
23	1	0	0.542427	-1.966966	1.611975
24	1	0	1.571644	-1.128179	2.815407
25	1	0	2.199261	-2.524155	1.895656
26	1	0	-3.643893	-0.803161	-0.437723
27	1	0	-3.644304	0.803595	0.437880
28	1	0	-2.317286	-0.104483	2.123862
29	1	0	-2.324761	-1.725374	1.241727

Xb

Zero-point correction= 0.267120
(Hartree/Particle)
Thermal correction to Energy= 0.285432
Thermal correction to Enthalpy= 0.286376
Thermal correction to Gibbs Free Energy= 0.219843
Sum of electronic and zero-point Energies= -1477.337541
Sum of electronic and thermal Energies= -1477.319229
Sum of electronic and thermal Enthalpies= -1477.318285
Sum of electronic and thermal Free Energies= -1477.384818

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.697224	-2.113790	0.993874
2	44	0	0.556261	0.091141	-0.042658
3	6	0	2.015245	-0.346058	-1.303268
4	17	0	0.312627	2.286129	-1.079158
5	6	0	-1.459808	-0.063649	0.021530
6	6	0	-3.648126	0.140625	0.771501
7	7	0	-2.254302	0.596741	0.875869
8	7	0	-2.203067	-0.838067	-0.781080
9	6	0	-3.638989	-0.595986	-0.579082
10	6	0	-1.711236	-1.596093	-1.917088
11	6	0	-1.801819	1.420172	1.982698
12	1	0	2.225633	-1.410046	-1.420384
13	1	0	2.021013	0.235791	-2.224577
14	1	0	-4.335023	0.991740	0.791928
15	1	0	-3.892880	-0.529072	1.607678
16	1	0	-4.038040	0.024873	-1.393249
17	1	0	-4.189961	-1.540836	-0.557384
18	1	0	-1.798455	-1.024796	-2.850726
19	1	0	-0.667205	-1.861562	-1.741573
20	1	0	-2.288495	-2.521750	-2.008458
21	1	0	-0.839247	1.864694	1.723056
22	1	0	-1.705266	0.835860	2.907213
23	1	0	-2.520357	2.230003	2.143620
24	6	0	2.856097	0.327593	-0.135973
25	6	0	1.994314	0.793389	1.115104
26	6	0	3.967473	-0.628307	0.324079
27	1	0	3.229463	1.258099	-0.570820
28	1	0	2.187987	0.204611	2.012579
29	1	0	2.000789	1.874220	1.254246
30	1	0	4.608624	-0.904203	-0.520026
31	1	0	3.530167	-1.538017	0.745973
32	1	0	4.590994	-0.150394	1.087170

Xc

```
Zero-point correction=                           0.323599
(Hartree/Particle)
 Thermal correction to Energy=                    0.344910
 Thermal correction to Enthalpy=                  0.345854
 Thermal correction to Gibbs Free Energy=         0.271282
 Sum of electronic and zero-point Energies=          -1555.904583
 Sum of electronic and thermal Energies=             -1555.883272
 Sum of electronic and thermal Enthalpies=           -1555.882328
 Sum of electronic and thermal Free Energies=        -1555.956900
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.244602	-1.867386	1.323543
2	44	0	-0.093039	0.129199	-0.090926
3	6	0	-1.546300	0.992697	0.929907
4	17	0	0.179737	2.096688	-1.489023
5	6	0	1.909822	-0.067590	0.042972
6	6	0	4.053296	-0.880366	-0.304452
7	7	0	2.668295	-0.793071	-0.792455
8	7	0	2.680612	0.502442	0.979561
9	6	0	4.107181	0.283181	0.698182
10	6	0	2.247331	1.539176	1.900032
11	6	0	2.154638	-1.752125	-1.756473
12	6	0	-2.396683	0.373532	-0.262055
13	6	0	-1.551066	-0.566939	-1.225049
14	6	0	-3.636998	-0.390552	0.292671
15	6	0	-4.497299	0.520921	1.183961
16	6	0	-4.504036	-0.943886	-0.850704
17	1	0	-1.746453	0.531837	1.896965
18	1	0	-1.543293	2.082611	0.923800
19	1	0	4.764787	-0.773374	-1.128158
20	1	0	4.218523	-1.851927	0.182244
21	1	0	4.547044	1.188855	0.257368
22	1	0	4.652002	0.037890	1.614408
23	1	0	2.433079	2.540317	1.490593
24	1	0	1.179090	1.426161	2.093088
25	1	0	2.783643	1.427604	2.847793
26	1	0	1.194072	-1.401779	-2.138707
27	1	0	2.019588	-2.741935	-1.302503
28	1	0	2.853535	-1.825287	-2.595501
29	1	0	-2.687718	1.228152	-0.880064
30	1	0	-1.755751	-1.628958	-1.093483
31	1	0	-1.545021	-0.216328	-2.257213
32	1	0	-3.257498	-1.226803	0.893517
33	1	0	-4.852367	1.395204	0.622848
34	1	0	-3.952694	0.882786	2.061196
35	1	0	-5.379089	-0.023042	1.541471
36	1	0	-3.964091	-1.659744	-1.477859
37	1	0	-4.863129	-0.132638	-1.497400
38	1	0	-5.383506	-1.456359	-0.444167

Xd

Zero-point correction= 0.295270
(Hartree/Particle)
Thermal correction to Energy= 0.315236
Thermal correction to Enthalpy= 0.316180
Thermal correction to Gibbs Free Energy= 0.246201
Sum of electronic and zero-point Energies= -1516.624357
Sum of electronic and thermal Energies= -1516.604392
Sum of electronic and thermal Enthalpies= -1516.603447
Sum of electronic and thermal Free Energies= -1516.673426

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.288634	2.314245	0.919733
2	44	0	-0.448130	0.097307	-0.103094
3	6	0	-1.766506	0.796609	-1.404261
4	17	0	-0.427735	-2.077592	-1.234754
5	6	0	1.565872	-0.060134	0.011665
6	6	0	3.680349	-0.614801	0.799236
7	7	0	2.231565	-0.855133	0.862446
8	7	0	2.438738	0.616214	-0.748879
9	6	0	3.814513	0.146138	-0.530357
10	6	0	2.094999	1.453041	-1.884777
11	6	0	1.634664	-1.633387	1.931942
12	1	0	-1.765676	1.880140	-1.522157
13	1	0	-1.853883	0.227927	-2.330673
14	1	0	4.229460	-1.560927	0.810812
15	1	0	4.004059	-0.009793	1.657749
16	1	0	4.126411	-0.511281	-1.353976
17	1	0	4.507271	0.990807	-0.474355
18	1	0	2.077117	0.876723	-2.819202
19	1	0	1.117809	1.906530	-1.709944
20	1	0	2.833468	2.256139	-1.973040
21	1	0	0.621868	-1.918416	1.640368
22	1	0	1.608213	-1.071702	2.875278
23	1	0	2.217389	-2.548503	2.078065
24	6	0	-2.739872	0.300376	-0.265856
25	6	0	-2.038418	-0.508193	0.929481
26	6	0	-2.349788	-0.032257	2.331504
27	6	0	-3.826588	-0.600014	-0.880286
28	1	0	-3.141408	1.203216	0.200960
29	1	0	-2.195697	-1.581615	0.795663
30	1	0	-2.173064	1.037121	2.455715
31	1	0	-1.735151	-0.572960	3.060751
32	1	0	-3.400905	-0.256648	2.572596
33	1	0	-4.537714	-0.923607	-0.112316
34	1	0	-3.371193	-1.485388	-1.333319
35	1	0	-4.379867	-0.054204	-1.652206

XIb

Zero-point correction= 0.263335
(Hartree/Particle)
Thermal correction to Energy= 0.283132
Thermal correction to Enthalpy= 0.284077
Thermal correction to Gibbs Free Energy= 0.214579
Sum of electronic and zero-point Energies= -1477.325146
Sum of electronic and thermal Energies= -1477.305349
Sum of electronic and thermal Enthalpies= -1477.304405

Sum of electronic and thermal Free Energies= -1477.373903

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.555085	-2.053463	1.294142
2	44	0	0.651073	-0.117073	-0.217521
3	6	0	0.762207	-1.141869	-1.715080
4	17	0	0.696994	1.910361	-1.616484
5	6	0	-1.371605	0.089969	0.027786
6	6	0	-3.347061	0.960107	0.922134
7	7	0	-1.914347	1.150644	0.662591
8	7	0	-2.360196	-0.754523	-0.314047
9	6	0	-3.688522	-0.190111	-0.033230
10	6	0	-2.220310	-1.991020	-1.061344
11	1	0	0.843626	-2.233959	-1.651151
12	1	0	0.810782	-0.693116	-2.714229
13	1	0	-3.903833	1.877548	0.708924
14	1	0	-3.510871	0.688920	1.975149
15	1	0	-4.156265	0.167269	-0.961490
16	1	0	-4.341759	-0.942796	0.417571
17	1	0	-2.111235	-1.808044	-2.138950
18	1	0	-1.361185	-2.545893	-0.683003
19	1	0	-3.119832	-2.592511	-0.900787
20	6	0	3.101962	-0.606373	-0.282055
21	6	0	2.876446	0.578939	0.360974
22	6	0	2.759456	0.724723	1.858589
23	1	0	3.408293	-0.611999	-1.323568
24	1	0	3.126002	-1.549401	0.255101
25	1	0	2.967302	1.499422	-0.210626
26	1	0	2.618789	-0.237873	2.355236
27	1	0	1.931885	1.389334	2.140366
28	1	0	3.674675	1.198539	2.240896
29	6	0	-1.184363	2.200943	1.348991
30	1	0	-0.252920	2.398995	0.814646
31	1	0	-0.982771	1.935997	2.396819
32	1	0	-1.780682	3.118846	1.329444

XIc

Zero-point correction= 0.320473
(Hartree/Particle)
Thermal correction to Energy= 0.342974
Thermal correction to Enthalpy= 0.343918
Thermal correction to Gibbs Free Energy= 0.267971
Sum of electronic and zero-point Energies= -1555.891067
Sum of electronic and thermal Energies= -1555.868566
Sum of electronic and thermal Enthalpies= -1555.867622
Sum of electronic and thermal Free Energies= -1555.943569

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.568167	0.786145	2.340182
2	44	0	-0.204234	-0.475715	0.259519
3	6	0	-2.571510	-0.612753	-0.390178
4	17	0	0.152335	-1.557975	-1.919133
5	6	0	-2.498853	-1.385755	0.734548

6	6	0	0.127039	-2.012047	1.171932
7	6	0	1.681419	0.309875	0.053601
8	6	0	3.313091	1.913418	-0.454138
9	7	0	1.890189	1.602027	-0.267164
10	7	0	2.871600	-0.325324	0.066278
11	6	0	3.945796	0.517927	-0.482196
12	6	0	0.933651	2.692559	-0.202855
13	6	0	3.079918	-1.763687	0.113801
14	6	0	-3.070332	0.821811	-0.418206
15	6	0	-2.489225	1.596242	-1.612872
16	6	0	-4.613736	0.811324	-0.489570
17	1	0	-2.485775	-1.107234	-1.356481
18	1	0	-2.420914	-2.465505	0.651584
19	1	0	-2.675452	-0.971961	1.722923
20	1	0	0.237795	-2.972970	0.654005
21	1	0	0.164012	-2.026700	2.268588
22	1	0	3.670515	2.521540	0.388700
23	1	0	3.473455	2.477436	-1.378516
24	1	0	4.851491	0.442855	0.127251
25	1	0	4.186225	0.194759	-1.504491
26	1	0	0.703406	3.071170	-1.206329
27	1	0	0.025186	2.360089	0.299324
28	1	0	1.356555	3.511116	0.392607
29	1	0	2.753771	-2.246385	-0.813851
30	1	0	4.145692	-1.947676	0.277345
31	1	0	2.530077	-2.193613	0.952872
32	1	0	-2.803131	1.142838	-2.560915
33	1	0	-1.393779	1.601637	-1.610910
34	1	0	-2.833675	2.636685	-1.603416
35	1	0	-5.047639	0.317743	0.386147
36	1	0	-4.964354	0.284810	-1.385989
37	1	0	-4.997529	1.837625	-0.531025
38	1	0	-2.776568	1.313900	0.516924

XIe

Zero-point correction= 0.348609
(Hartree/Particle)
Thermal correction to Energy= 0.372653
Thermal correction to Enthalpy= 0.373597
Thermal correction to Gibbs Free Energy= 0.294524
Sum of electronic and zero-point Energies= -1595.178313
Sum of electronic and thermal Energies= -1595.154269
Sum of electronic and thermal Enthalpies= -1595.153324
Sum of electronic and thermal Free Energies= -1595.232398

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.417182	0.798593	2.366015
2	44	0	-0.153935	-0.370788	0.211556
3	17	0	0.097914	-1.376963	-2.017374
4	6	0	0.069073	-1.952052	1.069896
5	6	0	1.817030	0.202446	0.089541
6	6	0	3.640495	1.637097	-0.244150
7	7	0	2.187004	1.486282	-0.097213
8	7	0	2.923421	-0.570950	0.029246
9	6	0	4.095832	0.187945	-0.433312
10	6	0	1.385902	2.682322	0.096985

11	6	0	2.963165	-2.018916	-0.092933
12	1	0	-0.023563	-2.905303	0.534807
13	1	0	0.245940	-2.000495	2.151780
14	1	0	4.055339	2.093639	0.665702
15	1	0	3.884218	2.281482	-1.094757
16	1	0	4.983361	-0.066753	0.153834
17	1	0	4.297310	-0.047308	-1.487832
18	1	0	1.261964	3.222628	-0.849462
19	1	0	0.417319	2.417773	0.518074
20	1	0	1.887995	3.342358	0.815432
21	1	0	2.650640	-2.345471	-1.090556
22	1	0	3.985988	-2.350153	0.110106
23	1	0	2.304530	-2.474281	0.647530
24	6	0	-2.508158	-0.129135	-0.503550
25	6	0	-2.661318	-0.961116	0.568599
26	6	0	-2.692460	1.379976	-0.468251
27	6	0	-1.914010	2.069688	-1.602097
28	6	0	-4.198142	1.704512	-0.587965
29	6	0	-2.968926	-2.431354	0.434168
30	1	0	-2.492862	-0.578657	-1.496566
31	1	0	-2.755304	-0.522609	1.560770
32	1	0	-2.344194	1.756466	0.501480
33	1	0	-2.283770	1.741559	-2.581162
34	1	0	-0.843068	1.838169	-1.578643
35	1	0	-2.027357	3.158406	-1.543240
36	1	0	-4.763317	1.274662	0.245628
37	1	0	-4.614855	1.308464	-1.522555
38	1	0	-4.354456	2.790015	-0.584099
39	1	0	-2.601895	-2.833633	-0.514902
40	1	0	-4.059671	-2.568853	0.460473
41	1	0	-2.553469	-3.020967	1.256994

TS(XI-XII)b

Zero-point correction= 0.264062
(Hartree/Particle)
Thermal correction to Energy= 0.282674
Thermal correction to Enthalpy= 0.283618
Thermal correction to Gibbs Free Energy= 0.216777
Sum of electronic and zero-point Energies= -1477.323784
Sum of electronic and thermal Energies= -1477.305173
Sum of electronic and thermal Enthalpies= -1477.304229
Sum of electronic and thermal Free Energies= -1477.371069

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.631529	2.075735	1.216743
2	44	0	-0.644413	0.059851	-0.188122
3	6	0	-1.066594	1.040169	-1.679643
4	17	0	-0.591820	-2.002101	-1.530068
5	6	0	1.391132	-0.056283	0.043198
6	6	0	3.425558	-0.793490	0.921958
7	7	0	1.993699	-1.052022	0.723893
8	7	0	2.331518	0.804314	-0.380956
9	6	0	3.689485	0.308634	-0.113102
10	6	0	2.119326	1.970420	-1.217451
11	1	0	-1.206771	2.125868	-1.629947

12	1	0	-1.199601	0.562323	-2.656155
13	1	0	4.011287	-1.700556	0.744662
14	1	0	3.613271	-0.451863	1.950095
15	1	0	4.139738	-0.087210	-1.034407
16	1	0	4.326588	1.112390	0.267501
17	1	0	2.131514	1.713822	-2.285674
18	1	0	1.168187	2.429960	-0.950185
19	1	0	2.919448	2.690998	-1.020999
20	6	0	-3.025432	0.398630	-0.492697
21	6	0	-2.738635	-0.626068	0.403920
22	6	0	-2.853084	-0.485202	1.904436
23	1	0	-3.348235	0.149164	-1.498980
24	1	0	-3.230087	1.402087	-0.131939
25	1	0	-2.763732	-1.640323	0.010936
26	1	0	-2.768790	0.553983	2.227169
27	1	0	-2.087516	-1.072345	2.426251
28	1	0	-3.826553	-0.887121	2.221280
29	6	0	1.316414	-2.083807	1.487419
30	1	0	0.373335	-2.332048	0.995193
31	1	0	1.139043	-1.770961	2.526176
32	1	0	1.934430	-2.987468	1.494114

TS(XI-XII)c

Zero-point correction= 0.320939
(Hartree/Particle)
Thermal correction to Energy= 0.342364
Thermal correction to Enthalpy= 0.343308
Thermal correction to Gibbs Free Energy= 0.269890
Sum of electronic and zero-point Energies= -1555.890212
Sum of electronic and thermal Energies= -1555.868787
Sum of electronic and thermal Enthalpies= -1555.867843
Sum of electronic and thermal Free Energies= -1555.941261

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.649437	0.993707	2.166728
2	44	0	-0.198689	-0.419005	0.208596
3	6	0	-2.454552	-0.565110	-0.442632
4	17	0	0.256180	-1.708447	-1.834848
5	6	0	-2.376287	-1.495098	0.580796
6	6	0	-0.110258	-1.909968	1.266641
7	6	0	1.712529	0.318088	0.041618
8	6	0	3.432878	1.810430	-0.504987
9	7	0	1.989400	1.564102	-0.386557
10	7	0	2.871013	-0.350212	0.204247
11	6	0	4.015078	0.400926	-0.337065
12	6	0	1.063011	2.679037	-0.474212
13	6	0	3.008224	-1.781769	0.424419
14	6	0	-3.158966	0.775822	-0.312346
15	6	0	-2.696301	1.761355	-1.395845
16	6	0	-4.683544	0.548088	-0.417794
17	1	0	-2.329217	-0.942723	-1.457259
18	1	0	-2.293319	-2.550680	0.341417
19	1	0	-2.683873	-1.231023	1.588750
20	1	0	0.060838	-2.906841	0.844113
21	1	0	-0.246648	-1.846154	2.352506

22	1	0	3.755435	2.497255	0.290010
23	1	0	3.677589	2.262946	-1.471253
24	1	0	4.866377	0.365874	0.349675
25	1	0	4.324872	-0.033491	-1.297461
26	1	0	0.851062	2.938055	-1.518996
27	1	0	0.141583	2.432732	0.055546
28	1	0	1.502624	3.553506	0.020819
29	1	0	2.686688	-2.351870	-0.453652
30	1	0	4.058165	-1.993411	0.645530
31	1	0	2.410615	-2.084105	1.286799
32	1	0	-2.905587	1.369737	-2.399396
33	1	0	-1.620682	1.956827	-1.336791
34	1	0	-3.215243	2.721011	-1.292976
35	1	0	-5.045175	-0.104588	0.383939
36	1	0	-4.951830	0.087552	-1.377001
37	1	0	-5.214382	1.504792	-0.344856
38	1	0	-2.935968	1.193381	0.674987

TS(XI-XII)e

Zero-point correction= 0.349334
(Hartree/Particle)
Thermal correction to Energy= 0.372117
Thermal correction to Enthalpy= 0.373061
Thermal correction to Gibbs Free Energy= 0.296908
Sum of electronic and zero-point Energies= -1595.175453
Sum of electronic and thermal Energies= -1595.152670
Sum of electronic and thermal Enthalpies= -1595.151726
Sum of electronic and thermal Free Energies= -1595.227879

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.427121	1.212681	2.129149
2	44	0	-0.130682	-0.277859	0.194540
3	17	0	0.223792	-1.653912	-1.813774
4	6	0	-0.343315	-1.727496	1.298334
5	6	0	1.865364	0.232927	0.048138
6	6	0	3.763593	1.500218	-0.480333
7	7	0	2.299151	1.431629	-0.382326
8	7	0	2.931927	-0.569926	0.234203
9	6	0	4.167404	0.032960	-0.290490
10	6	0	1.518722	2.652181	-0.485682
11	6	0	2.906295	-2.006391	0.448263
12	1	0	-0.279406	-2.751259	0.915907
13	1	0	-0.512386	-1.605934	2.373922
14	1	0	4.154869	2.151182	0.313861
15	1	0	4.074814	1.910682	-1.446234
16	1	0	4.995488	-0.099642	0.412777
17	1	0	4.439006	-0.447530	-1.240629
18	1	0	1.348273	2.926481	-1.534053
19	1	0	0.570945	2.524931	0.038974
20	1	0	2.060954	3.469132	0.005732
21	1	0	2.775959	-2.547955	-0.495668
22	1	0	3.847490	-2.302585	0.922551
23	1	0	2.083839	-2.261796	1.114837
24	6	0	-2.304802	-0.112551	-0.471932
25	6	0	-2.439158	-1.119678	0.496452
26	6	0	-2.887901	1.285631	-0.304196

27	6	0	-2.321971	2.260966	-1.346124
28	6	0	-4.424159	1.198255	-0.446306
29	6	0	-2.781003	-2.541243	0.097307
30	1	0	-2.247811	-0.463375	-1.504885
31	1	0	-2.731012	-0.797375	1.495463
32	1	0	-2.651124	1.652532	0.698972
33	1	0	-2.540032	1.917887	-2.365772
34	1	0	-1.236646	2.367052	-1.257340
35	1	0	-2.763828	3.256485	-1.224716
36	1	0	-4.862166	0.560344	0.329446
37	1	0	-4.711260	0.789065	-1.423484
38	1	0	-4.871952	2.195373	-0.356789
39	1	0	-2.201704	-2.848912	-0.777860
40	1	0	-3.846775	-2.576144	-0.167307
41	1	0	-2.620874	-3.258530	0.907422

XIIb

Zero-point correction= 0.266748
(Hartree/Particle)
Thermal correction to Energy= 0.284504
Thermal correction to Enthalpy= 0.285448
Thermal correction to Gibbs Free Energy= 0.220831
Sum of electronic and zero-point Energies= -1477.340255
Sum of electronic and thermal Energies= -1477.322500
Sum of electronic and thermal Enthalpies= -1477.321556
Sum of electronic and thermal Free Energies= -1477.386172

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.704076	1.856032	-1.512591
2	44	0	0.632257	0.094521	0.177182
3	6	0	1.860105	1.119426	1.345640
4	17	0	0.376014	-1.583706	1.945416
5	6	0	-1.373708	-0.033931	-0.078279
6	6	0	-3.441769	-0.731276	-0.877411
7	7	0	-2.007444	-1.017923	-0.732729
8	7	0	-2.268798	0.854492	0.375386
9	6	0	-3.645864	0.388318	0.157615
10	6	0	-1.980002	1.963994	1.265695
11	1	0	1.930983	2.182307	1.115388
12	1	0	1.814438	0.870794	2.404944
13	1	0	-4.037763	-1.624405	-0.667370
14	1	0	-3.661205	-0.395485	-1.900485
15	1	0	-4.070895	0.011199	1.098240
16	1	0	-4.276800	1.203049	-0.209771
17	1	0	-2.148175	1.689174	2.315338
18	1	0	-0.941844	2.270844	1.129350
19	1	0	-2.624494	2.810642	1.007985
20	6	0	2.875213	0.241447	0.526727
21	6	0	2.255932	-0.892311	-0.417601
22	6	0	2.734323	-0.902636	-1.852387
23	1	0	3.465954	-0.307083	1.263533
24	1	0	3.470105	0.900748	-0.105942
25	1	0	2.319855	-1.867079	0.070662
26	1	0	2.667911	0.082180	-2.317507
27	1	0	2.138663	-1.606923	-2.444964

28	1	0	3.776902	-1.254593	-1.892138
29	6	0	-1.363141	-2.076005	-1.488011
30	1	0	-0.390882	-2.290767	-1.040218
31	1	0	-1.233016	-1.798299	-2.542368
32	1	0	-1.973432	-2.982890	-1.429242

XIIc

Zero-point correction= 0.324015
(Hartree/Particle)
Thermal correction to Energy= 0.345262
Thermal correction to Enthalpy= 0.346206
Thermal correction to Gibbs Free Energy= 0.273488
Sum of electronic and zero-point Energies= -1555.909042
Sum of electronic and thermal Energies= -1555.887795
Sum of electronic and thermal Enthalpies= -1555.886851
Sum of electronic and thermal Free Energies= -1555.959570

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.415284	-0.827182	-2.241345
2	44	0	0.228530	-0.488338	0.174161
3	6	0	2.085348	0.196065	0.418683
4	17	0	-0.123255	-0.216348	2.584531
5	6	0	2.284043	-1.386204	0.547397
6	6	0	0.992107	-2.282977	0.501881
7	6	0	-1.646192	0.256283	-0.091398
8	6	0	-3.432354	1.738206	-0.263265
9	7	0	-2.030978	1.522631	0.123530
10	7	0	-2.702601	-0.470761	-0.487260
11	6	0	-3.952595	0.296740	-0.390533
12	6	0	-1.175089	2.630621	0.502434
13	6	0	-2.720155	-1.909012	-0.688546
14	6	0	2.903240	0.891589	-0.662013
15	6	0	2.349924	2.295154	-0.953609
16	6	0	4.379069	0.974138	-0.218118
17	1	0	2.189370	0.671657	1.398555
18	1	0	2.730312	-1.539369	1.531583
19	1	0	2.929254	-1.688926	-0.278109
20	1	0	0.735732	-2.731287	1.460889
21	1	0	0.967039	-2.957395	-0.353702
22	1	0	-3.485300	2.286318	-1.214052
23	1	0	-3.956656	2.318163	0.502302
24	1	0	-4.570123	0.139576	-1.279848
25	1	0	-4.524734	-0.018419	0.493228
26	1	0	-1.703449	3.262233	1.224427
27	1	0	-0.279252	2.239053	0.985329
28	1	0	-0.896232	3.239998	-0.367154
29	1	0	-3.019598	-2.438837	0.225684
30	1	0	-3.429512	-2.148051	-1.487330
31	1	0	-1.728543	-2.236151	-1.004540
32	1	0	2.309520	2.907154	-0.042381
33	1	0	1.343349	2.231805	-1.378788
34	1	0	2.989279	2.816531	-1.675571
35	1	0	4.805909	-0.018369	-0.032689
36	1	0	4.483433	1.562791	0.702316
37	1	0	4.982779	1.456991	-0.995607
38	1	0	2.838602	0.304728	-1.583177

XIIe

Zero-point correction= 0.352382
(Hartree/Particle)
Thermal correction to Energy= 0.375034
Thermal correction to Enthalpy= 0.375978
Thermal correction to Gibbs Free Energy= 0.300395
Sum of electronic and zero-point Energies= -1595.189400
Sum of electronic and thermal Energies= -1595.166747
Sum of electronic and thermal Enthalpies= -1595.165803
Sum of electronic and thermal Free Energies= -1595.241387

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.269910	1.044845	2.228300
2	44	0	-0.115028	-0.319005	0.206225
3	17	0	0.238146	-1.682503	-1.808354
4	6	0	-0.987907	-1.819583	1.137115
5	6	0	1.837374	0.230422	-0.005126
6	6	0	3.770759	1.430000	-0.510669
7	7	0	2.300550	1.396402	-0.475467
8	7	0	2.867538	-0.586462	0.268933
9	6	0	4.137677	-0.035550	-0.226782
10	6	0	1.534838	2.622212	-0.618847
11	6	0	2.771484	-2.003360	0.583088
12	6	0	-1.959708	0.107579	-0.475944
13	6	0	-2.257000	-1.119787	0.505521
14	6	0	-2.720868	1.403464	-0.213548
15	6	0	-2.317634	2.479967	-1.234481
16	6	0	-4.245913	1.168596	-0.304165
17	6	0	-3.067841	-2.180049	-0.264367
18	1	0	-0.797518	-2.810110	0.721470
19	1	0	-0.964434	-1.761082	2.225675
20	1	0	4.140088	2.113147	0.266288
21	1	0	4.133233	1.781523	-1.481589
22	1	0	4.928882	-0.144733	0.521352
23	1	0	4.441961	-0.569606	-1.137230
24	1	0	1.372340	2.869880	-1.674378
25	1	0	0.580471	2.510552	-0.103689
26	1	0	2.079954	3.445502	-0.142099
27	1	0	2.774602	-2.612484	-0.327903
28	1	0	3.617074	-2.278887	1.221870
29	1	0	1.846650	-2.195098	1.127414
30	1	0	-2.046001	-0.218150	-1.517230
31	1	0	-2.800721	-0.685587	1.347798
32	1	0	-2.482029	1.757669	0.794017
33	1	0	-2.533619	2.150659	-2.259162
34	1	0	-1.251922	2.716337	-1.179574
35	1	0	-2.876339	3.405948	-1.055803
36	1	0	-4.600414	0.457440	0.449284
37	1	0	-4.532535	0.788912	-1.293268
38	1	0	-4.777734	2.113788	-0.143561
39	1	0	-2.469651	-2.582894	-1.086745
40	1	0	-3.984636	-1.747891	-0.676602
41	1	0	-3.344656	-3.001461	0.405656