

Electronic supplementary information for

## Computational Studies on the Cyclization of Squalene to the Steroids and Hopenes

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### FIGURE 2

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```
-----  
#BB95/6-31G(d) IOp(3/76=0580004200) nopop freq(noraman) GUESS=READ GEO  
M=CHECK  
-----  
   1         6         0         0.744592    -0.562658    1.639802  
   2         6         0         0.411150     0.116785    0.321175  
   3         6         0         2.756904   -0.618410    0.413244  
   4         6         0         1.871935   -1.503473    1.267520  
   5         6         0        -0.120253    2.287560    1.525268  
   6         6         0        -0.169815    1.434136    0.332147  
   7         6         0        -3.145292   -0.793251    1.326760  
   8         6         0        -3.028741   -0.928463   -0.156605  
   9         6         0        -2.680429    0.064830   -0.982119  
  10         6         0        -2.408051    1.476362   -0.620405  
  11         6         0        -0.890500    1.903389   -0.833165  
  12         6         0        -3.375214   -2.278238   -0.694255  
  13         6         0         2.353781    1.504358   -0.881791  
  14         6         0         1.549111   -0.639527   -1.837501  
  15         6         0         3.901644   -1.337689   -0.273308  
  16         6         0         1.801708    0.126103   -0.552301  
  17         1         0         1.111092    0.154122    2.374413  
  18         1         0        -0.126989   -1.054434    2.066661  
  19         1         0        -0.263591   -0.506327   -0.277599  
  20         1         0         3.182477    0.143006    1.073733  
  21         1         0         2.390538   -1.909428    2.132290  
  22         1         0         1.496583   -2.346364    0.683701  
  23         1         0        -0.622981    1.781705    2.354248  
  24         1         0        -0.557460    3.267871    1.370934  
  25         1         0         0.917040    2.393631    1.852433  
  26         1         0        -2.735358    0.135057    1.718622  
  27         1         0        -2.644417   -1.623614    1.824209  
  28         1         0        -4.191904   -0.842532    1.630387  
  29         1         0        -2.636016   -0.151301   -2.043199  
  30         1         0        -2.948870    2.138692   -1.294721  
  31         1         0        -2.730721    1.732003    0.385120  
  32         1         0        -0.553703    1.432050   -1.752316  
  33         1         0        -0.853975    2.986016   -0.917842  
  34         1         0        -2.739266   -3.048668   -0.257015  
  35         1         0        -3.282180   -2.324208   -1.775745  
  36         1         0        -4.400903   -2.538745   -0.430749  
  37         1         0         1.743649    2.042207   -1.606546  
  38         1         0         3.339854    1.387224   -1.328912  
  39         1         0         2.481773    2.127105    0.003389  
  40         1         0         0.772376   -0.165304   -2.437217  
  41         1         0         1.243089   -1.666938   -1.645204  
  42         1         0         2.452467   -0.662439   -2.444680  
  43         1         0         4.592360   -1.724120    0.473093  
  44         1         0         4.468669   -0.676037   -0.926729  
  45         1         0         3.550947   -2.181337   -0.864531  
-----  
SCF Done: E(RB+HF-B95) = -626.534649983 A.U. after 1 cycles  
Frequencies -- 18.8810 48.0041 73.0893  
Zero-point correction= 0.426823 (Hartree/Particle)  
Thermal correction to Energy= 0.445744  
Thermal correction to Enthalpy= 0.446688
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Thermal correction to Gibbs Free Energy=      0.380744
Sum of electronic and zero-point Energies=    -626.107827
Sum of electronic and thermal Energies=       -626.088906
Sum of electronic and thermal Enthalpies=     -626.087962
Sum of electronic and thermal Free Energies=   -626.153906

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-----
#BB95/6-31G(d) IOp(3/76=0580004200) nopop freq(noraman) GUESS=READ GEOM=CHECK
-----
   1         6         0      -0.327546    1.378405   -0.732771
   2         6         0      0.097666    0.012610   -0.391700
   3         6         0     -1.622585   -0.756161    0.629076
   4         6         0     -2.350141    0.580033    0.447072
   5         6         0     -1.861345    1.316578   -0.785113
   6         6         0      0.476347    0.464446    2.046505
   7         6         0      0.273443   -0.476727    0.891492
   8         6         0      3.602310    1.303268   -0.013889
   9         6         0      3.191353    0.232505   -0.972683
  10         6         0      2.740265   -0.979859   -0.627391
  11         6         0      2.508522   -1.527654    0.738215
  12         6         0      1.010449   -1.780765    1.005754
  13         6         0      3.367608    0.592785   -2.413449
  14         6         0     -1.939896   -1.785006   -0.437640
  15         6         0     -1.872957   -1.355342    2.000521
  16         6         0     -3.863139    0.390413    0.384418
  17         1         0     -0.000671    2.096990    0.014937
  18         1         0      0.080251    1.667162   -1.699020
  19         1         0      0.158559   -0.703459   -1.199659
  20         1         0     -2.136050    1.193161    1.323893
  21         1         0     -2.275487    2.320964   -0.835231
  22         1         0     -2.182497    0.797937   -1.688540
  23         1         0     -0.274356    1.244498    2.117762
  24         1         0      1.441051    0.955419    1.925256
  25         1         0      0.501291   -0.078176    2.987094
  26         1         0      3.592506    0.990086    1.025592
  27         1         0      2.962435    2.182139   -0.117756
  28         1         0      4.613833    1.637980   -0.243866
  29         1         0      2.518644   -1.670269   -1.435919
  30         1         0      3.016759   -2.486642    0.840589
  31         1         0      2.916540   -0.881956    1.512074
  32         1         0      0.646653   -2.499769    0.273295
  33         1         0      0.885230   -2.216438    1.994173
  34         1         0      2.837015    1.515009   -2.657082
  35         1         0      3.021441   -0.193511   -3.079558
  36         1         0      4.419395    0.780335   -2.632104
  37         1         0     -1.954751   -1.381681   -1.446285
  38         1         0     -2.930642   -2.187362   -0.229903
  39         1         0     -1.254953   -2.628140   -0.409936
  40         1         0     -1.312224   -2.271002    2.163139
  41         1         0     -2.929369   -1.621760    2.039755
  42         1         0     -1.681994   -0.658108    2.810413
  43         1         0     -4.260352   -0.100662    1.268884
  44         1         0     -4.156659   -0.182751   -0.492941
  45         1         0     -4.343015    1.363723    0.314658
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```

SCF Done: E(RB+HF-B95) = -626.523284416 A.U. after 1 cycles
Frequencies -- -197.8394 47.4252 51.8203
Zero-point correction= 0.428330 (Hartree/Particle)
Thermal correction to Energy= 0.446402
Thermal correction to Enthalpy= 0.447346
Thermal correction to Gibbs Free Energy= 0.384425
Sum of electronic and zero-point Energies= -626.094955
Sum of electronic and thermal Energies= -626.076882
Sum of electronic and thermal Enthalpies= -626.075938
Sum of electronic and thermal Free Energies= -626.138860

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-----
#BB95/6-31G(d) IOp(3/76=0580004200) nopop freq(noraman) GUESS=READ GEO
M=CHECK
-----

```

1	6	0	0.136941	1.417115	-0.903145
2	6	0	0.295173	-0.026784	-0.498407
3	6	0	-2.115850	-0.362633	0.095054
4	6	0	-2.366864	1.063769	-0.465330
5	6	0	-1.289132	1.534214	-1.437362
6	6	0	-0.482459	0.476030	1.855890
7	6	0	-0.645563	-0.433727	0.637001
8	6	0	2.948715	1.116894	1.225990
9	6	0	2.643112	0.351305	0.012623
10	6	0	1.749828	-0.750974	-0.060106
11	6	0	1.380188	-1.633743	1.123716
12	6	0	-0.128102	-1.822125	1.004908
13	6	0	3.299121	0.800553	-1.222624
14	6	0	-2.391933	-1.422662	-0.968736
15	6	0	-3.077829	-0.626518	1.252806
16	6	0	-3.726891	1.233454	-1.127381
17	1	0	0.283757	2.091897	-0.058002
18	1	0	0.833661	1.709275	-1.688503
19	1	0	0.075654	-0.624607	-1.379541
20	1	0	-2.353951	1.743623	0.388851
21	1	0	-1.485516	2.569473	-1.713784
22	1	0	-1.359565	0.956990	-2.363011
23	1	0	-0.979190	1.434858	1.745222
24	1	0	0.561463	0.687344	2.071587
25	1	0	-0.895681	-0.004550	2.739803
26	1	0	2.724720	0.600296	2.150968
27	1	0	2.362621	2.042018	1.188227
28	1	0	3.990830	1.435705	1.209774
29	1	0	1.988351	-1.340657	-0.941796
30	1	0	1.925658	-2.572697	1.067105
31	1	0	1.638203	-1.174583	2.074012
32	1	0	-0.336819	-2.532795	0.206404
33	1	0	-0.562739	-2.216587	1.920063
34	1	0	3.424445	1.880842	-1.260801
35	1	0	2.820840	0.425621	-2.122152
36	1	0	4.310475	0.374859	-1.189321
37	1	0	-2.276764	-2.427644	-0.569181
38	1	0	-1.767799	-1.338174	-1.857894
39	1	0	-3.424046	-1.341683	-1.300460
40	1	0	-3.077579	0.182947	1.980410
41	1	0	-2.827997	-1.551727	1.771223
42	1	0	-4.095417	-0.735226	0.884886
43	1	0	-4.541052	0.885955	-0.495927
44	1	0	-3.782462	0.701238	-2.075710
45	1	0	-3.908545	2.286005	-1.337166

```

-----
SCF Done: E(RB+HF-B95) = -626.549381956 A.U. after 1 cycles
Frequencies -- 61.6977 109.5993 114.8201
Zero-point correction= 0.431283 (Hartree/Particle)
Thermal correction to Energy= 0.448401
Thermal correction to Enthalpy= 0.449345
Thermal correction to Gibbs Free Energy= 0.389666
Sum of electronic and zero-point Energies= -626.118099
Sum of electronic and thermal Energies= -626.100981
Sum of electronic and thermal Enthalpies= -626.100037
Sum of electronic and thermal Free Energies= -626.159716

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## FIGURE 4

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-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) guess=read geom=chec
k nopop
-----

```

1	6	0	0.727834	-2.528997	0.333349
2	6	0	-1.190322	-0.944841	-0.153216
3	6	0	-0.163436	-1.418037	0.770078
4	6	0	1.333083	0.917429	-1.357413
5	6	0	0.340232	1.556159	-0.735571
6	6	0	-1.085603	1.296779	-1.143088
7	6	0	-1.837799	0.393881	-0.156463
8	6	0	0.267932	-0.625917	1.951248
9	6	0	0.516548	2.573585	0.346872
10	8	0	-1.652506	-1.871946	0.946831

11	6	0	2.799598	1.051879	-1.132115
12	1	0	0.985799	-3.180416	1.164358
13	1	0	0.303754	-3.115222	-0.479808
14	1	0	1.648381	-2.078212	-0.036385
15	1	0	-1.219280	-1.463623	-1.104449
16	1	0	1.058336	0.253893	-2.173058
17	1	0	-1.117898	0.848609	-2.136600
18	1	0	-1.637363	2.234240	-1.209670
19	1	0	-1.849346	0.825070	0.841006
20	1	0	-2.873455	0.275301	-0.471869
21	1	0	1.108599	-0.008752	1.637710
22	1	0	-0.514827	0.022899	2.327330
23	1	0	0.598774	-1.284031	2.749981
24	1	0	1.520852	2.593489	0.758239
25	1	0	0.303561	3.570530	-0.041559
26	1	0	-0.178937	2.413876	1.172536
27	1	0	-1.801932	-2.776486	0.626862
28	1	0	3.270152	1.530172	-1.991668
29	1	0	3.048658	1.641337	-0.254790
30	1	0	3.275686	0.075948	-1.030146

```

-----
SCF Done: E(RB+HF-B95) = -467.165787203 A.U. after 1 cycles
Frequencies -- 57.1309 89.2677 110.1982
Zero-point correction= 0.280684 (Hartree/Particle)
Thermal correction to Energy= 0.293800
Thermal correction to Enthalpy= 0.294744
Thermal correction to Gibbs Free Energy= 0.242401
Sum of electronic and zero-point Energies= -466.885103
Sum of electronic and thermal Energies= -466.871987
Sum of electronic and thermal Enthalpies= -466.871043
Sum of electronic and thermal Free Energies= -466.923386

```

### 30(ts)

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-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop GUESS=READ GEO
M=CHECK

```

1	6	0	0.314160	-2.625570	0.477050
2	6	0	-1.848840	-1.321117	0.192209
3	6	0	-0.574710	-1.525237	0.899704
4	6	0	0.625290	0.374664	-0.947528
5	6	0	-0.345884	1.111592	-0.389483
6	6	0	-1.775019	0.919179	-0.815510
7	6	0	-2.527311	0.010999	0.157078
8	6	0	-0.240948	-0.808537	2.144075
9	6	0	-0.120614	2.163323	0.647246
10	8	0	-2.327641	-2.203021	1.229902
11	6	0	2.086395	0.444795	-0.665544
12	1	0	0.519937	-3.301223	1.305661
13	1	0	-0.061272	-3.176310	-0.380238
14	1	0	1.273189	-2.182693	0.202468
15	1	0	-1.866876	-1.805353	-0.780890
16	1	0	0.339081	-0.286049	-1.761134
17	1	0	-1.815011	0.487789	-1.815942
18	1	0	-2.288636	1.878172	-0.866263
19	1	0	-2.573374	0.443540	1.154641
20	1	0	-3.555430	-0.135538	-0.169080
21	1	0	0.719141	-0.312777	1.991604
22	1	0	-0.978403	-0.068355	2.427016
23	1	0	-0.105844	-1.521301	2.955728
24	1	0	0.838955	2.082859	1.150022
25	1	0	-0.153890	3.147240	0.176307
26	1	0	-0.906045	2.160472	1.403460
27	1	0	-2.436470	-3.100682	0.891655
28	1	0	2.587448	1.058147	-1.416021
29	1	0	2.317450	0.876791	0.305377
30	1	0	2.555653	-0.537580	-0.723929

```

-----
SCF Done: E(RB+HF-B95) = -467.160808911 A.U. after 1 cycles
Frequencies -- -241.4810 68.5864 116.7033
Zero-point correction= 0.278806 (Hartree/Particle)
Thermal correction to Energy= 0.291703
Thermal correction to Enthalpy= 0.292647
Thermal correction to Gibbs Free Energy= 0.241189
Sum of electronic and zero-point Energies= -466.882003

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Sum of electronic and thermal Energies= -466.869106  
 Sum of electronic and thermal Enthalpies= -466.868162  
 Sum of electronic and thermal Free Energies= -466.919620

### 31

-----  
 #BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop GUESS=READ GEO  
 M=CHECK

1	6	0	1.176593	-2.075861	0.024464
2	6	0	-1.084325	-1.038535	-0.116802
3	6	0	0.388779	-0.795773	0.247088
4	6	0	0.966345	0.293240	-0.805198
5	6	0	0.101327	1.422597	-0.559800
6	6	0	-1.278587	1.319101	-1.021053
7	6	0	-1.905330	0.237672	-0.093862
8	6	0	0.531797	-0.362815	1.697053
9	6	0	0.528730	2.569261	0.228454
10	8	0	-1.572124	-1.950932	0.820340
11	6	0	2.460241	0.520434	-0.689824
12	1	0	0.681462	-2.862681	0.590775
13	1	0	1.195166	-2.367360	-1.024920
14	1	0	2.198496	-1.992034	0.384636
15	1	0	-1.107479	-1.461998	-1.128385
16	1	0	0.712509	-0.142555	-1.772988
17	1	0	-1.316712	0.950091	-2.045443
18	1	0	-1.825123	2.253749	-0.938250
19	1	0	-1.985641	0.602943	0.927951
20	1	0	-2.918368	0.063685	-0.451916
21	1	0	1.569314	-0.149828	1.946579
22	1	0	-0.067163	0.506669	1.963110
23	1	0	0.205726	-1.182206	2.332134
24	1	0	1.338784	2.346059	0.916795
25	1	0	0.942004	3.269038	-0.515737
26	1	0	-0.294668	3.084695	0.715467
27	1	0	-2.380513	-2.354388	0.497031
28	1	0	2.774571	1.355846	-1.312060
29	1	0	2.780216	0.716989	0.330213
30	1	0	2.990150	-0.360098	-1.038995

-----  
 SCF Done: E(RB+HF-B95) = -467.196726438 A.U. after 1 cycles  
 Frequencies -- 83.2250 115.5440 172.5655  
 Zero-point correction= 0.281096 (Hartree/Particle)  
 Thermal correction to Energy= 0.293484  
 Thermal correction to Enthalpy= 0.294428  
 Thermal correction to Gibbs Free Energy= 0.244681  
 Sum of electronic and zero-point Energies= -466.915630  
 Sum of electronic and thermal Energies= -466.903243  
 Sum of electronic and thermal Enthalpies= -466.902298  
 Sum of electronic and thermal Free Energies= -466.952046

### Figure 5

### 32

-----  
 #BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop

1	6	0	-2.765121	-0.952576	-1.745316
2	6	0	-0.817902	0.392014	-0.918274
3	6	0	-2.125870	-0.150497	-0.703812
4	6	0	2.190781	-0.648819	-0.222229
5	6	0	1.743958	0.374512	0.521896
6	6	0	1.206223	1.604752	-0.149048
7	6	0	1.740280	0.397720	2.016754
8	6	0	2.766754	-1.939346	0.242889
9	6	0	-0.324509	1.604492	-0.149155
10	6	0	-2.840240	0.065842	0.556564
11	1	0	-3.608841	-0.356613	-2.119370
12	1	0	-2.113266	-1.183273	-2.580902
13	1	0	-3.216751	-1.853989	-1.331284
14	1	0	-0.181793	-0.468353	-0.541916
15	1	0	-0.567825	0.424728	-1.978882
16	1	0	2.205460	-0.502900	-1.298416

17	1	0	1.565170	1.665924	-1.176224
18	1	0	1.551987	2.502533	0.362534
19	1	0	1.882492	-0.581848	2.460770
20	1	0	2.543350	1.042297	2.377106
21	1	0	0.813675	0.815231	2.412262
22	1	0	3.833145	-1.972275	0.015869
23	1	0	2.652298	-2.101410	1.310089
24	1	0	2.315598	-2.781250	-0.281265
25	1	0	-0.689682	1.586090	0.876663
26	1	0	-0.712006	2.510910	-0.612213
27	1	0	-2.168747	-0.026169	1.410553
28	1	0	-3.174300	1.110229	0.567429
29	1	0	-3.704361	-0.577988	0.676956

-----  
SCF Done: E(RB+HF-B95) = -391.979108077 A.U. after 15 cycles  
Frequencies -- 41.1604 52.2883 60.6164  
Zero-point correction= 0.270745 (Hartree/Particle)  
Thermal correction to Energy= 0.284206  
Thermal correction to Enthalpy= 0.285150  
Thermal correction to Gibbs Free Energy= 0.230424  
Sum of electronic and zero-point Energies= -391.708363  
Sum of electronic and thermal Energies= -391.694902  
Sum of electronic and thermal Enthalpies= -391.693958  
Sum of electronic and thermal Free Energies= -391.748684

### 33ts

-----  
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop

1	6	0	-2.435898	-1.604309	-1.205994
2	6	0	-1.318054	0.634949	-1.146622
3	6	0	-1.768997	-0.554108	-0.440338
4	6	0	1.903366	-0.358780	-0.341736
5	6	0	1.405426	0.684906	0.327148
6	6	0	0.796890	1.837128	-0.420517
7	6	0	1.433838	0.839523	1.816483
8	6	0	2.572281	-1.572906	0.204773
9	6	0	-0.733170	1.837143	-0.420502
10	6	0	-1.548370	-0.761108	0.975525
11	1	0	-3.492950	-1.564957	-0.909454
12	1	0	-2.372223	-1.478348	-2.281662
13	1	0	-2.095490	-2.593277	-0.898056
14	1	0	-0.570633	0.209000	-1.843200
15	1	0	-2.128479	0.899567	-1.837570
16	1	0	1.885040	-0.301178	-1.426773
17	1	0	1.141708	1.831665	-1.455368
18	1	0	1.133148	2.779282	0.012985
19	1	0	1.676727	-0.078140	2.343948
20	1	0	2.181625	1.582230	2.097214
21	1	0	0.481827	1.209091	2.202988
22	1	0	3.629837	-1.569122	-0.060577
23	1	0	2.509796	-1.649460	1.286484
24	1	0	2.153625	-2.482712	-0.226074
25	1	0	-1.120270	1.909271	0.595505
26	1	0	-1.083084	2.732941	-0.929245
27	1	0	-0.462296	-0.952347	1.029465
28	1	0	-1.692963	0.143570	1.562515
29	1	0	-2.082031	-1.609894	1.388748

-----  
SCF Done: E(RB+HF-B95) = -391.974527808 A.U. after 16 cycles  
Frequencies -- -139.0343 68.2823 76.7091  
Zero-point correction= 0.270900 (Hartree/Particle)  
Thermal correction to Energy= 0.283415  
Thermal correction to Enthalpy= 0.284359  
Thermal correction to Gibbs Free Energy= 0.233035  
Sum of electronic and zero-point Energies= -391.703628  
Sum of electronic and thermal Energies= -391.691113  
Sum of electronic and thermal Enthalpies= -391.690169  
Sum of electronic and thermal Free Energies= -391.741492

### 34

-----  
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop

1	6	0	-1.208511	-1.875793	-0.940842
---	---	---	-----------	-----------	-----------

2	6	0	-1.323959	0.618134	-1.089371
3	6	0	-0.800629	-0.566238	-0.285095
4	6	0	0.834747	-0.513809	-0.375061
5	6	0	1.113770	0.782883	0.188431
6	6	0	0.762329	1.950394	-0.606354
7	6	0	1.597595	0.947845	1.553909
8	6	0	1.526184	-1.709579	0.248993
9	6	0	-0.802704	1.950378	-0.606400
10	6	0	-1.304138	-0.539154	1.149109
11	1	0	-2.294693	-1.901505	-1.018906
12	1	0	-0.797058	-1.973740	-1.944061
13	1	0	-0.905487	-2.736847	-0.350815
14	1	0	-1.068497	0.480392	-2.141708
15	1	0	-2.412827	0.615463	-1.031448
16	1	0	1.004288	-0.482468	-1.451508
17	1	0	1.088943	1.837189	-1.638626
18	1	0	1.139114	2.879211	-0.188293
19	1	0	1.388535	0.100281	2.199158
20	1	0	2.692825	1.000031	1.452774
21	1	0	1.288162	1.889206	2.001343
22	1	0	2.602676	-1.555573	0.287598
23	1	0	1.180130	-1.922943	1.257095
24	1	0	1.349625	-2.592773	-0.356491
25	1	0	-1.166718	2.187973	0.391266
26	1	0	-1.109924	2.764572	-1.258469
27	1	0	-0.861877	-1.330841	1.750427
28	1	0	-1.133270	0.408173	1.657700
29	1	0	-2.379059	-0.711212	1.145981

-----

SCF Done: E(RB+HF-B95) = -392.016873524 A.U. after 13 cycles  
Frequencies -- 79.5578 125.9027 161.0021  
Zero-point correction= 0.276727 (Hartree/Particle)  
Thermal correction to Energy= 0.287961  
Thermal correction to Enthalpy= 0.288906  
Thermal correction to Gibbs Free Energy= 0.241511  
Sum of electronic and zero-point Energies= -391.740146  
Sum of electronic and thermal Energies= -391.728912  
Sum of electronic and thermal Enthalpies= -391.727968  
Sum of electronic and thermal Free Energies= -391.775362

## FIGURE 6

### 35a-ts

#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop

1	6	0	0.305191	-1.197723	-2.430283
2	6	0	0.314407	-1.125244	-0.849716
3	6	0	1.694244	-1.428085	-2.982208
4	6	0	-1.079086	-0.991898	-0.259872
5	6	0	1.243011	-0.021378	-0.662537
6	6	0	2.649902	-0.353912	-2.512573
7	6	0	0.762238	1.330139	-0.439453
8	6	0	-1.076965	-1.019608	1.274368
9	6	0	2.643890	-0.277863	-0.940079
10	6	0	-1.439621	0.226349	2.050308
11	6	0	-2.079666	1.271667	1.524261
12	6	0	-1.077911	0.104126	3.497452
13	6	0	-2.545273	2.507233	2.215561
14	1	0	-0.132050	-0.281540	-2.828995
15	1	0	-0.375885	-2.011414	-2.673737
16	1	0	0.783768	-2.054321	-0.523605
17	1	0	1.657562	-1.431473	-4.071091
18	1	0	2.057144	-2.410034	-2.677567
19	1	0	-1.660736	-1.827759	-0.643250
20	1	0	-1.565338	-0.101181	-0.652969
21	1	0	3.678925	-0.552292	-2.803543
22	1	0	2.379318	0.618561	-2.922958
23	1	0	1.527710	2.092667	-0.527100
24	1	0	0.326400	1.341339	0.575394
25	1	0	-0.099091	1.554840	-1.070969
26	1	0	-0.091110	-1.347412	1.620087

27	1	0	-1.748672	-1.809906	1.615311
28	1	0	3.300903	0.520432	-0.608582
29	1	0	2.975616	-1.240829	-0.559341
30	1	0	-2.348969	1.235458	0.474380
31	1	0	-0.000305	-0.013321	3.624115
32	1	0	-1.538544	-0.786865	3.926849
33	1	0	-1.394409	0.954254	4.090332
34	1	0	-2.194962	3.398575	1.694916
35	1	0	-2.216736	2.573990	3.247253
36	1	0	-3.634674	2.554306	2.209457

```

-----
SCF Done: E(RB+HF-B95) = -508.659080278 A.U. after 14 cycles
Frequencies -- -36.5086 50.4701 70.3474
Zero-point correction= 0.340393 (Hartree/Particle)
Thermal correction to Energy= 0.354613
Thermal correction to Enthalpy= 0.355558
Thermal correction to Gibbs Free Energy= 0.299902
Sum of electronic and zero-point Energies= -508.318687
Sum of electronic and thermal Energies= -508.304467
Sum of electronic and thermal Enthalpies= -508.303523
Sum of electronic and thermal Free Energies= -508.359178

```

### 35b

```

-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop
-----

```

1	6	0	0.807953	-0.541794	-2.329849
2	6	0	0.825928	-0.448288	-0.731308
3	6	0	2.177185	-0.840744	-2.892578
4	6	0	-0.576248	-0.330429	-0.167908
5	6	0	1.734512	0.669174	-0.644913
6	6	0	3.160507	0.236252	-2.496918
7	6	0	1.279022	2.049332	-0.494629
8	6	0	-0.599045	-0.219452	1.354843
9	6	0	3.139847	0.418747	-0.940002
10	6	0	-1.991913	-0.191528	1.915939
11	6	0	-2.406372	-1.189529	2.694366
12	6	0	-2.814026	1.001083	1.540024
13	6	0	-3.733047	-1.361679	3.344650
14	1	0	0.396606	0.378159	-2.746338
15	1	0	0.087341	-1.333466	-2.528870
16	1	0	1.315750	-1.363800	-0.400314
17	1	0	2.114380	-0.900391	-3.978821
18	1	0	2.520386	-1.814575	-2.543213
19	1	0	-1.122818	-1.224777	-0.465515
20	1	0	-1.101257	0.507980	-0.626343
21	1	0	4.183640	-0.005020	-2.774368
22	1	0	2.909805	1.184235	-2.972412
23	1	0	1.888565	2.748428	-1.063919
24	1	0	1.455154	2.290146	0.562881
25	1	0	0.219971	2.191605	-0.681534
26	1	0	-0.067963	0.689758	1.657562
27	1	0	-0.048660	-1.059052	1.780289
28	1	0	3.781097	1.250839	-0.661743
29	1	0	3.491257	-0.504578	-0.485229
30	1	0	-1.698547	-1.987686	2.893295
31	1	0	-3.095367	0.986755	0.485092
32	1	0	-2.256012	1.924118	1.709412
33	1	0	-3.732849	1.069138	2.112198
34	1	0	-3.620422	-1.439728	4.426117
35	1	0	-4.200700	-2.289291	3.013458
36	1	0	-4.423447	-0.550247	3.136307

```

-----
SCF Done: E(RB+HF-B95) = -508.663090467 A.U. after 15 cycles
Frequencies -- 31.9891 39.9782 65.3806
Zero-point correction= 0.340536 (Hartree/Particle)
Thermal correction to Energy= 0.355742
Thermal correction to Enthalpy= 0.356686
Thermal correction to Gibbs Free Energy= 0.297732
Sum of electronic and zero-point Energies= -508.322554
Sum of electronic and thermal Energies= -508.307348
Sum of electronic and thermal Enthalpies= -508.306404
Sum of electronic and thermal Free Energies= -508.365358

```

### 35c



```

-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop
-----

```

1	6	0	-0.226257	-1.442322	-2.264969
2	6	0	-0.109528	-1.078552	-0.722549
3	6	0	1.132416	-1.599426	-2.910675
4	6	0	-1.472534	-1.037140	-0.048050
5	6	0	0.656387	0.148438	-0.852188
6	6	0	1.960800	-0.345261	-2.740753
7	6	0	0.012741	1.453766	-0.873032
8	6	0	-1.439789	-1.035172	1.480408
9	6	0	2.057770	0.020844	-1.216187
10	6	0	-0.818893	0.179092	2.127441
11	6	0	-1.582916	1.227722	2.441376
12	6	0	0.643295	0.081833	2.429764
13	6	0	-1.189545	2.501114	3.105667
14	1	0	-0.821747	-0.681595	-2.770721
15	1	0	-0.800720	-2.366776	-2.286255
16	1	0	0.515259	-1.861800	-0.291321
17	1	0	1.007706	-1.816086	-3.971130
18	1	0	1.652969	-2.452637	-2.475067
19	1	0	-2.012802	-1.925583	-0.374359
20	1	0	-2.051727	-0.185806	-0.405975
21	1	0	2.981781	-0.465317	-3.095703
22	1	0	1.523117	0.489410	-3.287796
23	1	0	0.648666	2.246231	-1.252029
24	1	0	-0.253418	1.660110	0.176834
25	1	0	-0.946579	1.430222	-1.388916
26	1	0	-0.922211	-1.934662	1.820908
27	1	0	-2.470398	-1.135162	1.816589
28	1	0	2.615372	0.944916	-1.095276
29	1	0	2.550156	-0.801071	-0.702469
30	1	0	-2.642151	1.144104	2.218872
31	1	0	1.233795	-0.201111	1.551758
32	1	0	0.824966	-0.704407	3.164093
33	1	0	1.063370	1.002090	2.822449
34	1	0	-1.676056	2.581573	4.078094
35	1	0	-1.523773	3.361145	2.525009
36	1	0	-0.119705	2.596771	3.265762

```

-----
SCF Done: E(RB+HF-B95) = -508.663579870 A.U. after 14 cycles
Frequencies -- 55.1614 60.4357 103.0126
Zero-point correction= 0.341073 (Hartree/Particle)
Thermal correction to Energy= 0.355761
Thermal correction to Enthalpy= 0.356705
Thermal correction to Gibbs Free Energy= 0.300316
Sum of electronic and zero-point Energies= -508.322507
Sum of electronic and thermal Energies= -508.307819
Sum of electronic and thermal Enthalpies= -508.306875
Sum of electronic and thermal Free Energies= -508.363264
-----

```

### 35d-ts

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-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop
-----

```

1	6	0	0.347382	0.362869	-2.414886
2	6	0	0.389587	0.210083	-0.829865
3	6	0	1.718170	0.218719	-3.034363
4	6	0	-0.998398	0.229706	-0.221054
5	6	0	1.286438	1.309479	-0.548264
6	6	0	2.668915	1.250168	-2.470963
7	6	0	0.797394	2.611389	-0.109344
8	6	0	-0.975662	0.173584	1.321350
9	6	0	2.687088	1.145691	-0.903824
10	6	0	-1.650681	-1.047623	1.878891
11	6	0	-0.928253	-1.988693	2.483459
12	6	0	-3.135468	-1.075211	1.704910
13	6	0	-1.399887	-3.256729	3.102509
14	1	0	-0.106262	1.320267	-2.673965
15	1	0	-0.343018	-0.415222	-2.736832
16	1	0	0.889755	-0.740479	-0.643753
17	1	0	1.641144	0.342484	-4.114182
18	1	0	2.103989	-0.785614	-2.859039
19	1	0	-1.523529	-0.639511	-0.613937
20	1	0	-1.552078	1.096481	-0.582703

21	1	0	3.693634	1.106903	-2.805100
22	1	0	2.369217	2.256454	-2.762711
23	1	0	1.458191	3.430450	-0.378754
24	1	0	0.796800	2.544785	0.989227
25	1	0	-0.232574	2.807968	-0.394302
26	1	0	-1.458481	1.068298	1.719421
27	1	0	0.056839	0.196900	1.677994
28	1	0	3.322449	1.924255	-0.491165
29	1	0	3.062531	0.159653	-0.639694
30	1	0	0.141510	-1.818939	2.560028
31	1	0	-3.419708	-0.924194	0.661697
32	1	0	-3.600998	-0.268433	2.273651
33	1	0	-3.581300	-2.008820	2.030121
34	1	0	-1.164658	-3.270462	4.167068
35	1	0	-0.891403	-4.113831	2.660355
36	1	0	-2.469009	-3.412552	2.997818

```

-----
SCF Done: E(RB+HF-B95) = -508.658794881 A.U. after 15 cycles
Zero-point correction= 0.340513 (Hartree/Particle)
Thermal correction to Energy= 0.354739
Thermal correction to Enthalpy= 0.355683
Thermal correction to Gibbs Free Energy= 0.299622
Sum of electronic and zero-point Energies= -508.318282
Sum of electronic and thermal Energies= -508.304056
Sum of electronic and thermal Enthalpies= -508.303112
Sum of electronic and thermal Free Energies= -508.359173

```

### 35e-ts

```

-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop

```

1	6	0	-0.093582	-1.518753	-2.192276
2	6	0	-0.114868	-1.048462	-0.667648
3	6	0	1.321762	-1.642807	-2.711273
4	6	0	-1.510406	-1.067520	-0.066269
5	6	0	0.563034	0.214966	-0.862700
6	6	0	2.064300	-0.332016	-2.578613
7	6	0	-0.156326	1.463150	-1.098846
8	6	0	-1.507355	-1.055252	1.462509
9	6	0	1.997467	0.169327	-1.090256
10	6	0	-0.854736	0.153015	2.090744
11	6	0	-1.563782	1.270569	2.258743
12	6	0	0.557449	-0.033768	2.555374
13	6	0	-1.140182	2.555954	2.880905
14	1	0	-0.685700	-0.833130	-2.798813
15	1	0	-0.615112	-2.474197	-2.183289
16	1	0	0.539352	-1.752090	-0.152557
17	1	0	1.299408	-1.947600	-3.757095
18	1	0	1.846939	-2.427673	-2.166565
19	1	0	-2.008011	-1.974152	-0.409271
20	1	0	-2.102936	-0.232956	-0.440048
21	1	0	3.118744	-0.419724	-2.829651
22	1	0	1.636368	0.426331	-3.233765
23	1	0	0.437332	2.198898	-1.632523
24	1	0	-0.372559	1.850861	-0.094345
25	1	0	-1.126114	1.315735	-1.567688
26	1	0	-1.017868	-1.963455	1.819122
27	1	0	-2.544632	-1.124069	1.786255
28	1	0	2.472763	1.143204	-1.014511
29	1	0	2.499588	-0.559708	-0.459320
30	1	0	-2.600082	1.245834	1.934509
31	1	0	1.191635	-0.482651	1.786743
32	1	0	0.583847	-0.726242	3.398376
33	1	0	1.030151	0.888474	2.877563
34	1	0	-1.713760	2.739151	3.789963
35	1	0	-1.344437	3.398163	2.218704
36	1	0	-0.087906	2.582062	3.147583

```

-----
SCF Done: E(RB+HF-B95) = -508.663279914 A.U. after 15 cycles
Frequencies -- -26.1214 54.7478 72.8467
Zero-point correction= 0.340378 (Hartree/Particle)
Thermal correction to Energy= 0.354588
Thermal correction to Enthalpy= 0.355532
Thermal correction to Gibbs Free Energy= 0.300196
Sum of electronic and zero-point Energies= -508.322902

```

Sum of electronic and thermal Energies= -508.308692  
 Sum of electronic and thermal Enthalpies= -508.307747  
 Sum of electronic and thermal Free Energies= -508.363084

### 36a

```
-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop
-----
```

1	6	0	-1.743576	-1.592194	-0.084549
2	6	0	-0.342941	-0.994263	-0.063873
3	6	0	-2.669891	-0.790588	-0.980270
4	6	0	0.591782	-1.841248	0.786148
5	6	0	-0.342987	0.484070	0.359924
6	6	0	-2.691772	0.668716	-0.569153
7	6	0	-0.767258	0.673126	1.811539
8	6	0	1.918579	-1.084000	1.203751
9	6	0	-1.285858	1.260483	-0.557159
10	6	0	2.047485	-0.105362	0.145660
11	6	0	1.177612	1.060318	0.191589
12	6	0	2.936569	-0.376389	-0.977661
13	6	0	1.412781	2.087784	-0.898041
14	1	0	-2.141068	-1.626953	0.931992
15	1	0	-1.683853	-2.626373	-0.423615
16	1	0	0.022903	-1.011154	-1.099564
17	1	0	-3.673523	-1.210175	-0.949753
18	1	0	-2.330002	-0.870773	-2.015457
19	1	0	0.866806	-2.748138	0.254974
20	1	0	0.110565	-2.133835	1.717468
21	1	0	-3.299164	1.248535	-1.262131
22	1	0	-3.161514	0.777206	0.408707
23	1	0	-1.769135	0.287140	1.976974
24	1	0	-0.782089	1.731552	2.067093
25	1	0	-0.112244	0.171509	2.520432
26	1	0	2.748520	-1.780975	1.254822
27	1	0	1.761124	-0.613617	2.168732
28	1	0	-1.325943	2.306305	-0.254333
29	1	0	-0.907333	1.234589	-1.579254
30	1	0	1.365524	1.523438	1.165924
31	1	0	3.250931	-1.414093	-1.032120
32	1	0	3.836914	0.224518	-0.776642
33	1	0	2.552917	-0.015747	-1.928436
34	1	0	2.448364	2.423721	-0.888367
35	1	0	0.791092	2.961487	-0.732971
36	1	0	1.189285	1.711060	-1.892883

```
-----
SCF Done: E(RB+HF-B95) = -508.685892852 A.U. after 15 cycles
Frequencies -- 40.8678 85.7082 107.2044
Zero-point correction= 0.343972 (Hartree/Particle)
Thermal correction to Energy= 0.357251
Thermal correction to Enthalpy= 0.358195
Thermal correction to Gibbs Free Energy= 0.305427
Sum of electronic and zero-point Energies= -508.341921
Sum of electronic and thermal Energies= -508.328642
Sum of electronic and thermal Enthalpies= -508.327698
Sum of electronic and thermal Free Energies= -508.380465
-----
```

### 36b

```
-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop
-----
```

1	6	0	-1.757309	-1.744934	0.349396
2	6	0	-0.377609	-1.151627	0.136673
3	6	0	-2.714400	-1.114365	-0.654037
4	6	0	0.788910	-1.818481	0.846893
5	6	0	-0.377594	0.358109	0.389252
6	6	0	-2.692993	0.405609	-0.603745
7	6	0	-0.853409	0.733292	1.788788
8	6	0	2.036911	-1.409973	0.089233
9	6	0	-1.282852	0.991302	-0.669968
10	6	0	2.037186	-0.015778	-0.358719
11	6	0	1.115768	0.910095	0.265823
12	6	0	2.999374	0.411377	-1.369019
13	6	0	1.229996	2.367264	-0.126282
14	1	0	-2.097229	-1.587555	1.372986
15	1	0	-1.716583	-2.823334	0.199020

16	1	0	-0.172577	-1.271225	-0.938568
17	1	0	-3.728302	-1.474838	-0.491379
18	1	0	-2.427170	-1.444382	-1.655289
19	1	0	0.701370	-2.902222	0.836807
20	1	0	0.842163	-1.520142	1.894440
21	1	0	-3.271683	0.810059	-1.432785
22	1	0	-3.191147	0.753876	0.300476
23	1	0	-1.905991	0.515167	1.931091
24	1	0	-0.721832	1.800674	1.963867
25	1	0	-0.303589	0.199539	2.563629
26	1	0	2.217911	-2.043060	-0.784653
27	1	0	2.964142	-1.516373	0.674118
28	1	0	-1.336060	2.071457	-0.541519
29	1	0	-0.861908	0.805573	-1.662079
30	1	0	1.469330	0.786163	1.310394
31	1	0	3.719223	-0.353134	-1.639969
32	1	0	3.500046	1.333710	-1.072571
33	1	0	2.416931	0.691696	-2.256668
34	1	0	2.227432	2.760696	0.057159
35	1	0	0.538589	2.963806	0.462036
36	1	0	0.985138	2.521774	-1.175034

-----

SCF Done: E(RB+HF-B95) = -508.689838925 A.U. after 15 cycles  
Frequencies -- 21.1002 90.4295 129.8044  
Zero-point correction= 0.342851 (Hartree/Particle)  
Thermal correction to Energy= 0.356003  
Thermal correction to Enthalpy= 0.356947  
Thermal correction to Gibbs Free Energy= 0.304085  
Sum of electronic and zero-point Energies= -508.346988  
Sum of electronic and thermal Energies= -508.333836  
Sum of electronic and thermal Enthalpies= -508.332892  
Sum of electronic and thermal Free Energies= -508.385754

## FIGURE 7

35f

-----

#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop

-----

1	6	0	-2.376495	-2.266983	1.619034
2	6	0	2.313583	-0.242828	-2.934006
3	6	0	0.917068	-0.296524	-2.360565
4	6	0	0.928253	-0.337204	-0.759491
5	6	0	1.577225	0.937668	-0.571228
6	6	0	3.000870	1.018845	-0.869766
7	6	0	3.045959	0.982208	-2.436218
8	6	0	-0.461838	-0.567917	-0.199615
9	6	0	-2.520859	0.063980	2.540634
10	6	0	-0.495972	-0.591690	1.326950
11	6	0	-1.864975	-0.884277	1.874283
12	6	0	-3.870926	-0.004913	3.161835
13	6	0	0.835663	2.168640	-0.310059
14	1	0	-3.299927	-2.473236	2.148941
15	1	0	-2.570236	-2.441040	0.559021
16	1	0	-1.643800	-3.011688	1.933746
17	1	0	2.861786	-1.146393	-2.666855
18	1	0	2.255219	-0.220062	-4.021851
19	1	0	0.311798	0.543869	-2.701600
20	1	0	0.383987	-1.205994	-2.633575
21	1	0	1.605408	-1.151200	-0.501740
22	1	0	3.544006	0.154709	-0.494110
23	1	0	3.452316	1.940887	-0.513443
24	1	0	2.592743	1.891922	-2.829590
25	1	0	4.094406	0.991653	-2.723648
26	1	0	-1.162323	0.178406	-0.575958
27	1	0	-0.806229	-1.524658	-0.589798
28	1	0	-2.017563	1.018051	2.664871
29	1	0	-0.151443	0.366730	1.719238
30	1	0	0.212234	-1.347321	1.678879
31	1	0	-4.524460	0.758926	2.739532
32	1	0	-4.357590	-0.965866	3.029633
33	1	0	-3.809036	0.195633	4.231659
34	1	0	0.941483	2.333984	0.771393
35	1	0	1.287262	3.034149	-0.790253

```

36          1          0      -0.227142    2.099213   -0.516495
-----
SCF Done:  E(RB+HF-B95) = -508.663021843    A.U. after 15 cycles
Frequencies --    22.3554          40.2273          65.0049
Zero-point correction=                0.340230 (Hartree/Particle)
Thermal correction to Energy=          0.355636
Thermal correction to Enthalpy=        0.356580
Thermal correction to Gibbs Free Energy= 0.296578
Sum of electronic and zero-point Energies= -508.322792
Sum of electronic and thermal Energies= -508.307386
Sum of electronic and thermal Enthalpies= -508.306442
Sum of electronic and thermal Free Energies= -508.366444

```

### 35g

```

-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop
-----
  1          6          0      0.512756   -0.401825    2.569336
  2          6          0      0.976761    0.045441   -2.971573
  3          6          0     -0.393021    0.143784   -2.344070
  4          6          0     -0.316269    0.150757   -0.752563
  5          6          0      0.489044    1.341080   -0.588165
  6          6          0      1.893173    1.257813   -0.967072
  7          6          0      1.843979    1.201721   -2.533157
  8          6          0     -1.698883    0.088470   -0.128357
  9          6          0     -1.088608   -2.233536    1.956421
 10          6          0     -1.687851    0.086807    1.398788
 11          6          0     -0.750381   -0.945450    1.982300
 12          6          0     -0.325821   -3.405090    2.466415
 13          6          0     -0.083328    2.641739   -0.257538
 14          1          0      1.206711   -1.171890    2.889465
 15          1          0      1.044891    0.239807    1.857315
 16          1          0      0.293610    0.226624    3.434158
 17          1          0      1.444977   -0.901138   -2.701736
 18          1          0      0.879105    0.051437   -4.056839
 19          1          0     -0.925018    1.031494   -2.688370
 20          1          0     -1.022736   -0.714844   -2.571472
 21          1          0      0.261658   -0.735245   -0.487427
 22          1          0      2.353119    0.337952   -0.612610
 23          1          0      2.467712    2.122620   -0.646927
 24          1          0      1.456207    2.145126   -2.917191
 25          1          0      2.871964    1.111450   -2.875717
 26          1          0     -2.332611    0.889893   -0.510696
 27          1          0     -2.146912   -0.842712   -0.473633
 28          1          0     -2.059753   -2.476547    1.534760
 29          1          0     -2.707642   -0.091293    1.736542
 30          1          0     -1.422836    1.077576    1.773529
 31          1          0     -0.206787   -4.157410    1.686554
 32          1          0      0.661087   -3.148468    2.839386
 33          1          0     -0.871704   -3.886353    3.278244
 34          1          0      0.085052    2.745117    0.824539
 35          1          0      0.452087    3.465317   -0.724762
 36          1          0     -1.154251    2.710098   -0.417800

```

```

-----
SCF Done:  E(RB+HF-B95) = -508.662278120    A.U. after 15 cycles
Frequencies --    32.4915          44.4301          77.8492
Zero-point correction=                0.340427 (Hartree/Particle)
Thermal correction to Energy=          0.355483
Thermal correction to Enthalpy=        0.356428
Thermal correction to Gibbs Free Energy= 0.298236
Sum of electronic and zero-point Energies= -508.321851
Sum of electronic and thermal Energies= -508.306795
Sum of electronic and thermal Enthalpies= -508.305851
Sum of electronic and thermal Free Energies= -508.364042

```

### 35h-TS

```

-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop guess=read geom=check
-----
  1          6          0     -0.584419   -1.796162    2.074434
  2          6          0      1.071389    0.503054   -2.493451
  3          6          0     -0.371659    0.460422   -2.052498
  4          6          0     -0.505867    0.368622   -0.459935
  5          6          0      0.150706    1.619633   -0.161431

```

6	6	0	1.596642	1.674499	-0.329705
7	6	0	1.778720	1.693752	-1.887175
8	6	0	-1.949989	0.163272	-0.042994
9	6	0	-3.022390	-1.892474	2.623033
10	6	0	-2.187814	0.098807	1.473181
11	6	0	-1.980062	-1.253909	2.093059
12	6	0	-3.053123	-3.227389	3.277761
13	6	0	-0.582683	2.859195	0.084060
14	1	0	-0.440007	-2.595158	2.794295
15	1	0	-0.318688	-2.204866	1.095795
16	1	0	0.141254	-1.014612	2.310595
17	1	0	1.575671	-0.420829	-2.209501
18	1	0	1.114857	0.564348	-3.580528
19	1	0	-0.928289	1.324136	-2.417752
20	1	0	-0.892740	-0.428649	-2.404093
21	1	0	0.129969	-0.467152	-0.176957
22	1	0	2.085364	0.783742	0.058156
23	1	0	2.035712	2.570915	0.099917
24	1	0	1.378781	2.626424	-2.284619
25	1	0	2.848659	1.691595	-2.080418
26	1	0	-2.564604	0.951488	-0.479276
27	1	0	-2.295458	-0.764323	-0.498446
28	1	0	-3.983050	-1.390601	2.578918
29	1	0	-3.211271	0.415693	1.662933
30	1	0	-1.546320	0.833908	1.972970
31	1	0	-3.720334	-3.898663	2.736102
32	1	0	-2.080494	-3.706246	3.335383
33	1	0	-3.450623	-3.146137	4.289420
34	1	0	-0.628907	2.949458	1.178434
35	1	0	-0.047340	3.736209	-0.271970
36	1	0	-1.609204	2.843495	-0.267776

-----  
SCF Done: E(RB+HF-B95) = -508.659775760 A.U. after 1 cycles  
Frequencies -- -28.3113 34.8039 57.0010  
Zero-point correction= 0.340589 (Hartree/Particle)  
Thermal correction to Energy= 0.354809  
Thermal correction to Enthalpy= 0.355753  
Thermal correction to Gibbs Free Energy= 0.299695  
Sum of electronic and zero-point Energies= -508.319187  
Sum of electronic and thermal Energies= -508.304967  
Sum of electronic and thermal Enthalpies= -508.304022  
Sum of electronic and thermal Free Energies= -508.360081

### 35i-ts

-----  
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop  
-----

1	6	0	-2.946548	-0.989349	1.631531
2	6	0	2.194473	-0.488876	-2.986115
3	6	0	0.864258	-0.939941	-2.425293
4	6	0	0.832458	-0.842926	-0.845917
5	6	0	1.128357	0.571884	-0.681046
6	6	0	2.481140	1.008209	-0.972809
7	6	0	2.519196	0.920242	-2.543991
8	6	0	-0.465591	-1.355606	-0.248947
9	6	0	-1.249756	0.483841	2.747864
10	6	0	-0.458496	-1.336334	1.294052
11	6	0	-1.557022	-0.521942	1.924774
12	6	0	-2.170578	1.360641	3.522644
13	6	0	0.067764	1.537567	-0.451889
14	1	0	-3.109421	-1.973663	2.073730
15	1	0	-3.707626	-0.322571	2.021729
16	1	0	-3.122284	-1.099716	0.560745
17	1	0	2.983322	-1.170807	-2.667709
18	1	0	2.163361	-0.531418	-4.074371
19	1	0	0.042221	-0.352798	-2.836456
20	1	0	0.655060	-1.984741	-2.648804
21	1	0	1.681595	-1.436462	-0.503876
22	1	0	3.232376	0.324539	-0.584595
23	1	0	2.680832	2.027466	-0.656418
24	1	0	1.813538	1.636093	-2.964676
25	1	0	3.516327	1.235077	-2.842804
26	1	0	-1.302460	-0.776108	-0.639679
27	1	0	-0.613113	-2.367737	-0.620285
28	1	0	-0.193451	0.670135	2.925140

29	1	0	0.505875	-0.973526	1.656616
30	1	0	-0.535522	-2.363434	1.654205
31	1	0	-1.944855	2.412918	3.350327
32	1	0	-3.217422	1.200256	3.285629
33	1	0	-2.043488	1.188110	4.591797
34	1	0	-0.294876	1.357208	0.575821
35	1	0	0.380936	2.569962	-0.558212
36	1	0	-0.810211	1.323471	-1.063110

-----  
SCF Done: E(RB+HF-B95) = -508.661060184 A.U. after 15 cycles  
Frequencies -- -35.6412 66.1586 69.2351  
Zero-point correction= 0.340586 (Hartree/Particle)  
Thermal correction to Energy= 0.354697  
Thermal correction to Enthalpy= 0.355641  
Thermal correction to Gibbs Free Energy= 0.300394  
Sum of electronic and zero-point Energies= -508.320474  
Sum of electronic and thermal Energies= -508.306363  
Sum of electronic and thermal Enthalpies= -508.305419  
Sum of electronic and thermal Free Energies= -508.360666

### 35j-ts

-----  
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop

1	6	0	0.547958	0.991211	2.281708
2	6	0	0.330612	-1.408798	-2.653519
3	6	0	-0.864975	-0.658813	-2.112717
4	6	0	-0.570419	-0.028305	-0.675583
5	6	0	0.539703	0.809647	-1.067017
6	6	0	1.807266	0.152756	-1.341721
7	6	0	1.540573	-0.506760	-2.742218
8	6	0	-1.807358	0.606369	-0.056519
9	6	0	-0.633636	-1.169907	2.721481
10	6	0	-1.834473	0.594437	1.496719
11	6	0	-0.612122	0.053925	2.190094
12	6	0	0.434219	-1.873795	3.482285
13	6	0	0.365555	2.215698	-1.443619
14	1	0	1.403915	0.569565	2.797546
15	1	0	0.897873	1.312546	1.293869
16	1	0	0.259644	1.904724	2.803802
17	1	0	0.548096	-2.265579	-2.015656
18	1	0	0.093689	-1.803757	-3.641144
19	1	0	-1.191620	0.123978	-2.798004
20	1	0	-1.717712	-1.312820	-1.940400
21	1	0	-0.218506	-0.860489	-0.065247
22	1	0	2.026779	-0.636429	-0.627274
23	1	0	2.637878	0.848541	-1.420059
24	1	0	1.391968	0.274261	-3.487700
25	1	0	2.446793	-1.043716	-3.012360
26	1	0	-1.944107	1.618240	-0.431213
27	1	0	-2.669083	0.049072	-0.417786
28	1	0	-1.559143	-1.728043	2.623900
29	1	0	-2.695480	0.009674	1.810165
30	1	0	-2.018600	1.609848	1.847504
31	1	0	0.637146	-2.851822	3.045898
32	1	0	1.370285	-1.325485	3.528687
33	1	0	0.106796	-2.057037	4.505997
34	1	0	0.387329	2.793579	-0.511719
35	1	0	1.168716	2.581329	-2.075851
36	1	0	-0.605347	2.412476	-1.892441

-----  
SCF Done: E(RB+HF-B95) = -508.655634482 A.U. after 15 cycles  
Frequencies -- -115.4967 48.1169 55.5480  
Zero-point correction= 0.340568 (Hartree/Particle)  
Thermal correction to Energy= 0.354944  
Thermal correction to Enthalpy= 0.355888  
Thermal correction to Gibbs Free Energy= 0.299572  
Sum of electronic and zero-point Energies= -508.315066  
Sum of electronic and thermal Energies= -508.300691  
Sum of electronic and thermal Enthalpies= -508.299746  
Sum of electronic and thermal Free Energies= -508.356062

### 35k

-----  
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop

1	6	0	2.610931	-1.532242	-0.786224
2	6	0	-2.527817	0.220276	0.326187
3	6	0	-1.213700	0.483963	1.021072
4	6	0	-0.028305	0.730072	-0.014206
5	6	0	-0.582947	1.858704	-0.724380
6	6	0	-1.719742	1.616928	-1.599091
7	6	0	-2.893875	1.365479	-0.588821
8	6	0	1.314163	0.889297	0.679900
9	6	0	0.936859	-2.631882	0.727631
10	6	0	1.790588	-0.410202	1.333633
11	6	0	1.728455	-1.602615	0.420273
12	6	0	0.746689	-3.909912	-0.011520
13	6	0	-0.156128	3.226913	-0.448975
14	1	0	2.583282	-2.437241	-1.383148
15	1	0	2.338211	-0.701202	-1.441574
16	1	0	3.646729	-1.363159	-0.489151
17	1	0	-2.467148	-0.709274	-0.240021
18	1	0	-3.309128	0.084198	1.073639
19	1	0	-1.281662	1.332138	1.703018
20	1	0	-0.877441	-0.377029	1.595261
21	1	0	-0.039307	-0.164520	-0.639893
22	1	0	-1.592789	0.715347	-2.194122
23	1	0	-1.952850	2.467712	-2.232971
24	1	0	-3.085205	2.274765	-0.019363
25	1	0	-3.781097	1.163925	-1.184433
26	1	0	2.048233	1.218231	-0.056763
27	1	0	1.265625	1.669250	1.439987
28	1	0	0.383163	-2.564941	1.659882
29	1	0	1.211594	-0.606216	2.235504
30	1	0	2.817444	-0.246780	1.665039
31	1	0	-0.310806	-4.091248	-0.204880
32	1	0	1.269485	-3.940933	-0.962265
33	1	0	1.097977	-4.749329	0.589066
34	1	0	0.734192	3.373535	-1.079071
35	1	0	-0.887360	3.973816	-0.742279
36	1	0	0.184128	3.374435	0.572662

SCF Done: E(RB+HF-B95) = -508.665550604 A.U. after 14 cycles  
 Frequencies -- 33.7795 52.5560 65.4949  
 Zero-point correction= 0.340709 (Hartree/Particle)  
 Thermal correction to Energy= 0.355795  
 Thermal correction to Enthalpy= 0.356739  
 Thermal correction to Gibbs Free Energy= 0.298290  
 Sum of electronic and zero-point Energies= -508.324841  
 Sum of electronic and thermal Energies= -508.309756  
 Sum of electronic and thermal Enthalpies= -508.308812  
 Sum of electronic and thermal Free Energies= -508.367260

### 36c

#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop

1	6	0	2.760635	1.453354	-0.128616
2	6	0	-2.715485	-1.327576	0.749847
3	6	0	-1.501877	-1.104324	1.636078
4	6	0	-0.239395	-1.004745	0.783585
5	6	0	-0.347366	0.144348	-0.220825
6	6	0	-1.563690	-0.083038	-1.120010
7	6	0	-2.842850	-0.242905	-0.301987
8	6	0	1.016647	-0.917191	1.616592
9	6	0	0.965103	0.024460	-1.207825
10	6	0	2.274796	-0.885361	0.690018
11	6	0	2.028564	0.197205	-0.254288
12	6	0	0.933960	0.952454	-2.404541
13	6	0	-0.423172	1.514847	0.434891
14	1	0	2.221649	2.312805	-0.514847
15	1	0	3.134949	1.626190	0.877304
16	1	0	3.644577	1.324768	-0.771912
17	1	0	-2.623795	-2.299911	0.260971
18	1	0	-3.618454	-1.369095	1.356110
19	1	0	-1.623260	-0.198120	2.232483
20	1	0	-1.392105	-1.926697	2.341782
21	1	0	-0.185089	-1.928131	0.195938
22	1	0	-1.402191	-0.988647	-1.709702



23	1	0	-1.675049	0.743881	-1.819504
24	1	0	-3.110428	0.703705	0.167908
25	1	0	-3.655350	-0.475113	-0.988998
26	1	0	1.010574	-0.042007	2.264481
27	1	0	1.129471	-1.786804	2.260406
28	1	0	0.917236	-1.018311	-1.520309
29	1	0	2.319611	-1.844009	0.175461
30	1	0	3.175461	-0.733200	1.277695
31	1	0	0.161972	0.633011	-3.097397
32	1	0	0.733826	1.987289	-2.138031
33	1	0	1.881546	0.920670	-2.938873
34	1	0	-0.373520	2.311020	-0.305725
35	1	0	-1.372925	1.630020	0.948669
36	1	0	0.355927	1.694687	1.173508

---

SCF Done: E(RB+HF-B95) = -508.699948625 A.U. after 14 cycles  
Frequencies -- 88.7290 111.4817 150.8873  
Zero-point correction= 0.344399 (Hartree/Particle)  
Thermal correction to Energy= 0.357513  
Thermal correction to Enthalpy= 0.358457  
Thermal correction to Gibbs Free Energy= 0.306826  
Sum of electronic and zero-point Energies= -508.355550  
Sum of electronic and thermal Energies= -508.342436  
Sum of electronic and thermal Enthalpies= -508.341492  
Sum of electronic and thermal Free Energies= -508.393123

## FIGURE 8

### 37a

---

#BB95/6-31G(d) IOp(3/76=0580004200) nopop freq(noraman) guess=read geo  
m=check

---

1	6	0	-4.811216	1.415626	-0.326110
2	6	0	-2.910546	0.060164	0.585822
3	6	0	-3.951814	0.233172	-0.378201
4	6	0	0.222588	0.831357	0.543072
5	6	0	-0.039486	-0.483156	0.445017
6	6	0	-0.925190	-1.143762	1.460033
7	6	0	-2.343608	-1.310990	0.908403
8	6	0	-4.166680	-0.745527	-1.448021
9	6	0	0.507125	-1.375223	-0.621456
10	6	0	3.851048	0.126753	-1.004471
11	6	0	3.297203	0.550063	0.130574
12	6	0	1.062698	1.667268	-0.362292
13	6	0	2.508906	1.835626	0.131207
14	6	0	3.405241	-0.147291	1.448837
15	6	0	4.652971	-1.105240	-1.242426
16	1	0	-5.816337	1.060985	-0.061857
17	1	0	-4.500918	2.148762	0.410505
18	1	0	-4.920732	1.866904	-1.312477
19	1	0	-2.058662	0.599888	0.057706
20	1	0	-3.071171	0.678920	1.468590
21	1	0	-0.149676	1.340606	1.428201
22	1	0	-0.963488	-0.553754	2.375739
23	1	0	-0.538749	-2.126549	1.728146
24	1	0	-2.315493	-1.936863	0.017608
25	1	0	-2.986413	-1.809585	1.632482
26	1	0	-3.218490	-1.079582	-1.870203
27	1	0	-4.609747	-1.639403	-0.994095
28	1	0	-4.827042	-0.387276	-2.229924
29	1	0	0.919238	-0.829963	-1.463789
30	1	0	1.319674	-1.972819	-0.203940
31	1	0	-0.241415	-2.079085	-0.988223
32	1	0	3.722264	0.758260	-1.879043
33	1	0	1.091626	1.249719	-1.367328
34	1	0	0.610958	2.657261	-0.442504
35	1	0	2.989487	2.565446	-0.519172
36	1	0	2.499444	2.270769	1.131660
37	1	0	2.422275	-0.282976	1.902293
38	1	0	3.883186	-1.119701	1.382021
39	1	0	3.985987	0.456690	2.148390
40	1	0	4.741769	-1.735128	-0.362112

41	1	0	4.214949	-1.705284	-2.041327
42	1	0	5.662035	-0.849278	-1.567259

---

SCF Done: E(RB+HF-B95) = -587.205176275 A.U. after 1 cycles  
Frequencies -- 28.6471 37.6365 42.3924  
Zero-point correction= 0.393275 (Hartree/Particle)  
Thermal correction to Energy= 0.412552  
Thermal correction to Enthalpy= 0.413496  
Thermal correction to Gibbs Free Energy= 0.344726  
Sum of electronic and zero-point Energies= -586.811901  
Sum of electronic and thermal Energies= -586.792624  
Sum of electronic and thermal Enthalpies= -586.791680  
Sum of electronic and thermal Free Energies= -586.860450

### 39a-ts

---

#BB95/6-31G(d) IOp(3/76=0580004200) nopop freq(noraman) guess=read geom=check

1	6	0	-2.357073	-0.612463	3.697321
2	6	0	-3.044958	-0.833466	1.300326
3	6	0	-2.594459	0.009744	2.396712
4	6	0	-0.005714	-0.046802	-0.217250
5	6	0	-1.107250	0.514561	-0.722309
6	6	0	-2.296283	-0.334027	-1.073094
7	6	0	-3.436511	-0.265234	-0.055420
8	6	0	-2.328299	1.423799	2.245947
9	6	0	-1.253093	1.972078	-1.035237
10	6	0	2.041566	0.479212	-2.656139
11	6	0	2.742150	-0.239753	-1.782283
12	6	0	1.280895	0.605559	0.177374
13	6	0	2.499379	-0.174051	-0.298990
14	6	0	3.860928	-1.165000	-2.143820
15	6	0	2.194973	0.531949	-4.137350
16	1	0	-3.169453	-0.263730	4.349130
17	1	0	-2.366935	-1.697135	3.679212
18	1	0	-1.445404	-0.229049	4.156249
19	1	0	-2.194138	-1.532312	1.189879
20	1	0	-3.809832	-1.494406	1.728164
21	1	0	-0.007579	-1.129346	-0.108883
22	1	0	-1.989220	-1.375610	-1.177754
23	1	0	-2.693196	-0.029889	-2.042125
24	1	0	-3.811116	0.753642	0.039471
25	1	0	-4.274552	-0.850538	-0.427973
26	1	0	-1.401803	1.429030	1.644689
27	1	0	-3.057399	1.929273	1.616222
28	1	0	-2.155611	1.947416	3.179640
29	1	0	-0.465698	2.586487	-0.608617
30	1	0	-1.239223	2.122332	-2.115970
31	1	0	-2.210723	2.368510	-0.690341
32	1	0	1.257155	1.119757	-2.270314
33	1	0	1.333579	1.631836	-0.181631
34	1	0	1.339415	0.660006	1.268965
35	1	0	3.388571	0.245922	0.177803
36	1	0	2.431367	-1.196392	0.086685
37	1	0	3.625885	-2.189040	-1.848090
38	1	0	4.086925	-1.170176	-3.204426
39	1	0	4.772921	-0.889294	-1.611976
40	1	0	2.980745	-0.116531	-4.511153
41	1	0	1.266466	0.244254	-4.632512
42	1	0	2.420691	1.547622	-4.464510

---

SCF Done: E(RB+HF-B95) = -587.200372649 A.U. after 1 cycles  
Frequencies -- -103.6734 23.2577 40.2239  
Zero-point correction= 0.392670 (Hartree/Particle)  
Thermal correction to Energy= 0.411463  
Thermal correction to Enthalpy= 0.412407  
Thermal correction to Gibbs Free Energy= 0.345114  
Sum of electronic and zero-point Energies= -586.807703  
Sum of electronic and thermal Energies= -586.788910  
Sum of electronic and thermal Enthalpies= -586.787966  
Sum of electronic and thermal Free Energies= -586.855259

```
-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop guess=read geo
m=check
```

```
-----
```

1	6	0	2.502774	1.807524	-0.719624
2	6	0	2.269423	-0.605774	-1.190992
3	6	0	2.000620	0.483823	-0.146261
4	6	0	0.472213	0.564460	0.000979
5	6	0	-0.244817	-0.746267	0.356953
6	6	0	0.052668	-1.749661	-0.755559
7	6	0	1.558855	-1.920612	-0.926034
8	6	0	2.759545	0.228570	1.151928
9	6	0	0.100979	-1.346268	1.717219
10	6	0	-1.821211	-0.441130	0.432889
11	6	0	-2.209116	0.823766	-0.151026
12	6	0	-0.098580	1.704631	0.837247
13	6	0	-1.459404	2.016405	0.247012
14	6	0	-3.341311	0.952357	-1.062042
15	6	0	-2.712009	-1.631585	0.151682
16	1	0	3.531213	1.693680	-1.058449
17	1	0	1.909000	2.128987	-1.576640
18	1	0	2.499999	2.606538	0.020463
19	1	0	1.949797	-0.224639	-2.165321
20	1	0	3.344059	-0.772928	-1.266850
21	1	0	0.141570	0.773910	-1.029944
22	1	0	-0.373110	-1.391458	-1.697276
23	1	0	-0.403394	-2.715173	-0.541953
24	1	0	1.982962	-2.409690	-0.049382
25	1	0	1.736915	-2.603391	-1.755668
26	1	0	2.387529	0.855669	1.963014
27	1	0	2.722407	-0.804981	1.481339
28	1	0	3.810032	0.477142	1.009984
29	1	0	0.159095	-0.590877	2.499819
30	1	0	-0.658392	-2.070054	2.011417
31	1	0	1.044094	-1.876595	1.704718
32	1	0	-1.912266	-0.151537	1.499109
33	1	0	-0.176725	1.424889	1.888750
34	1	0	0.516424	2.598487	0.799686
35	1	0	-2.130837	2.549295	0.939234
36	1	0	-1.394339	2.686840	-0.614364
37	1	0	-3.043912	0.452273	-1.993985
38	1	0	-4.204840	0.387113	-0.711521
39	1	0	-3.609145	1.979863	-1.283331
40	1	0	-2.728114	-1.882222	-0.906775
41	1	0	-2.349311	-2.504324	0.687209
42	1	0	-3.734489	-1.458264	0.480492

```
-----
```

```
SCF Done: E(RB+HF-B95) = -587.264289213 A.U. after 1 cycles
Frequencies -- 41.7396 84.4740 117.0392
Zero-point correction= 0.400265 (Hartree/Particle)
Thermal correction to Energy= 0.416096
Thermal correction to Enthalpy= 0.417041
Thermal correction to Gibbs Free Energy= 0.359525
Sum of electronic and zero-point Energies= -586.864025
Sum of electronic and thermal Energies= -586.848193
Sum of electronic and thermal Enthalpies= -586.847249
Sum of electronic and thermal Free Energies= -586.904764
```

## **FIGURE 10**

### **37b**

```
-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop guess=read geo
m=check
```

```
-----
```

1	6	0	-4.531179	-1.412081	-1.252519
2	6	0	-2.731066	0.226616	-0.657637
3	6	0	-3.947930	-0.446769	-0.321690
4	6	0	0.395990	-0.406618	-0.100289
5	6	0	-0.116043	0.618141	0.599977
6	6	0	-0.830672	1.724550	-0.119971
7	6	0	-0.048576	0.756568	2.087360

8	6	0	4.682492	1.316791	-1.352835
9	6	0	3.719269	-0.139827	1.220588
10	6	0	1.148755	-1.594084	0.394812
11	6	0	3.799756	0.120411	-1.271213
12	6	0	2.497530	-1.731913	-0.321163
13	6	0	3.376958	-0.522211	-0.184190
14	6	0	-2.348641	1.551639	-0.022871
15	6	0	-4.624677	-0.205091	0.955483
16	1	0	-5.460065	-0.960187	-1.626179
17	1	0	-3.896086	-1.638224	-2.102248
18	1	0	-4.844505	-2.320136	-0.737641
19	1	0	-1.971784	-0.515347	-0.252865
20	1	0	-2.538970	0.193526	-1.730363
21	1	0	0.328568	-0.339832	-1.183381
22	1	0	-0.538243	1.743921	-1.169492
23	1	0	-0.564272	2.692914	0.302655
24	1	0	0.343390	-0.125552	2.582209
25	1	0	0.589285	1.600887	2.352173
26	1	0	-1.028685	0.970504	2.516938
27	1	0	4.986118	1.691991	-0.380239
28	1	0	5.585726	1.089038	-1.919684
29	1	0	4.182584	2.130131	-1.880567
30	1	0	4.067762	-1.008054	1.782068
31	1	0	4.492520	0.619272	1.274637
32	1	0	2.845231	0.246963	1.749716
33	1	0	1.300569	-1.544180	1.470645
34	1	0	0.570138	-2.501884	0.206977
35	1	0	3.481919	-0.273775	-2.231140
36	1	0	2.323094	-1.938920	-1.377457
37	1	0	3.003472	-2.608455	0.090094
38	1	0	-2.654379	1.583323	1.021636
39	1	0	-2.865549	2.362655	-0.534093
40	1	0	-3.908865	-0.141225	1.775223
41	1	0	-5.085087	0.788370	0.899609
42	1	0	-5.395681	-0.934453	1.177720

-----  
SCF Done: E(RB+HF-B95) = -587.206387527 A.U. after 1 cycles  
Frequencies -- 14.9881 29.6745 39.5816  
Zero-point correction= 0.392926 (Hartree/Particle)  
Thermal correction to Energy= 0.412473  
Thermal correction to Enthalpy= 0.413417  
Thermal correction to Gibbs Free Energy= 0.342917  
Sum of electronic and zero-point Energies= -586.813461  
Sum of electronic and thermal Energies= -586.793915  
Sum of electronic and thermal Enthalpies= -586.792971  
Sum of electronic and thermal Free Energies= -586.863471

### 39b-ts

-----  
#BB95/6-31G(d) Iop(3/76=0580004200) nopop freq(noraman) guess=read geo  
m=check

1	6	0	-4.279820	-1.216223	2.020465
2	6	0	-2.780095	-2.145982	0.243803
3	6	0	-3.631532	-1.066901	0.719736
4	6	0	-0.191830	0.169948	0.421919
5	6	0	-0.607260	-0.168543	-0.802092
6	6	0	-0.737884	-1.618374	-1.176468
7	6	0	-0.943484	0.796915	-1.897131
8	6	0	4.587375	-0.114541	0.131486
9	6	0	2.562068	2.126417	-0.622070
10	6	0	0.042288	1.530526	0.990439
11	6	0	3.421239	0.354216	0.929823
12	6	0	1.445151	1.649019	1.596767
13	6	0	2.546273	1.312967	0.632615
14	6	0	-2.173809	-2.146396	-1.151784
15	6	0	-3.825412	0.162771	-0.017307
16	1	0	-5.347407	-1.364346	1.808601
17	1	0	-3.920519	-2.058868	2.601719
18	1	0	-4.233748	-0.288391	2.591251
19	1	0	-1.980800	-2.153143	1.009692
20	1	0	-3.311385	-3.075928	0.482877
21	1	0	0.084165	-0.643931	1.088870
22	1	0	-0.134374	-2.229116	-0.503546
23	1	0	-0.340339	-1.777554	-2.179116
24	1	0	-0.972238	1.831420	-1.568730
25	1	0	-0.204970	0.724615	-2.696348
26	1	0	-1.906580	0.566446	-2.358797
27	1	0	4.694249	0.403296	-0.816856

28	1	0	5.513657	0.020182	0.690904
29	1	0	4.506364	-1.181433	-0.080603
30	1	0	2.497520	3.191320	-0.392722
31	1	0	3.455928	1.970782	-1.216757
32	1	0	1.702941	1.886041	-1.252660
33	1	0	-0.100646	2.302096	0.236483
34	1	0	-0.684197	1.736251	1.781958
35	1	0	3.292407	-0.151415	1.881485
36	1	0	1.514611	0.999088	2.469652
37	1	0	1.566547	2.672645	1.959074
38	1	0	-2.803636	-1.596566	-1.850944
39	1	0	-2.173223	-3.174393	-1.508219
40	1	0	-2.840375	0.657068	0.066666
41	1	0	-3.948484	-0.002840	-1.086023
42	1	0	-4.593922	0.810652	0.389101

```

-----
SCF Done: E(RB+HF-B95) = -587.201840950 A.U. after 1 cycles
Frequencies -- -98.2023 24.6508 38.9784
Zero-point correction= 0.393320 (Hartree/Particle)
Thermal correction to Energy= 0.411770
Thermal correction to Enthalpy= 0.412714
Thermal correction to Gibbs Free Energy= 0.346658
Sum of electronic and zero-point Energies= -586.808521
Sum of electronic and thermal Energies= -586.790071
Sum of electronic and thermal Enthalpies= -586.789127
Sum of electronic and thermal Free Energies= -586.855183

```

### 38b

```

-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) guess=read geom=cheCk nopop
k nopop

```

1	6	0	-2.684650	-0.446123	1.843143
2	6	0	-1.980152	-1.921102	-0.008192
3	6	0	-1.986081	-0.472957	0.484940
4	6	0	-0.507406	-0.046127	0.681621
5	6	0	0.414390	-0.280422	-0.526695
6	6	0	0.329827	-1.740272	-0.969891
7	6	0	0.188352	0.643293	-1.715026
8	6	0	3.044673	-0.537076	-0.911928
9	6	0	2.509316	2.339768	-0.363408
10	6	0	-0.349699	1.354948	1.230767
11	6	0	1.960879	-0.102652	0.052182
12	6	0	1.137390	1.617399	1.626598
13	6	0	1.917436	1.276698	0.443707
14	6	0	-1.114697	-2.146334	-1.229725
15	6	0	-2.784463	0.417486	-0.461793
16	1	0	-3.646917	-0.950049	1.768195
17	1	0	-2.102262	-0.962306	2.607045
18	1	0	-2.884211	0.567567	2.187356
19	1	0	-1.623168	-2.562773	0.802226
20	1	0	-3.006100	-2.227388	-0.213653
21	1	0	-0.141545	-0.732833	1.454672
22	1	0	0.738264	-2.379856	-0.183740
23	1	0	0.931012	-1.898068	-1.864124
24	1	0	-0.011516	1.676078	-1.435184
25	1	0	1.048040	0.638940	-2.382674
26	1	0	-0.651804	0.303512	-2.309788
27	1	0	2.937307	-0.110007	-1.905761
28	1	0	4.025102	-0.256460	-0.531934
29	1	0	3.034469	-1.617662	-1.013477
30	1	0	3.492928	2.520405	0.095737
31	1	0	2.693425	2.062007	-1.395690
32	1	0	1.963171	3.277184	-0.286481
33	1	0	-0.676270	2.111590	0.520007
34	1	0	-0.929741	1.501269	2.137653
35	1	0	1.945824	-0.740683	0.933962
36	1	0	1.376984	0.949941	2.452740
37	1	0	1.269121	2.651765	1.931428
38	1	0	-1.516513	-1.610665	-2.089772
39	1	0	-1.126304	-3.199787	-1.506212
40	1	0	-2.708132	1.470741	-0.193467
41	1	0	-2.497140	0.314130	-1.503699
42	1	0	-3.837781	0.149250	-0.396291

```

-----
SCF Done: E(RB+HF-B95) = -587.274856910 A.U. after 1 cycles
Frequencies -- 78.1656 114.5204 130.6187
Zero-point correction= 0.402145 (Hartree/Particle)

```

```

Thermal correction to Energy=          0.417791
Thermal correction to Enthalpy=        0.418736
Thermal correction to Gibbs Free Energy= 0.362360
Sum of electronic and zero-point Energies= -586.872711
Sum of electronic and thermal Energies=   -586.857066
Sum of electronic and thermal Enthalpies= -586.856121
Sum of electronic and thermal Free Energies= -586.912497

```

### FIGURE 13

#### 40a-ts

```

-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop
-----
   1         6         0      -0.155182   -0.852539   -3.007507
   2         6         0       0.735214    0.194031   -2.346313
   3         6         0       0.453247    0.314255   -0.778458
   4         6         0       1.079819   -0.941284   -0.483826
   5         6         0       0.407440   -2.158798   -0.959885
   6         6         0      -0.674850   -1.866669   -1.984711
   7         6         0       0.976181    1.589798   -0.159821
   8         6         0      -1.321777    0.778076    2.048752
   9         6         0       0.982651    1.597092    1.382538
  10         6         0       0.007660    0.666733    2.051331
  11         6         0      -2.046936    1.869186    1.329102
  12         6         0      -2.187164   -0.185516    2.793884
  13         6         0       2.397202   -1.031952    0.147308
  14         1         0      -0.999191   -0.372177   -3.496124
  15         1         0       0.407898   -1.364029   -3.784760
  16         1         0       1.794342    0.011520   -2.533737
  17         1         0       0.544769    1.204254   -2.707245
  18         1         0      -0.628250    0.237000   -0.688965
  19         1         0      -0.016312   -2.626953   -0.059967
  20         1         0       1.155900   -2.866913   -1.318024
  21         1         0      -0.979233   -2.791077   -2.467270
  22         1         0      -1.561722   -1.479111   -1.487305
  23         1         0       1.977493    1.808655   -0.534958
  24         1         0       0.343765    2.390839   -0.539322
  25         1         0       0.810120    2.622284    1.709671
  26         1         0       1.983459    1.354752    1.734604
  27         1         0       0.436279   -0.137253    2.640381
  28         1         0      -2.765808    2.349594    1.992523
  29         1         0      -1.383133    2.639923    0.946228
  30         1         0      -2.628448    1.470581    0.494156
  31         1         0      -2.750763    0.331848    3.570770
  32         1         0      -2.925156   -0.646393    2.135422
  33         1         0      -1.607666   -0.973373    3.268951
  34         1         0       2.937149   -1.937408   -0.109726
  35         1         0       3.002090   -0.144867   -0.024643
  36         1         0       2.198700   -1.053650    1.226410
-----
SCF Done: E(RB+HF-B95) = -508.656761269 A.U. after 15 cycles
Frequencies -- -28.0474 43.0053 59.6410
Zero-point correction= 0.339587 (Hartree/Particle)
Thermal correction to Energy= 0.354138
Thermal correction to Enthalpy= 0.355083
Thermal correction to Gibbs Free Energy= 0.298019
Sum of electronic and zero-point Energies= -508.317174
Sum of electronic and thermal Energies= -508.302623
Sum of electronic and thermal Enthalpies= -508.301679
Sum of electronic and thermal Free Energies= -508.358743

```

#### 40b

```

-----
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop guess=read geo
m=check
-----
   1         6         0      -2.862746   -0.982204    0.910253
   2         6         0      -2.072166    0.263997    0.523056
   3         6         0      -0.776305   -0.025381   -0.331151
   4         6         0      -1.134618   -1.055391   -1.278174
   5         6         0      -1.616604   -2.320506   -0.724904
   6         6         0      -2.020691   -2.237787    0.734229

```

7	6	0	-0.106686	1.238141	-0.835328
8	6	0	2.560207	1.135992	1.111456
9	6	0	1.384024	1.059204	-1.129184
10	6	0	2.140546	0.476684	0.029798
11	6	0	2.349225	2.598762	1.334281
12	6	0	3.317316	0.435633	2.193109
13	6	0	-1.110901	-0.861017	-2.722928
14	1	0	-3.211350	-0.898431	1.936081
15	1	0	-3.752282	-1.072537	0.286497
16	1	0	-2.680402	0.970945	-0.037107
17	1	0	-1.698815	0.785874	1.400144
18	1	0	-0.110055	-0.522343	0.393068
19	1	0	-0.779081	-3.019026	-0.888098
20	1	0	-2.408877	-2.714123	-1.367820
21	1	0	-2.574889	-3.131259	1.008001
22	1	0	-1.143005	-2.204607	1.379747
23	1	0	-0.637987	1.632876	-1.703324
24	1	0	-0.211760	1.987934	-0.051701
25	1	0	1.788810	2.029760	-1.412006
26	1	0	1.528345	0.420088	-2.001677
27	1	0	2.383491	-0.578129	-0.034073
28	1	0	3.305617	3.094328	1.502519
29	1	0	1.857884	3.099482	0.504514
30	1	0	1.755228	2.769159	2.233386
31	1	0	4.311648	0.869192	2.305010
32	1	0	2.820235	0.550049	3.157225
33	1	0	3.433408	-0.625934	1.989016
34	1	0	-1.227882	-1.782425	-3.284722
35	1	0	-1.978495	-0.221520	-2.943157
36	1	0	-0.244322	-0.293794	-3.053612

-----  
SCF Done: E(RB+HF-B95) = -508.659172640 A.U. after 1 cycles  
Frequencies -- 35.7509 41.8597 62.8044  
Zero-point correction= 0.339851 (Hartree/Particle)  
Thermal correction to Energy= 0.354919  
Thermal correction to Enthalpy= 0.355863  
Thermal correction to Gibbs Free Energy= 0.297199  
Sum of electronic and zero-point Energies= -508.319322  
Sum of electronic and thermal Energies= -508.304253  
Sum of electronic and thermal Enthalpies= -508.303309  
Sum of electronic and thermal Free Energies= -508.361973

## 40c-ts

-----  
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop  
-----

1	6	0	-1.116959	-1.840851	-3.173615
2	6	0	-0.480087	-0.593002	-2.559738
3	6	0	-0.270630	-0.674347	-0.990692
4	6	0	0.385452	-1.950302	-0.812820
5	6	0	-0.356567	-3.139038	-1.226898
6	6	0	-1.555588	-2.830612	-2.101517
7	6	0	0.384674	0.561676	-0.413177
8	6	0	0.038971	2.735443	2.455658
9	6	0	0.395859	0.598846	1.130203
10	6	0	-0.391251	1.742432	1.679123
11	6	0	1.439117	2.901886	2.950455
12	6	0	-0.907013	3.800613	2.911133
13	6	0	1.762238	-2.062225	-0.347809
14	1	0	-1.966049	-1.562271	-3.791855
15	1	0	-0.403519	-2.335129	-3.831665
16	1	0	0.479309	-0.358109	-3.015427
17	1	0	-1.110764	0.283966	-2.684189
18	1	0	-1.291016	-0.790085	-0.606918
19	1	0	-0.644730	-3.626419	-0.280670
20	1	0	0.336502	-3.850784	-1.683762
21	1	0	-1.928680	-3.749908	-2.544357
22	1	0	-2.372772	-2.420166	-1.509048
23	1	0	1.395264	0.659073	-0.812683
24	1	0	-0.159851	1.425766	-0.789886
25	1	0	1.419968	0.633316	1.493362
26	1	0	-0.026932	-0.336670	1.515137
27	1	0	-1.439056	1.747513	1.396011
28	1	0	1.459152	2.872879	4.040359
29	1	0	2.130981	2.148346	2.586349

30	1	0	1.826630	3.878922	2.660600
31	1	0	-0.952576	3.835541	4.000214
32	1	0	-0.569794	4.784210	2.581970
33	1	0	-1.914078	3.641083	2.534286
34	1	0	2.105072	-3.085403	-0.238510
35	1	0	2.389800	-1.552521	-1.091232
36	1	0	1.908417	-1.493774	0.571167

-----  
SCF Done: E(RB+HF-B95) = -508.654288007 A.U. after 17 cycles  
Frequencies -- -42.1972 36.1489 41.4500  
Zero-point correction= 0.339178 (Hartree/Particle)  
Thermal correction to Energy= 0.353804  
Thermal correction to Enthalpy= 0.354748  
Thermal correction to Gibbs Free Energy= 0.296757  
Sum of electronic and zero-point Energies= -508.315110  
Sum of electronic and thermal Energies= -508.300484  
Sum of electronic and thermal Enthalpies= -508.299540  
Sum of electronic and thermal Free Energies= -508.357531

#### 40d

-----  
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop

1	6	0	-1.886871	-1.612473	-3.021744
2	6	0	-1.349487	-0.322433	-2.402893
3	6	0	-0.994553	-0.436264	-0.853210
4	6	0	-0.195770	-1.637085	-0.835281
5	6	0	-0.877700	-2.886139	-1.176697
6	6	0	-2.165543	-2.664749	-1.956207
7	6	0	-0.406204	0.839844	-0.290741
8	6	0	1.368652	2.313034	2.389267
9	6	0	-0.361191	0.856735	1.237061
10	6	0	0.211472	2.134200	1.754883
11	6	0	2.342819	1.230133	2.726456
12	6	0	1.785583	3.677597	2.837143
13	6	0	1.250595	-1.628600	-0.644333
14	1	0	-2.790436	-1.405609	-3.589096
15	1	0	-1.162384	-2.016815	-3.727844
16	1	0	-0.469788	0.050125	-2.922668
17	1	0	-2.091583	0.472015	-2.421677
18	1	0	-1.959015	-0.668533	-0.391830
19	1	0	-1.070328	-3.363785	-0.201965
20	1	0	-0.183075	-3.561462	-1.679977
21	1	0	-2.485275	-3.603485	-2.399811
22	1	0	-2.971481	-2.343140	-1.297928
23	1	0	0.589569	1.010956	-0.701096
24	1	0	-1.014587	1.674789	-0.637390
25	1	0	0.197144	-0.002167	1.610260
26	1	0	-1.380386	0.736053	1.612808
27	1	0	-0.402390	3.009598	1.574982
28	1	0	2.503235	1.186142	3.804108
29	1	0	2.031250	0.239853	2.403381
30	1	0	3.315063	1.441620	2.279617
31	1	0	1.920258	3.704208	3.919098
32	1	0	2.744003	3.956192	2.396957
33	1	0	1.053726	4.434631	2.568024
34	1	0	1.655014	-2.617325	-0.447800
35	1	0	1.669357	-1.296829	-1.606277
36	1	0	1.579880	-0.901016	0.092178

-----  
SCF Done: E(RB+HF-B95) = -508.658111104 A.U. after 17 cycles  
Frequencies -- 24.3924 37.7604 57.1718  
Zero-point correction= 0.339836 (Hartree/Particle)  
Thermal correction to Energy= 0.355122  
Thermal correction to Enthalpy= 0.356066  
Thermal correction to Gibbs Free Energy= 0.296181  
Sum of electronic and zero-point Energies= -508.318275  
Sum of electronic and thermal Energies= -508.302989  
Sum of electronic and thermal Enthalpies= -508.302045  
Sum of electronic and thermal Free Energies= -508.361930

#### 40e-ts

-----  
#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop



1	6	0	-1.809784	-1.141251	-3.256287
2	6	0	-1.329971	0.151550	-2.596619
3	6	0	-1.066879	0.028000	-1.041412
4	6	0	-0.314270	-1.202286	-0.906357
5	6	0	-0.981506	-2.430800	-1.332413
6	6	0	-2.191376	-2.186539	-2.215881
7	6	0	-0.459946	1.270981	-0.430206
8	6	0	1.565475	1.482544	2.590439
9	6	0	-0.483505	1.247635	1.105789
10	6	0	0.702164	1.945084	1.685806
11	6	0	1.494217	0.140884	3.248703
12	6	0	2.702835	2.335403	3.056168
13	6	0	1.080795	-1.234451	-0.486969
14	1	0	-2.653625	-0.936508	-3.909637
15	1	0	-1.022461	-1.552704	-3.887436
16	1	0	-0.420609	0.530533	-3.057861
17	1	0	-2.075806	0.938980	-2.670654
18	1	0	-2.063538	-0.172195	-0.629623
19	1	0	-1.255432	-2.927078	-0.386337
20	1	0	-0.249023	-3.106735	-1.780716
21	1	0	-2.491898	-3.119659	-2.684235
22	1	0	-3.042313	-1.848602	-1.625168
23	1	0	0.563995	1.382263	-0.790039
24	1	0	-0.998413	2.140381	-0.803223
25	1	0	-0.533615	0.218750	1.465530
26	1	0	-1.406479	1.717896	1.450211
27	1	0	0.861938	2.950806	1.312714
28	1	0	1.330002	0.258804	4.320343
29	1	0	0.699829	-0.497803	2.870728
30	1	0	2.441315	-0.389664	3.142075
31	1	0	2.639404	2.506897	4.131302
32	1	0	3.659790	1.844086	2.875626
33	1	0	2.715836	3.302231	2.560043
34	1	0	1.429200	-2.232834	-0.239288
35	1	0	1.644669	-0.906128	-1.374527
36	1	0	1.318665	-0.508881	0.289886

SCF Done: E(RB+HF-B95) = -508.657135335 A.U. after 14 cycles  
Frequencies -- -22.6459 44.7549 58.2588  
Zero-point correction= 0.340127 (Hartree/Particle)  
Thermal correction to Energy= 0.354249  
Thermal correction to Enthalpy= 0.355194  
Thermal correction to Gibbs Free Energy= 0.299433  
Sum of electronic and zero-point Energies= -508.317008  
Sum of electronic and thermal Energies= -508.302886  
Sum of electronic and thermal Enthalpies= -508.301942  
Sum of electronic and thermal Free Energies= -508.357702

## 41

#BB95/6-31G(d) IOp(3/76=0580004200) freq(noraman) nopop

1	6	0	-2.603806	-1.160782	-0.722092
2	6	0	-2.370407	0.339096	-0.957825
3	6	0	-1.106888	0.836548	-0.261200
4	6	0	0.026535	-0.167236	-0.473984
5	6	0	-0.281754	-1.460266	0.312408
6	6	0	-1.797852	-1.669846	0.459412
7	6	0	-0.582443	2.195755	-0.656937
8	6	0	1.864075	0.114777	0.972931
9	6	0	0.758575	2.251465	0.059113
10	6	0	1.365631	0.868622	-0.105743
11	6	0	1.448456	0.371292	2.360687
12	6	0	2.821487	-0.973221	0.730270
13	6	0	0.293991	-0.516220	-1.927277
14	1	0	-3.659744	-1.350174	-0.543976
15	1	0	-2.352264	-1.736023	-1.612671
16	1	0	-2.304337	0.555511	-2.023895
17	1	0	-3.208740	0.921127	-0.579163
18	1	0	-1.304016	0.864014	0.815842
19	1	0	0.129730	-1.471420	1.319672
20	1	0	0.170135	-2.302017	-0.212311
21	1	0	-1.985458	-2.729095	0.621490
22	1	0	-2.139755	-1.163177	1.362427

23	1	0	-0.452194	2.262711	-1.737137
24	1	0	-1.243271	3.006210	-0.360275
25	1	0	0.605148	2.491394	1.109497
26	1	0	1.436768	3.000000	-0.343826
27	1	0	1.993805	0.779282	-0.984650
28	1	0	2.088257	1.180786	2.731750
29	1	0	0.427078	0.738037	2.427261
30	1	0	1.591675	-0.487320	3.009583
31	1	0	3.776855	-0.661621	1.167435
32	1	0	2.533325	-1.881042	1.258865
33	1	0	2.982483	-1.174622	-0.324005
34	1	0	1.206360	-1.104691	-2.018860
35	1	0	-0.515640	-1.131683	-2.312927
36	1	0	0.388046	0.363388	-2.559647

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SCF Done: E(RB+HF-B95) = -508.680408447 A.U. after 15 cycles  
Frequencies -- 74.9574 102.0916 130.8657  
Zero-point correction= 0.344171 (Hartree/Particle)  
Thermal correction to Energy= 0.357617  
Thermal correction to Enthalpy= 0.358561  
Thermal correction to Gibbs Free Energy= 0.305992  
Sum of electronic and zero-point Energies= -508.336238  
Sum of electronic and thermal Energies= -508.322792  
Sum of electronic and thermal Enthalpies= -508.321848  
Sum of electronic and thermal Free Energies= -508.374416