

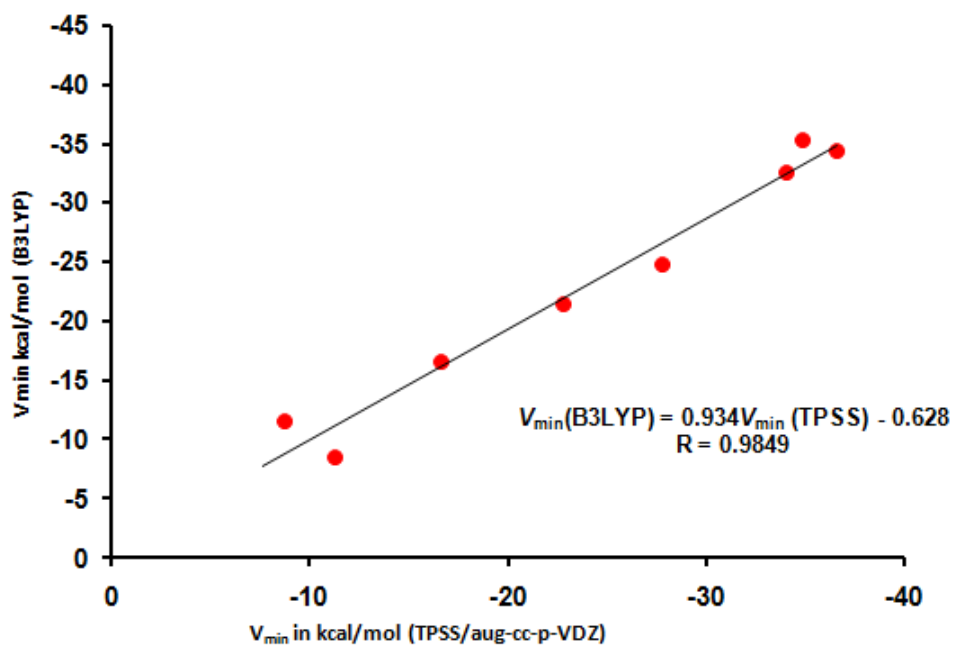
## Designing metal hydride complexes for water splitting reactions: A molecular electrostatic potential approach

*K. S. Sandhya and Cherumuttathu H. Suresh\**

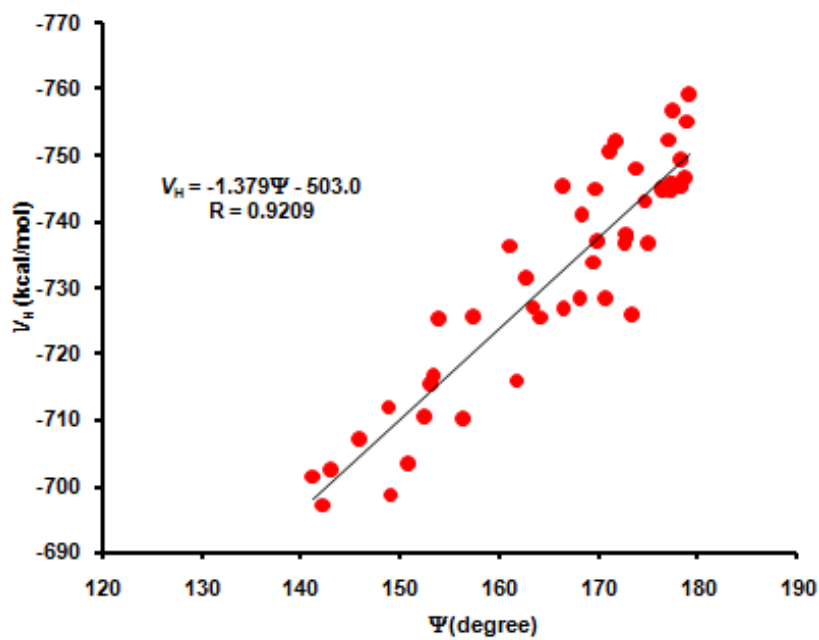
Inorganic and Theoretical Chemistry Section, CSTD, CSIR-National Institute for  
Interdisciplinary Science and Technology, Trivandrum-695019, India

\* To whom correspondence should be addressed. E-mail: sureshch@gmail.com, Phone: +91-471-2535506

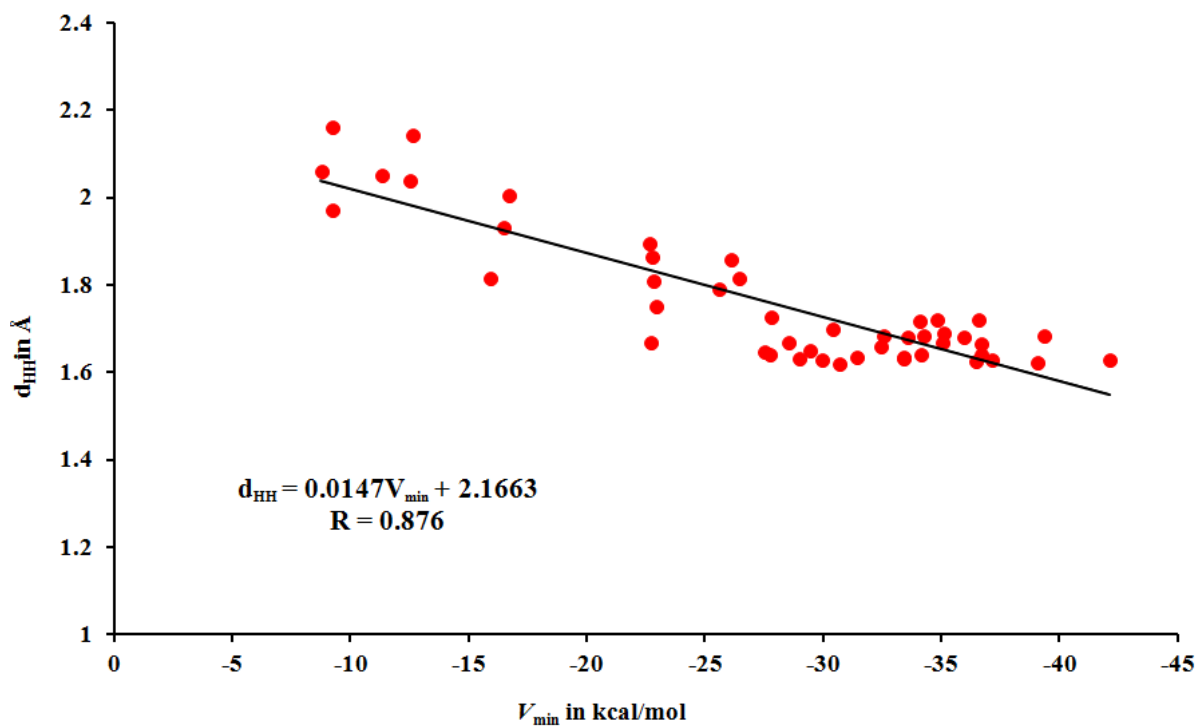
1. **Figure S1.** Correlation between  $V_{\min}$  of Ru hydride complexes at B3LYP and TPSS level. S2
2. **Figure S2.** Correlation between  $V_{\text{H}}$  (kcal/mol) and  $\Psi$  (in angle) of DHB complexes. S2
3. **Figure S3.** Correlation between  $d_{\text{H-H}}$  (kcal/mol) and  $V_{\min}$  (in kcal/mol) of DHB complexes. S3
4. **Figure S4.** Higher derivative of W complexes with  $V_{\min}$  Studied at B3LYP level. S3
5. Cartesian coordinates (Ångstrom) of all optimized geometric structure with energy values (A.U) at the bottom of each geometry. S4



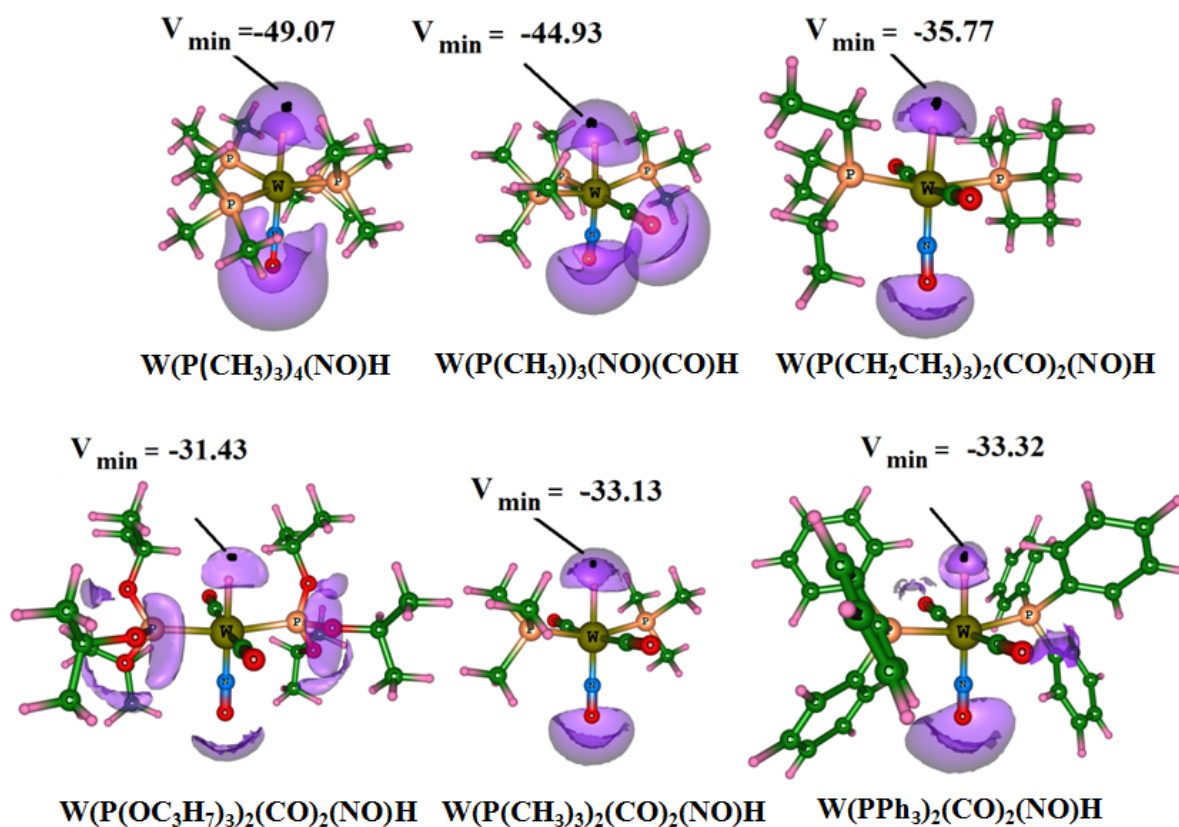
**Figure S1.** Correlation between  $V_{\text{H}}$  of Ru hydride complexes at B3LYP and TPSS level.



**Figure S2.** Correlation between  $V_{\text{H}}$  (kcal/mol) and H...H-O angle  $\Psi$  (in degrees) of DHB complexes.



**Figure S3.** Correlation between  $d_{\text{H-H}}$  (kcal/mol) and  $V_{\text{min}}$  (in kcal/mol) of DHB complexes.



**Figure S4.**  $V_{\text{min}}$  values of the higher derivatives of W complexes.

5. Cartesian coordinates (Ångstrom) of all optimized geometric structure with energy values (A.U.) at the bottom of each geometry.

**1**

25	-0.000210000	0.002267000	-0.146952000
6	0.001913000	-0.007594000	1.686278000
8	0.003022000	-0.021676000	2.836586000
6	-1.815407000	0.277972000	-0.359430000
8	-2.934640000	0.446428000	-0.548000000
6	1.815098000	-0.273866000	-0.364383000
8	2.933953000	-0.442479000	-0.554433000
6	-0.276671000	-1.807639000	-0.391836000
8	-0.446915000	-2.920881000	-0.612080000
6	0.275617000	1.813911000	-0.380204000
8	0.445263000	2.929177000	-0.590543000
1	-0.003516000	0.002075000	-1.720998000

E(RB3LYP) = -671.225718681

Zero-point correction= 0.050601 (Hartree/Particle)

Thermal correction to Energy= 0.062352

Thermal correction to Enthalpy= 0.063296

Thermal correction to Gibbs Free Energy= 0.011400

Sum of electronic and zero-point Energies= -671.175118

Sum of electronic and thermal Energies= -671.163367

Sum of electronic and thermal Enthalpies= -671.162422

Sum of electronic and thermal Free Energies= -671.214318

**2a**

25	0.097605000	0.000410000	-0.135372000
15	-2.209932000	-0.000622000	-0.302070000
8	3.026038000	-0.001645000	-0.577937000
8	0.034811000	-2.938266000	-0.643689000
8	0.201364000	0.000525000	2.840002000
6	1.891163000	-0.000609000	-0.380894000
6	0.062677000	-1.812450000	-0.402974000
6	0.158741000	0.000485000	1.686645000
1	-3.058998000	-0.006042000	0.831797000
1	-2.823972000	-1.063309000	-1.000828000
1	-2.826240000	1.066448000	-0.992172000
1	-0.016349000	0.000715000	-1.711775000
6	0.063202000	1.813307000	-0.403299000
8	0.035252000	2.938995000	-0.644445000

E(RB3LYP) = -901.042762274

Zero-point correction= 0.070401 (Hartree/Particle)

Thermal correction to Energy= 0.082861

Thermal correction to Enthalpy= 0.083805

Thermal correction to Gibbs Free Energy= 0.030474

Sum of electronic and zero-point Energies= -900.972361

Sum of electronic and thermal Energies= -900.959901

Sum of electronic and thermal Enthalpies= -900.958957

Sum of electronic and thermal Free Energies= -901.012288

**2b**

25	0.006393000	0.000555000	-0.232875000
----	-------------	-------------	--------------

1	0.024004000	0.001993000	-1.777695000
15	-0.048718000	-0.004393000	2.052442000
1	-0.742533000	1.014527000	2.748950000
1	-0.622874000	-1.096731000	2.746625000
1	1.145490000	0.062496000	2.810224000
6	-1.813919000	-0.118057000	-0.467680000
8	-2.941015000	-0.191158000	-0.691555000
6	1.832776000	0.119992000	-0.419720000
8	2.966372000	0.193827000	-0.605352000
6	-0.106451000	1.824236000	-0.445219000
8	-0.173890000	2.954814000	-0.651657000
6	0.131554000	-1.822172000	-0.446367000
8	0.211421000	-2.951763000	-0.653803000

E(RB3LYP) = -901.036542997

Zero-point correction=	0.069609 (Hartree/Particle)
Thermal correction to Energy=	0.082470
Thermal correction to Enthalpy=	0.083414
Thermal correction to Gibbs Free Energy=	0.026870
Sum of electronic and zero-point Energies=	-900.966934
Sum of electronic and thermal Energies=	-900.954073
Sum of electronic and thermal Enthalpies=	-900.953129
Sum of electronic and thermal Free Energies=	-901.009673

### 3a

25	0.000085000	-0.000090000	-0.112745000
8	-0.001593000	0.002225000	2.855988000
8	0.001934000	-2.939432000	-0.599565000
6	-0.000715000	0.001226000	1.697571000
6	0.001222000	-1.807415000	-0.367762000
1	0.000274000	-0.001151000	-1.705065000
15	-2.251771000	-0.001434000	-0.383591000
1	-2.847643000	1.059750000	-1.103951000
1	-3.154361000	-0.000321000	0.710694000
1	-2.846659000	-1.065238000	-1.100901000
6	-0.000698000	1.806994000	-0.369401000
8	-0.001182000	2.938849000	-0.601997000
15	2.252054000	0.000692000	-0.382419000
1	2.848089000	-1.062032000	-1.100396000
1	3.154271000	0.001549000	0.712184000
1	2.847538000	1.062872000	-1.101657000

E(RB3LYP) = -1130.85204547

Zero-point correction=	0.089693 (Hartree/Particle)
Thermal correction to Energy=	0.103012
Thermal correction to Enthalpy=	0.103957
Thermal correction to Gibbs Free Energy=	0.048641
Sum of electronic and zero-point Energies=	-1130.762352
Sum of electronic and thermal Energies=	-1130.749033
Sum of electronic and thermal Enthalpies=	-1130.748089
Sum of electronic and thermal Free Energies=	-1130.803404

### 3b

25	0.075736000	0.000063000	-0.216688000
15	-2.230244000	-0.003695000	-0.319561000
1	-2.870092000	-1.073826000	-0.985385000

1	-3.067103000	0.008272000	0.829815000
1	-2.870612000	1.051592000	-1.008029000
1	-0.101908000	0.000438000	-1.762491000
15	0.268937000	-0.001405000	2.048230000
1	0.940580000	1.053901000	2.714652000
1	-0.876371000	-0.003435000	2.889949000
1	0.943163000	-1.056150000	2.712886000
6	0.032293000	1.811298000	-0.456437000
8	-0.002038000	2.941902000	-0.691540000
6	0.040372000	-1.811051000	-0.458513000
8	0.010789000	-2.941510000	-0.694871000
6	1.849476000	0.004586000	-0.522155000
8	2.978214000	0.007749000	-0.773790000

E(RB3LYP) = -1130.84929664

Zero-point correction=	0.089396 (Hartree/Particle)
Thermal correction to Energy=	0.102769
Thermal correction to Enthalpy=	0.103713
Thermal correction to Gibbs Free Energy=	0.048388
Sum of electronic and zero-point Energies=	-1130.759900
Sum of electronic and thermal Energies=	-1130.746527
Sum of electronic and thermal Enthalpies=	-1130.745583
Sum of electronic and thermal Free Energies=	-1130.800909

### 3c

25	-0.000043000	0.111306000	-0.122418000
8	-0.000684000	0.207057000	2.851004000
8	-2.077430000	2.160046000	-0.610120000
6	-0.000403000	0.166758000	1.694184000
6	-1.271351000	1.362008000	-0.388480000
1	0.000438000	-0.036211000	-1.701709000
15	-1.630526000	-1.486057000	-0.363571000
1	-2.757442000	-1.156105000	-1.149754000
1	-2.342729000	-2.061478000	0.720882000
1	-1.309936000	-2.702142000	-1.015997000
6	1.268582000	1.364656000	-0.388714000
8	2.072895000	2.164362000	-0.610756000
15	1.633768000	-1.482746000	-0.362717000
1	1.315836000	-2.699607000	-1.015008000
1	2.346787000	-2.056558000	0.722048000
1	2.760280000	-1.150755000	-1.148632000

E(RB3LYP) = -1130.85315317

Zero-point correction=	0.089897 (Hartree/Particle)
Thermal correction to Energy=	0.103031
Thermal correction to Enthalpy=	0.103975
Thermal correction to Gibbs Free Energy=	0.049560
Sum of electronic and zero-point Energies=	-1130.763256
Sum of electronic and thermal Energies=	-1130.750122
Sum of electronic and thermal Enthalpies=	-1130.749178
Sum of electronic and thermal Free Energies=	-1130.803593

### 4a

25	0.000022000	0.009663000	-0.186531000
15	-2.241505000	0.000392000	-0.480671000
1	-2.802833000	-0.989170000	-1.322654000

1	-3.182698000	-0.144719000	0.578826000
1	-2.861318000	1.118523000	-1.089014000
15	2.241548000	0.000440000	-0.480687000
1	2.861125000	1.118029000	-1.090253000
1	3.182904000	-0.143476000	0.578832000
1	2.802929000	-0.989914000	-1.321707000
1	0.000168000	0.025396000	-1.756600000
15	0.000021000	-0.029601000	2.077169000
1	-1.051736000	-0.663481000	2.794804000
1	1.051092000	-0.664666000	2.794747000
1	0.000701000	1.155632000	2.859766000
6	-0.000009000	-1.795577000	-0.426264000
8	-0.000069000	-2.931210000	-0.662475000
6	-0.000037000	1.819389000	-0.397703000
8	-0.000128000	2.959326000	-0.607130000

E(RB3LYP) = -1360.65336915

Zero-point correction=	0.108328 (Hartree/Particle)
Thermal correction to Energy=	0.122616
Thermal correction to Enthalpy=	0.123560
Thermal correction to Gibbs Free Energy=	0.065538
Sum of electronic and zero-point Energies=	-1360.545041
Sum of electronic and thermal Energies=	-1360.530753
Sum of electronic and thermal Enthalpies=	-1360.529809
Sum of electronic and thermal Free Energies=	-1360.587832

#### 4b

25	0.000002000	0.067240000	-0.102573000
8	-0.000982000	0.094538000	2.866105000
8	-0.002658000	2.991328000	-0.527127000
6	-0.000543000	0.083101000	1.704409000
6	-0.001638000	1.847705000	-0.331215000
1	0.000465000	-0.028731000	-1.701006000
15	2.235486000	0.109956000	-0.423796000
1	2.873229000	-0.969066000	-1.090054000
1	3.181003000	0.223509000	0.631099000
1	2.769629000	1.142287000	-1.230368000
15	-2.235483000	0.105896000	-0.424483000
1	-2.770913000	1.135476000	-1.233708000
1	-3.181132000	0.220978000	0.630114000
1	-2.871899000	-0.975622000	-1.087995000
15	0.002200000	-2.210727000	-0.345534000
1	-1.054256000	-2.823520000	-1.066386000
1	0.003241000	-3.133573000	0.735453000
1	1.059744000	-2.821376000	-1.066616000

E(RB3LYP) = -1360.65779169

Zero-point correction=	0.109164
Thermal correction to Energy=	0.122981
Thermal correction to Enthalpy=	0.123925
Thermal correction to Gibbs Free Energy=	0.068393
Sum of electronic and zero-point Energies=	-1360.548627
Sum of electronic and thermal Energies=	-1360.534810
Sum of electronic and thermal Enthalpies=	-1360.533866
Sum of electronic and thermal Free Energies=	-1360.589399

**4c**

25	0.000042000	0.090995000	-0.201717000
15	1.631957000	-1.506920000	-0.386441000
1	2.739002000	-1.220034000	-1.218137000
1	2.388221000	-2.016503000	0.707936000
1	1.317113000	-2.768408000	-0.953526000
15	-1.632966000	-1.505896000	-0.386201000
1	-1.319216000	-2.767489000	-0.953644000
1	-2.389597000	-2.015045000	0.708121000
1	-2.739819000	-1.217859000	-1.217751000
1	-0.000332000	-0.128296000	-1.753505000
15	0.000280000	0.266088000	2.056109000
1	0.000665000	1.541533000	2.676538000
1	-1.052047000	-0.274994000	2.846288000
1	1.052357000	-0.275591000	2.846216000
6	-1.262659000	1.333128000	-0.494833000
8	-2.067261000	2.130263000	-0.747360000
6	1.263395000	1.332432000	-0.494959000
8	2.068401000	2.129159000	-0.747497000

E(RB3LYP) = -1360.65601507

Zero-point correction= 0.108733

Thermal correction to Energy= 0.122678

Thermal correction to Enthalpy= 0.123622

Thermal correction to Gibbs Free Energy= 0.067824

Sum of electronic and zero-point Energies= -1360.547282

Sum of electronic and thermal Energies= -1360.533337

Sum of electronic and thermal Enthalpies= -1360.532393

Sum of electronic and thermal Free Energies= -1360.588191

**5a**

25	-0.000020000	0.000007000	-0.091470000
6	-0.000526000	-0.000435000	1.707110000
8	-0.000924000	-0.000766000	2.873247000
15	-1.180593000	1.900198000	-0.384403000
1	-2.400055000	1.862872000	-1.112589000
1	-1.676042000	2.701872000	0.682284000
1	-0.607209000	2.975115000	-1.115634000
15	1.900317000	1.180698000	-0.383465000
1	1.863002000	2.400834000	-1.110556000
1	2.701991000	1.675184000	0.683657000
1	2.975258000	0.608007000	-1.115210000
15	1.181050000	-1.899846000	-0.384525000
15	-1.900230000	-1.180619000	-0.384395000
1	2.397581000	-1.862741000	-1.117564000
1	1.681611000	-2.698389000	0.682121000
1	0.606138000	-2.977243000	-1.110946000
1	-1.862720000	-2.400417000	-1.112024000
1	-2.701915000	-1.675652000	0.682469000
1	-2.975155000	-0.607637000	-1.115919000
1	0.000394000	0.000291000	-1.710158000

E(RB3LYP) = -1590.45715731

Zero-point correction= 0.128048 (Hartree/Particle)

Thermal correction to Energy= 0.142531

Thermal correction to Enthalpy= 0.143475



Thermal correction to Gibbs Free Energy= 0.086874  
 Sum of electronic and zero-point Energies= -1590.329109  
 Sum of electronic and thermal Energies= -1590.314626  
 Sum of electronic and thermal Enthalpies= -1590.313682  
 Sum of electronic and thermal Free Energies= -1590.370283

**5b**

25	0.000107000	0.052870000	-0.176500000
15	2.226184000	0.094491000	-0.503873000
1	2.742706000	1.064396000	-1.397005000
1	3.191786000	0.316703000	0.523279000
1	2.890805000	-1.022233000	-1.080325000
15	-0.002217000	-2.226618000	-0.361917000
15	-2.225855000	0.098770000	-0.504083000
1	1.053389000	-2.866807000	-1.062869000
1	-0.004423000	-3.130326000	0.742278000
1	-1.058095000	-2.864151000	-1.064861000
1	-2.892205000	-1.015637000	-1.082988000
1	-3.191315000	0.320485000	0.523326000
1	-2.740594000	1.071423000	-1.395262000
1	-0.000050000	-0.086347000	-1.754559000
15	-0.000032000	0.141801000	2.076073000
1	1.051306000	0.784140000	2.789773000
1	-1.049608000	0.787602000	2.789231000
1	-0.002171000	-1.030315000	2.888297000
6	0.001802000	1.825812000	-0.418775000
8	0.002971000	2.970972000	-0.635774000

E(RB3LYP) = -1590.45632850

Zero-point correction= 0.127787 (Hartree/Particle)  
 Thermal correction to Energy= 0.142393  
 Thermal correction to Enthalpy= 0.143337  
 Thermal correction to Gibbs Free Energy= 0.086533  
 Sum of electronic and zero-point Energies= -1590.328541  
 Sum of electronic and thermal Energies= -1590.313936  
 Sum of electronic and thermal Enthalpies= -1590.312992  
 Sum of electronic and thermal Free Energies= -1590.369795

**6**

25	0.000486000	0.001746000	-0.157018000
15	-0.266833000	2.219183000	-0.424642000
1	-1.388061000	2.704087000	-1.154227000
1	-0.375126000	3.188829000	0.620834000
1	0.704519000	2.950029000	-1.164364000
15	2.213784000	0.290611000	-0.430483000
1	2.681627000	1.379609000	-1.217518000
1	3.156518000	0.488739000	0.626391000
1	2.983741000	-0.702391000	-1.098825000
15	0.278653000	-2.201311000	-0.493817000
15	-2.212325000	-0.253756000	-0.456067000
1	1.389267000	-2.666160000	-1.251441000
1	0.424097000	-3.166346000	0.552320000
1	-0.700824000	-2.940260000	-1.214306000
1	-2.715438000	-1.401580000	-1.130073000
1	-3.179333000	-0.290645000	0.596989000

1	-2.924287000	0.692173000	-1.245183000
1	0.007167000	0.034518000	-1.760595000
15	-0.014171000	-0.059079000	2.087040000
1	0.891026000	0.711527000	2.877689000
1	-1.165836000	0.308940000	2.846542000
1	0.212167000	-1.269443000	2.810731000

E(RB3LYP) = -1820.25114302

Zero-point correction=	0.146197 (Hartree/Particle)
Thermal correction to Energy=	0.161534
Thermal correction to Enthalpy=	0.162478
Thermal correction to Gibbs Free Energy=	0.103775
Sum of electronic and zero-point Energies=	-1820.104946
Sum of electronic and thermal Energies=	-1820.089609
Sum of electronic and thermal Enthalpies=	-1820.088665
Sum of electronic and thermal Free Energies=	-1820.147368

7

25	0.764112000	0.000058000	-0.158066000
15	-0.853730000	-1.597034000	-0.435331000
15	-0.853783000	1.597319000	-0.434350000
8	2.812492000	-2.106220000	-0.499695000
8	0.663119000	-0.000246000	2.813147000
8	2.812464000	2.106126000	-0.501009000
6	2.015357000	-1.284447000	-0.334307000
6	0.683917000	-0.000166000	1.652412000
6	2.015413000	1.284469000	-0.334638000
6	-2.581978000	-1.298128000	0.202340000
1	-3.206168000	-2.156912000	-0.063463000
1	-2.514973000	-1.271326000	1.296554000
6	-3.228519000	-0.000122000	-0.314647000
1	-3.241263000	0.000048000	-1.413183000
1	-4.281035000	-0.000225000	-0.006171000
6	-2.582143000	1.297776000	0.202769000
1	-2.515222000	1.270637000	1.296979000
1	-3.206408000	2.156581000	-0.062785000
1	0.819121000	0.000494000	-1.732158000
1	-1.155551000	2.025980000	-1.748973000
1	-0.634955000	2.883251000	0.119861000
1	-0.634583000	-2.883540000	0.117406000
1	-1.155956000	-2.024290000	-1.750309000

E(RB3LYP) = -1247.60584047

Zero-point correction=	0.159283 (Hartree/Particle)
Thermal correction to Energy=	0.174108
Thermal correction to Enthalpy=	0.175052
Thermal correction to Gibbs Free Energy=	0.116478
Sum of electronic and zero-point Energies=	-1247.446558
Sum of electronic and thermal Energies=	-1247.431733
Sum of electronic and thermal Enthalpies=	-1247.430789
Sum of electronic and thermal Free Energies=	-1247.489362

8

25	-0.000024000	-0.000049000	0.131776000
15	1.584587000	-1.526528000	-0.249419000
15	1.652345000	1.488848000	-0.137437000

S10

15	-1.652464000	-1.488750000	-0.137914000
15	-1.584566000	1.526704000	-0.248652000
6	0.000132000	-0.000576000	1.923570000
8	0.000263000	-0.000976000	3.092093000
1	2.242771000	-2.280900000	0.765877000
1	1.376486000	-2.621675000	-1.129103000
6	3.072184000	-0.724972000	-1.070853000
6	3.311271000	0.639633000	-0.413758000
1	1.619803000	2.388759000	-1.236216000
1	2.051249000	2.454675000	0.827864000
1	-2.051495000	-2.454737000	0.827176000
1	-1.619950000	-2.388450000	-1.236869000
6	-3.311335000	-0.639346000	-0.414062000
6	-3.072176000	0.725566000	-1.070481000
1	-1.376306000	2.622111000	-1.127969000
1	-2.242705000	2.280832000	0.766860000
1	-0.000217000	0.000416000	-1.487231000
1	2.806570000	-0.600131000	-2.125709000
1	3.957988000	-1.364945000	-1.015536000
1	3.758332000	0.507473000	0.578237000
1	3.989831000	1.265747000	-1.000343000
1	-3.758530000	-0.507659000	0.577935000
1	-3.989823000	-1.265180000	-1.001030000
1	-2.806521000	0.601229000	-2.125385000
1	-3.957963000	1.365539000	-1.014889000

E(RB3LYP) = -1745.33232773

Zero-point correction= 0.208417 (Hartree/Particle)

Thermal correction to Energy= 0.223988

Thermal correction to Enthalpy= 0.224932

Thermal correction to Gibbs Free Energy= 0.165888

Sum of electronic and zero-point Energies= -1745.123911

Sum of electronic and thermal Energies= -1745.108339

Sum of electronic and thermal Enthalpies= -1745.107395

Sum of electronic and thermal Free Energies= -1745.166440

**9**

25	-0.000267000	-0.000024000	0.158267000
15	-1.587605000	1.529058000	-0.229620000
15	-1.662188000	-1.486690000	-0.118943000
15	1.662351000	1.486627000	-0.117478000
15	1.587719000	-1.528439000	-0.230598000
7	-0.000010000	-0.001201000	2.008033000
7	0.000414000	-0.001930000	3.135941000
1	-2.290020000	2.260083000	0.777520000
1	-1.361127000	2.642790000	-1.080955000
6	-3.040974000	0.731817000	-1.114752000
6	-3.307007000	-0.636403000	-0.475456000
1	-1.592625000	-2.416130000	-1.190225000
1	-2.108011000	-2.425018000	0.856840000
1	2.108438000	2.423890000	0.859230000
1	1.592696000	2.417336000	-1.187664000
6	3.307095000	0.636775000	-0.475481000
6	3.040756000	-0.730814000	-1.115851000
1	1.361763000	-2.642504000	-1.081690000

S11

1	2.290503000	-2.258989000	0.776646000
1	-0.000381000	0.001281000	-1.450154000
1	-2.732787000	0.613834000	-2.158583000
1	-3.928628000	1.371257000	-1.091342000
1	-3.802072000	-0.508334000	0.494136000
1	-3.956830000	-1.260840000	-1.095364000
1	3.802677000	0.507838000	0.493742000
1	3.956481000	1.261952000	-1.095089000
1	2.732093000	-0.612054000	-2.159445000
1	3.928288000	-1.370455000	-1.093261000

E(RB3LYP) = -1741.50817876

Zero-point correction= 0.208114

Thermal correction to Energy= 0.223875

Thermal correction to Enthalpy= 0.224819

Thermal correction to Gibbs Free Energy= 0.165638

Sum of electronic and zero-point Energies= -1741.300065

Sum of electronic and thermal Energies= -1741.284304

Sum of electronic and thermal Enthalpies= -1741.283360

Sum of electronic and thermal Free Energies= -1741.342541

## 10

25	0.000004000	0.000124000	-0.095803000
15	0.888820000	2.058683000	-0.375276000
1	0.163625000	3.044678000	-1.096700000
1	1.264651000	2.917445000	0.699653000
1	2.099554000	2.206553000	-1.103799000
15	2.059087000	-0.888695000	-0.373096000
1	3.044726000	-0.165124000	-1.096639000
1	2.917840000	-1.260567000	0.703168000
1	2.207891000	-2.101551000	-1.097963000
15	-0.888587000	-2.058580000	-0.375256000
15	-2.059063000	0.888310000	-0.373516000
1	-0.163000000	-3.044331000	-1.096599000
1	-1.263949000	-2.917355000	0.699822000
1	-2.099239000	-2.206944000	-1.103810000
1	-3.043519000	0.165522000	-1.099388000
1	-2.919033000	1.257152000	0.702849000
1	-2.208203000	2.102749000	-1.095675000
1	-0.000164000	0.000060000	-1.702281000
7	-0.000204000	0.000292000	1.760940000
7	-0.000529000	0.000114000	2.887573000

E(RB3LYP) = -1586.63468934

Zero-point correction= 0.127730 (Hartree/Particle)

Thermal correction to Energy= 0.142400

Thermal correction to Enthalpy= 0.143345

Thermal correction to Gibbs Free Energy= 0.086582

Sum of electronic and zero-point Energies= -1586.506959

Sum of electronic and thermal Energies= -1586.492289

Sum of electronic and thermal Enthalpies= -1586.491345

Sum of electronic and thermal Free Energies= -1586.548108

## 11

75	-0.000019000	0.000429000	-0.131673000
6	-0.000279000	-0.002805000	1.864944000

8	-0.000355000	-0.005118000	3.017817000
6	1.993329000	-0.008882000	-0.321062000
8	3.129484000	-0.014671000	-0.488651000
6	-0.009171000	-1.991963000	-0.328623000
8	-0.014345000	-3.127205000	-0.502517000
1	0.000387000	0.005285000	-1.862626000
6	0.009262000	1.993097000	-0.324588000
8	0.014929000	3.128511000	-0.497351000
6	-1.993322000	0.009430000	-0.321157000
8	-3.129447000	0.014643000	-0.489169000

E(RB+HF-LYP) = -646.482251401

Zero-point correction=	0.049442 (Hartree/Particle)
Thermal correction to Energy=	0.061599
Thermal correction to Enthalpy=	0.062544
Thermal correction to Gibbs Free Energy=	0.008760
Sum of electronic and zero-point Energies=	-646.432809
Sum of electronic and thermal Energies=	-646.420652
Sum of electronic and thermal Enthalpies=	-646.419708
Sum of electronic and thermal Free Energies=	-646.473491

## 12

75	0.000020000	0.000082000	0.107219000
15	-2.379119000	-0.000351000	0.398308000
15	2.379172000	0.000032000	0.398233000
6	-0.000037000	0.000047000	-1.856343000
8	-0.000121000	-0.000262000	-3.018392000
6	-0.000192000	1.974334000	0.280057000
8	-0.000345000	3.120057000	0.435855000
6	0.000163000	-1.974172000	0.280193000
8	0.000205000	-3.119897000	0.435968000
1	-2.959946000	-1.065461000	1.123249000
1	-2.960804000	1.065402000	1.121622000
1	-3.284423000	-0.001526000	-0.692049000
1	2.960162000	-1.064868000	1.123349000
1	2.960678000	1.066006000	1.121367000
1	3.284492000	-0.001194000	-0.692111000
1	0.000011000	-0.000121000	1.854170000

E(RB+HF-LYP) = -1106.1089267

Zero-point correction=	0.089159
Thermal correction to Energy=	0.102749
Thermal correction to Enthalpy=	0.103693
Thermal correction to Gibbs Free Energy=	0.046784
Sum of electronic and zero-point Energies=	-1106.019768
Sum of electronic and thermal Energies=	-1106.006178
Sum of electronic and thermal Enthalpies=	-1106.005234
Sum of electronic and thermal Free Energies=	-1106.062143

## 13

75	0.000081000	0.082225000	-0.119487000
15	-1.736815000	-1.638125000	-0.293260000
15	1.734894000	-1.640206000	-0.293156000
6	-0.000280000	0.185625000	1.846268000

8	-0.000665000	0.227199000	3.006327000
6	-1.371414000	1.436100000	-0.366500000
8	-2.187234000	2.237703000	-0.550958000
6	1.373393000	1.434384000	-0.365830000
8	2.190376000	2.234892000	-0.549903000
1	-2.864731000	-1.339125000	-1.087884000
1	-1.402164000	-2.873506000	-0.897603000
1	-2.428855000	-2.166556000	0.824355000
1	2.863091000	-1.342481000	-1.087876000
1	1.398804000	-2.875212000	-0.897452000
1	2.426430000	-2.169443000	0.824418000
1	0.000180000	-0.160602000	-1.847585000

E(RB+HF-LYP) = -1106.11192

Zero-point correction=	0.089180
Thermal correction to Energy=	0.102691
Thermal correction to Enthalpy=	0.103635
Thermal correction to Gibbs Free Energy=	0.047252
Sum of electronic and zero-point Energies=	-1106.022745
Sum of electronic and thermal Energies=	-1106.009234
Sum of electronic and thermal Enthalpies=	-1106.008290
Sum of electronic and thermal Free Energies=	-1106.064673

#### 14

75	-0.000015000	-0.000061000	-0.090942000
6	-0.000049000	0.000598000	1.845305000
8	0.000253000	0.001129000	3.016072000
15	2.259266000	-0.664699000	-0.348985000
1	3.152121000	0.177123000	-1.065297000
1	3.128166000	-0.921131000	0.745776000
1	2.554755000	-1.854070000	-1.067720000
15	-0.664620000	-2.259239000	-0.349480000
1	0.177441000	-3.152057000	-1.065541000
1	-0.921799000	-3.128404000	0.744916000
1	-1.853673000	-2.554309000	-1.068913000
15	-2.259295000	0.664456000	-0.349078000
15	0.664617000	2.259039000	-0.350279000
1	-3.152333000	-0.177625000	-1.064842000
1	-3.128074000	0.921659000	0.745599000
1	-2.554536000	1.853493000	-1.068464000
1	-0.177579000	3.151582000	-1.066515000
1	0.922070000	3.128581000	0.743748000
1	1.853541000	2.553673000	-1.070073000
1	-0.000257000	0.000083000	-1.855084000

E(RB+HF-LYP) = -1565.71626

Zero-point correction=	0.128602
Thermal correction to Energy=	0.143090
Thermal correction to Enthalpy=	0.144035
Thermal correction to Gibbs Free Energy=	0.086571
Sum of electronic and zero-point Energies=	-1565.587656
Sum of electronic and thermal Energies=	-1565.573167
Sum of electronic and thermal Enthalpies=	-1565.572223

Sum of electronic and thermal Free Energies= -1565.629686

**15**

75	-0.000187000	0.000235000	-0.098955000
7	-0.004598000	-0.003458000	1.902575000
7	-0.004562000	-0.006322000	3.032263000
15	0.556497000	-2.281787000	-0.342873000
1	1.653183000	-2.645817000	-1.168669000
1	0.902283000	-3.126861000	0.751347000
1	-0.384767000	-3.170313000	-0.930297000
15	-2.284918000	-0.553423000	-0.330035000
1	-2.646936000	-1.763076000	-0.982435000
1	-3.165196000	-0.708315000	0.779726000
1	-3.139095000	0.293961000	-1.085647000
15	-0.552906000	2.284310000	-0.339501000
15	2.284800000	0.553456000	-0.324613000
1	-1.675351000	2.652317000	-1.128401000
1	-0.852291000	3.139492000	0.760104000
1	0.373906000	3.160571000	-0.966491000
1	2.647382000	1.762260000	-0.978351000
1	3.165220000	0.709088000	0.785045000
1	3.138485000	-0.295271000	-1.079111000
1	0.009217000	0.004479000	-1.823706000

E(RB+HF-LYP) = -1561.88254

Zero-point correction= 0.128655

Thermal correction to Energy= 0.143250

Thermal correction to Enthalpy= 0.144194

Thermal correction to Gibbs Free Energy= 0.086634

Sum of electronic and zero-point Energies= -1561.753886

Sum of electronic and thermal Energies= -1561.739291

Sum of electronic and thermal Enthalpies= -1561.738346

Sum of electronic and thermal Free Energies= -1561.795906

**16**

75	0.000018000	-0.053640000	-0.103110000
15	-2.365282000	-0.071682000	-0.398045000
15	2.365246000	-0.071341000	-0.398259000
15	-0.000283000	2.381299000	-0.263564000
8	0.000067000	-3.126999000	-0.461058000
8	0.000243000	-0.120134000	3.013350000
6	0.000152000	-1.973809000	-0.306021000
6	0.000194000	-0.105893000	1.847533000
1	-2.919608000	-1.061757000	-1.241940000
1	-2.997825000	1.047325000	-0.999083000
1	-3.278891000	-0.222937000	0.677022000
1	2.998715000	1.050682000	-0.992728000
1	2.918949000	-1.056863000	-1.247876000
1	3.278602000	-0.229528000	0.676006000
1	-0.001141000	3.243690000	0.862643000
1	-1.060115000	3.012970000	-0.960567000
1	1.060450000	3.013119000	-0.959084000

1 -0.000275000 0.107442000 -1.850531000  
E(RB+HF-LYP) = -1335.91679

Zero-point correction= 0.109059  
Thermal correction to Energy= 0.123089  
Thermal correction to Enthalpy= 0.124033  
Thermal correction to Gibbs Free Energy= 0.067010  
Sum of electronic and zero-point Energies= -1335.807733  
Sum of electronic and thermal Energies= -1335.793703  
Sum of electronic and thermal Enthalpies= -1335.792759  
Sum of electronic and thermal Free Energies= -1335.849782

### 17

75 -0.002544000 -0.035838000 -0.164104000  
15 0.001764000 2.333910000 -0.253950000  
15 -2.357661000 -0.040111000 -0.387209000  
15 2.340397000 -0.072313000 -0.456964000  
15 0.058239000 -0.201342000 2.217004000  
7 -0.030368000 -1.995839000 -0.425025000  
7 -0.053846000 -3.107490000 -0.613427000  
1 -1.025335000 2.992010000 -0.982371000  
1 -0.059492000 3.190644000 0.883300000  
1 1.087037000 3.005583000 -0.879610000  
1 -2.959084000 -1.172435000 -0.995751000  
1 -3.286861000 0.067005000 0.688798000  
1 -2.974287000 0.942816000 -1.205563000  
1 2.919391000 -1.182106000 -1.125314000  
1 3.277082000 -0.029468000 0.618101000  
1 2.960986000 0.940503000 -1.234969000  
1 -0.749831000 0.625887000 3.050371000  
1 -0.271544000 -1.414155000 2.888626000  
1 1.257967000 0.023719000 2.955743000  
1 -0.036786000 0.119003000 -1.867601000

E(RB+HF-LYP) = -1561.88040

Zero-point correction= 0.128178  
Thermal correction to Energy= 0.143016  
Thermal correction to Enthalpy= 0.143961  
Thermal correction to Gibbs Free Energy= 0.085489  
Sum of electronic and zero-point Energies= -1561.752224  
Sum of electronic and thermal Energies= -1561.737386  
Sum of electronic and thermal Enthalpies= -1561.736441  
Sum of electronic and thermal Free Energies= -1561.794913

### 18

26 -0.000077000 0.000127000 -0.347672000  
15 -2.253644000 -0.000787000 -0.127258000  
1 -3.118176000 0.000808000 -1.248331000  
1 -2.811671000 -1.076447000 0.590756000  
1 -2.811732000 1.072672000 0.593973000  
6 0.000740000 -1.790633000 -0.583655000  
8 0.001263000 -2.916468000 -0.814259000



1	-0.000295000	0.000447000	-1.853676000
15	2.253651000	0.000984000	-0.127464000
6	-0.000839000	1.790950000	-0.582901000
1	3.118074000	-0.000718000	-1.248622000
1	2.811740000	1.076721000	0.590380000
1	2.811710000	-1.072432000	0.593833000
8	-0.001342000	2.916835000	-0.813286000
17	0.000204000	-0.000714000	2.050687000
E(RB+HF-LYP) = -1497.25554			
Zero-point correction=			0.082544
Thermal correction to Energy=			0.095581
Thermal correction to Enthalpy=			0.096525
Thermal correction to Gibbs Free Energy=			0.042189
Sum of electronic and zero-point Energies=			-1497.172997
Sum of electronic and thermal Energies=			-1497.159960
Sum of electronic and thermal Enthalpies=			-1497.159016
Sum of electronic and thermal Free Energies=			-1497.213300

## 19

26	-0.000013000	0.000066000	-0.170151000
15	-2.204563000	-0.004179000	0.279812000
1	-3.255764000	-0.008245000	-0.669313000
1	-2.626194000	-1.077054000	1.088506000
1	-2.631641000	1.069141000	1.085087000
6	0.003559000	-1.760256000	-0.538157000
8	0.006284000	-2.850589000	-0.909430000
1	-0.001317000	0.000057000	-1.699678000
15	2.203839000	0.004154000	0.279479000
6	-0.003569000	1.760120000	-0.538333000
1	3.254013000	0.003058000	-0.670945000
1	2.627437000	1.080144000	1.082833000
1	2.629509000	-1.067111000	1.087947000
8	-0.006170000	2.850582000	-0.909305000
9	0.001590000	-0.000053000	1.748771000
E(RB+HF-LYP) = -1136.86589			
Zero-point correction=			0.083259
Thermal correction to Energy=			0.095760
Thermal correction to Enthalpy=			0.096704
Thermal correction to Gibbs Free Energy=			0.044443
Sum of electronic and zero-point Energies=			-1136.782626
Sum of electronic and thermal Energies=			-1136.770125
Sum of electronic and thermal Enthalpies=			-1136.769181
Sum of electronic and thermal Free Energies=			-1136.821443

## 20

26	-0.000218000	-0.560146000	0.000287000
15	-1.624112000	-0.763329000	-1.514330000
15	-1.646326000	-0.664026000	1.513047000
15	1.623749000	-0.764059000	1.514605000

15	1.645283000	-0.665773000	-1.512984000
7	0.000673000	1.482472000	-0.000098000
1	-2.053332000	0.344902000	-2.290281000
1	-1.561076000	-1.712096000	-2.564663000
1	-1.811819000	-1.837591000	2.291048000
1	-1.812842000	0.277634000	2.558880000
6	-3.313007000	-0.541773000	0.667132000
6	-3.230888000	-1.261849000	-0.685398000
1	1.560605000	-1.712944000	2.564829000
1	2.053601000	0.343898000	2.290589000
1	1.809990000	-1.839925000	-2.290267000
1	1.811769000	0.275104000	-2.559513000
6	3.230180000	-1.263217000	0.685291000
6	3.312218000	-0.543714000	-0.667559000
6	-0.034031000	2.309666000	-1.096185000
6	-0.020430000	3.645193000	-0.708113000
6	0.023732000	3.645362000	0.707339000
6	0.036119000	2.309928000	1.095769000
1	-4.117328000	-0.936612000	1.294410000
1	-3.495565000	0.527908000	0.517175000
1	-4.093441000	-1.037464000	-1.319483000
1	-3.190603000	-2.347038000	-0.542164000
1	4.092959000	-1.038814000	1.319064000
1	3.189613000	-2.348453000	0.542488000
1	4.116258000	-0.939110000	-1.294847000
1	3.495171000	0.525969000	-0.518108000
1	-0.069391000	1.903182000	-2.099722000
1	-0.040153000	4.505784000	-1.365715000
1	0.044227000	4.506112000	1.364708000
1	0.071085000	1.903674000	2.099412000
1	-0.001036000	-2.117399000	0.000658000

E(RB+HF-LYP) = -1861.08041

Zero-point correction=	0.271544
Thermal correction to Energy=	0.290128
Thermal correction to Enthalpy=	0.291072
Thermal correction to Gibbs Free Energy=	0.224659
Sum of electronic and zero-point Energies=	-1860.808869
Sum of electronic and thermal Energies=	-1860.790284
Sum of electronic and thermal Enthalpies=	-1860.789340
Sum of electronic and thermal Free Energies=	-1860.855753

**21**

26	-0.000205000	-0.000014000	-0.163244000
15	-1.626073000	1.512721000	-0.184245000
15	-1.611857000	-1.514148000	-0.314419000
15	1.625829000	-1.512725000	-0.186075000
15	1.611242000	1.514219000	-0.315881000
6	-3.271003000	0.666858000	0.109721000
1	-3.338223000	0.510780000	1.191748000
1	-4.112200000	1.295651000	-0.195853000
6	-3.263708000	-0.680055000	-0.625590000
1	-3.340328000	-0.526733000	-1.707575000

S18

1	-4.096929000	-1.317836000	-0.317139000
6	3.270364000	-0.666882000	0.109834000
1	3.336356000	-0.511319000	1.192004000
1	4.111958000	-1.295414000	-0.195187000
6	3.263658000	0.680333000	-0.624906000
1	3.341862000	0.527434000	-1.706840000
1	4.096317000	1.318192000	-0.315109000
7	0.002691000	-0.000384000	2.959403000
6	0.001441000	-0.000203000	1.786547000
1	-0.001367000	0.000090000	-1.718100000
1	1.625503000	2.516140000	-1.317138000
1	-1.924804000	-2.349221000	0.788735000
1	-1.688663000	2.565371000	0.760803000
1	1.905465000	-2.282372000	-1.344269000
1	1.688173000	-2.566669000	0.757534000
1	1.922923000	2.351543000	0.785909000
1	-1.905241000	2.283982000	-1.341478000
1	-1.625940000	-2.517865000	-1.313881000

E(RB+HF-LYP) = -1744.36783

Zero-point correction=	0.208857
Thermal correction to Energy=	0.224841
Thermal correction to Enthalpy=	0.225785
Thermal correction to Gibbs Free Energy=	0.165753
Sum of electronic and zero-point Energies=	-1744.158971
Sum of electronic and thermal Energies=	-1744.142987
Sum of electronic and thermal Enthalpies=	-1744.142043
Sum of electronic and thermal Free Energies=	-1744.202075

## 22

26	-0.001284000	-0.002078000	-0.263582000
15	-1.627237000	1.518084000	-0.357533000
15	-1.640666000	-1.520598000	-0.244943000
15	1.630400000	-1.517173000	-0.361096000
15	1.635776000	1.520722000	-0.244900000
1	-1.882145000	2.342137000	0.767236000
1	-1.691667000	2.523137000	-1.354585000
1	-1.974418000	-2.262276000	-1.407903000
1	-1.669241000	-2.589875000	0.682231000
6	-3.266924000	-0.669812000	0.130548000
6	-3.290161000	0.681100000	-0.598193000
1	1.698711000	-2.519912000	-1.360278000
1	1.887131000	-2.342893000	0.761958000
1	1.966309000	2.268388000	-1.404942000
1	1.659642000	2.586039000	0.686857000
6	3.291109000	-0.675700000	-0.600291000
6	3.264422000	0.674540000	0.129288000
1	-4.124650000	-1.293454000	-0.137732000
1	-3.278244000	-0.518900000	1.214987000
1	-4.111391000	1.315653000	-0.252855000
1	-3.413598000	0.531796000	-1.676640000
1	4.113742000	-1.308499000	-0.255074000
1	3.414689000	-0.525545000	-1.678619000

1	4.120516000	1.300713000	-0.138290000
1	3.275682000	0.522893000	1.213632000
1	-0.003729000	-0.002469000	-1.796620000
17	0.004779000	-0.002895000	2.161690000

E(RB+HF-LYP) = -2111.75349

Zero-point correction=	0.201388
Thermal correction to Energy=	0.216999
Thermal correction to Enthalpy=	0.217943
Thermal correction to Gibbs Free Energy=	0.158120
Sum of electronic and zero-point Energies=	-2111.552106
Sum of electronic and thermal Energies=	-2111.536495
Sum of electronic and thermal Enthalpies=	-2111.535551
Sum of electronic and thermal Free Energies=	-2111.595374

### 23

44	0.303775000	0.000002000	-0.118365000
15	-0.056603000	2.322774000	-0.337557000
15	-0.057273000	-2.322647000	-0.337720000
8	-3.985683000	0.000258000	-0.399202000
8	1.095864000	-0.000353000	2.941779000
8	3.122797000	-0.000338000	-1.272833000
7	-1.744150000	0.000223000	0.454720000
6	-2.855215000	0.000258000	-0.011180000
6	0.806833000	-0.000194000	1.831813000
6	2.068404000	-0.000196000	-0.801021000
1	0.901495000	3.177603000	-0.928671000
1	-0.340552000	3.081858000	0.818133000
1	-1.180002000	2.660602000	-1.113173000
1	-1.180565000	-2.660111000	-1.113647000
1	0.900698000	-3.177820000	-0.928547000
1	-0.341806000	-3.081584000	0.817919000
1	-0.192119000	0.000145000	-1.673455000

E(RB+HF-LYP) = -1175.62399

Zero-point correction=	0.094235
Thermal correction to Energy=	0.109408
Thermal correction to Enthalpy=	0.110352
Thermal correction to Gibbs Free Energy=	0.049333
Sum of electronic and zero-point Energies=	-1175.529752
Sum of electronic and thermal Energies=	-1175.514579
Sum of electronic and thermal Enthalpies=	-1175.513635
Sum of electronic and thermal Free Energies=	-1175.574654

### 24

44	0.069394000	0.000008000	-0.119439000
15	2.486269000	-0.000618000	-0.319388000
14	-2.382486000	0.000462000	-0.516737000
8	-0.217125000	3.054088000	-0.544838000
8	-0.290543000	0.000143000	2.988733000
8	-0.218736000	-3.053943000	-0.544753000
6	-0.098947000	1.928788000	-0.346580000

6	-0.129612000	0.000034000	1.850534000
6	-0.099930000	-1.928696000	-0.346559000
1	3.094708000	-1.062219000	-1.025211000
1	3.359091000	-0.000964000	0.795692000
1	3.095329000	1.060750000	-1.025028000
1	-3.174298000	-0.001255000	0.749444000
1	-2.831240000	1.194525000	-1.287882000
1	-2.831141000	-1.191559000	-1.291083000
1	0.077148000	0.000109000	-1.773002000

E(RB+HF-LYP) = -1069.01789

Zero-point correction=	0.085794
Thermal correction to Energy=	0.099895
Thermal correction to Enthalpy=	0.100839
Thermal correction to Gibbs Free Energy=	0.043241
Sum of electronic and zero-point Energies=	-1068.932094
Sum of electronic and thermal Energies=	-1068.917993
Sum of electronic and thermal Enthalpies=	-1068.917049
Sum of electronic and thermal Free Energies=	-1068.974647

## 25

44	-0.000537000	0.208450000	-0.221674000
15	-2.316288000	-0.008772000	-0.546541000
15	0.000951000	-0.413008000	2.171181000
15	2.315983000	-0.000124000	-0.546784000
8	-0.005695000	3.221611000	0.028971000
17	0.004695000	-2.286478000	-0.529476000
1	-2.682607000	-0.735608000	-1.694865000
1	-3.148621000	1.122407000	-0.720860000
1	-3.109716000	-0.696618000	0.402173000
1	-1.055703000	-1.229894000	2.636786000
1	1.062136000	-1.223654000	2.637502000
1	-0.002044000	0.509726000	3.249626000
1	3.111082000	-0.686831000	0.401300000
1	3.144644000	1.134097000	-0.718988000
1	2.685352000	-0.723888000	-1.696059000
6	-0.003941000	2.064337000	-0.054419000
1	-0.001215000	0.398234000	-1.814954000

E(RB+HF-LYP) = -1697.58877

Zero-point correction=	0.101872
Thermal correction to Energy=	0.115983
Thermal correction to Enthalpy=	0.116927
Thermal correction to Gibbs Free Energy=	0.059924
Sum of electronic and zero-point Energies=	-1697.486903
Sum of electronic and thermal Energies=	-1697.472792
Sum of electronic and thermal Enthalpies=	-1697.471848
Sum of electronic and thermal Free Energies=	-1697.528851

## 26

44	0.016249000	0.158203000	-0.207346000
----	-------------	-------------	--------------

15	-2.284342000	0.189939000	-0.624367000
15	2.290467000	-0.136771000	-0.655819000
8	0.267463000	2.848292000	1.169682000
6	0.174103000	1.813402000	0.649888000
1	-3.110536000	1.323857000	-0.445038000
1	-3.121260000	-0.767881000	-0.002045000
1	-2.600345000	-0.109674000	-1.962845000
1	2.517908000	-0.734602000	-1.911734000
1	3.181212000	0.955256000	-0.758859000
1	3.122035000	-0.985132000	0.119880000
1	0.071947000	0.917026000	-1.618274000
15	-0.108867000	-1.417599000	1.692963000
1	0.829543000	-2.475638000	1.674104000
1	-0.020386000	-1.133371000	3.080958000
1	-1.264013000	-2.232038000	1.756743000
9	-0.218250000	-1.657666000	-1.139788000

E(RB+HF-LYP) = -1337.19813

Zero-point correction=	0.102451
Thermal correction to Energy=	0.116335
Thermal correction to Enthalpy=	0.117279
Thermal correction to Gibbs Free Energy=	0.060310
Sum of electronic and zero-point Energies=	-1337.095679
Sum of electronic and thermal Energies=	-1337.081794
Sum of electronic and thermal Enthalpies=	-1337.080850
Sum of electronic and thermal Free Energies=	-1337.137820

**27**

44	0.080949000	-0.000363000	-0.184372000
15	2.451666000	-0.009140000	-0.254866000
15	-0.095176000	-2.294744000	-0.469789000
15	-0.243875000	-0.002146000	2.171857000
15	-0.075155000	2.296407000	-0.466010000
14	-2.346929000	0.010996000	-0.521901000
1	3.134485000	-1.068321000	-0.910678000
1	3.287781000	-0.006382000	0.899109000
1	3.140485000	1.040247000	-0.919979000
1	-0.809201000	-2.787561000	-1.583623000
1	1.067183000	-3.097259000	-0.639473000
1	-0.711387000	-3.118640000	0.509782000
1	-0.973050000	-1.058847000	2.777812000
1	0.812506000	0.001650000	3.128270000
1	-0.981920000	1.047838000	2.778594000
1	-0.683706000	3.124952000	0.514447000
1	1.093947000	3.089131000	-0.635386000
1	-0.785286000	2.796695000	-1.579051000
1	-3.177448000	0.023820000	0.736679000
1	-2.893519000	-1.171686000	-1.271668000
1	-2.880059000	1.189774000	-1.287126000
1	0.092534000	0.000968000	-1.816608000

E(RB+HF-LYP) = -1758.45983

Zero-point correction=	0.144543
------------------------	----------

Thermal correction to Energy=	0.160480
Thermal correction to Enthalpy=	0.161424
Thermal correction to Gibbs Free Energy=	0.101095
Sum of electronic and zero-point Energies=	-1758.315290
Sum of electronic and thermal Energies=	-1758.299353
Sum of electronic and thermal Enthalpies=	-1758.298408
Sum of electronic and thermal Free Energies=	-1758.358738

## 28

44	-0.000049000	0.000029000	-0.328301000
15	1.733867000	-1.552154000	-0.308552000
15	1.726987000	1.561115000	-0.264164000
15	-1.733960000	1.552197000	-0.307864000
15	-1.727043000	-1.561068000	-0.264002000
1	1.910554000	-2.338467000	0.856112000
1	1.908302000	-2.580794000	-1.268096000
1	2.149815000	2.276955000	-1.414337000
1	1.711142000	2.649334000	0.640664000
6	3.308121000	0.693628000	0.246331000
6	3.391373000	-0.677273000	-0.438589000
1	-1.908605000	2.581044000	-1.267147000
1	-1.910418000	2.338256000	0.857008000
1	-2.150092000	-2.276782000	-1.414171000
1	-1.710979000	-2.649394000	0.640694000
6	-3.391483000	0.677333000	-0.437739000
6	-3.308095000	-0.693687000	0.246935000
1	4.187076000	1.307015000	0.026364000
1	3.235616000	0.573544000	1.332275000
1	4.189253000	-1.290373000	-0.009393000
1	3.601560000	-0.559290000	-1.507577000
1	-4.189295000	1.290350000	-0.008295000
1	-3.601859000	0.559527000	-1.506708000
1	-4.187084000	-1.307043000	0.027022000
1	-3.235399000	-0.573786000	1.332887000
1	-0.000272000	0.000157000	-1.936825000
17	0.000328000	-0.000168000	2.266581000

E(RB+HF-LYP) = -2082.26656

Zero-point correction=	0.201570
Thermal correction to Energy=	0.217406
Thermal correction to Enthalpy=	0.218350
Thermal correction to Gibbs Free Energy=	0.157256
Sum of electronic and zero-point Energies=	-2082.064995
Sum of electronic and thermal Energies=	-2082.049158
Sum of electronic and thermal Enthalpies=	-2082.048214
Sum of electronic and thermal Free Energies=	-2082.109308

## 29

44	-0.217508000	0.014597000	-0.302040000
17	0.320844000	-0.112598000	2.234031000
15	-1.788785000	-1.624618000	-0.330015000
15	-1.778916000	1.650119000	-0.145175000

7	1.477493000	-1.386518000	-0.462569000
1	1.344054000	-2.100272000	0.250920000
1	1.492663000	-1.836982000	-1.373732000
7	1.470047000	1.408791000	-0.265717000
1	1.316717000	2.297512000	-0.734489000
1	1.564645000	1.575208000	0.740363000
6	2.747163000	-0.663478000	-0.195883000
1	3.618650000	-1.204194000	-0.585318000
1	2.837859000	-0.586047000	0.890602000
6	2.675819000	0.735182000	-0.796826000
1	3.596771000	1.286768000	-0.563403000
1	2.574831000	0.682702000	-1.885365000
1	-2.925703000	-1.563355000	-1.179739000
1	-2.481996000	-2.004797000	0.850952000
1	-1.394414000	-2.940359000	-0.709190000
1	-2.941108000	1.668249000	-0.962208000
1	-2.430959000	1.929665000	1.086026000
1	-1.383544000	2.990497000	-0.423137000
1	-0.327643000	0.108665000	-1.908932000

E(RB+HF-LYP) = -1431.63750

Zero-point correction=	0.181447
Thermal correction to Energy=	0.195306
Thermal correction to Enthalpy=	0.196251
Thermal correction to Gibbs Free Energy=	0.140326
Sum of electronic and zero-point Energies=	-1431.456055
Sum of electronic and thermal Energies=	-1431.442195
Sum of electronic and thermal Enthalpies=	-1431.441251
Sum of electronic and thermal Free Energies=	-1431.497175

### 30

44	-0.000378000	0.000395000	-0.404033000
17	0.003085000	-0.002729000	2.197441000
15	1.893357000	-1.385130000	-0.315076000
15	1.893035000	1.385990000	-0.311985000
15	-1.894232000	-1.385334000	-0.313229000
15	-1.893977000	1.386039000	-0.311507000
1	-0.001633000	0.002175000	-2.005877000
6	3.055075000	-0.000024000	0.191793000
1	4.057902000	0.000633000	-0.240876000
1	3.116453000	-0.001289000	1.282938000
6	-3.055291000	0.000091000	0.194050000
1	-4.058694000	0.000465000	-0.237317000
1	-3.115595000	-0.000544000	1.285252000
1	2.546044000	-1.966346000	-1.430165000
1	2.143553000	-2.414724000	0.624092000
1	2.545827000	1.969669000	-1.425712000
1	2.142937000	2.413657000	0.629400000
1	-2.144301000	-2.414792000	0.626194000
1	-2.547872000	-1.966533000	-1.427727000
1	-2.144851000	2.414693000	0.628569000
1	-2.547023000	1.968073000	-1.425923000

E(RB+HF-LYP) = -2003.59175



Zero-point correction=	0.142534
Thermal correction to Energy=	0.156420
Thermal correction to Enthalpy=	0.157364
Thermal correction to Gibbs Free Energy=	0.101071
Sum of electronic and zero-point Energies=	-2003.449213
Sum of electronic and thermal Energies=	-2003.435327
Sum of electronic and thermal Enthalpies=	-2003.434383
Sum of electronic and thermal Free Energies=	-2003.490675

### 31

42	0.000498000	0.002166000	-0.075526000
15	2.441913000	-0.056212000	-0.530683000
15	-2.442614000	0.048282000	-0.525447000
7	0.003879000	0.000777000	1.776932000
8	0.006503000	0.000537000	2.957155000
6	0.047202000	2.049920000	-0.299136000
8	0.069895000	3.189189000	-0.475148000
1	2.975259000	-1.123719000	-1.288610000
1	3.381040000	-0.095252000	0.529237000
1	3.034595000	0.998760000	-1.261939000
1	-3.004517000	-0.960414000	-1.340720000
1	-3.381524000	-0.025319000	0.532830000
1	-3.007671000	1.158172000	-1.194982000
1	-0.002027000	0.004200000	-1.889727000
6	-0.050004000	-2.045244000	-0.299204000
8	-0.078384000	-3.184970000	-0.472075000

E(RB+HF-LYP) = -1111.09080

Zero-point correction=	0.086272
Thermal correction to Energy=	0.100606
Thermal correction to Enthalpy=	0.101550
Thermal correction to Gibbs Free Energy=	0.043146
Sum of electronic and zero-point Energies=	-1111.004529
Sum of electronic and thermal Energies=	-1110.990195
Sum of electronic and thermal Enthalpies=	-1110.989251
Sum of electronic and thermal Free Energies=	-1111.047655

### 32

42	-0.498724000	0.005414000	-0.065899000
1	-0.020291000	0.155595000	-1.809054000
15	1.446936000	-1.592197000	-0.128848000
15	1.428206000	1.615615000	-0.005244000
6	-1.785274000	-1.405858000	-0.755502000
6	-1.817655000	1.474505000	-0.541541000
7	-0.969676000	-0.129585000	1.721419000
8	-1.284869000	-0.208546000	2.856023000
6	3.070051000	-0.666554000	0.066808000
1	3.248937000	-0.589286000	1.145372000
1	3.896395000	-1.241328000	-0.361405000
1	3.873687000	1.325173000	-0.310831000
6	2.987930000	0.733056000	-0.559100000

1	2.924461000	0.662045000	-1.649602000
1	1.649553000	-2.652057000	0.788269000
1	1.673772000	-2.330465000	-1.311673000
1	1.458649000	2.758660000	-0.834253000
1	1.878928000	2.242934000	1.185134000
8	-2.552373000	2.310921000	-0.845421000
8	-2.501181000	-2.204089000	-1.182695000

E(RB+HF-LYP) = -1188.52808

Zero-point correction=	0.126717
Thermal correction to Energy=	0.141336
Thermal correction to Enthalpy=	0.142281
Thermal correction to Gibbs Free Energy=	0.083652
Sum of electronic and zero-point Energies=	-1188.401363
Sum of electronic and thermal Energies=	-1188.386743
Sum of electronic and thermal Enthalpies=	-1188.385799
Sum of electronic and thermal Free Energies=	-1188.444428

### 33

42	0.000027000	-0.067393000	-0.075163000
15	-2.434675000	-0.072665000	-0.501711000
15	-0.002304000	2.445570000	-0.276904000
15	2.435172000	-0.067477000	-0.500444000
7	-0.000673000	-0.169316000	1.765248000
8	-0.001493000	-0.218182000	2.949532000
6	0.002587000	-2.057451000	-0.372749000
8	0.004222000	-3.199143000	-0.570780000
1	-3.074351000	1.062502000	-1.065002000
1	-3.364575000	-0.284604000	0.547522000
1	-2.964902000	-1.024464000	-1.403216000
1	-0.002955000	3.301289000	0.854761000
1	1.053543000	3.092007000	-0.967994000
1	-1.059040000	3.090559000	-0.968023000
1	3.072979000	1.068892000	-1.063433000
1	3.364775000	-0.277447000	0.549439000
1	2.967889000	-1.018298000	-1.401517000
1	-0.000034000	0.107164000	-1.890084000

E(RB+HF-LYP) = -1340.90499

Zero-point correction=	0.105916
Thermal correction to Energy=	0.120810
Thermal correction to Enthalpy=	0.121754
Thermal correction to Gibbs Free Energy=	0.062754
Sum of electronic and zero-point Energies=	-1340.799069
Sum of electronic and thermal Energies=	-1340.784175
Sum of electronic and thermal Enthalpies=	-1340.783231
Sum of electronic and thermal Free Energies=	-1340.842231

### 34

42	0.000016000	-0.000024000	0.165918000
15	1.857726000	-1.558343000	-0.199311000

15	1.783781000	1.599911000	-0.318512000
15	-1.857688000	1.558473000	-0.198650000
15	-1.783756000	-1.599706000	-0.319156000
6	3.482997000	-0.636100000	-0.475113000
1	3.918343000	-0.487207000	0.519871000
1	4.184930000	-1.243311000	-1.054517000
6	3.229394000	0.719540000	-1.146831000
1	2.935342000	0.578932000	-2.192363000
1	4.127350000	1.344847000	-1.129304000
6	-3.482930000	0.636369000	-0.475122000
1	-3.918473000	0.487102000	0.519719000
1	-4.184734000	1.243830000	-1.054420000
6	-3.229251000	-0.719019000	-1.147324000
1	-2.935054000	-0.578018000	-2.192763000
1	-4.127215000	-1.344326000	-1.130156000
8	-0.000314000	-0.000990000	3.193258000
7	-0.000115000	-0.000544000	1.999207000
1	-0.000014000	0.000341000	-1.671723000
1	-1.646817000	-2.701010000	-1.203024000
1	2.467874000	2.303371000	0.710395000
1	2.295635000	-2.519163000	0.749500000
1	-1.854288000	2.429571000	-1.318209000
1	-2.295743000	2.518788000	0.750606000
1	-2.467949000	-2.303338000	0.709566000
1	1.854467000	-2.428844000	-1.319335000
1	1.646804000	2.701413000	-1.202128000

E(RB+HF-LYP) = -1725.58318

Zero-point correction=	0.205799
Thermal correction to Energy=	0.222224
Thermal correction to Enthalpy=	0.223168
Thermal correction to Gibbs Free Energy=	0.161401
Sum of electronic and zero-point Energies=	-1725.377380
Sum of electronic and thermal Energies=	-1725.360955
Sum of electronic and thermal Enthalpies=	-1725.360011
Sum of electronic and thermal Free Energies=	-1725.421778

### 35

42	-0.000475000	0.000285000	-0.059849000
15	2.431773000	0.037456000	-0.408317000
15	0.030488000	-2.423989000	-0.447155000
15	-2.432726000	-0.021754000	-0.408694000
7	-0.000117000	-0.020400000	1.772451000
8	0.000309000	-0.039301000	2.964022000
1	3.078511000	-1.011373000	-1.116592000
1	3.334559000	0.068753000	0.686709000
1	3.033516000	1.096257000	-1.140658000
1	0.043517000	-3.347238000	0.631326000
1	-1.014764000	-3.049210000	-1.178906000
1	1.094169000	-3.018892000	-1.177919000
1	-3.052455000	-1.087894000	-1.115506000
1	-3.336266000	-0.012519000	0.686127000

1	-3.060773000	1.020295000	-1.142649000
1	-0.000556000	0.016281000	-1.895350000
15	-0.028716000	2.430442000	-0.417247000
1	-1.096928000	3.034949000	-1.133655000
1	-0.028166000	3.346609000	0.667346000
1	1.011657000	3.056901000	-1.154738000

E(RB+HF-LYP) = -1570.71350

Zero-point correction=	0.125557
Thermal correction to Energy=	0.140839
Thermal correction to Enthalpy=	0.141783
Thermal correction to Gibbs Free Energy=	0.082728
Sum of electronic and zero-point Energies=	-1570.587941
Sum of electronic and thermal Energies=	-1570.572659
Sum of electronic and thermal Enthalpies=	-1570.571715
Sum of electronic and thermal Free Energies=	-1570.630771

### 36

42	-0.000006000	-0.000301000	0.440488000
1	-0.000436000	0.000407000	-1.398569000
15	1.848144000	-1.597400000	0.079504000
15	1.807109000	1.604931000	-0.026024000
15	-1.807505000	-1.605048000	-0.026433000
15	-1.848094000	1.597190000	0.080968000
7	0.000369000	-0.000772000	2.272207000
8	0.000600000	-0.000924000	3.467447000
6	3.452672000	-0.651286000	-0.100231000
1	3.730760000	-0.403502000	0.936277000
6	4.678532000	-1.229676000	-0.826382000
1	5.227510000	-1.951074000	-0.213991000
1	4.355285000	-1.755117000	-1.732754000
6	5.536324000	0.019898000	-1.201641000
1	5.872855000	-0.041442000	-2.241141000
1	6.436978000	0.085380000	-0.583633000
6	4.619503000	1.262883000	-0.975504000
1	4.894189000	1.771720000	-0.043842000
1	4.698892000	1.999214000	-1.780735000
6	3.204202000	0.676374000	-0.848873000
1	2.815225000	0.436358000	-1.849166000
1	2.242558000	-2.598236000	1.007152000
1	1.885440000	-2.420211000	-1.077009000
1	1.681550000	2.720985000	-0.895259000
1	2.518879000	2.279500000	1.004316000
6	-3.452736000	0.651411000	-0.099490000
1	-3.730889000	0.403004000	0.936846000
6	-4.678505000	1.230544000	-0.825289000
1	-5.227904000	1.950749000	-0.211876000
1	-4.355117000	1.757638000	-1.730641000
6	-5.535870000	-0.018660000	-1.203013000
1	-5.869949000	0.043355000	-2.243266000
1	-6.437979000	-0.084311000	-0.587153000

6	-4.619811000	-1.261926000	-0.975778000
1	-4.699278000	-1.998746000	-1.780557000
1	-4.895044000	-1.769987000	-0.043843000
6	-3.204400000	-0.675851000	-0.848873000
1	-2.815378000	-0.435375000	-1.849039000
1	-2.519407000	-2.279561000	1.003854000
1	-1.682492000	-2.720982000	-0.895907000
1	-2.242360000	2.597306000	1.009461000
1	-1.885304000	2.420985000	-1.074849000

E(RB+HF-LYP) = -1959.04110

Zero-point correction=	0.335003
Thermal correction to Energy=	0.356637
Thermal correction to Enthalpy=	0.357581
Thermal correction to Gibbs Free Energy=	0.283218
Sum of electronic and zero-point Energies=	-1958.706099
Sum of electronic and thermal Energies=	-1958.684465
Sum of electronic and thermal Enthalpies=	-1958.683521
Sum of electronic and thermal Free Energies=	-1958.757884

### 37

74	0.060892000	0.000029000	-0.098816000
1	-0.127259000	0.000204000	-1.901500000
8	0.002098000	3.185717000	-0.505988000
8	0.004063000	-3.185635000	-0.506253000
8	3.186891000	0.000965000	-0.708675000
8	0.286794000	-0.000028000	2.926539000
15	-2.459795000	-0.000714000	-0.313668000
6	0.028025000	2.048543000	-0.330711000
6	0.029294000	-2.048498000	-0.330609000
6	2.059945000	0.000555000	-0.470396000
7	0.201667000	-0.000094000	1.750436000
1	-3.294716000	-0.001040000	0.828414000
1	-3.070904000	1.065395000	-1.008545000
1	-3.070252000	-1.067097000	-1.008694000

E(RB+HF-LYP) = -881.57934

Zero-point correction=	0.067043
Thermal correction to Energy=	0.080450
Thermal correction to Enthalpy=	0.081394
Thermal correction to Gibbs Free Energy=	0.024655
Sum of electronic and zero-point Energies=	-881.512297
Sum of electronic and thermal Energies=	-881.498890
Sum of electronic and thermal Enthalpies=	-881.497946
Sum of electronic and thermal Free Energies=	-881.554685

### 38

74	0.000023000	0.000066000	0.079263000
15	-2.442725000	0.000009000	0.484275000
15	2.442684000	0.000219000	0.484762000
7	0.000404000	-0.000375000	-1.766482000

8	0.000562000	-0.001189000	-2.952331000
6	-0.000271000	2.040116000	0.273113000
8	-0.000503000	3.186017000	0.421600000
1	-3.020386000	-1.063454000	1.215055000
1	-3.020294000	1.064427000	1.213740000
1	-3.344523000	-0.000658000	-0.606819000
1	3.020189000	-1.063083000	1.215889000
1	3.344482000	-0.000861000	-0.606320000
1	3.020377000	1.064786000	1.213917000
1	-0.000513000	-0.000299000	1.901658000
6	-0.000019000	-2.039926000	0.273888000
8	-0.000250000	-3.185787000	0.422638000

E(RB+HF-LYP) = -1111.39355

Zero-point correction=	0.086899
Thermal correction to Energy=	0.100995
Thermal correction to Enthalpy=	0.101939
Thermal correction to Gibbs Free Energy=	0.043700
Sum of electronic and zero-point Energies=	-1111.306647
Sum of electronic and thermal Energies=	-1111.292550
Sum of electronic and thermal Enthalpies=	-1111.291606
Sum of electronic and thermal Free Energies=	-1111.349845

### 39

74	0.001076000	0.003960000	-0.071812000
15	0.124894000	2.423953000	-0.398195000
15	2.425262000	-0.139071000	-0.369943000
15	-0.130607000	-2.416773000	-0.394080000
7	0.003006000	0.003700000	1.754903000
8	0.002768000	0.001870000	2.953035000
1	1.239938000	3.009984000	-1.058479000
1	0.108601000	3.303092000	0.715122000
1	-0.867586000	3.097574000	-1.160827000
1	3.274785000	-0.277526000	0.757473000
1	2.992809000	-1.189507000	-1.141437000
1	3.150555000	0.911025000	-0.998462000
1	0.908835000	-3.118214000	-1.064895000
1	-0.227228000	-3.287216000	0.721956000
1	-1.196545000	-2.983922000	-1.144727000
1	-0.005756000	0.001329000	-1.912013000
15	-2.424760000	0.116092000	-0.366577000
1	-3.028179000	1.200680000	-1.061381000
1	-3.111310000	-0.907005000	-1.076959000
1	-3.283602000	0.142828000	0.762025000

E(RB+HF-LYP) = -1571.00724

Zero-point correction=	0.125921
Thermal correction to Energy=	0.141088
Thermal correction to Enthalpy=	0.142032
Thermal correction to Gibbs Free Energy=	0.082668
Sum of electronic and zero-point Energies=	-1570.881318

Sum of electronic and thermal Energies=	-1570.866151
Sum of electronic and thermal Enthalpies=	-1570.865207
Sum of electronic and thermal Free Energies=	-1570.924571

**40**

74	-0.124708000	0.044119000	0.024232000
15	1.840137000	-1.359029000	0.661391000
15	-1.236530000	-2.006019000	-0.918360000
15	-1.829511000	1.447512000	-1.068716000
7	-0.935248000	-0.017675000	1.667497000
8	-1.517166000	-0.063230000	2.705743000
6	0.953678000	1.677494000	0.420747000
8	1.617941000	2.611913000	0.620876000
1	2.393684000	-2.280250000	-0.253350000
1	1.629687000	-2.254491000	1.739994000
1	3.040932000	-0.779201000	1.118281000
1	-2.091842000	-2.809976000	-0.124139000
1	-2.105156000	-1.872116000	-2.031389000
1	-0.451816000	-3.057406000	-1.452282000
1	-2.685602000	0.914571000	-2.069762000
1	-2.834244000	2.069249000	-0.287824000
1	-1.415914000	2.589125000	-1.794009000
1	0.513832000	0.055942000	-1.697996000
8	3.244116000	0.170777000	-1.603926000
1	2.288713000	0.175428000	-1.797127000
1	3.400194000	1.050441000	-1.236801000

E(RB+HF-LYP) = -1341.20361

Zero-point correction=	0.106518
Thermal correction to Energy=	0.121181
Thermal correction to Enthalpy=	0.122125
Thermal correction to Gibbs Free Energy=	0.063254
Sum of electronic and zero-point Energies=	-1341.097095
Sum of electronic and thermal Energies=	-1341.082432
Sum of electronic and thermal Enthalpies=	-1341.081488
Sum of electronic and thermal Free Energies=	-1341.140359

**41**

74	0.000002000	-0.000001000	0.107523000
15	1.854573000	-1.554395000	-0.219718000
15	1.792427000	1.589829000	-0.329205000
15	-1.854569000	1.554393000	-0.219716000
15	-1.792418000	-1.589829000	-0.329232000
6	3.496684000	-0.646304000	-0.453278000
1	3.913428000	-0.512068000	0.551588000
1	4.201951000	-1.256160000	-1.025689000
6	3.268262000	0.717842000	-1.116242000
1	3.012535000	0.591465000	-2.173764000
1	4.163648000	1.344162000	-1.057322000
6	-3.496678000	0.646303000	-0.453295000
1	-3.913428000	0.512057000	0.551566000
1	-4.201942000	1.256163000	-1.025706000

6	-3.268249000	-0.717837000	-1.116270000
1	-3.012517000	-0.591451000	-2.173789000
1	-4.163635000	-1.344160000	-1.057360000
8	-0.000071000	0.000026000	3.136359000
7	0.000002000	-0.000017000	1.935793000
1	0.000015000	0.000002000	-1.735194000
1	-1.676405000	-2.690626000	-1.216673000
1	2.430864000	2.288418000	0.730252000
1	2.248615000	-2.511681000	0.750260000
1	-1.872343000	2.426083000	-1.338779000
1	-2.248619000	2.511672000	0.750265000
1	-2.430859000	-2.288429000	0.730214000
1	1.872353000	-2.426077000	-1.338786000
1	1.676421000	2.690636000	-1.216635000

E(RB+HF-LYP) = -1725.87872

Zero-point correction=	0.206126
Thermal correction to Energy=	0.222452
Thermal correction to Enthalpy=	0.223396
Thermal correction to Gibbs Free Energy=	0.161451
Sum of electronic and zero-point Energies=	-1725.672592
Sum of electronic and thermal Energies=	-1725.656266
Sum of electronic and thermal Enthalpies=	-1725.655322
Sum of electronic and thermal Free Energies=	-1725.717267

## 42

74	-0.000007000	-0.000054000	0.259188000
15	-1.858561000	1.551254000	-0.092340000
15	-1.780609000	-1.594096000	-0.238789000
15	1.858721000	-1.551176000	-0.092474000
15	1.780699000	1.594194000	-0.237990000
6	-3.500519000	0.637226000	-0.304181000
1	-3.896426000	0.487104000	0.706716000
1	-4.220253000	1.249376000	-0.856257000
6	-3.273909000	-0.715857000	-0.989646000
1	-3.034835000	-0.570837000	-2.048800000
1	-4.164788000	-1.348548000	-0.928510000
6	3.500595000	-0.637061000	-0.304767000
1	3.896980000	-0.487305000	0.705996000
1	4.220057000	-1.249042000	-0.857385000
6	3.273754000	0.716274000	-0.989660000
1	3.034336000	0.571653000	-2.048792000
1	4.164647000	1.348950000	-0.928579000
6	-0.000426000	-0.000482000	2.083772000
1	0.000056000	0.000068000	-1.637706000
1	1.654387000	2.654513000	-1.172826000
1	-2.406114000	-2.346079000	0.787378000
1	-2.250312000	2.525537000	0.857842000
1	1.894798000	-2.400290000	-1.229931000
1	2.250727000	-2.525195000	0.857872000
1	2.406394000	2.345383000	0.788638000
1	-1.894692000	2.400091000	-1.229999000



1	-1.654312000	-2.653752000	-1.174377000
1	-0.000836000	-0.000875000	3.179594000
E(RB+HF-LYP) = -1634.56270			
Zero-point correction=			0.211206
Thermal correction to Energy=			0.227028
Thermal correction to Enthalpy=			0.227972
Thermal correction to Gibbs Free Energy=			0.167632
Sum of electronic and zero-point Energies=			-1634.351497
Sum of electronic and thermal Energies=			-1634.335676
Sum of electronic and thermal Enthalpies=			-1634.334731
Sum of electronic and thermal Free Energies=			-1634.395071

**1<sup>+</sup>**

25	-0.000066000	0.000071000	-0.316085000
6	0.000191000	-0.000154000	1.526511000
8	0.000615000	-0.000541000	2.665269000
6	1.375243000	1.335891000	-0.381619000
8	2.189670000	2.125931000	-0.418082000
6	-1.375384000	-1.335743000	-0.381581000
8	-2.189782000	-2.125815000	-0.418022000
6	-1.336460000	1.374797000	-0.382105000
8	-2.127875000	2.187830000	-0.419835000
6	1.336296000	-1.374659000	-0.382560000
8	2.127665000	-2.187725000	-0.420548000

E(RB3LYP) = -670.346342423

Zero-point correction=			0.042168
Thermal correction to Energy=			0.054342
Thermal correction to Enthalpy=			0.055286
Thermal correction to Gibbs Free Energy=			0.002813
Sum of electronic and zero-point Energies=			-670.304174
Sum of electronic and thermal Energies=			-670.292001
Sum of electronic and thermal Enthalpies=			-670.291057
Sum of electronic and thermal Free Energies=			-670.343529

**2a<sup>+</sup>**

25	0.091771000	0.000137000	-0.285371000
15	-2.310976000	-0.002738000	-0.315505000
8	3.080922000	0.003601000	-0.620832000
8	0.040914000	-3.031370000	-0.360364000
8	0.286088000	0.000188000	2.678274000
6	1.948934000	0.002332000	-0.491175000
6	0.059910000	-1.892929000	-0.336507000
6	0.222197000	0.000291000	1.537762000
1	-2.993749000	-1.087289000	0.267453000
1	-2.886601000	-0.003593000	-1.604079000
1	-2.995928000	1.080651000	0.267062000
6	0.055206000	1.893093000	-0.336409000
8	0.033219000	3.031477000	-0.360280000

E(RB3LYP) = -900.185161578

Zero-point correction=			0.062003
------------------------	--	--	----------

Thermal correction to Energy=	0.074873
Thermal correction to Enthalpy=	0.075817
Thermal correction to Gibbs Free Energy=	0.021687
Sum of electronic and zero-point Energies=	-900.123158
Sum of electronic and thermal Energies=	-900.110289
Sum of electronic and thermal Enthalpies=	-900.109345
Sum of electronic and thermal Free Energies=	-900.163475

**2b<sup>+</sup>**

25	0.001090000	0.006267000	-0.413676000
15	-0.004853000	-0.030875000	1.934132000
1	1.063206000	0.595283000	2.606305000
1	-1.099871000	0.557860000	2.596789000
1	0.013981000	-1.294836000	2.556213000
6	1.388719000	1.305737000	-0.447496000
8	2.219982000	2.083855000	-0.463103000
6	-1.387015000	-1.290335000	-0.467693000
8	-2.219328000	-2.067119000	-0.502295000
6	1.299843000	-1.380082000	-0.465521000
8	2.078117000	-2.211034000	-0.498017000
6	-1.296701000	1.395252000	-0.449615000
8	-2.073879000	2.227387000	-0.467513000

E(RB3LYP) = -900.177024880

Zero-point correction=	0.061644
Thermal correction to Energy=	0.074766
Thermal correction to Enthalpy=	0.075710
Thermal correction to Gibbs Free Energy=	0.020070
Sum of electronic and zero-point Energies=	-900.115381
Sum of electronic and thermal Energies=	-900.102259
Sum of electronic and thermal Enthalpies=	-900.101315
Sum of electronic and thermal Free Energies=	-900.156955

**3a<sup>+</sup>**

25	0.000000000	0.000031000	-0.246784000
8	0.001320000	-0.000462000	2.713863000
8	-0.000921000	3.021947000	-0.274005000
6	0.000682000	-0.000170000	1.567408000
6	-0.000432000	1.879205000	-0.276103000
15	2.351643000	0.000342000	-0.463696000
1	2.832582000	0.000389000	-1.791725000
1	3.088772000	-1.080573000	0.058559000
1	3.088910000	1.081051000	0.058764000
6	0.000036000	-1.879114000	-0.276345000
8	-0.000198000	-3.021859000	-0.274447000
15	-2.351828000	-0.000168000	-0.462804000
1	-3.089042000	1.080728000	0.059327000
1	-3.088836000	-1.080935000	0.059907000
1	-2.832932000	-0.000577000	-1.790769000

E(RB3LYP) = -1130.01504362

Zero-point correction=	0.081286
Thermal correction to Energy=	0.095070
Thermal correction to Enthalpy=	0.096014

Thermal correction to Gibbs Free Energy=	0.039866
Sum of electronic and zero-point Energies=	-1129.933758
Sum of electronic and thermal Energies=	-1129.919974
Sum of electronic and thermal Enthalpies=	-1129.919029
Sum of electronic and thermal Free Energies=	-1129.975177

**3b<sup>+</sup>**

25	0.048303000	0.000743000	-0.363778000
15	-2.357972000	-0.001630000	-0.323216000
1	-2.956324000	-0.004259000	-1.602283000
1	-3.051370000	-1.080440000	0.261415000
1	-3.053271000	1.077892000	0.257824000
15	0.414270000	-0.003134000	1.939094000
1	1.095137000	1.093952000	2.504540000
1	-0.704184000	-0.050812000	2.798340000
1	1.171575000	-1.058874000	2.485713000
6	0.017366000	1.879416000	-0.371667000
8	0.003223000	3.022096000	-0.362962000
6	0.021334000	-1.877910000	-0.374738000
8	0.009400000	-3.020672000	-0.368810000
6	1.867333000	0.003164000	-0.693271000
8	2.988650000	0.004504000	-0.919630000

E(RB3LYP) = -1130.00983427

Zero-point correction=	0.081271
Thermal correction to Energy=	0.095172
Thermal correction to Enthalpy=	0.096116
Thermal correction to Gibbs Free Energy=	0.038916
Sum of electronic and zero-point Energies=	-1129.928564
Sum of electronic and thermal Energies=	-1129.914662
Sum of electronic and thermal Enthalpies=	-1129.913718
Sum of electronic and thermal Free Energies=	-1129.970918

**3c<sup>+</sup>**

25	-0.000096000	0.108309000	-0.254646000
8	0.000184000	0.299354000	2.702237000
8	-2.129470000	2.202360000	-0.530619000
6	0.000051000	0.244025000	1.557621000
6	-1.320780000	1.401284000	-0.425618000
15	-1.709870000	-1.553902000	-0.297929000
1	-2.159089000	-1.928841000	-1.583636000
1	-2.947481000	-1.249880000	0.302302000
1	-1.484362000	-2.832712000	0.251821000
6	1.320204000	1.401635000	-0.425896000
8	2.128648000	2.202926000	-0.531148000
15	1.710404000	-1.553218000	-0.297820000
1	1.485889000	-2.831916000	0.252589000
1	2.947788000	-1.247938000	0.302244000
1	2.159918000	-1.928422000	-1.583342000

E(RB3LYP) = -1130.01548731

Zero-point correction=	0.081258
Thermal correction to Energy=	0.095042

Thermal correction to Enthalpy=	0.095986
Thermal correction to Gibbs Free Energy=	0.039854
Sum of electronic and zero-point Energies=	-1129.934230
Sum of electronic and thermal Energies=	-1129.920446
Sum of electronic and thermal Enthalpies=	-1129.919501
Sum of electronic and thermal Free Energies=	-1129.975634

**4a<sup>+</sup>**

25	-0.000074000	0.007985000	-0.314396000
15	-2.339623000	0.005699000	-0.610100000
1	-2.751555000	-0.039298000	-1.961603000
1	-3.122514000	-1.054195000	-0.106180000
1	-3.122652000	1.096511000	-0.177872000
15	2.339458000	0.009278000	-0.610441000
1	3.120096000	1.104596000	-0.185354000
1	3.124503000	-1.045555000	-0.099265000
1	2.751760000	-0.043954000	-1.961525000
15	0.000315000	-0.032864000	2.009504000
1	-1.067824000	-0.675349000	2.674018000
1	1.069674000	-0.673679000	2.673669000
1	-0.000536000	1.182586000	2.726712000
6	0.001695000	-1.857080000	-0.308578000
8	0.002463000	-3.004261000	-0.279206000
6	-0.001829000	1.873479000	-0.280406000
8	-0.002533000	3.019089000	-0.223702000

E(RB3LYP) = -1359.8332224

Zero-point correction=	0.100485
Thermal correction to Energy=	0.115299
Thermal correction to Enthalpy=	0.116243
Thermal correction to Gibbs Free Energy=	0.057261
Sum of electronic and zero-point Energies=	-1359.732738
Sum of electronic and thermal Energies=	-1359.717924
Sum of electronic and thermal Enthalpies=	-1359.716980
Sum of electronic and thermal Free Energies=	-1359.775961

**4b<sup>+</sup>**

25	-0.000082000	0.067852000	-0.224622000
8	0.000008000	0.159880000	2.730494000
8	-0.000508000	3.049297000	-0.415693000
6	-0.000007000	0.136671000	1.580264000
6	-0.000337000	1.903277000	-0.349716000
15	2.343623000	0.107580000	-0.417724000
1	3.133256000	-0.957147000	0.067923000
1	3.041232000	1.188976000	0.157569000
1	2.860723000	0.182649000	-1.731400000
15	-2.343648000	0.106775000	-0.417656000
1	-3.041977000	1.187726000	0.157603000
1	-3.133174000	-0.958391000	0.067204000
1	-2.860107000	0.182096000	-1.731585000
15	0.000426000	-2.311704000	-0.258037000
1	-1.071364000	-3.019251000	0.327054000

1	1.072815000	-3.018344000	0.327067000
1	0.000718000	-2.937482000	-1.526305000
E(RB3LYP) = -1359.83925969			
Zero-point correction=		0.100451	
Thermal correction to Energy=		0.115144	
Thermal correction to Enthalpy=		0.116089	
Thermal correction to Gibbs Free Energy=		0.058075	
Sum of electronic and zero-point Energies=		-1359.738809	
Sum of electronic and thermal Energies=		-1359.724115	
Sum of electronic and thermal Enthalpies=		-1359.723171	
Sum of electronic and thermal Free Energies=		-1359.781185	

**4c<sup>+</sup>**

25	-0.000018000	-0.059373000	-0.320475000
15	-1.714143000	1.604934000	-0.271956000
1	-2.177548000	2.031724000	-1.537162000
1	-2.956331000	1.285790000	0.314984000
1	-1.509223000	2.871746000	0.317604000
15	1.713866000	1.605208000	-0.272150000
1	1.508804000	2.872047000	0.317306000
1	2.956123000	1.286293000	0.314765000
1	2.177150000	2.031942000	-1.537417000
15	0.000173000	-0.491696000	1.955629000
1	0.000316000	-1.838457000	2.375667000
1	1.070999000	-0.020042000	2.747149000
1	-1.070605000	-0.020225000	2.747326000
6	1.307002000	-1.324433000	-0.586077000
8	2.117280000	-2.118552000	-0.761815000
6	-1.306893000	-1.324657000	-0.585761000
8	-2.117069000	-2.118778000	-0.761956000

E(RB3LYP) = -1359.83439477

Zero-point correction=		0.100414
Thermal correction to Energy=		0.115230
Thermal correction to Enthalpy=		0.116174
Thermal correction to Gibbs Free Energy=		0.057415
Sum of electronic and zero-point Energies=		-1359.733981
Sum of electronic and thermal Energies=		-1359.719165
Sum of electronic and thermal Enthalpies=		-1359.718220
Sum of electronic and thermal Free Energies=		-1359.776980

**5a<sup>+</sup>**

25	0.000070000	0.000097000	-0.204556000
6	0.000071000	-0.000458000	1.592826000
8	0.000178000	-0.000898000	2.748385000
15	-1.586744000	-1.715634000	-0.356834000
1	-1.979120000	-2.141070000	-1.649151000
1	-1.307175000	-2.986533000	0.193902000
1	-2.876235000	-1.535746000	0.192456000
15	-1.715864000	1.586770000	-0.355915000
1	-2.986396000	1.306691000	0.195444000
1	-1.536362000	2.876481000	0.192971000
1	-2.142280000	1.978565000	-1.648099000

15	1.586717000	1.715908000	-0.356411000
15	1.715724000	-1.586645000	-0.356409000
1	1.977179000	2.142434000	-1.648969000
1	1.307782000	2.986382000	0.195666000
1	2.877089000	1.535773000	0.190728000
1	2.986255000	-1.306982000	0.195164000
1	1.535940000	-2.876523000	0.191981000
1	2.142216000	-1.977967000	-1.648709000

E(RB3LYP) = -1589.66

Zero-point correction=	0.119549
Thermal correction to Energy=	0.135132
Thermal correction to Enthalpy=	0.136076
Thermal correction to Gibbs Free Energy=	0.076341
Sum of electronic and zero-point Energies=	-1589.536527
Sum of electronic and thermal Energies=	-1589.520943
Sum of electronic and thermal Enthalpies=	-1589.519999
Sum of electronic and thermal Free Energies=	-1589.579734

### 5b<sup>+</sup>

25	-0.001200000	-0.037481000	-0.280777000
15	-2.336153000	-0.045660000	-0.510769000
1	-2.821506000	-0.117195000	-1.837931000
1	-3.074717000	-1.119135000	0.032937000
1	-3.151421000	1.018153000	-0.058663000
15	0.021475000	2.346237000	-0.225756000
15	2.331658000	-0.087867000	-0.516965000
1	-1.045743000	3.064953000	0.359614000
1	1.090116000	3.041052000	0.385347000
1	0.043670000	3.017486000	-1.471557000
1	3.168874000	0.955814000	-0.058213000
1	3.052902000	-1.180465000	0.011661000
1	2.809213000	-0.154558000	-1.847281000
15	0.003028000	-0.303044000	2.012105000
1	-1.097531000	-0.932820000	2.638476000
1	1.025464000	-1.073960000	2.612039000
1	0.088007000	0.821661000	2.866627000
6	-0.019026000	-1.848817000	-0.493872000
8	-0.030410000	-2.994506000	-0.628702000

E(RB3LYP) = -1589.65173062

Zero-point correction=	0.119507
Thermal correction to Energy=	0.135199
Thermal correction to Enthalpy=	0.136143
Thermal correction to Gibbs Free Energy=	0.075803
Sum of electronic and zero-point Energies=	-1589.532224
Sum of electronic and thermal Energies=	-1589.516532
Sum of electronic and thermal Enthalpies=	-1589.515587
Sum of electronic and thermal Free Energies=	-1589.575927

### 6<sup>+</sup>

25	-0.001534000	0.006834000	-0.254656000
15	1.620266000	1.675135000	-0.429886000

1	1.377454000	2.992276000	0.030734000
1	2.897374000	1.506638000	0.158623000
1	2.066938000	2.022125000	-1.729876000
15	1.666335000	-1.611310000	-0.451713000
1	2.023620000	-2.010995000	-1.764365000
1	2.980179000	-1.384668000	0.026423000
1	1.496796000	-2.909516000	0.088615000
15	-1.617781000	-1.663864000	-0.446365000
15	-1.674823000	1.624544000	-0.425619000
1	-1.953524000	-2.091742000	-1.755766000
1	-1.409439000	-2.948630000	0.112199000
1	-2.941280000	-1.473525000	0.020824000
1	-2.952067000	1.408162000	0.146623000
1	-1.476304000	2.940706000	0.058287000
1	-2.118628000	1.978358000	-1.724689000
15	0.006886000	-0.028397000	2.047010000
1	1.100145000	0.506869000	2.773522000
1	-1.012596000	0.618487000	2.789740000
1	-0.053559000	-1.267004000	2.734103000

E(RB3LYP) = -1819.46180266

Zero-point correction=	0.138415
Thermal correction to Energy=	0.154943
Thermal correction to Enthalpy=	0.155888
Thermal correction to Gibbs Free Energy=	0.092918
Sum of electronic and zero-point Energies=	-1819.323387
Sum of electronic and thermal Energies=	-1819.306859
Sum of electronic and thermal Enthalpies=	-1819.305915
Sum of electronic and thermal Free Energies=	-1819.368885

7<sup>+</sup>

E(RB3LYP) = -1246.78222758

25	-0.778024000	-0.000021000	-0.274841000
15	0.912024000	1.638071000	-0.446315000
15	0.912056000	-1.638032000	-0.446562000
8	-2.858918000	2.152829000	-0.393953000
8	-0.742127000	-0.000322000	2.680117000
8	-2.859280000	-2.152502000	-0.393957000
6	-2.064719000	1.330140000	-0.349276000
6	-0.778799000	-0.000157000	1.532111000
6	-2.064887000	-1.330002000	-0.349228000
6	2.590115000	1.303698000	0.274448000
1	3.229482000	2.157761000	0.033681000
1	2.471143000	1.288891000	1.363938000
6	3.246694000	0.000023000	-0.216097000
1	3.322743000	0.000115000	-1.310751000
1	4.279186000	0.000005000	0.149363000
6	2.590157000	-1.303758000	0.274224000
1	2.471218000	-1.289160000	1.363720000
1	3.229538000	-2.157759000	0.033274000
1	1.212383000	-1.965927000	-1.789659000
1	0.616356000	-2.929007000	0.037234000
1	0.616209000	2.928858000	0.037912000

1 1.212384000 1.966457000 -1.789282000

Zero-point correction=	0.151029
Thermal correction to Energy=	0.166208
Thermal correction to Enthalpy=	0.167152
Thermal correction to Gibbs Free Energy=	0.108107
Sum of electronic and zero-point Energies=	-1246.631198
Sum of electronic and thermal Energies=	-1246.616020
Sum of electronic and thermal Enthalpies=	-1246.615076
Sum of electronic and thermal Free Energies=	-1246.674120

**8<sup>+</sup>**

25	-0.000014000	-0.000020000	-0.188687000
15	-1.736835000	1.546678000	-0.277913000
15	-1.717094000	-1.541009000	-0.327247000
15	1.717056000	1.540987000	-0.327256000
15	1.736866000	-1.546663000	-0.277945000
6	0.000009000	-0.000009000	1.593959000
8	0.000055000	-0.000023000	2.753346000
1	-1.941390000	2.335176000	0.876305000
1	-1.823409000	2.580594000	-1.239774000
6	-3.385522000	0.678713000	-0.499499000
6	-3.332297000	-0.719824000	0.134171000
1	-2.013760000	-2.078914000	-1.605180000
1	-1.751206000	-2.746192000	0.408248000
1	1.751116000	2.746217000	0.408166000
1	2.013713000	2.078831000	-1.605216000
6	3.332280000	0.719869000	0.134185000
6	3.385539000	-0.678660000	-0.499512000
1	1.823483000	-2.580593000	-1.239788000
1	1.941441000	-2.335127000	0.876296000
1	-3.557653000	0.602940000	-1.578897000
1	-4.198612000	1.277528000	-0.081592000
1	-3.349013000	-0.652545000	1.227345000
1	-4.185701000	-1.329659000	-0.173392000
1	3.349000000	0.652582000	1.227358000
1	4.185656000	1.329748000	-0.173371000
1	3.557683000	-0.602855000	-1.578906000
1	4.198628000	-1.277480000	-0.081613000

E(RB3LYP) = -1744.53991365

Zero-point correction=	0.20079
Thermal correction to Energy=	0.21696
Thermal correction to Enthalpy=	0.21790
Thermal correction to Gibbs Free Energy=	0.15735
Sum of electronic and zero-point Energies=	-1744.33913
Sum of electronic and thermal Energies=	-1744.32296
Sum of electronic and thermal Enthalpies=	-1744.32201
Sum of electronic and thermal Free Energies=	-1744.38256

**9<sup>+</sup>**

25	-0.000001000	0.000004000	-0.166871000
----	--------------	-------------	--------------



15	-1.750624000	1.549220000	-0.235459000
15	-1.732217000	-1.545001000	-0.330481000
15	1.732208000	1.545017000	-0.330435000
15	1.750630000	-1.549203000	-0.235511000
7	0.000001000	-0.000051000	1.695357000
7	0.000014000	-0.000102000	2.816646000
1	-1.997046000	2.241570000	0.973210000
1	-1.827904000	2.653671000	-1.115303000
6	-3.385376000	0.686489000	-0.555968000
6	-3.363010000	-0.717135000	0.067923000
1	-1.985382000	-2.086214000	-1.615606000
1	-1.806681000	-2.749046000	0.406175000
1	1.806679000	2.749075000	0.406198000
1	1.985364000	2.086207000	-1.615572000
6	3.363004000	0.717149000	0.067948000
6	3.385376000	-0.686452000	-0.555996000
1	1.827929000	-2.653654000	-1.115353000
1	1.997053000	-2.241546000	0.973162000
1	-3.499640000	0.620644000	-1.643822000
1	-4.220432000	1.280375000	-0.175934000
1	-3.425524000	-0.656289000	1.160050000
1	-4.206056000	-1.321045000	-0.277446000
1	3.425517000	0.656262000	1.160073000
1	4.206048000	1.321075000	-0.277398000
1	3.499637000	-0.620565000	-1.643848000
1	4.220436000	-1.280348000	-0.175985000

E(RB3LYP) = -1740.71676597

Zero-point correction=	0.200297
Thermal correction to Energy=	0.216799
Thermal correction to Enthalpy=	0.217743
Thermal correction to Gibbs Free Energy=	0.156573
Sum of electronic and zero-point Energies=	-1740.516469
Sum of electronic and thermal Energies=	-1740.499967
Sum of electronic and thermal Enthalpies=	-1740.499023
Sum of electronic and thermal Free Energies=	-1740.560193

**10<sup>+</sup>**

25	-0.000001000	0.000004000	-0.166871000
15	-1.750624000	1.549220000	-0.235459000
15	-1.732217000	-1.545001000	-0.330481000
15	1.732208000	1.545017000	-0.330435000
15	1.750630000	-1.549203000	-0.235511000
7	0.000001000	-0.000051000	1.695357000
7	0.000014000	-0.000102000	2.816646000
1	-1.997046000	2.241570000	0.973210000
1	-1.827904000	2.653671000	-1.115303000
6	-3.385376000	0.686489000	-0.555968000
6	-3.363010000	-0.717135000	0.067923000
1	-1.985382000	-2.086214000	-1.615606000
1	-1.806681000	-2.749046000	0.406175000
1	1.806679000	2.749075000	0.406198000

1	1.985364000	2.086207000	-1.615572000
6	3.363004000	0.717149000	0.067948000
6	3.385376000	-0.686452000	-0.555996000
1	1.827929000	-2.653654000	-1.115353000
1	1.997053000	-2.241546000	0.973162000
1	-3.499640000	0.620644000	-1.643822000
1	-4.220432000	1.280375000	-0.175934000
1	-3.425524000	-0.656289000	1.160050000
1	-4.206056000	-1.321045000	-0.277446000
1	3.425517000	0.656262000	1.160073000
1	4.206048000	1.321075000	-0.277398000
1	3.499637000	-0.620565000	-1.643848000
1	4.220436000	-1.280348000	-0.175985000

E(RB3LYP) = -1740.71676597

Zero-point correction=	0.118742
Thermal correction to Energy=	0.134936
Thermal correction to Enthalpy=	0.135880
Thermal correction to Gibbs Free Energy=	0.073668
Sum of electronic and zero-point Energies=	-1585.714987
Sum of electronic and thermal Energies=	-1585.698793
Sum of electronic and thermal Enthalpies=	-1585.697849
Sum of electronic and thermal Free Energies=	-1585.760061

**11<sup>+</sup>**

75	-0.000590000	0.000111000	-0.227015000
6	-0.001019000	0.000094000	1.683224000
8	-0.001283000	0.000014000	2.829339000
6	-1.669175000	-1.166017000	-0.270013000
8	-2.600939000	-1.819207000	-0.289075000
6	-1.164961000	1.669927000	-0.269956000
8	-1.814350000	2.604340000	-0.289150000
6	1.165551000	-1.668435000	-0.269426000
8	1.818809000	-2.600160000	-0.288288000
6	1.669199000	1.164491000	-0.269305000
8	2.603597000	1.813924000	-0.287952000

E(RB3LYP) = -645.595884511

Zero-point correction=	0.042442
Thermal correction to Energy=	0.054401
Thermal correction to Enthalpy=	0.055345
Thermal correction to Gibbs Free Energy=	0.002306
Sum of electronic and zero-point Energies=	-645.553442
Sum of electronic and thermal Energies=	-645.541484
Sum of electronic and thermal Enthalpies=	-645.540540
Sum of electronic and thermal Free Energies=	-645.593579

**12<sup>+</sup>**

75	0.000011000	0.000018000	-0.195672000
----	-------------	-------------	--------------

15	2.449720000	-0.001781000	-0.331014000
15	-2.449721000	0.001984000	-0.330933000
6	0.000070000	-0.000238000	1.688441000
8	0.000126000	-0.000589000	2.844188000
6	0.001670000	2.006807000	-0.215141000
8	0.002604000	3.152626000	-0.211458000
6	-0.001741000	-2.006740000	-0.215473000
8	-0.002832000	-3.152561000	-0.211993000
1	3.008586000	-0.001447000	-1.627915000
1	3.148412000	1.080739000	0.237403000
1	3.147033000	-1.085803000	0.236225000
1	-3.008660000	0.001348000	-1.627801000
1	-3.146841000	1.086259000	0.236059000
1	-3.148546000	-1.080283000	0.237799000

E(RB3LYP) = -1105.26347078

Zero-point correction=	0.082134
Thermal correction to Energy=	0.095591
Thermal correction to Enthalpy=	0.096535
Thermal correction to Gibbs Free Energy=	0.040104
Sum of electronic and zero-point Energies=	-1105.181337
Sum of electronic and thermal Energies=	-1105.167880
Sum of electronic and thermal Enthalpies=	-1105.166935
Sum of electronic and thermal Free Energies=	-1105.223367

**13<sup>+</sup>**

75	-0.000006000	0.073028000	-0.196773000
15	-1.793003000	-1.679420000	-0.193285000
15	1.792960000	-1.679460000	-0.193341000
6	0.000016000	0.250240000	1.682219000
8	0.000075000	0.336161000	2.833567000
6	-1.396735000	1.450363000	-0.342394000
8	-2.209941000	2.255458000	-0.428244000
6	1.396761000	1.450326000	-0.342388000
8	2.209993000	2.255396000	-0.428241000
1	-2.294327000	-2.079131000	-1.451005000
1	-1.526279000	-2.944110000	0.369202000
1	-2.999951000	-1.364495000	0.459978000
1	2.294217000	-2.079163000	-1.451090000
1	1.526235000	-2.944151000	0.369143000
1	2.999943000	-1.364566000	0.459871000

E(RB3LYP) = -1105.26509911

Zero-point correction=	0.081934
Thermal correction to Energy=	0.095463
Thermal correction to Enthalpy=	0.096407
Thermal correction to Gibbs Free Energy=	0.039729
Sum of electronic and zero-point Energies=	-1105.183165
Sum of electronic and thermal Energies=	-1105.169636
Sum of electronic and thermal Enthalpies=	-1105.168692
Sum of electronic and thermal Free Energies=	-1105.225370

**14<sup>+</sup>**

75	-0.00002000	0.000045000	-0.178781000
6	0.000085000	0.000063000	1.683036000
8	0.000059000	-0.000065000	2.849053000
15	1.710568000	-1.703737000	-0.264708000
1	2.153716000	-2.144467000	-1.535085000
1	2.972586000	-1.448307000	0.317952000
1	1.460051000	-2.967054000	0.317261000
15	-1.703746000	-1.710471000	-0.264696000
1	-1.448869000	-2.972234000	0.318752000
1	-2.967484000	-1.459598000	0.316228000
1	-2.143583000	-2.154183000	-1.535192000
15	-1.710593000	1.703557000	-0.264638000
15	1.703746000	1.710491000	-0.264725000
1	-2.154390000	2.143163000	-1.535190000
1	-2.972297000	1.448324000	0.318796000
1	-1.460171000	2.967430000	0.316180000
1	1.448865000	2.972241000	0.318747000
1	2.967476000	1.459588000	0.316204000
1	2.143613000	2.154225000	-1.535204000

E(RB3LYP) = -1564.90258269

Zero-point correction=	0.121280
Thermal correction to Energy=	0.136186
Thermal correction to Enthalpy=	0.137131
Thermal correction to Gibbs Free Energy=	0.078173
Sum of electronic and zero-point Energies=	-1564.781303
Sum of electronic and thermal Energies=	-1564.766396
Sum of electronic and thermal Enthalpies=	-1564.765452
Sum of electronic and thermal Free Energies=	-1564.824409

**15<sup>+</sup>**

75	-0.000198000	-0.000419000	-0.200338000
7	-0.001251000	-0.000489000	1.707978000
7	-0.002099000	-0.000448000	2.836398000
15	1.730551000	-1.689960000	-0.232279000
1	2.849975000	-1.545828000	-1.085151000
1	2.418885000	-1.919648000	0.981840000
1	1.412643000	-3.031784000	-0.551119000
15	-1.700736000	-1.719848000	-0.238389000
1	-1.357216000	-3.058883000	-0.541683000
1	-2.403271000	-1.950962000	0.967281000
1	-2.809708000	-1.599766000	-1.108574000
15	-1.728077000	1.692104000	-0.233049000
15	1.700145000	1.719523000	-0.237142000
1	-2.853192000	1.546762000	-1.078179000
1	-2.408207000	1.930462000	0.984046000
1	-1.408055000	3.031173000	-0.561179000
1	1.355699000	3.059007000	-0.537402000
1	2.405091000	1.948812000	0.967468000
1	2.807432000	1.601372000	-1.109760000

E(RB3LYP) = -1561.05458428

Zero-point correction=	0.120996
Thermal correction to Energy=	0.136226

Thermal correction to Enthalpy=	0.137170
Thermal correction to Gibbs Free Energy=	0.076510
Sum of electronic and zero-point Energies=	-1560.933589
Sum of electronic and thermal Energies=	-1560.918358
Sum of electronic and thermal Enthalpies=	-1560.917414
Sum of electronic and thermal Free Energies=	-1560.978074

**16<sup>+</sup>**

75	-0.000009000	-0.046380000	-0.184610000
15	-2.434409000	-0.076036000	-0.292160000
15	2.434433000	-0.077839000	-0.292061000
15	0.000922000	2.447501000	-0.182480000
8	-0.001249000	-3.141817000	-0.382683000
8	-0.000230000	-0.208832000	2.844801000
6	-0.000768000	-1.991196000	-0.310642000
6	-0.000142000	-0.155994000	1.685742000
1	-3.024608000	-0.168611000	-1.573236000
1	-3.176790000	1.010858000	0.218220000
1	-3.101144000	-1.139810000	0.347645000
1	3.177625000	1.008667000	0.217982000
1	3.024538000	-0.171253000	-1.573119000
1	3.100378000	-1.141902000	0.348080000
1	-1.074534000	3.131142000	0.423332000
1	0.001833000	3.103257000	-1.434524000
1	1.076478000	3.130065000	0.424373000

E(RB3LYP) = -1335.08780829

Zero-point correction=	0.101755
Thermal correction to Energy=	0.115969
Thermal correction to Enthalpy=	0.116913
Thermal correction to Gibbs Free Energy=	0.059070
Sum of electronic and zero-point Energies=	-1334.986053
Sum of electronic and thermal Energies=	-1334.971840
Sum of electronic and thermal Enthalpies=	-1334.970895
Sum of electronic and thermal Free Energies=	-1335.028739

**17<sup>+</sup>**

75	0.000039000	-0.035754000	-0.219946000
15	-0.000417000	2.374695000	-0.224600000
15	-2.407799000	-0.068181000	-0.341405000
15	2.407876000	-0.067685000	-0.341533000
15	0.000139000	-0.184434000	2.073671000
7	0.000102000	-2.022334000	-0.387603000
7	0.000062000	-3.140060000	-0.492580000
1	-0.000812000	3.016649000	-1.487371000
1	-1.067961000	3.097046000	0.359342000
1	1.066961000	3.097600000	0.358956000
1	-3.082055000	-1.292346000	-0.128340000
1	-3.171713000	0.752154000	0.521965000
1	-3.026564000	0.296809000	-1.561567000
1	3.082386000	-1.291689000	-0.128345000
1	3.171617000	0.752899000	0.521756000
1	3.026557000	0.297302000	-1.561736000

1	-1.070113000	0.378108000	2.812463000
1	-0.000249000	-1.479586000	2.645797000
1	1.070854000	0.377414000	2.812325000
E(RB3LYP) = -1561.06121176			
Zero-point correction=			0.121662
Thermal correction to Energy=			0.136466
Thermal correction to Enthalpy=			0.137410
Thermal correction to Gibbs Free Energy=			0.079010
Sum of electronic and zero-point Energies=			-1560.939550
Sum of electronic and thermal Energies=			-1560.924746
Sum of electronic and thermal Enthalpies=			-1560.923802
Sum of electronic and thermal Free Energies=			-1560.982202

**18<sup>+</sup>**

26	-0.000055000	0.000014000	-0.431906000
15	2.350070000	-0.001373000	-0.350290000
1	3.097727000	-0.003008000	-1.547139000
1	2.914107000	1.087677000	0.336003000
1	2.912575000	-1.089865000	0.338127000
6	0.001227000	1.876462000	-0.352559000
8	0.002271000	3.007204000	-0.246136000
15	-2.350169000	0.001420000	-0.350283000
6	-0.001151000	-1.876440000	-0.352644000
1	-3.097707000	0.003616000	-1.547206000
1	-2.914352000	-1.087897000	0.335468000
1	-2.912663000	1.089659000	0.338540000
8	-0.001895000	-3.007184000	-0.246238000
17	-0.000013000	-0.000091000	1.862033000

E(RB3LYP) = -1496.39487650

Zero-point correction=	0.074353
Thermal correction to Energy=	0.087590
Thermal correction to Enthalpy=	0.088534
Thermal correction to Gibbs Free Energy=	0.034034
Sum of electronic and zero-point Energies=	-1496.320523
Sum of electronic and thermal Energies=	-1496.307287
Sum of electronic and thermal Enthalpies=	-1496.306343
Sum of electronic and thermal Free Energies=	-1496.360843

**19<sup>+</sup>**

26	-0.000055000	0.000014000	-0.431906000
15	2.350070000	-0.001373000	-0.350290000
1	3.097727000	-0.003008000	-1.547139000
1	2.914107000	1.087677000	0.336003000
1	2.912575000	-1.089865000	0.338127000
6	0.001227000	1.876462000	-0.352559000
8	0.002271000	3.007204000	-0.246136000
15	-2.350169000	0.001420000	-0.350283000
6	-0.001151000	-1.876440000	-0.352644000
1	-3.097707000	0.003616000	-1.547206000

1	-2.914352000	-1.087897000	0.335468000
1	-2.912663000	1.089659000	0.338540000
8	-0.001895000	-3.007184000	-0.246238000
17	-0.000013000	-0.000091000	1.862033000

E(RB3LYP) = -1136.02039997

Zero-point correction=	0.075000
Thermal correction to Energy=	0.088046
Thermal correction to Enthalpy=	0.088990
Thermal correction to Gibbs Free Energy=	0.034954
Sum of electronic and zero-point Energies=	-1135.945400
Sum of electronic and thermal Energies=	-1135.932354
Sum of electronic and thermal Enthalpies=	-1135.931410
Sum of electronic and thermal Free Energies=	-1135.985446

**20+**

26	0.000028000	0.754579000	0.000014000
15	-1.703704000	0.686348000	1.585162000
15	-1.773679000	0.864117000	-1.491619000
15	1.703750000	0.686298000	-1.585148000
15	1.773739000	0.863964000	1.491650000
7	-0.000026000	-1.200777000	-0.000015000
1	-1.680730000	-0.495343000	2.349611000
1	-1.888864000	1.641886000	2.610635000
1	-2.231778000	2.166835000	-1.806926000
1	-1.765776000	0.319000000	-2.791558000
6	-3.255235000	0.095746000	-0.671129000
6	-3.379447000	0.665520000	0.750894000
1	1.888921000	1.641801000	-2.610652000
1	1.680748000	-0.495417000	-2.349561000
1	2.231869000	2.166644000	1.807069000
1	1.765817000	0.318735000	2.791542000
6	3.379494000	0.665452000	-0.750888000
6	3.255282000	0.095618000	0.671111000
6	0.271862000	-2.026964000	1.071322000
6	0.175853000	-3.356540000	0.684778000
6	-0.176155000	-3.356503000	-0.684860000
6	-0.271998000	-2.026906000	-1.071375000
1	-4.164674000	0.272842000	-1.251213000
1	-3.060938000	-0.981239000	-0.650131000
1	-4.095028000	0.094236000	1.347488000
1	-3.733039000	1.701778000	0.720410000
1	4.095081000	0.094199000	-1.347503000
1	3.733076000	1.701713000	-0.720360000
1	4.164725000	0.272675000	1.251198000
1	3.060975000	-0.981365000	0.650063000
1	0.466530000	-1.630582000	2.058661000
1	0.328759000	-4.217522000	1.321479000
1	-0.329156000	-4.217453000	-1.321582000
1	-0.466607000	-1.630476000	-2.058706000

E(RB3LYP) = -1860.28182380

Zero-point correction=	0.264425
------------------------	----------

Thermal correction to Energy=	0.283194
Thermal correction to Enthalpy=	0.284138
Thermal correction to Gibbs Free Energy=	0.217929
Sum of electronic and zero-point Energies=	-1860.017399
Sum of electronic and thermal Energies=	-1859.998630
Sum of electronic and thermal Enthalpies=	-1859.997686
Sum of electronic and thermal Free Energies=	-1860.063895

## 21+

26	0.000067000	0.000063000	-0.418975000
15	1.684181000	-1.555010000	-0.306138000
15	1.717992000	1.538348000	-0.342225000
15	-1.684087000	1.555098000	-0.306195000
15	-1.717852000	-1.538249000	-0.343008000
6	3.146403000	-0.721187000	0.488497000
1	2.893406000	-0.618762000	1.548099000
1	4.043269000	-1.340901000	0.408195000
6	3.357766000	0.655329000	-0.161836000
1	3.771108000	0.548000000	-1.170575000
1	4.058583000	1.264376000	0.414653000
6	-3.146364000	0.721122000	0.488171000
1	-2.893454000	0.618535000	1.547774000
1	-4.043239000	1.340825000	0.407875000
6	-3.357647000	-0.655295000	-0.162401000
1	-3.771010000	-0.547812000	-1.171114000
1	-4.058429000	-1.264475000	0.413990000
7	-0.000746000	-0.000477000	2.643494000
6	-0.000279000	-0.000183000	1.472557000
1	-1.972821000	-2.473371000	-1.371418000
1	1.656946000	2.408452000	0.763313000
1	1.503157000	-2.730014000	0.449720000
1	-2.221087000	2.115394000	-1.489951000
1	-1.503177000	2.730013000	0.449830000
1	-1.656913000	-2.408923000	0.762082000
1	2.221297000	-2.115167000	-1.489907000
1	1.973056000	2.474008000	-1.370121000

E(RB3LYP) = -1743.56326028

Zero-point correction=	0.201375
Thermal correction to Energy=	0.217629
Thermal correction to Enthalpy=	0.218574
Thermal correction to Gibbs Free Energy=	0.158353
Sum of electronic and zero-point Energies=	-1743.361885
Sum of electronic and thermal Energies=	-1743.345631
Sum of electronic and thermal Enthalpies=	-1743.344687
Sum of electronic and thermal Free Energies=	-1743.404908

## 22+

E(RB3LYP) = -2110.94832864

26	0.000003000	0.000003000	-0.444852000
15	-1.730600000	1.546747000	-0.377452000



15	-1.699500000	-1.561801000	-0.334669000
15	1.730572000	-1.546726000	-0.377537000
15	1.699507000	1.561809000	-0.334719000
1	-1.674774000	2.406134000	0.735546000
1	-1.984810000	2.485866000	-1.402795000
1	-2.229882000	-2.133472000	-1.516316000
1	-1.523202000	-2.726942000	0.436322000
6	-3.170205000	-0.718416000	0.433944000
6	-3.369254000	0.657035000	-0.222279000
1	1.984801000	-2.485650000	-1.403056000
1	1.674717000	-2.406337000	0.735287000
1	2.229917000	2.133440000	-1.516372000
1	1.523210000	2.726975000	0.436235000
6	3.369236000	-0.657049000	-0.222194000
6	3.170172000	0.718426000	0.433973000
1	-4.067287000	-1.336086000	0.340146000
1	-2.932079000	-0.613063000	1.495961000
1	-4.083388000	1.264958000	0.338939000
1	-3.762660000	0.547399000	-1.238834000
1	4.083285000	-1.264985000	0.339119000
1	3.762761000	-0.547456000	-1.238706000
1	4.067268000	1.336080000	0.340195000
1	2.931992000	0.613112000	1.495981000
17	0.000040000	-0.000027000	1.883145000

E(RB3LYP) = -2110.94832864

Zero-point correction=	0.194292
Thermal correction to Energy=	0.209917
Thermal correction to Enthalpy=	0.210862
Thermal correction to Gibbs Free Energy=	0.152038
Sum of electronic and zero-point Energies=	-2110.754037
Sum of electronic and thermal Energies=	-2110.738411
Sum of electronic and thermal Enthalpies=	-2110.737467
Sum of electronic and thermal Free Energies=	-2110.796291

### 23<sup>+</sup>

44	0.241226000	-0.000022000	-0.144086000
15	0.000365000	2.416932000	-0.228725000
15	-0.001231000	-2.416719000	-0.228804000
8	-4.100993000	0.000482000	0.020995000
8	1.202894000	-0.000408000	2.706170000
8	3.150730000	-0.000903000	-1.152720000
7	-1.732255000	0.000878000	-0.310397000
6	-2.933561000	0.000616000	-0.124308000
6	0.882084000	-0.000308000	1.605596000
6	2.081069000	-0.000708000	-0.748193000
1	1.105796000	3.266876000	-0.034899000
1	-0.934226000	2.937336000	0.683119000
1	-0.505431000	2.879443000	-1.457461000
1	-0.508681000	-2.878756000	-1.457039000
1	1.103869000	-3.267392000	-0.036328000
1	-0.935097000	-2.936854000	0.683961000

E(RB3LYP) = -1174.78052340  
 Zero-point correction= 0.086444  
 Thermal correction to Energy= 0.101436  
 Thermal correction to Enthalpy= 0.102380  
 Thermal correction to Gibbs Free Energy= 0.041072  
 Sum of electronic and zero-point Energies= -1174.694079  
 Sum of electronic and thermal Energies= -1174.679088  
 Sum of electronic and thermal Enthalpies= -1174.678144  
 Sum of electronic and thermal Free Energies= -1174.739451

**24<sup>+</sup>**

44	0.051853000	0.000072000	-0.368656000
15	-2.411963000	-0.000300000	-0.242755000
14	0.312586000	0.001042000	2.066042000
8	0.016684000	3.121876000	-0.266453000
8	3.130484000	-0.001659000	-0.606336000
8	0.015760000	-3.121675000	-0.264958000
6	0.031765000	1.984283000	-0.315188000
6	1.993740000	-0.000798000	-0.512366000
6	0.031169000	-1.984113000	-0.314251000
1	-3.038018000	-1.083721000	0.400780000
1	-3.085428000	-0.001965000	-1.481736000
1	-3.038836000	1.084087000	0.398353000
1	1.043597000	-1.223128000	2.465503000
1	1.052546000	1.220402000	2.463682000
1	-1.055630000	0.006509000	2.643824000

E(RB3LYP) = -1068.17230358

Zero-point correction= 0.078718  
 Thermal correction to Energy= 0.092700  
 Thermal correction to Enthalpy= 0.093644  
 Thermal correction to Gibbs Free Energy= 0.036190  
 Sum of electronic and zero-point Energies= -1068.093585  
 Sum of electronic and thermal Energies= -1068.079604  
 Sum of electronic and thermal Enthalpies= -1068.078660  
 Sum of electronic and thermal Free Energies= -1068.136113

**25<sup>+</sup>**

44	-0.001139000	0.097585000	-0.244051000
15	-2.396868000	-0.117724000	-0.422318000
15	0.009328000	0.148263000	2.018100000
15	2.392711000	-0.130695000	-0.430880000
8	0.007819000	3.144767000	-0.520440000
17	-0.008313000	-2.293314000	-0.289173000
1	-2.785432000	-0.623999000	-1.677766000
1	-3.257513000	0.992383000	-0.302125000
1	-3.013138000	-1.041729000	0.441525000
1	-1.129314000	-0.383294000	2.652738000
1	1.037990000	-0.592735000	2.629041000
1	0.133536000	1.398340000	2.653423000

1	3.007395000	-1.069478000	0.417970000
1	3.261951000	0.971823000	-0.302915000
1	2.770889000	-0.624634000	-1.694458000
6	0.004163000	2.001683000	-0.412209000

E(RB3LYP) = -1696.74860040

Zero-point correction=	0.094710
Thermal correction to Energy=	0.108617
Thermal correction to Enthalpy=	0.109561
Thermal correction to Gibbs Free Energy=	0.051945
Sum of electronic and zero-point Energies=	-1696.653891
Sum of electronic and thermal Energies=	-1696.639984
Sum of electronic and thermal Enthalpies=	-1696.639040
Sum of electronic and thermal Free Energies=	-1696.696655

### 26<sup>+</sup>

44	0.000016000	-0.120469000	-0.210703000
15	-2.380979000	-0.456441000	-0.358938000
15	2.381126000	-0.455969000	-0.358894000
8	-0.000400000	2.825680000	-1.019839000
6	-0.000270000	1.731382000	-0.665983000
1	-3.332034000	0.580134000	-0.286078000
1	-2.913309000	-1.386904000	0.553214000
1	-2.728207000	-1.063459000	-1.581212000
1	2.728085000	-1.063540000	-1.580969000
1	3.332129000	0.580696000	-0.286731000
1	2.913744000	-1.385954000	0.553580000
15	-0.000101000	0.442608000	1.976472000
1	0.000057000	-0.690239000	2.815499000
1	1.085464000	1.182341000	2.485301000
1	-1.085914000	1.181971000	2.485314000
9	0.000382000	-2.064567000	-0.290218000

E(RB3LYP) = -1336.36713201

Zero-point correction=	0.095218
Thermal correction to Energy=	0.108869
Thermal correction to Enthalpy=	0.109813
Thermal correction to Gibbs Free Energy=	0.053306
Sum of electronic and zero-point Energies=	-1336.271914
Sum of electronic and thermal Energies=	-1336.258263
Sum of electronic and thermal Enthalpies=	-1336.257319
Sum of electronic and thermal Free Energies=	-1336.313826

### 27<sup>+</sup>

44	-0.077596000	-0.009701000	-0.211706000
15	-2.547281000	-0.211138000	-0.231212000
15	-0.133496000	2.362033000	-0.349881000
15	0.388723000	0.037211000	1.979328000
15	0.276901000	-2.352645000	-0.345026000
14	2.319688000	0.195001000	-0.620513000
1	-3.250112000	-0.056394000	-1.450189000
1	-3.315438000	0.693806000	0.537280000

1	-3.178133000	-1.403779000	0.192506000
1	0.253721000	2.888499000	-1.602130000
1	-1.331012000	3.092002000	-0.168725000
1	0.711327000	3.122949000	0.486177000
1	1.054280000	1.168114000	2.501998000
1	-0.692075000	-0.032484000	2.889969000
1	1.206595000	-0.980779000	2.517924000
1	1.247326000	-2.955902000	0.483000000
1	-0.777096000	-3.276195000	-0.155764000
1	0.739369000	-2.804946000	-1.600952000
1	3.181549000	-0.916652000	-0.123137000
1	2.968354000	1.466047000	-0.184777000
1	2.347208000	0.160638000	-2.119049000

E(RB3LYP) = -1757.63686158

Zero-point correction=	0.137253
Thermal correction to Energy=	0.153427
Thermal correction to Enthalpy=	0.154371
Thermal correction to Gibbs Free Energy=	0.092982
Sum of electronic and zero-point Energies=	-1757.499609
Sum of electronic and thermal Energies=	-1757.483434
Sum of electronic and thermal Enthalpies=	-1757.482490
Sum of electronic and thermal Free Energies=	-1757.543880

**28<sup>+</sup>**

44	0.000071000	0.000017000	-0.415070000
15	-1.786853000	1.573710000	-0.276456000
15	-1.772938000	-1.581709000	-0.280857000
15	1.786822000	-1.573590000	-0.276358000
15	1.772970000	1.581667000	-0.280645000
1	-1.785169000	2.352777000	0.897757000
1	-2.017018000	2.581972000	-1.239367000
1	-2.264472000	-2.181014000	-1.464907000
1	-1.647771000	-2.727967000	0.529441000
6	-3.267263000	-0.711473000	0.417871000
6	-3.426362000	0.671042000	-0.232546000
1	2.016642000	-2.581613000	-1.239606000
1	1.785233000	-2.353026000	0.897617000
1	2.264333000	2.181087000	-1.464707000
1	1.647873000	2.727846000	0.529780000
6	3.426447000	-0.671103000	-0.232457000
6	3.267463000	0.711469000	0.417856000
1	-4.165894000	-1.318663000	0.279173000
1	-3.083387000	-0.616451000	1.492459000
1	-4.174134000	1.270133000	0.293906000
1	-3.758551000	0.573765000	-1.272046000
1	4.174110000	-1.270277000	0.294048000
1	3.758682000	-0.573925000	-1.271951000
1	4.166019000	1.318708000	0.278863000
1	3.083876000	0.616620000	1.492508000
17	-0.000307000	-0.000089000	1.983560000

E(RB3LYP) = -2081.44555643  
 Zero-point correction= 0.194324  
 Thermal correction to Energy= 0.209916  
 Thermal correction to Enthalpy= 0.210860  
 Thermal correction to Gibbs Free Energy= 0.151546  
 Sum of electronic and zero-point Energies= -2081.251233  
 Sum of electronic and thermal Energies= -2081.235640  
 Sum of electronic and thermal Enthalpies= -2081.234696  
 Sum of electronic and thermal Free Energies= -2081.294010

**29<sup>+</sup>**

44	-0.141540000	0.018555000	-0.356092000
17	-0.098648000	-0.101910000	2.007891000
15	-1.770146000	-1.660265000	-0.374670000
15	-1.759608000	1.697942000	-0.210426000
7	1.541155000	-1.393120000	-0.347607000
1	1.342853000	-2.140133000	0.317774000
1	1.690656000	-1.843500000	-1.251468000
7	1.541895000	1.406769000	-0.183715000
1	1.473996000	2.285464000	-0.695915000
1	1.551152000	1.646857000	0.811228000
6	2.784960000	-0.681683000	0.080635000
1	3.682073000	-1.245176000	-0.194402000
1	2.748994000	-0.602472000	1.169910000
6	2.808287000	0.705430000	-0.543041000
1	3.687226000	1.262311000	-0.200744000
1	2.857853000	0.641375000	-1.635241000
1	-2.479543000	-1.966801000	-1.559575000
1	-2.854951000	-1.545050000	0.519386000
1	-1.349916000	-2.967104000	-0.036731000
1	-2.490643000	2.098019000	-1.353539000
1	-2.826178000	1.516924000	0.694509000
1	-1.323317000	2.972134000	0.218814000

E(RB3LYP) = -1430.82344291  
 Zero-point correction= 0.174764  
 Thermal correction to Energy= 0.188349  
 Thermal correction to Enthalpy= 0.189294  
 Thermal correction to Gibbs Free Energy= 0.134183  
 Sum of electronic and zero-point Energies= -1430.648679  
 Sum of electronic and thermal Energies= -1430.635093  
 Sum of electronic and thermal Enthalpies= -1430.634149  
 Sum of electronic and thermal Free Energies= -1430.689260

**30<sup>+</sup>**

44	-0.000004000	0.000003000	-0.447850000
17	0.000034000	-0.000031000	1.950332000
15	-1.941822000	1.399966000	-0.270846000
15	-1.941834000	-1.399955000	-0.270880000
15	1.941814000	1.399962000	-0.270869000
15	1.941822000	-1.399955000	-0.270883000

6	-3.064926000	0.000004000	0.265448000
1	-4.070061000	0.000013000	-0.159818000
1	-3.131904000	-0.000009000	1.356069000
6	3.064920000	0.000005000	0.265433000
1	4.070054000	0.000010000	-0.159834000
1	3.131896000	-0.000001000	1.356054000
1	-2.599477000	1.978158000	-1.378962000
1	-2.095620000	2.423381000	0.685076000
1	-2.599499000	-1.978118000	-1.379006000
1	-2.095639000	-2.423388000	0.685020000
1	2.095631000	2.423397000	0.685027000
1	2.599448000	1.978124000	-1.379013000
1	2.095617000	-2.423378000	0.685029000
1	2.599478000	-1.978130000	-1.379008000

E(RB3LYP) = -2002.76576276

Zero-point correction=	0.135313
Thermal correction to Energy=	0.148965
Thermal correction to Enthalpy=	0.149909
Thermal correction to Gibbs Free Energy=	0.094751
Sum of electronic and zero-point Energies=	-2002.630449
Sum of electronic and thermal Energies=	-2002.616798
Sum of electronic and thermal Enthalpies=	-2002.615853
Sum of electronic and thermal Free Energies=	-2002.671012

**31<sup>+</sup>**

42	-0.000119000	-0.000001000	-0.219599000
15	2.541734000	-0.001841000	-0.428723000
15	-2.541993000	0.001835000	-0.428102000
7	0.000534000	-0.000121000	1.566549000
8	0.000695000	-0.000187000	2.734199000
6	0.001430000	2.091127000	-0.275802000
8	0.002799000	3.234359000	-0.276936000
1	3.070122000	0.000847000	-1.738544000
1	3.266704000	-1.082621000	0.1111783000
1	3.267659000	1.075840000	0.116693000
1	-3.068580000	0.003290000	-1.738678000
1	-3.268982000	-1.077284000	0.112995000
1	-3.267376000	1.081152000	0.114756000
6	-0.001563000	-2.091035000	-0.275997000
8	-0.002696000	-3.234272000	-0.277075000

E(RB3LYP) = -1110.26794286

Zero-point correction=	0.079933
Thermal correction to Energy=	0.094129
Thermal correction to Enthalpy=	0.095073
Thermal correction to Gibbs Free Energy=	0.036808
Sum of electronic and zero-point Energies=	-1110.188010
Sum of electronic and thermal Energies=	-1110.173814
Sum of electronic and thermal Enthalpies=	-1110.172869
Sum of electronic and thermal Free Energies=	-1110.231135

Energies=

**32<sup>+</sup>**

42	-0.528540000	0.003119000	-0.237462000
15	1.461898000	-1.619893000	-0.271233000
15	1.472613000	1.625985000	-0.156530000
6	-1.950572000	-1.471029000	-0.475079000
6	-1.938443000	1.497088000	-0.436838000
7	-0.731542000	-0.025339000	1.535518000
8	-0.852894000	-0.039611000	2.697899000
6	3.004161000	-0.710833000	0.268225000
1	2.956881000	-0.637107000	1.360084000
1	3.892499000	-1.297129000	0.017777000
1	3.905532000	1.260323000	0.049257000
6	3.076890000	0.684894000	-0.372235000
1	3.253301000	0.606761000	-1.450926000
1	1.478337000	-2.800432000	0.497687000
1	1.831153000	-2.156423000	-1.525733000
1	1.637259000	2.734795000	-1.012445000
1	1.627099000	2.270087000	1.088758000
8	-2.715201000	2.332604000	-0.525814000
8	-2.735963000	-2.296318000	-0.583046000

E(RB3LYP) = -1187.71042096

Zero-point correction=	0.120451
Thermal correction to Energy=	0.134864
Thermal correction to Enthalpy=	0.135809
Thermal correction to Gibbs Free Energy=	0.077872
Sum of electronic and zero-point Energies=	-1187.589970
Sum of electronic and thermal Energies=	-1187.575556
Sum of electronic and thermal Enthalpies=	-1187.574612
Sum of electronic and thermal Free Energies=	-1187.632549

**33<sup>+</sup>**

42	0.000036000	-0.056497000	-0.204557000
15	-2.529207000	-0.091282000	-0.371999000
15	-0.000225000	2.529554000	-0.239014000
15	2.529377000	-0.090737000	-0.371611000
7	-0.000287000	-0.184278000	1.569472000
8	-0.000556000	-0.258837000	2.740501000
6	0.000329000	-2.081745000	-0.395469000
8	0.000499000	-3.227564000	-0.483771000
1	-3.311034000	1.035833000	-0.034347000
1	-3.197338000	-1.066423000	0.395937000
1	-3.096202000	-0.373677000	-1.635165000
1	-1.072297000	3.231941000	0.352755000
1	1.071172000	3.232017000	0.353886000
1	0.000409000	3.174030000	-1.497269000
1	3.310994000	1.036508000	-0.033913000
1	3.197656000	-1.065777000	0.396323000
1	3.096469000	-0.373003000	-1.634764000

E(RB3LYP) = -1340.09610442

Zero-point correction=	0.099367
Thermal correction to Energy=	0.114406
Thermal correction to Enthalpy=	0.115350
Thermal correction to Gibbs Free Energy=	0.055348
Sum of electronic and zero-point Energies=	-1339.996738
Sum of electronic and thermal Energies=	-1339.981699
Sum of electronic and thermal Enthalpies=	-1339.980754
Sum of electronic and thermal Free Energies=	-1340.040757

**34<sup>+</sup>**

42	-0.000009000	-0.000065000	-0.164906000
15	-1.914150000	1.597205000	-0.331402000
15	-1.926550000	-1.600746000	-0.248096000
15	1.914280000	-1.597162000	-0.331482000
15	1.926385000	1.600765000	-0.248134000
6	-3.508931000	0.712551000	0.107954000
1	-3.531369000	0.642844000	1.201203000
1	-4.373739000	1.305160000	-0.202573000
6	-3.545846000	-0.686158000	-0.525965000
1	-3.681985000	-0.611696000	-1.611115000
1	-4.382203000	-1.271168000	-0.134174000
6	3.508956000	-0.712367000	0.107975000
1	3.531326000	-0.642680000	1.201226000
1	4.373830000	-1.304901000	-0.202513000
6	3.545793000	0.686354000	-0.525914000
1	3.682011000	0.611927000	-1.611056000
1	4.382067000	1.271437000	-0.134054000
8	0.000104000	-0.000130000	2.787837000
7	0.000054000	-0.000095000	1.602563000
1	2.069975000	2.697755000	-1.128914000
1	-2.155692000	-2.280029000	0.968719000
1	-2.010021000	2.790106000	0.417967000
1	2.220688000	-2.131834000	-1.607339000
1	2.010308000	-2.790107000	0.417799000
1	2.155425000	2.280218000	0.968605000
1	-2.220458000	2.132006000	-1.607227000
1	-2.070313000	-2.697813000	-1.128752000

E(RB3LYP) = -1724.79788413

Zero-point correction=	0.199579
Thermal correction to Energy=	0.216048
Thermal correction to Enthalpy=	0.216992
Thermal correction to Gibbs Free Energy=	0.155113
Sum of electronic and zero-point Energies=	-1724.598305
Sum of electronic and thermal Energies=	-1724.581836
Sum of electronic and thermal Enthalpies=	-1724.580892
Sum of electronic and thermal Free Energies=	-1724.642771

**35<sup>+</sup>**

42	0.000015000	-0.000015000	-0.192371000
15	1.744912000	1.802089000	-0.338665000
15	1.802255000	-1.744687000	-0.338767000
15	-1.744864000	-1.801966000	-0.339082000



7	-0.000244000	-0.000235000	1.579228000
8	-0.000469000	-0.000421000	2.759832000
1	2.159092000	2.228817000	-1.623130000
1	3.025116000	1.588506000	0.221988000
1	1.489412000	3.075138000	0.220703000
1	3.074776000	-1.489288000	0.221861000
1	1.588676000	-3.025483000	0.220540000
1	2.230167000	-2.157520000	-1.623274000
1	-1.489834000	-3.074840000	0.220896000
1	-3.025344000	-1.588020000	0.220816000
1	-2.158413000	-2.229066000	-1.623630000
15	-1.802044000	1.744858000	-0.338800000
1	-2.229675000	2.158133000	-1.623257000
1	-3.074689000	1.489433000	0.221535000
1	-1.588338000	3.025423000	0.220972000

E(RB3LYP) = -1569.91717391

Zero-point correction=	0.118605
Thermal correction to Energy=	0.134461
Thermal correction to Enthalpy=	0.135406
Thermal correction to Gibbs Free Energy=	0.073772
Sum of electronic and zero-point Energies=	-1569.798569
Sum of electronic and thermal Energies=	-1569.782712
Sum of electronic and thermal Enthalpies=	-1569.781768
Sum of electronic and thermal Free Energies=	-1569.843402

### 36<sup>+</sup>

42	-0.000005000	-0.000028000	-0.116772000
15	-1.923155000	1.616516000	-0.269925000
15	-1.926783000	-1.626146000	-0.210879000
15	1.926741000	1.626128000	-0.210900000
15	1.923196000	-1.616525000	-0.269953000
7	0.000012000	-0.000035000	1.648487000
8	0.000030000	-0.000046000	2.835567000
6	-3.474780000	0.685615000	0.167967000
1	-3.384633000	0.497205000	1.248393000
6	-4.871493000	1.253707000	-0.138094000
1	-5.176374000	2.017005000	0.582050000
1	-4.872309000	1.722267000	-1.128905000
6	-5.805766000	0.004355000	-0.127534000
1	-6.494162000	0.032681000	-0.975847000
1	-6.419564000	-0.022459000	0.776281000
6	-4.875388000	-1.247350000	-0.191828000
1	-4.823790000	-1.735347000	0.787883000
1	-5.220661000	-1.996255000	-0.908951000
6	-3.493116000	-0.678958000	-0.562051000
1	-3.462011000	-0.484295000	-1.645841000
1	-2.003828000	2.794975000	0.505662000
1	-2.257789000	2.175988000	-1.529009000
1	-2.043728000	-2.748055000	-1.065926000
1	-2.210519000	-2.268211000	1.016154000
6	3.474790000	-0.685583000	0.167956000
1	3.384626000	-0.497174000	1.248382000

6	4.871520000	-1.253643000	-0.138087000
1	5.176410000	-2.016934000	0.582062000
1	4.872360000	-1.722203000	-1.128897000
6	5.805763000	-0.004268000	-0.127515000
1	6.494172000	-0.032579000	-0.975819000
1	6.419549000	0.022561000	0.776308000
6	4.875357000	1.247415000	-0.191823000
1	5.220622000	1.996326000	-0.908943000
1	4.823736000	1.735413000	0.787887000
6	3.493103000	0.678989000	-0.562061000
1	3.462015000	0.484326000	-1.645852000
1	2.210461000	2.268235000	1.016114000
1	2.043628000	2.748021000	-1.065976000
1	2.003917000	-2.794995000	0.505613000
1	2.257851000	-2.175963000	-1.529046000

E(RB3LYP) = -1958.26214553

Zero-point correction=	0.328906
Thermal correction to Energy=	0.350539
Thermal correction to Enthalpy=	0.351483
Thermal correction to Gibbs Free Energy=	0.277178
Sum of electronic and zero-point Energies=	-1957.933240
Sum of electronic and thermal Energies=	-1957.911607
Sum of electronic and thermal Enthalpies=	-1957.910663
Sum of electronic and thermal Free Energies=	-1957.984967

**37<sup>+</sup>**

74	0.052861000	-0.000076000	-0.182062000
8	0.043012000	3.227872000	-0.281770000
8	0.032036000	-3.227952000	-0.281725000
8	3.225235000	-0.005142000	-0.600764000
8	0.325971000	-0.000458000	2.766212000
15	-2.533925000	0.003956000	-0.256635000
6	0.043647000	2.086356000	-0.258649000
6	0.036648000	-2.086445000	-0.258609000
6	2.091617000	-0.003359000	-0.456104000
7	0.228932000	-0.000357000	1.604047000
1	-3.210958000	1.090939000	0.328570000
1	-3.121533000	0.004485000	-1.539476000
1	-3.214375000	-1.080520000	0.329251000

E(RB3LYP) = -880.725322792

Zero-point correction=	0.060676
Thermal correction to Energy=	0.073830
Thermal correction to Enthalpy=	0.074774
Thermal correction to Gibbs Free Energy=	0.018453
Sum of electronic and zero-point Energies=	-880.664647
Sum of electronic and thermal Energies=	-880.651493
Sum of electronic and thermal Enthalpies=	-880.650549
Sum of electronic and thermal Free Energies=	-880.706870

**38+**

74	0.000065000	-0.000029000	-0.162590000
15	2.518744000	0.000968000	-0.399396000
15	-2.518542000	-0.000808000	-0.399853000
7	-0.000376000	-0.000011000	1.625242000
8	-0.000657000	-0.000001000	2.798516000
6	-0.000794000	2.068710000	-0.233458000
8	-0.001348000	3.214841000	-0.253341000
1	3.027363000	0.001650000	-1.716967000
1	3.242966000	1.083970000	0.136850000
1	3.243986000	-1.081724000	0.136102000
1	-3.242950000	-1.083880000	0.136012000
1	-3.243511000	1.081796000	0.136191000
1	-3.027272000	-0.000862000	-1.717373000
6	0.000830000	-2.068789000	-0.233474000
8	0.001251000	-3.214917000	-0.253365000

E(RB3LYP) = -1110.55656229

Zero-point correction=	0.080413
Thermal correction to Energy=	0.094367
Thermal correction to Enthalpy=	0.095311
Thermal correction to Gibbs Free Energy=	0.037088
Sum of electronic and zero-point Energies=	-1110.476150
Sum of electronic and thermal Energies=	-1110.462196
Sum of electronic and thermal Enthalpies=	-1110.461251
Sum of electronic and thermal Free Energies=	-1110.519475

**39+**

74	0.000030000	-0.000022000	-0.148008000
15	1.467236000	2.003651000	-0.308769000
15	2.003729000	-1.467256000	-0.308679000
15	-1.467332000	-2.003623000	-0.308748000
7	-0.000023000	0.000044000	1.626400000
8	-0.000087000	0.000113000	2.813272000
1	1.826737000	2.462914000	-1.598570000
1	2.760561000	1.966903000	0.262447000
1	1.036143000	3.237498000	0.232395000
1	3.237983000	-1.035688000	0.231190000
1	1.967242000	-2.759955000	0.263926000
1	2.462121000	-1.828125000	-1.598408000
1	-1.035936000	-3.238079000	0.230761000
1	-2.759890000	-1.966975000	0.264167000
1	-1.828592000	-2.461660000	-1.598467000
15	-2.003666000	1.467227000	-0.308759000
1	-1.967026000	2.760210000	0.263198000
1	-2.462521000	1.827469000	-1.598493000
1	-3.237723000	1.035926000	0.231769000

E(RB3LYP) = -1570.19759214

Zero-point correction=	0.119488
Thermal correction to Energy=	0.134888
Thermal correction to Enthalpy=	0.135832

Thermal correction to Gibbs Free Energy=	0.075206
Sum of electronic and zero-point Energies=	-1570.078104
Sum of electronic and thermal Energies=	-1570.062704
Sum of electronic and thermal Enthalpies=	-1570.061760
Sum of electronic and thermal Free Energies=	-1570.122387

**40<sup>+</sup>**

74	0.000007000	-0.041681000	-0.153623000
15	-2.505629000	-0.081432000	-0.335700000
15	0.000992000	2.519511000	-0.217544000
15	2.505514000	-0.083467000	-0.335786000
7	0.000042000	-0.173682000	1.621734000
8	0.000051000	-0.249034000	2.798910000
6	-0.000929000	-2.046998000	-0.361677000
8	-0.001490000	-3.194774000	-0.472409000
1	-3.290334000	1.052761000	-0.027495000
1	-3.165895000	-1.043457000	0.454801000
1	-3.062482000	-0.394123000	-1.596142000
1	-1.073949000	3.223517000	0.367116000
1	1.076387000	3.222924000	0.366999000
1	0.001102000	3.143611000	-1.485891000
1	3.291015000	1.049328000	-0.024514000
1	3.165355000	-1.048181000	0.451795000
1	3.061896000	-0.392958000	-1.597236000

E(RB3LYP) = -1340.38111070

Zero-point correction=	0.099908
Thermal correction to Energy=	0.114655
Thermal correction to Enthalpy=	0.115599
Thermal correction to Gibbs Free Energy=	0.055925
Sum of electronic and zero-point Energies=	-1340.281203
Sum of electronic and thermal Energies=	-1340.266456
Sum of electronic and thermal Enthalpies=	-1340.265511
Sum of electronic and thermal Free Energies=	-1340.325186

**41<sup>+</sup>**

74	-0.000001000	0.000000000	0.125465000
15	-1.897307000	-1.583330000	0.309919000
15	-1.908257000	1.587860000	0.230470000
15	1.897303000	1.583330000	0.309925000
15	1.908256000	-1.587858000	0.230497000
6	-3.507308000	-0.715359000	-0.112572000
1	-3.547484000	-0.659305000	-1.206017000
1	-4.361458000	-1.310964000	0.220716000
6	-3.539907000	0.689957000	0.505712000
1	-3.686099000	0.629196000	1.590380000
1	-4.366008000	1.279373000	0.099310000
6	3.507308000	0.715360000	-0.112545000
1	3.547495000	0.659299000	-1.205990000
1	4.361454000	1.310968000	0.220746000
6	3.539903000	-0.689952000	0.505748000

1	3.686085000	-0.629184000	1.590416000	
1	4.366008000	-1.279370000	0.099356000	
8	0.000013000	-0.000009000	-2.836472000	
7	0.000008000	-0.000006000	-1.644671000	
1	2.031284000	-2.670215000	1.132189000	
1	-2.125896000	2.286461000	-0.977196000	
1	-1.976064000	-2.770269000	-0.450338000	
1	2.183602000	2.129030000	1.585807000	
1	1.976065000	2.770265000	-0.450341000	
1	2.125906000	-2.286465000	-0.977164000	
1	-2.183619000	-2.129018000	1.585803000	
1	-2.031291000	2.670222000	1.132156000	
E(RB3LYP) = -1725.08064597				
Zero-point correction=				0.199809
Thermal correction to Energy=				0.216134
Thermal correction to Enthalpy=				0.217078
Thermal correction to Gibbs Free Energy=				0.155124
Sum of electronic and zero-point Energies=				-1724.880837
Sum of electronic and thermal Energies=				-1724.864512
Sum of electronic and thermal Enthalpies=				-1724.863568
Sum of electronic and thermal Free Energies=				-1724.925522

**42+**

74	0.000000000	-0.000008000	0.028032000	
15	-1.895092000	1.580357000	-0.180254000	
15	-1.903661000	-1.587834000	-0.192638000	
15	1.895108000	-1.580296000	-0.180641000	
15	1.903657000	1.587896000	-0.192035000	
6	-3.502720000	0.711189000	0.250155000	
1	-3.526156000	0.635554000	1.342458000	
1	-4.359920000	1.313975000	-0.062158000	
6	-3.545921000	-0.681612000	-0.395058000	
1	-3.721573000	-0.595552000	-1.473567000	
1	-4.360193000	-1.282842000	0.017700000	
6	3.502689000	-0.711258000	0.250200000	
1	3.526017000	-0.635974000	1.342529000	
1	4.359922000	-1.313943000	-0.062223000	
6	3.545951000	0.681750000	-0.394560000	
1	3.721727000	0.596042000	-1.473076000	
1	4.360170000	1.282852000	0.018486000	
6	-0.000033000	-0.000284000	1.787583000	
1	2.011209000	2.556775000	-1.217915000	
1	-2.126569000	-2.429923000	0.914430000	
1	-1.980174000	2.776114000	0.563183000	
1	2.195102000	-2.107195000	-1.462496000	
1	1.980149000	-2.776307000	0.562395000	
1	2.126465000	2.429718000	0.915257000	
1	-2.194974000	2.107696000	-1.461954000	
1	-2.011157000	-2.556458000	-1.218765000	
1	-0.000053000	-0.000456000	2.874933000	
E(RB3LYP) = -1633.79259448				
Zero-point correction=				0.205710
Thermal correction to Energy=				0.221262

Thermal correction to Enthalpy=	0.222206
Thermal correction to Gibbs Free Energy=	0.162611
Sum of electronic and zero-point Energies=	-1633.586885
Sum of electronic and thermal Energies=	-1633.571333
Sum of electronic and thermal Enthalpies=	-1633.570389
Sum of electronic and thermal Free Energies=	-1633.629984

### 1...H<sub>2</sub>O

25	-0.300250000	0.005193000	-0.048960000
6	-1.125456000	-0.025013000	1.587227000
8	-1.646294000	-0.041160000	2.613058000
6	0.914891000	-1.352419000	0.330015000
8	1.642352000	-2.214444000	0.525029000
6	-1.340094000	1.342134000	-0.780491000
8	-1.954911000	2.169864000	-1.285558000
6	0.983756000	1.263252000	0.354752000
8	1.787418000	2.063991000	0.539427000
6	-1.372656000	-1.246402000	-0.882938000
8	-2.002693000	-2.014740000	-1.457473000
1	0.403640000	0.027139000	-1.456547000
8	3.635723000	-0.069879000	-0.776251000
1	3.790964000	0.860943000	-0.572806000
1	3.256259000	-0.056273000	-1.663875000

E(RB3LYP) = -747.649484709

Zero-point correction=	0.073604 (Hartree/Particle)
Thermal correction to Energy=	0.089571
Thermal correction to Enthalpy=	0.090515
Thermal correction to Gibbs Free Energy=	0.027865
Sum of electronic and zero-point Energies=	-747.575880
Sum of electronic and thermal Energies=	-747.559914
Sum of electronic and thermal Enthalpies=	-747.558969
Sum of electronic and thermal Free Energies=	-747.621620

### 2a ...H<sub>2</sub>O

25	0.322210000	0.059889000	-0.063001000
15	-1.366419000	-1.413348000	0.624912000
8	2.236553000	1.962761000	-1.281967000
8	1.425285000	-2.168693000	-1.711557000
8	1.887337000	-0.313475000	2.443378000
6	1.505725000	1.219572000	-0.791849000
6	1.030167000	-1.320627000	-1.040395000
6	1.272745000	-0.173162000	1.476838000
1	-0.963497000	-2.490102000	1.450999000
1	-2.088057000	-2.146043000	-0.335286000
1	-2.441737000	-0.949332000	1.406059000
1	-0.493430000	0.227767000	-1.406408000
6	-0.744589000	1.445547000	0.462802000
8	-1.464915000	2.310426000	0.717162000
8	-3.332778000	0.274301000	-1.075334000
1	-3.448974000	1.155601000	-0.697501000
1	-2.519409000	0.354561000	-1.594357000

E(RB3LYP) = -977.471575924

Zero-point correction=	0.094685 (Hartree/Particle)
------------------------	-----------------------------

Thermal correction to Energy=	0.110518
Thermal correction to Enthalpy=	0.111462
Thermal correction to Gibbs Free Energy=	0.050674
Sum of electronic and zero-point Energies=	-977.376891
Sum of electronic and thermal Energies=	-977.361058
Sum of electronic and thermal Enthalpies=	-977.360114
Sum of electronic and thermal Free Energies=	-977.420902

### 2b... H<sub>2</sub>O

25	0.200235000	0.008897000	-0.108050000
1	-0.693162000	0.087589000	-1.368423000
15	1.580139000	-0.099098000	1.716493000
1	1.715779000	1.017849000	2.575370000
1	1.371644000	-1.066337000	2.728801000
1	2.963320000	-0.339477000	1.535542000
6	-0.950920000	1.295345000	0.510955000
8	-1.714849000	2.103472000	0.814975000
6	1.045953000	-1.265211000	-1.130392000
8	1.513702000	-2.048217000	-1.832380000
6	1.192608000	1.315701000	-0.938566000
8	1.774816000	2.133615000	-1.502160000
6	-0.949585000	-1.303566000	0.517247000
8	-1.650437000	-2.133438000	0.888809000
8	-3.620272000	-0.003287000	-0.892298000
1	-3.686521000	0.925699000	-0.638775000
1	-2.831037000	-0.032057000	-1.449717000

E(RB3LYP) = -977.460883545

Zero-point correction=	0.092943 (Hartree/Particle)
Thermal correction to Energy=	0.109798
Thermal correction to Enthalpy=	0.110742
Thermal correction to Gibbs Free Energy=	0.045044
Sum of electronic and zero-point Energies=	-977.367940
Sum of electronic and thermal Energies=	-977.351086
Sum of electronic and thermal Enthalpies=	-977.350142
Sum of electronic and thermal Free Energies=	-977.415840

### 3a... H<sub>2</sub>O

25	-0.244011000	-0.012197000	-0.008514000
8	-1.776987000	-0.570386000	2.473008000
8	-1.340159000	-2.156730000	-1.765940000
6	-1.169587000	-0.359682000	1.509841000
6	-0.941003000	-1.341231000	-1.052136000
1	0.504042000	0.313269000	-1.380131000
15	-1.770059000	1.439605000	-0.857518000
1	-1.369604000	2.769488000	-1.125122000
1	-2.979917000	1.750158000	-0.186418000
1	-2.334855000	1.161391000	-2.123712000
6	0.752110000	1.382224000	0.602765000
8	1.434574000	2.263483000	0.915723000
15	1.476208000	-1.436780000	0.532163000
1	2.211126000	-2.075316000	-0.486134000
1	1.140402000	-2.586397000	1.288900000
1	2.556049000	-0.992723000	1.322602000
8	3.324137000	0.470935000	-1.171063000

1	3.375966000	1.291263000	-0.664155000
1	2.423188000	0.485136000	-1.529298000
E(RB3LYP) = -1207.28093836			
Zero-point correction=		0.114037 (Hartree/Particle)	
Thermal correction to Energy=		0.130668	
Thermal correction to Enthalpy=		0.131612	
Thermal correction to Gibbs Free Energy=		0.068982	
Sum of electronic and zero-point Energies=		-1207.166902	
Sum of electronic and thermal Energies=		-1207.150271	
Sum of electronic and thermal Enthalpies=		-1207.149327	
Sum of electronic and thermal Free Energies=		-1207.211957	

### 3b...H<sub>2</sub>O

25	0.244789000	0.068350000	-0.128881000
15	-1.389074000	-1.402128000	0.679232000
1	-2.114543000	-2.197477000	-0.228910000
1	-0.961630000	-2.440440000	1.548136000
1	-2.468045000	-0.938126000	1.458052000
1	-0.658959000	0.221855000	-1.385515000
15	1.629974000	-0.203101000	1.663031000
1	1.850631000	0.852295000	2.582343000
1	1.406547000	-1.211350000	2.639392000
1	2.996177000	-0.507506000	1.443658000
6	-0.760291000	1.450714000	0.500192000
8	-1.461748000	2.315906000	0.815323000
6	0.889910000	-1.315923000	-1.135319000
8	1.236539000	-2.167701000	-1.834049000
6	1.360964000	1.218369000	-0.948192000
8	2.044742000	1.961782000	-1.511001000
8	-3.406095000	0.267629000	-1.019056000
1	-2.550901000	0.313929000	-1.474419000
1	-3.483490000	1.136606000	-0.604493000
E(RB3LYP) = -1207.27870292			
Zero-point correction=		0.113851 (Hartree/Particle)	
Thermal correction to Energy=		0.130520	
Thermal correction to Enthalpy=		0.131464	
Thermal correction to Gibbs Free Energy=		0.068833	
Sum of electronic and zero-point Energies=		-1207.164852	
Sum of electronic and thermal Energies=		-1207.148183	
Sum of electronic and thermal Enthalpies=		-1207.147239	
Sum of electronic and thermal Free Energies=		-1207.209870	

### 3c... H<sub>2</sub>O

25	-0.308787000	-0.000151000	-0.087882000
8	-1.988569000	-0.002674000	2.367479000
8	-1.797478000	-2.092782000	-1.555783000
6	-1.320591000	-0.001505000	1.421846000
6	-1.233417000	-1.281141000	-0.956574000
1	0.570123000	0.000390000	-1.406868000
15	1.131759000	1.663965000	0.659360000
1	2.323292000	1.344280000	1.348177000
1	0.639417000	2.627179000	1.574238000
1	1.684508000	2.564248000	-0.275127000
6	-1.236135000	1.279651000	-0.955410000



8	-1.802055000	2.090797000	-1.553540000
15	1.134629000	-1.661641000	0.660344000
1	1.687462000	-2.562960000	-0.273100000
1	0.643961000	-2.623855000	1.577195000
1	2.326227000	-1.339494000	1.347794000
8	3.170741000	0.002184000	-1.151426000
1	3.689935000	-0.004376000	-1.964721000
1	2.238665000	0.001268000	-1.439107000

E(RB3LYP) = -1207.28314477

Zero-point correction= 0.114044 (Hartree/Particle)

Thermal correction to Energy= 0.130636

Thermal correction to Enthalpy= 0.131580

Thermal correction to Gibbs Free Energy= 0.069249

Sum of electronic and zero-point Energies= -1207.169100

Sum of electronic and thermal Energies= -1207.152509

Sum of electronic and thermal Enthalpies= -1207.151564

Sum of electronic and thermal Free Energies= -1207.213896

#### 4a ...H<sub>2</sub>O

25	0.188841000	0.018511000	-0.067209000
15	1.577384000	1.597768000	-0.906998000
1	1.133961000	2.940378000	-0.979951000
1	2.864588000	1.882994000	-0.369151000
1	1.991618000	1.478796000	-2.255009000
15	-1.439228000	-1.517907000	0.427685000
1	-2.147497000	-2.143243000	-0.619606000
1	-1.059911000	-2.700411000	1.120051000
1	-2.545118000	-1.185455000	1.239757000
1	-0.637168000	0.394230000	-1.352155000
15	1.480977000	-0.522384000	1.716855000
1	2.870238000	-0.218914000	1.715833000
1	1.231008000	-0.018718000	3.020562000
1	1.636873000	-1.876881000	2.119064000
6	-0.816264000	1.308432000	0.722035000
8	-1.517983000	2.131114000	1.146247000
6	0.904660000	-1.198538000	-1.222250000
8	1.305458000	-1.942427000	-2.015456000
8	-3.404994000	0.467313000	-1.085117000
1	-3.444280000	1.211555000	-0.470975000
1	-2.492571000	0.503391000	-1.415420000

E(RB3LYP) = -1437.08324660

Zero-point correction= 0.133055 (Hartree/Particle)

Thermal correction to Energy= 0.150448

Thermal correction to Enthalpy= 0.151392

Thermal correction to Gibbs Free Energy= 0.087299

Sum of electronic and zero-point Energies= -1436.950192

Sum of electronic and thermal Energies= -1436.932798

Sum of electronic and thermal Enthalpies= -1436.931854

Sum of electronic and thermal Free Energies= -1436.995947

#### 4b...H<sub>2</sub>O

25	0.251882000	0.060643000	-0.026119000
8	1.925312000	0.296050000	2.414082000
8	1.579988000	2.208372000	-1.559203000

6	1.257630000	0.206420000	1.467539000
6	1.073725000	1.371542000	-0.934720000
1	-0.595055000	-0.139684000	-1.371680000
15	1.549497000	-1.442231000	-1.106442000
1	1.012583000	-2.702249000	-1.477581000
1	2.777490000	-1.940113000	-0.592855000
1	2.039423000	-1.087922000	-2.385498000
15	-1.313532000	1.599710000	0.611046000
1	-1.911950000	2.424289000	-0.367165000
1	-0.923585000	2.636138000	1.497185000
1	-2.500950000	1.227828000	1.285499000
15	-1.059845000	-1.662899000	0.802346000
1	-2.381725000	-1.406006000	1.233429000
1	-0.652517000	-2.416410000	1.934079000
1	-1.360570000	-2.766951000	-0.030627000
8	-3.202284000	-0.258066000	-1.271293000
1	-3.613225000	-0.000928000	-2.105569000
1	-2.241047000	-0.201371000	-1.436076000

E(RB3LYP) = -1437.08800023

Zero-point correction=	0.133358 (Hartree/Particle)
Thermal correction to Energy=	0.150683
Thermal correction to Enthalpy=	0.151628
Thermal correction to Gibbs Free Energy=	0.087759
Sum of electronic and zero-point Energies=	-1436.954642
Sum of electronic and thermal Energies=	-1436.937317
Sum of electronic and thermal Enthalpies=	-1436.936373
Sum of electronic and thermal Free Energies=	-1437.000242

#### 4c...H<sub>2</sub>O

25	-0.239435000	-0.000173000	0.148764000
15	1.136883000	-1.655405000	-0.719062000
1	1.654236000	-2.631791000	0.160188000
1	0.636084000	-2.557417000	-1.697150000
1	2.348966000	-1.342545000	-1.377174000
15	1.133448000	1.658819000	-0.716943000
1	2.346155000	1.349239000	-1.375499000
1	0.631193000	2.561688000	-1.693497000
1	1.649057000	2.634578000	0.164032000
1	0.763751000	0.000739000	1.349455000
15	-1.713517000	-0.001001000	-1.574798000
1	-3.103788000	-0.006935000	-1.296070000
1	-1.763716000	1.054721000	-2.527480000
1	-1.756048000	-1.051366000	-2.533791000
6	-1.091211000	1.271246000	1.086277000
8	-1.602897000	2.081921000	1.740271000
6	-1.087857000	-1.274252000	1.085701000
8	-1.597349000	-2.086516000	1.739426000
8	3.335521000	0.001428000	1.030683000
1	3.825238000	-0.000419000	1.862071000
1	2.394759000	0.001010000	1.292959000

E(RB3LYP) = -1437.08630804

Zero-point correction=	0.132921 (Hartree/Particle)
Thermal correction to Energy=	0.150381

Thermal correction to Enthalpy= 0.151325  
 Thermal correction to Gibbs Free Energy= 0.087069  
 Sum of electronic and zero-point Energies= -1436.953387  
 Sum of electronic and thermal Energies= -1436.935927  
 Sum of electronic and thermal Enthalpies= -1436.934983  
 Sum of electronic and thermal Free Energies= -1436.999240

### 5a...H<sub>2</sub>O

25	0.211946000	0.000002000	0.015367000
6	1.209122000	0.000395000	1.510167000
8	1.880815000	0.000531000	2.463629000
15	-1.234098000	-1.617447000	0.730679000
1	-1.671504000	-2.625273000	-0.164940000
1	-0.860419000	-2.496350000	1.783327000
1	-2.513337000	-1.287829000	1.241533000
15	-1.237879000	1.613324000	0.732948000
1	-2.513827000	1.280018000	1.249611000
1	-0.863000000	2.495217000	1.782668000
1	-1.682381000	2.618085000	-0.162556000
15	1.369703000	1.598879000	-1.075651000
15	1.374106000	-1.594562000	-1.077415000
1	0.691417000	2.748213000	-1.562319000
1	2.470366000	2.308263000	-0.518149000
1	2.010200000	1.278940000	-2.303268000
1	2.012142000	-1.271818000	-2.305560000
1	2.477916000	-2.300118000	-0.521283000
1	0.699436000	-2.746149000	-1.563757000
1	-0.583372000	-0.000450000	-1.399680000
8	-3.198266000	-0.001884000	-1.336563000
1	-3.540200000	0.006094000	-2.238676000
1	-2.224671000	-0.001331000	-1.437074000

E(RB3LYP) = -1666.88760539

Zero-point correction= 0.151951 (Hartree/Particle)  
 Thermal correction to Energy= 0.170125  
 Thermal correction to Enthalpy= 0.171070  
 Thermal correction to Gibbs Free Energy= 0.105322  
 Sum of electronic and zero-point Energies= -1666.735654  
 Sum of electronic and thermal Energies= -1666.717480  
 Sum of electronic and thermal Enthalpies= -1666.716536  
 Sum of electronic and thermal Free Energies= -1666.782283

### 5b...H<sub>2</sub>O

25	0.194727000	0.037355000	-0.081520000
15	1.447081000	-1.405337000	-1.276935000
1	1.712049000	-1.076092000	-2.628420000
1	2.785521000	-1.781107000	-0.954768000
1	0.985864000	-2.726779000	-1.522897000
15	-0.976966000	-1.711913000	0.864386000
15	-1.357024000	1.517740000	0.687459000
1	-1.143053000	-2.914092000	0.130791000
1	-0.588409000	-2.334726000	2.085393000
1	-2.340824000	-1.538196000	1.201727000
1	-2.521135000	1.117569000	1.389293000

1	-0.960617000	2.535866000	1.600434000
1	-2.000471000	2.377266000	-0.232723000
1	-0.767548000	-0.237986000	-1.310146000
15	1.638493000	0.310946000	1.630890000
1	3.039650000	0.184562000	1.417600000
1	1.725105000	1.542452000	2.340405000
1	1.612468000	-0.506753000	2.798754000
6	0.869210000	1.369905000	-1.064215000
8	1.268410000	2.226486000	-1.746704000
8	-3.365494000	-0.271876000	-1.158183000
1	-3.721669000	0.158727000	-1.944945000
1	-2.397462000	-0.262447000	-1.295103000
E(RB3LYP) = -1666.88697977			
Zero-point correction=		0.151920 (Hartree/Particle)	
Thermal correction to Energy=		0.170061	
Thermal correction to Enthalpy=		0.171005	
Thermal correction to Gibbs Free Energy=		0.105483	
Sum of electronic and zero-point Energies=		-1666.735060	
Sum of electronic and thermal Energies=		-1666.716919	
Sum of electronic and thermal Enthalpies=		-1666.715974	
Sum of electronic and thermal Free Energies=		-1666.781497	

## 6...H<sub>2</sub>O

25	-0.168287000	-0.000010000	-0.035982000
15	1.210655000	1.603356000	0.790740000
1	1.609970000	2.690497000	-0.031720000
1	0.829508000	2.407183000	1.907911000
1	2.508692000	1.291969000	1.269445000
15	1.210251000	-1.603924000	0.790275000
1	2.508509000	-1.293022000	1.268679000
1	0.829119000	-2.407790000	1.907429000
1	1.608954000	-2.691108000	-0.032428000
15	-1.222619000	-1.581289000	-1.237424000
15	-1.222163000	1.581999000	-1.236939000
1	-0.532648000	-2.773920000	-1.592145000
1	-2.434402000	-2.245506000	-0.870746000
1	-1.649245000	-1.271606000	-2.559137000
1	-1.648618000	1.272938000	-2.558851000
1	-2.433927000	2.246161000	-0.870123000
1	-0.532003000	2.774709000	-1.591027000
1	0.745304000	-0.000155000	-1.358905000
15	-1.574874000	-0.000108000	1.710572000
1	-1.591178000	-1.050043000	2.678549000
1	-1.589572000	1.048291000	2.680248000
1	-2.989202000	0.001127000	1.522352000
8	3.361027000	-0.000045000	-1.213652000
1	3.675611000	0.000267000	-2.125721000
1	2.385327000	0.000091000	-1.293403000
E(RB3LYP) = -1896.68195255			
Zero-point correction=		0.170464 (Hartree/Particle)	
Thermal correction to Energy=		0.189313	
Thermal correction to Enthalpy=		0.190258	
Thermal correction to Gibbs Free Energy=		0.122385	
Sum of electronic and zero-point Energies=		-1896.511488	

Sum of electronic and thermal Energies= -1896.492639  
 Sum of electronic and thermal Enthalpies= -1896.491695  
 Sum of electronic and thermal Free Energies= -1896.559568

### 7...H<sub>2</sub>O

25	-0.853125000	-0.000039000	0.067682000
15	0.772171000	-1.640239000	-0.053517000
15	0.772064000	1.640263000	-0.053078000
8	-2.791353000	-2.105133000	0.817754000
8	-1.414758000	-0.000209000	-2.851164000
8	-2.791125000	2.105450000	0.817234000
6	-2.040828000	-1.286143000	0.495682000
6	-1.177564000	-0.000120000	-1.715857000
6	-2.040730000	1.286241000	0.495405000
6	2.438077000	-1.291222000	-0.815224000
1	3.085028000	-2.152112000	-0.620785000
1	2.284725000	-1.241629000	-1.900235000
6	3.110894000	0.000186000	-0.316641000
1	3.161978000	0.000117000	0.777929000
1	4.145445000	0.000272000	-0.681594000
6	2.437908000	1.291581000	-0.815041000
1	2.284431000	1.242091000	-1.900040000
1	3.084799000	2.152515000	-0.620581000
1	-0.574778000	0.000013000	1.626871000
1	1.160596000	2.253236000	1.157273000
1	0.444815000	2.820894000	-0.764142000
1	0.445027000	-2.820563000	-0.765130000
1	1.160585000	-2.253745000	1.156606000
8	1.808886000	-0.000645000	2.756516000
1	1.733509000	0.001628000	3.718320000
1	0.888705000	-0.000938000	2.429733000

E(RB3LYP) = -1324.03830043

Zero-point correction= 0.183401 (Hartree/Particle)

Thermal correction to Energy= 0.201736

Thermal correction to Enthalpy= 0.202680

Thermal correction to Gibbs Free Energy= 0.136105

Sum of electronic and zero-point Energies= -1323.854900

Sum of electronic and thermal Energies= -1323.836565

Sum of electronic and thermal Enthalpies= -1323.835620

Sum of electronic and thermal Free Energies= -1323.902196

### 8...H<sub>2</sub>O

25	0.141892000	-0.265989000	-0.017953000
15	1.708913000	0.293961000	-1.512634000
15	1.746098000	0.087411000	1.510663000
15	-1.549351000	-0.176873000	-1.503552000
15	-1.504940000	-0.243152000	1.525102000
6	0.340031000	-2.043955000	-0.100992000
8	0.487141000	-3.201887000	-0.155807000
1	2.440524000	-0.646370000	-2.294095000
1	1.459230000	1.201130000	-2.576241000
6	3.126293000	1.181828000	-0.655597000
6	3.391042000	0.494489000	0.689573000
1	1.622187000	1.161395000	2.429977000

1	2.195814000	-0.871839000	2.458971000
1	-1.693774000	-1.088112000	-2.584325000
1	-1.794088000	0.994904000	-2.268917000
6	-3.212143000	-0.417691000	-0.659703000
6	-3.151731000	0.202570000	0.741901000
1	-1.500276000	0.645186000	2.630418000
1	-1.861460000	-1.406129000	2.263046000
1	0.052034000	1.348654000	0.055254000
1	2.791453000	2.212517000	-0.498420000
1	4.022324000	1.207643000	-1.282868000
1	3.898693000	-0.463701000	0.529851000
1	4.026677000	1.100475000	1.341590000
1	-3.368842000	-1.500915000	-0.598972000
1	-4.026848000	0.002938000	-1.256327000
1	-3.156077000	1.295020000	0.669147000
1	-3.990583000	-0.117719000	1.366732000
8	-1.822297000	3.156571000	0.185687000
1	-1.094857000	2.502226000	0.151140000
1	-1.859955000	3.511297000	-0.710967000

E(RB3LYP) = -1821.76386360

Zero-point correction= 0.232683 (Hartree/Particle)

Thermal correction to Energy= 0.251707

Thermal correction to Enthalpy= 0.252651

Thermal correction to Gibbs Free Energy= 0.185195

Sum of electronic and zero-point Energies= -1821.531180

Sum of electronic and thermal Energies= -1821.512157

Sum of electronic and thermal Enthalpies= -1821.511213

Sum of electronic and thermal Free Energies= -1821.578669

## 9...H<sub>2</sub>O

25	-0.126295000	-0.325663000	-0.050544000
15	1.557714000	0.166513000	-1.475548000
15	1.535719000	-0.659204000	1.437697000
15	-1.706056000	0.508793000	-1.422831000
15	-1.733783000	-0.245055000	1.511017000
7	-0.318310000	-2.098079000	-0.544450000
7	-0.443508000	-3.177966000	-0.844374000
1	2.036528000	-0.774258000	-2.433582000
1	1.523081000	1.279373000	-2.353591000
6	3.132532000	0.536581000	-0.526041000
6	3.236038000	-0.438960000	0.653835000
1	1.640747000	0.180939000	2.577877000
1	1.767355000	-1.877508000	2.137801000
1	-2.191768000	-0.120626000	-2.604486000
1	-1.512124000	1.788322000	-2.003618000
6	-3.345327000	0.752029000	-0.523522000
6	-3.080743000	0.950887000	0.974409000
1	-1.493876000	0.233252000	2.826380000
1	-2.535076000	-1.358620000	1.905895000
1	-0.018172000	1.215734000	0.399642000
1	3.017636000	1.566488000	-0.171966000
1	4.012639000	0.483778000	-1.173843000
1	3.540422000	-1.432382000	0.304146000

1	3.974929000	-0.111382000	1.391004000
1	-3.923352000	-0.165219000	-0.684772000
1	-3.918184000	1.579829000	-0.951296000
1	-2.688802000	1.955586000	1.163125000
1	-3.991461000	0.824520000	1.567479000
8	1.526943000	3.306403000	0.395604000
1	0.905887000	2.550926000	0.355600000
1	1.669252000	3.434988000	1.341633000

E(RB3LYP) = -1817.93929065

Zero-point correction=	0.232225 (Hartree/Particle)
Thermal correction to Energy=	0.251528
Thermal correction to Enthalpy=	0.252472
Thermal correction to Gibbs Free Energy=	0.183710
Sum of electronic and zero-point Energies=	-1817.707066
Sum of electronic and thermal Energies=	-1817.687763
Sum of electronic and thermal Enthalpies=	-1817.686818
Sum of electronic and thermal Free Energies=	-1817.755581

### 10...H<sub>2</sub>O

25	0.211875000	0.000002000	0.019379000
15	-1.240855000	-1.612738000	0.740990000
1	-1.547645000	-2.714037000	-0.098149000
1	-0.946102000	-2.380511000	1.903334000
1	-2.577557000	-1.299144000	1.088345000
15	-1.240148000	1.613543000	0.740574000
1	-2.576986000	1.300588000	1.087980000
1	-0.945155000	2.381572000	1.902693000
1	-1.546476000	2.714702000	-0.098915000
15	1.392599000	1.597329000	-1.060627000
15	1.391798000	-1.598064000	-1.060422000
1	0.733804000	2.770244000	-1.516853000
1	2.516582000	2.273559000	-0.501784000
1	2.013247000	1.288404000	-2.301018000
1	2.012502000	-1.289634000	-2.300906000
1	2.515517000	-2.274688000	-0.501521000
1	0.732456000	-2.770772000	-1.516388000
1	-0.586088000	0.000114000	-1.380603000
8	-3.195468000	0.000121000	-1.422162000
1	-3.478868000	0.000039000	-2.344433000
1	-2.217508000	0.000187000	-1.464075000
7	1.227831000	-0.000203000	1.571283000
7	1.859919000	-0.000181000	2.504060000

E(RB3LYP) = -1663.06490865

Zero-point correction=	0.151878 (Hartree/Particle)
Thermal correction to Energy=	0.170090
Thermal correction to Enthalpy=	0.171035
Thermal correction to Gibbs Free Energy=	0.105153
Sum of electronic and zero-point Energies=	-1662.913030
Sum of electronic and thermal Energies=	-1662.894818
Sum of electronic and thermal Enthalpies=	-1662.893874
Sum of electronic and thermal Free Energies=	-1662.959756

### 11...H<sub>2</sub>O

75	-0.170555000	0.002891000	-0.057318000
----	--------------	-------------	--------------

S71

6	-1.061880000	-0.014272000	1.726337000
8	-1.583935000	-0.023121000	2.754251000
6	1.201157000	1.372396000	0.452187000
8	1.984251000	2.176203000	0.696527000
6	1.126574000	-1.464584000	0.414189000
8	1.852419000	-2.318256000	0.652427000
1	0.584096000	0.012565000	-1.619975000
6	-1.319824000	1.455351000	-0.807992000
8	-1.953007000	2.287256000	-1.284824000
6	-1.381278000	-1.362900000	-0.879698000
8	-2.045942000	-2.141207000	-1.400742000
8	3.514480000	-0.090433000	-1.018617000
1	2.746374000	-0.047467000	-1.604396000
1	3.926535000	0.778601000	-1.099122000

E(RB3LYP) = -722.906662431

Zero-point correction=	0.072787 (Hartree/Particle)
Thermal correction to Energy=	0.088917
Thermal correction to Enthalpy=	0.089861
Thermal correction to Gibbs Free Energy=	0.026587
Sum of electronic and zero-point Energies=	-722.833876
Sum of electronic and thermal Energies=	-722.817746
Sum of electronic and thermal Enthalpies=	-722.816801
Sum of electronic and thermal Free Energies=	-722.880075

## 12...H<sub>2</sub>O

75	-0.158729000	-0.002927000	-0.031261000
15	-1.775997000	1.549467000	-0.887636000
15	1.653470000	-1.529186000	0.473834000
6	-1.055089000	-0.286471000	1.689709000
8	-1.605595000	-0.446274000	2.700405000
6	-1.096243000	-1.489731000	-0.954187000
8	-1.612618000	-2.344632000	-1.535117000
6	0.962339000	1.498267000	0.594952000
8	1.660328000	2.370010000	0.902473000
1	-1.340705000	2.846474000	-1.242984000
1	-2.433194000	1.229755000	-2.097266000
1	-2.920768000	1.932647000	-0.146418000
1	2.746761000	-1.084467000	1.242205000
1	2.357072000	-2.150594000	-0.575431000
1	1.329783000	-2.685542000	1.223566000
1	0.569336000	0.255022000	-1.603739000
8	3.381955000	0.371869000	-1.292416000
1	2.452476000	0.408089000	-1.573267000
1	3.523201000	1.223789000	-0.860692000

E(RB3LYP) = -1182.53855780

Zero-point correction=	0.113682 (Hartree/Particle)
Thermal correction to Energy=	0.130515
Thermal correction to Enthalpy=	0.131459
Thermal correction to Gibbs Free Energy=	0.067258
Sum of electronic and zero-point Energies=	-1182.424876
Sum of electronic and thermal Energies=	-1182.408043
Sum of electronic and thermal Enthalpies=	-1182.407099
Sum of electronic and thermal Free Energies=	-1182.471300



**13...H<sub>2</sub>O**

75	0.221070000	0.000213000	-0.092575000
15	-1.380303000	1.748798000	0.612258000
15	-1.375157000	-1.753994000	0.608881000
6	1.165726000	-0.000452000	1.630991000
8	1.728466000	-0.001392000	2.646727000
6	1.337304000	1.384727000	-0.872503000
8	1.985307000	2.210591000	-1.362949000
6	1.341739000	-1.379104000	-0.875218000
8	1.992724000	-2.201632000	-1.367330000
1	-1.919919000	2.609426000	-0.364024000
1	-2.580461000	1.393071000	1.263242000
1	-0.938402000	2.734244000	1.526370000
1	-1.912004000	-2.614877000	-0.368756000
1	-2.576801000	-1.402326000	1.259461000
1	-0.931632000	-2.739489000	1.522147000
1	-0.659988000	0.000630000	-1.602067000
8	-3.282385000	-0.001432000	-1.212803000
1	-2.359888000	-0.000558000	-1.532281000
1	-3.830768000	0.001762000	-2.006812000

E(RB3LYP) = -1182.54372112

Zero-point correction= 0.113731 (Hartree/Particle)

Thermal correction to Energy= 0.130463

Thermal correction to Enthalpy= 0.131407

Thermal correction to Gibbs Free Energy= 0.067938

Sum of electronic and zero-point Energies= -1182.429991

Sum of electronic and thermal Energies= -1182.413258

Sum of electronic and thermal Enthalpies= -1182.412314

Sum of electronic and thermal Free Energies= -1182.475783

**14...H<sub>2</sub>O**

75	0.144668000	0.000002000	-0.007882000
6	1.145889000	-0.000153000	1.643340000
8	1.773216000	-0.000246000	2.632127000
15	-1.392053000	1.677401000	0.710594000
1	-2.712732000	1.322290000	1.077468000
1	-1.103063000	2.488093000	1.839488000
1	-1.735594000	2.734058000	-0.170293000
15	1.448185000	1.674015000	-1.064252000
1	0.815301000	2.834607000	-1.583332000
1	2.511844000	2.351766000	-0.410840000
1	2.167857000	1.350010000	-2.246792000
15	1.446638000	-1.675558000	-1.063661000
15	-1.393461000	-1.675807000	0.711409000
1	2.166643000	-1.352621000	-2.246291000
1	2.509651000	-2.354095000	-0.410011000
1	0.812668000	-2.835715000	-1.582380000
1	-1.737825000	-2.732654000	-0.168916000
1	-1.104984000	-2.486101000	1.840718000
1	-2.713830000	-1.319467000	1.078152000
1	-0.680596000	0.000054000	-1.574099000
8	-3.338061000	0.000280000	-1.417774000
1	-2.365070000	0.000580000	-1.516667000
1	-3.676573000	-0.001099000	-2.321270000

E(RB3LYP) = -1642.14717911  
 Zero-point correction= 0.152768 (Hartree/Particle)  
 Thermal correction to Energy= 0.170790  
 Thermal correction to Enthalpy= 0.171735  
 Thermal correction to Gibbs Free Energy= 0.105660  
 Sum of electronic and zero-point Energies= -1641.994411  
 Sum of electronic and thermal Energies= -1641.976389  
 Sum of electronic and thermal Enthalpies= -1641.975445  
 Sum of electronic and thermal Free Energies= -1642.041519

### 15...H<sub>2</sub>O

75	0.140919000	0.000158000	-0.011984000
7	1.168736000	-0.022479000	1.697734000
7	1.765457000	-0.037541000	2.657050000
15	-1.288289000	1.772443000	0.667619000
1	-2.666510000	1.526961000	0.883029000
1	-1.047782000	2.497936000	1.868294000
1	-1.445529000	2.902475000	-0.176238000
15	1.549555000	1.569305000	-1.080831000
1	1.005162000	2.788780000	-1.565558000
1	2.683609000	2.147996000	-0.442661000
1	2.214310000	1.206462000	-2.283605000
15	1.356212000	-1.765113000	-1.003555000
15	-1.472094000	-1.563035000	0.771531000
1	2.060532000	-1.533636000	-2.216580000
1	2.415807000	-2.442740000	-0.335231000
1	0.677043000	-2.933584000	-1.441408000
1	-1.793226000	-2.694540000	-0.021811000
1	-1.255968000	-2.270314000	1.987711000
1	-2.800564000	-1.152842000	1.035909000
1	-0.675189000	0.015865000	-1.536151000
8	-3.335682000	0.039987000	-1.473123000
1	-3.616061000	-0.209126000	-2.362190000
1	-2.359215000	0.034704000	-1.514692000

E(RB3LYP) = -1638.31332487  
 Zero-point correction= 0.152492 (Hartree/Particle)  
 Thermal correction to Energy= 0.170718  
 Thermal correction to Enthalpy= 0.171662  
 Thermal correction to Gibbs Free Energy= 0.105129  
 Sum of electronic and zero-point Energies= -1638.160833  
 Sum of electronic and thermal Energies= -1638.142607  
 Sum of electronic and thermal Enthalpies= -1638.141663  
 Sum of electronic and thermal Free Energies= -1638.208196

### 16...H<sub>2</sub>O

75	-0.179658000	0.041551000	-0.049279000
15	1.408560000	1.752155000	0.508362000
15	-1.546242000	-1.659189000	-1.015536000
15	1.380698000	-1.670122000	0.789084000
8	-1.922118000	2.195752000	-1.422809000
8	-1.723609000	0.192587000	2.649943000
6	-1.274434000	1.386245000	-0.893829000
6	-1.138202000	0.147108000	1.642334000
1	1.940734000	2.557596000	-0.522013000
1	2.627644000	1.424435000	1.145895000

1	1.012266000	2.797677000	1.378118000
1	-0.973090000	-2.909766000	-1.361394000
1	-2.147816000	-1.392478000	-2.267426000
1	-2.698472000	-2.176118000	-0.369584000
1	1.049246000	-2.433338000	1.936259000
1	2.686365000	-1.296895000	1.176666000
1	1.734884000	-2.751097000	-0.050551000
1	0.664485000	-0.144068000	-1.582202000
8	3.309224000	-0.157833000	-1.327209000
1	3.747704000	-0.040943000	-2.178723000
1	2.353021000	-0.138191000	-1.528196000
E(RB3LYP) = -1412.34822211			
Zero-point correction=		0.133373 (Hartree/Particle)	
Thermal correction to Energy=		0.150803	
Thermal correction to Enthalpy=		0.151748	
Thermal correction to Gibbs Free Energy=		0.086774	
Sum of electronic and zero-point Energies=		-1412.214850	
Sum of electronic and thermal Energies=		-1412.197419	
Sum of electronic and thermal Enthalpies=		-1412.196475	
Sum of electronic and thermal Free Energies=		-1412.261448	

### 17...H<sub>2</sub>O

75	-0.131538000	-0.028525000	-0.090574000
15	1.176409000	1.650453000	0.972404000
15	-1.486050000	1.626639000	-1.105081000
15	1.454795000	-1.686849000	0.535570000
15	-1.517854000	-0.361365000	1.819774000
7	-1.070615000	-1.397154000	-1.172598000
7	-1.580673000	-2.161714000	-1.826340000
1	1.395239000	2.886488000	0.310709000
1	0.794520000	2.208181000	2.226772000
1	2.529545000	1.393267000	1.302933000
1	-2.023593000	1.337941000	-2.386499000
1	-2.691360000	2.144364000	-0.547881000
1	-0.923571000	2.887376000	-1.436677000
1	1.886056000	-2.616540000	-0.442983000
1	1.163095000	-2.644348000	1.549727000
1	2.733720000	-1.311801000	1.009627000
1	-1.462977000	0.541029000	2.922385000
1	-2.939749000	-0.362656000	1.727867000
1	-1.443719000	-1.541225000	2.619227000
1	0.830145000	0.250473000	-1.483411000
8	3.476311000	0.356819000	-1.190418000
1	3.847285000	0.275342000	-2.077457000
1	2.509720000	0.315793000	-1.325374000
E(RB3LYP) = -1638.31099454			
Zero-point correction=		0.152324	
Thermal correction to Energy=		0.170732	
Thermal correction to Enthalpy=		0.171676	
Thermal correction to Gibbs Free Energy=		0.104162	
Sum of electronic and zero-point Energies=		-1638.158670	
Sum of electronic and thermal Energies=		-1638.140263	
Sum of electronic and thermal Enthalpies=		-1638.139318	
Sum of electronic and thermal Free Energies=		-1638.206832	

**18...H<sub>2</sub>O**

26	0.132656000	0.007585000	-0.208838000
15	-1.527450000	1.262118000	0.736916000
1	-2.454071000	1.978790000	-0.044214000
1	-2.405824000	0.630581000	1.635863000
1	-1.033638000	2.291803000	1.562103000
6	-0.739355000	-1.510790000	0.235935000
8	-1.321354000	-2.474810000	0.467439000
1	-0.547998000	-0.115784000	-1.553736000
15	1.952275000	-1.183676000	-0.851504000
6	0.836944000	1.515296000	-0.923805000
1	2.070948000	-1.722494000	-2.155566000
1	3.194710000	-0.526480000	-0.761761000
1	2.247467000	-2.337720000	-0.099794000
8	1.250805000	2.461411000	-1.425803000
17	1.295792000	0.160167000	1.878907000
8	-3.365683000	-0.330355000	-1.131216000
1	-2.509810000	-0.305190000	-1.585760000
1	-3.507367000	-1.267191000	-0.946092000

E(RB3LYP) = -1573.68438956

Zero-point correction=	0.106907
Thermal correction to Energy=	0.123299
Thermal correction to Enthalpy=	0.124243
Thermal correction to Gibbs Free Energy=	0.062317
Sum of electronic and zero-point Energies=	-1573.577483
Sum of electronic and thermal Energies=	-1573.561091
Sum of electronic and thermal Enthalpies=	-1573.560147
Sum of electronic and thermal Free Energies=	-1573.622073

**19...H<sub>2</sub>O**

26	0.249697000	-0.023467000	-0.038108000
15	-1.504194000	-1.075118000	0.954736000
1	-2.384818000	-0.296267000	1.728698000
1	-2.435556000	-1.895383000	0.289703000
1	-1.041352000	-1.965036000	1.944882000
6	0.862722000	-1.596682000	-0.674192000
8	1.196548000	-2.568708000	-1.191692000
1	-0.273827000	0.026977000	-1.484021000
15	2.262558000	0.954812000	-0.271464000
6	-0.591731000	1.562490000	0.019384000
1	2.826164000	1.455619000	-1.472136000
1	2.451124000	2.078118000	0.554152000
1	3.334488000	0.156643000	0.167786000
8	-1.173607000	2.553795000	-0.066934000
9	0.991401000	-0.029960000	1.727302000
8	-3.188569000	0.262785000	-1.221983000
1	-2.322356000	0.124015000	-1.633981000
1	-3.245005000	1.221870000	-1.125352000

E(RB3LYP) = -1213.29493421

Zero-point correction=	0.107421 (Hartree/Particle)
Thermal correction to Energy=	0.123372
Thermal correction to Enthalpy=	0.124316
Thermal correction to Gibbs Free Energy=	0.063919
Sum of electronic and zero-point Energies=	-1213.187513
Sum of electronic and thermal Energies=	-1213.171563

Sum of electronic and thermal Enthalpies= -1213.170619  
 Sum of electronic and thermal Free Energies= -1213.231015

**20...H<sub>2</sub>O**

26	-0.062056000	-0.415896000	-0.000795000
15	1.364733000	-1.213659000	1.523458000
15	1.410284000	-1.171152000	-1.514777000
15	-1.620573000	0.160552000	-1.525261000
15	-1.615513000	0.223982000	1.511332000
7	0.764748000	1.457074000	-0.002649000
1	2.190855000	-0.344909000	2.280999000
1	0.944711000	-2.052155000	2.584873000
1	1.101039000	-2.333699000	-2.264991000
1	1.927646000	-0.396374000	-2.581624000
6	2.996072000	-1.693172000	-0.664817000
6	2.645258000	-2.306636000	0.697690000
1	-2.072620000	-0.719806000	-2.538132000
1	-1.372737000	1.287883000	-2.345508000
1	-2.394998000	-0.747279000	2.182833000
1	-1.307179000	1.034366000	2.629593000
6	-3.235973000	0.624330000	-0.699770000
6	-2.925057000	1.255196000	0.664716000
6	1.094119000	2.214983000	1.095730000
6	1.661601000	3.424612000	0.710280000
6	1.687847000	3.416088000	-0.705080000
6	1.133203000	2.202545000	-1.096908000
1	3.581434000	-2.378807000	-1.284168000
1	3.581093000	-0.776725000	-0.530468000
1	3.530626000	-2.431074000	1.327708000
1	2.183599000	-3.291451000	0.567752000
1	-3.826673000	1.292598000	-1.332710000
1	-3.777147000	-0.316930000	-0.565688000
1	-3.823409000	1.345024000	1.282160000
1	-2.489167000	2.252909000	0.545638000
1	0.917559000	1.848895000	2.099408000
1	2.010551000	4.209451000	1.370173000
1	2.061437000	4.192882000	-1.360995000
1	0.977405000	1.832571000	-2.102414000
1	-0.616483000	-1.876498000	0.007970000
8	-3.136820000	-2.533382000	0.076816000
1	-2.181249000	-2.314338000	0.073800000
1	-3.217896000	-3.259232000	-0.553832000

E(RB3LYP) = -1937.51354699

Zero-point correction= 0.296301 (Hartree/Particle)

Thermal correction to Energy= 0.318134

Thermal correction to Enthalpy= 0.319078

Thermal correction to Gibbs Free Energy= 0.245044

Sum of electronic and zero-point Energies= -1937.217246

Sum of electronic and thermal Energies= -1937.195413

Sum of electronic and thermal Enthalpies= -1937.194469

Sum of electronic and thermal Free Energies= -1937.268503

**21...H<sub>2</sub>O**

26	0.133489000	0.013834000	-0.052371000
----	-------------	-------------	--------------

15	-1.494970000	1.421830000	0.574687000
15	-1.508394000	-1.494288000	-0.290646000
15	1.747499000	-1.415943000	-0.595677000
15	1.732139000	1.550838000	0.052407000
6	-2.991238000	0.419509000	1.076306000
1	-2.763926000	0.028712000	2.073383000
1	-3.885905000	1.044851000	1.145992000
6	-3.177503000	-0.724247000	0.068909000
1	-3.527127000	-0.331676000	-0.890152000
1	-3.888680000	-1.472082000	0.430783000
6	3.410243000	-0.647455000	-0.209087000
1	3.554021000	-0.773466000	0.869242000
1	4.226463000	-1.162839000	-0.723432000
6	3.354964000	0.843661000	-0.570839000
1	3.359367000	0.974356000	-1.658612000
1	4.209949000	1.392064000	-0.165565000
7	0.485828000	-0.769692000	2.949518000
6	0.348897000	-0.475238000	1.822463000
1	0.040176000	0.405171000	-1.560289000
1	1.674303000	2.766443000	-0.671430000
1	-1.495990000	-2.616763000	0.572121000
1	-1.321991000	2.256311000	1.703645000
1	1.938336000	-1.850258000	-1.932358000
1	1.876725000	-2.678304000	0.032033000
1	2.122479000	2.095169000	1.301909000
1	-2.054099000	2.381783000	-0.302362000
1	-1.774949000	-2.182678000	-1.497974000
8	-2.297866000	0.773093000	-2.675374000
1	-1.414938000	0.661903000	-2.263081000
1	-2.179081000	0.470782000	-3.583916000

E(RB3LYP) = -1820.80182859

Zero-point correction= 0.233356 (Hartree/Particle)

Thermal correction to Energy= 0.252680

Thermal correction to Enthalpy= 0.253624

Thermal correction to Gibbs Free Energy= 0.185915

Sum of electronic and zero-point Energies= -1820.568473

Sum of electronic and thermal Energies= -1820.549148

Sum of electronic and thermal Enthalpies= -1820.548204

Sum of electronic and thermal Free Energies= -1820.615913

## 22...H<sub>2</sub>O

26	-0.115157000	-0.026072000	0.141998000
15	-1.731120000	-1.567011000	0.131258000
15	-1.744340000	1.448559000	0.573249000
15	1.532633000	1.508031000	0.198480000
15	1.511925000	-1.475181000	-0.441507000
1	-2.079703000	-2.202177000	-1.085772000
1	-1.710290000	-2.717741000	0.957477000
1	-1.974243000	1.938983000	1.885174000
1	-1.849648000	2.680039000	-0.115986000
6	-3.396531000	0.662576000	0.177472000
6	-3.366681000	-0.800154000	0.644661000
1	1.840633000	2.302826000	1.329199000
1	1.474692000	2.542485000	-0.765375000

1	2.109382000	-2.358627000	0.489864000
1	1.311215000	-2.393479000	-1.498078000
6	3.193288000	0.713333000	-0.147879000
6	2.984116000	-0.502566000	-1.062119000
1	-4.228235000	1.215867000	0.623314000
1	-3.493000000	0.714145000	-0.911739000
1	-4.214353000	-1.368697000	0.251761000
1	-3.409746000	-0.853068000	1.738372000
1	3.895438000	1.430949000	-0.581772000
1	3.567185000	0.392353000	0.828699000
1	3.881311000	-1.126122000	-1.115098000
1	2.719509000	-0.186291000	-2.075941000
1	0.009653000	-0.302574000	1.649990000
17	-0.452880000	0.407779000	-2.220079000
8	2.380030000	-0.563119000	2.739824000
1	1.485128000	-0.503416000	2.344090000
1	2.296262000	-0.109983000	3.587623000

E(RB3LYP) = -2188.18753310

Zero-point correction=	0.226014 (Hartree/Particle)
Thermal correction to Energy=	0.244847
Thermal correction to Enthalpy=	0.245791
Thermal correction to Gibbs Free Energy=	0.179206
Sum of electronic and zero-point Energies=	-2187.961519
Sum of electronic and thermal Energies=	-2187.942687
Sum of electronic and thermal Enthalpies=	-2187.941742
Sum of electronic and thermal Free Energies=	-2188.008327

### 23...H<sub>2</sub>O

44	-0.093821000	-0.260052000	0.016149000
15	1.081225000	-1.743742000	-1.400838000
15	-0.799463000	1.730941000	1.115310000
8	3.459657000	2.050340000	-0.640005000
8	0.271320000	-1.931820000	2.668756000
8	-2.905473000	-1.174093000	-0.700758000
7	1.841509000	0.560378000	0.316462000
6	2.628530000	1.317093000	-0.194343000
6	0.136183000	-1.319888000	1.708343000
6	-1.833031000	-0.865056000	-0.392999000
1	0.419162000	-2.648261000	-2.262361000
1	2.011199000	-2.634873000	-0.824076000
1	1.921837000	-1.108016000	-2.331938000
1	-0.559414000	2.936429000	0.438377000
1	-2.123019000	1.940814000	1.547457000
1	-0.104866000	1.980784000	2.316818000
1	-0.173952000	0.630033000	-1.354988000
8	-2.669780000	2.135287000	-1.304446000
1	-1.877463000	1.740594000	-1.696633000
1	-3.338223000	1.443529000	-1.389914000

E(RB3LYP) = -1252.05258290

Zero-point correction=	0.118672 (Hartree/Particle)
Thermal correction to Energy=	0.137112
Thermal correction to Enthalpy=	0.138056
Thermal correction to Gibbs Free Energy=	0.070053
Sum of electronic and zero-point Energies=	-1251.933911

Sum of electronic and thermal Energies= -1251.915471  
 Sum of electronic and thermal Enthalpies= -1251.914527  
 Sum of electronic and thermal Free Energies= -1251.982530

**24...H<sub>2</sub>O**

44	-0.165856000	-0.057308000	-0.019234000
15	1.727799000	-1.538182000	0.466190000
14	-1.873087000	1.514852000	-0.901153000
8	1.355948000	2.517449000	0.769676000
8	-1.755665000	-0.431200000	2.644417000
8	-1.708815000	-2.174581000	-1.674308000
6	0.778780000	1.553372000	0.523695000
6	-1.144488000	-0.313560000	1.677930000
6	-1.148520000	-1.411213000	-1.024810000
1	2.485253000	-2.075811000	-0.590987000
1	1.448261000	-2.745371000	1.150792000
1	2.784941000	-1.088034000	1.280166000
1	-2.982322000	1.773041000	0.064735000
1	-1.293976000	2.848443000	-1.234015000
1	-2.514391000	1.014497000	-2.150452000
1	0.494708000	0.255313000	-1.506692000
8	3.384861000	0.519583000	-1.140345000
1	3.533673000	1.418737000	-0.821948000
1	2.522482000	0.563948000	-1.578413000

E(RB3LYP) = -1145.44607879

Zero-point correction= 0.109854 (Hartree/Particle)

Thermal correction to Energy= 0.127478

Thermal correction to Enthalpy= 0.128422

Thermal correction to Gibbs Free Energy= 0.062812

Sum of electronic and zero-point Energies= -1145.336225

Sum of electronic and thermal Energies= -1145.318601

Sum of electronic and thermal Enthalpies= -1145.317657

Sum of electronic and thermal Free Energies= -1145.383267

**25...H<sub>2</sub>O**

44	-0.035082000	0.141652000	-0.058023000
15	-1.456205000	1.800719000	-0.925427000
15	-1.455884000	-0.429074000	1.874589000
15	1.343244000	-1.776295000	0.151865000
8	1.944485000	2.005102000	1.258764000
17	-1.597171000	-1.415034000	-1.252283000
1	-1.686888000	1.711135000	-2.310829000
1	-1.132149000	3.175732000	-0.837953000
1	-2.799444000	1.881381000	-0.489301000
1	-2.835693000	-0.136475000	1.773198000
1	-1.590843000	-1.796297000	2.208441000
1	-1.265159000	0.061356000	3.192279000
1	0.693574000	-2.927395000	0.651054000
1	2.501512000	-1.800730000	0.956016000
1	1.868632000	-2.307085000	-1.037995000
6	1.162889000	1.294251000	0.772711000
1	0.735053000	0.373566000	-1.450751000
8	3.590561000	0.091097000	-1.028810000



1	3.741431000	0.789110000	-0.378473000
1	2.740458000	0.333246000	-1.425171000
E(RB3LYP) = -1774.01721458			
Zero-point correction=		0.126330 (Hartree/Particle)	
Thermal correction to Energy=		0.143742	
Thermal correction to Enthalpy=		0.144686	
Thermal correction to Gibbs Free Energy=		0.080350	
Sum of electronic and zero-point Energies=		-1773.890885	
Sum of electronic and thermal Energies=		-1773.873472	
Sum of electronic and thermal Enthalpies=		-1773.872528	
Sum of electronic and thermal Free Energies=		-1773.936864	

### 26...H<sub>2</sub>O

44	-0.099228000	-0.101394000	-0.049010000
15	1.619614000	1.513595000	-0.108061000
15	-1.623467000	-1.712588000	-0.789228000
8	0.692133000	-1.453529000	2.549065000
6	0.390438000	-0.932074000	1.556551000
1	2.748236000	1.506239000	0.734037000
1	1.227535000	2.864486000	0.059966000
1	2.243047000	1.635199000	-1.361521000
1	-1.447517000	-2.053817000	-2.144336000
1	-1.712285000	-3.011585000	-0.238028000
1	-3.009463000	-1.422551000	-0.836317000
1	0.931976000	-1.034350000	-0.855846000
15	-1.808119000	1.490946000	0.723906000
1	-3.078139000	1.379708000	0.111407000
1	-2.268149000	1.702515000	2.049245000
1	-1.584945000	2.847859000	0.393299000
9	-0.656256000	0.821601000	-1.795490000
8	3.629391000	-0.919455000	-0.586284000
1	3.786063000	-0.961420000	-1.538233000
1	2.700744000	-1.188324000	-0.498627000
E(RB3LYP) = -1413.62632925			
Zero-point correction=		0.126587 (Hartree/Particle)	
Thermal correction to Energy=		0.143935	
Thermal correction to Enthalpy=		0.144879	
Thermal correction to Gibbs Free Energy=		0.080086	
Sum of electronic and zero-point Energies=		-1413.499743	
Sum of electronic and thermal Energies=		-1413.482394	
Sum of electronic and thermal Enthalpies=		-1413.481450	
Sum of electronic and thermal Free Energies=		-1413.546244	

### 27...H<sub>2</sub>O

44	-0.091901000	-0.055379000	-0.053478000
15	1.532264000	-1.607224000	0.763457000
15	-1.264968000	-1.650020000	-1.263540000
15	-1.523750000	-0.080780000	1.835383000
15	1.134296000	1.809320000	0.631640000
14	-1.567103000	1.576896000	-1.127756000
1	2.032984000	-2.634984000	-0.075234000
1	1.245601000	-2.451894000	1.872520000
1	2.790570000	-1.156382000	1.230699000
1	-1.460875000	-1.431438000	-2.644725000

1	-0.797875000	-2.989316000	-1.363997000
1	-2.610328000	-1.979489000	-0.948082000
1	-2.884200000	-0.446066000	1.663312000
1	-1.307707000	-0.884080000	2.992473000
1	-1.781592000	1.121617000	2.543815000
1	0.531300000	2.748518000	1.508918000
1	2.354669000	1.666809000	1.338436000
1	1.582446000	2.728777000	-0.338336000
1	-2.765344000	1.999637000	-0.315983000
1	-2.179408000	1.127870000	-2.425067000
1	-0.920264000	2.887923000	-1.477657000
1	0.705805000	0.098019000	-1.477282000
8	3.388014000	0.269320000	-1.244419000
1	3.746890000	0.548104000	-2.095749000
1	2.428665000	0.182512000	-1.395192000

E(RB3LYP) = -1834.88993224

Zero-point correction= 0.168861 (Hartree/Particle)

Thermal correction to Energy= 0.188162

Thermal correction to Enthalpy= 0.189107

Thermal correction to Gibbs Free Energy= 0.121161

Sum of electronic and zero-point Energies= -1834.721072

Sum of electronic and thermal Energies= -1834.701770

Sum of electronic and thermal Enthalpies= -1834.700826

Sum of electronic and thermal Free Energies= -1834.768772

## 28...H<sub>2</sub>O

44	-0.098001000	0.137348000	0.145532000
15	-1.829311000	-0.812361000	1.380385000
15	-1.808917000	1.372439000	-0.842020000
15	1.632855000	0.987266000	-1.187634000
15	1.590926000	-1.252909000	0.980764000
1	-2.133240000	-2.174075000	1.142359000
1	-1.898458000	-0.836373000	2.795732000
1	-2.101229000	2.712487000	-0.476446000
1	-1.884257000	1.535769000	-2.245345000
6	-3.436877000	0.516587000	-0.487165000
6	-3.458671000	0.028663000	0.968044000
1	2.008891000	2.350398000	-1.261257000
1	1.533938000	0.729913000	-2.575439000
1	2.237103000	-1.012048000	2.217371000
1	1.366969000	-2.640702000	1.137023000
6	3.264704000	0.187490000	-0.730103000
6	3.020327000	-1.241705000	-0.226854000
1	-4.286915000	1.170121000	-0.704995000
1	-3.468879000	-0.334748000	-1.174647000
1	-4.300579000	-0.645478000	1.150500000
1	-3.557801000	0.876549000	1.655302000
1	3.954457000	0.199203000	-1.579098000
1	3.674303000	0.809266000	0.071489000
1	3.921279000	-1.662304000	0.229788000
1	2.710008000	-1.895107000	-1.048710000
1	0.095325000	1.261727000	1.291652000
17	-0.522211000	-1.648166000	-1.675983000
8	2.617601000	1.949444000	1.945043000

1	2.547977000	2.903602000	2.069601000
1	1.709727000	1.669020000	1.717111000
E(RB3LYP) = -2158.69977976			
Zero-point correction=		0.225985 (Hartree/Particle)	
Thermal correction to Energy=		0.245093	
Thermal correction to Enthalpy=		0.246037	
Thermal correction to Gibbs Free Energy=		0.178200	
Sum of electronic and zero-point Energies=		-2158.473795	
Sum of electronic and thermal Energies=		-2158.454687	
Sum of electronic and thermal Enthalpies=		-2158.453742	
Sum of electronic and thermal Free Energies=		-2158.521580	

### 29...H<sub>2</sub>O

44	-0.225987000	0.047343000	-0.213266000
17	-0.539348000	-1.560031000	1.771187000
15	-2.170177000	-0.564896000	-1.233692000
15	-1.208939000	1.770071000	0.902602000
7	0.939368000	-1.599259000	-1.087339000
1	0.395691000	-2.455271000	-0.997715000
1	1.116205000	-1.435066000	-2.075262000
7	1.723531000	0.410495000	0.705199000
1	1.963115000	1.403604000	0.698988000
1	1.606753000	0.071977000	1.661428000
6	2.211777000	-1.747761000	-0.332219000
1	2.950538000	-2.338439000	-0.888452000
1	1.961735000	-2.273750000	0.592640000
6	2.764691000	-0.367549000	-0.001817000
1	3.681004000	-0.465878000	0.595147000
1	3.018451000	0.179031000	-0.915341000
1	-2.890112000	0.302834000	-2.097369000
1	-3.281570000	-1.009362000	-0.470379000
1	-2.141750000	-1.672500000	-2.129102000
1	-1.727510000	2.923570000	0.253204000
1	-2.326732000	1.533047000	1.743379000
1	-0.427424000	2.470468000	1.861193000
1	0.106052000	0.989489000	-1.500162000
8	1.837690000	2.888087000	-0.701995000
1	1.443605000	3.766830000	-0.752166000
1	1.150403000	2.277754000	-1.044998000
E(RB3LYP) = -1508.07406696			
Zero-point correction=		0.206250 (Hartree/Particle)	
Thermal correction to Energy=		0.223147	
Thermal correction to Enthalpy=		0.224091	
Thermal correction to Gibbs Free Energy=		0.161434	
Sum of electronic and zero-point Energies=		-1507.867817	
Sum of electronic and thermal Energies=		-1507.850920	
Sum of electronic and thermal Enthalpies=		-1507.849976	
Sum of electronic and thermal Free Energies=		-1507.912633	

### 30...H<sub>2</sub>O

44	-0.083199000	-0.205063000	0.016054000
17	-0.880039000	2.243022000	-0.130766000
15	-1.929724000	-0.704251000	-1.360245000
15	-1.945181000	-0.556746000	1.414295000

15	1.716390000	0.365683000	-1.393550000
15	1.695157000	0.502703000	1.387144000
1	0.323639000	-1.765588000	0.108728000
6	-3.192273000	-0.482595000	0.012258000
1	-4.023235000	-1.190584000	0.044850000
1	-3.572537000	0.540034000	-0.044585000
6	2.906770000	0.815167000	-0.013950000
1	3.720324000	0.089408000	0.026685000
1	3.297508000	1.833324000	-0.061566000
1	-2.252873000	-1.976495000	-1.894673000
1	-2.419961000	0.092904000	-2.421370000
1	-2.270355000	-1.767105000	2.075152000
1	-2.448321000	0.345843000	2.380796000
1	1.645053000	1.528884000	-2.193633000
1	2.487381000	-0.444623000	-2.260341000
1	1.631756000	1.730693000	2.084460000
1	2.448301000	-0.242123000	2.324927000
8	2.957159000	-2.338393000	0.120651000
1	1.993171000	-2.180081000	0.135684000
1	3.067683000	-3.102233000	-0.458197000

E(RB3LYP) = -2080.02373960

Zero-point correction= 0.166541 (Hartree/Particle)

Thermal correction to Energy= 0.183906

Thermal correction to Enthalpy= 0.184850

Thermal correction to Gibbs Free Energy= 0.120337

Sum of electronic and zero-point Energies= -2079.857198

Sum of electronic and thermal Energies= -2079.839834

Sum of electronic and thermal Enthalpies= -2079.838890

Sum of electronic and thermal Free Energies= -2079.903403

### 31...H<sub>2</sub>O

42	-0.201386000	-0.017952000	0.020359000
15	1.876153000	-1.345670000	0.559645000
15	-1.976044000	1.344440000	-1.063118000
7	-1.065466000	-0.286318000	1.631015000
8	-1.679977000	-0.428578000	2.628303000
6	0.784580000	1.700734000	0.568282000
8	1.379107000	2.657091000	0.821651000
1	2.533593000	-2.067705000	-0.454353000
1	1.685682000	-2.406021000	1.478759000
1	3.002524000	-0.754868000	1.166367000
1	-2.575341000	0.876024000	-2.254763000
1	-3.168106000	1.662728000	-0.367111000
1	-1.671496000	2.649126000	-1.514965000
1	0.491787000	0.301870000	-1.634922000
8	3.221521000	0.468926000	-1.489845000
1	2.276942000	0.439245000	-1.726440000
1	3.344917000	1.366680000	-1.156709000
6	-0.956019000	-1.692835000	-0.916411000
8	-1.355278000	-2.614664000	-1.481008000

E(RB+HF-LYP) = -1187.52107961

Zero-point correction= 0.111019 (Hartree/Particle)

Thermal correction to Energy= 0.128453

Thermal correction to Enthalpy= 0.129397  
 Thermal correction to Gibbs Free Energy= 0.063881  
 Sum of electronic and zero-point Energies= -1187.410061  
 Sum of electronic and thermal Energies= -1187.392627  
 Sum of electronic and thermal Enthalpies= -1187.391683  
 Sum of electronic and thermal Free Energies= -1187.457199

### 32...H<sub>2</sub>O

42	-0.643186000	0.011511000	0.037543000
1	0.001629000	0.513546000	1.662287000
15	1.333027000	1.286727000	-0.928580000
15	1.205413000	-1.707484000	0.234067000
6	-1.778515000	1.683640000	0.228449000
6	-1.908576000	-1.042496000	1.222696000
7	-1.405098000	-0.539574000	-1.553558000
8	-1.945824000	-0.903022000	-2.537633000
6	2.773553000	0.119674000	-1.217712000
1	2.584810000	-0.369979000	-2.180045000
1	3.706506000	0.683252000	-1.308524000
1	3.620841000	-1.676920000	-0.313699000
6	2.871158000	-0.913556000	-0.085795000
1	3.143488000	-0.412068000	0.848869000
1	1.275933000	1.960328000	-2.171073000
1	1.928273000	2.311317000	-0.164179000
1	1.455789000	-2.403685000	1.436860000
1	1.235824000	-2.823910000	-0.638169000
8	-2.608021000	-1.635277000	1.923429000
8	-2.405272000	2.643638000	0.360241000
8	2.459929000	1.196034000	2.286996000
1	2.558662000	1.321479000	3.238439000
1	1.508920000	1.006973000	2.154926000

E(RB3LYP) = -1264.96148132

Zero-point correction= 0.150868 (Hartree/Particle)  
 Thermal correction to Energy= 0.168940  
 Thermal correction to Enthalpy= 0.169884  
 Thermal correction to Gibbs Free Energy= 0.102901  
 Sum of electronic and zero-point Energies= -1264.810614  
 Sum of electronic and thermal Energies= -1264.792541  
 Sum of electronic and thermal Enthalpies= -1264.791597  
 Sum of electronic and thermal Free Energies= -1264.858580

### 33...H<sub>2</sub>O

42	-0.163398000	0.050645000	0.048431000
15	1.865435000	-1.274071000	0.723333000
15	-1.175620000	-2.074462000	-0.873824000
15	-1.898793000	1.356954000	-1.130375000
7	-0.983209000	0.038185000	1.694097000
8	-1.573995000	0.050663000	2.721123000
6	0.873242000	1.736482000	0.373340000
8	1.509042000	2.694633000	0.527836000
1	2.444078000	-2.211877000	-0.158176000
1	1.695405000	-2.138568000	1.834847000
1	3.052953000	-0.647529000	1.152700000
1	-2.020495000	-2.912327000	-0.101809000

1	-2.014070000	-2.000920000	-2.014590000
1	-0.331019000	-3.099649000	-1.365376000
1	-2.679279000	0.764369000	-2.157542000
1	-2.973969000	1.943028000	-0.416121000
1	-1.516814000	2.508059000	-1.857612000
1	0.473625000	0.065487000	-1.670953000
8	3.184144000	0.194936000	-1.630307000
1	2.222395000	0.170888000	-1.792981000
1	3.334064000	1.097605000	-1.321448000
E(RB+HF-LYP) = -1417.33587737			
Zero-point correction=		0.130727 (Hartree/Particle)	
Thermal correction to Energy=		0.148730	
Thermal correction to Enthalpy=		0.149674	
Thermal correction to Gibbs Free Energy=		0.083300	
Sum of electronic and zero-point Energies=		-1417.205150	
Sum of electronic and thermal Energies=		-1417.187148	
Sum of electronic and thermal Enthalpies=		-1417.186204	
Sum of electronic and thermal Free Energies=		-1417.252578	

### 34...H<sub>2</sub>O

42	0.135210000	-0.252122000	-0.005536000
15	1.947531000	0.294078000	-1.565050000
15	1.909161000	0.253051000	1.601819000
15	-1.765184000	-0.229458000	1.571607000
15	-1.747384000	-0.053876000	-1.588584000
6	3.573919000	0.569176000	-0.643897000
1	4.035496000	-0.420578000	-0.547056000
1	4.255242000	1.195016000	-1.227992000
6	3.316878000	1.167946000	0.744984000
1	2.989793000	2.209670000	0.657794000
1	4.222609000	1.149451000	1.358728000
6	-3.397592000	-0.447985000	0.656709000
1	-3.516867000	-1.526882000	0.502591000
1	-4.234110000	-0.104665000	1.272571000
6	-3.363068000	0.292177000	-0.687455000
1	-3.371096000	1.374268000	-0.519022000
1	-4.218893000	0.020535000	-1.312800000
8	0.522962000	-3.245880000	-0.117086000
7	0.337602000	-2.067001000	-0.073100000
1	0.086541000	1.592244000	0.069618000
1	-1.834649000	0.911387000	-2.623217000
1	2.632132000	-0.784356000	2.250209000
1	2.407518000	-0.570671000	-2.592222000
1	-2.041998000	0.920092000	2.349978000
1	-1.932188000	-1.186337000	2.604791000
1	-2.102635000	-1.177745000	-2.379178000
1	1.888418000	1.470256000	-2.354727000
1	1.750725000	1.082237000	2.741259000
8	-2.015353000	3.134301000	0.141097000
1	-1.849786000	3.782162000	-0.554838000
1	-1.211858000	2.569862000	0.136712000
E(RB3LYP) = -1802.01666245			
Zero-point correction=		0.230368	
Thermal correction to Energy=		0.250064	

Thermal correction to Enthalpy=	0.251008
Thermal correction to Gibbs Free Energy=	0.181475
Sum of electronic and zero-point Energies=	-1801.786294
Sum of electronic and thermal Energies=	-1801.766599
Sum of electronic and thermal Enthalpies=	-1801.765654
Sum of electronic and thermal Free Energies=	-1801.835188

### 35...H<sub>2</sub>O

42	-0.163398000	0.050645000	0.048431000
15	1.865435000	-1.274071000	0.723333000
15	-1.175620000	-2.074462000	-0.873824000
15	-1.898793000	1.356954000	-1.130375000
7	-0.983209000	0.038185000	1.694097000
8	-1.573995000	0.050663000	2.721123000
6	0.873242000	1.736482000	0.373340000
8	1.509042000	2.694633000	0.527836000
1	2.444078000	-2.211877000	-0.158176000
1	1.695405000	-2.138568000	1.834847000
1	3.052953000	-0.647529000	1.152700000
1	-2.020495000	-2.912327000	-0.101809000
1	-2.014070000	-2.000920000	-2.014590000
1	-0.331019000	-3.099649000	-1.365376000
1	-2.679279000	0.764369000	-2.157542000
1	-2.973969000	1.943028000	-0.416121000
1	-1.516814000	2.508059000	-1.857612000
1	0.473625000	0.065487000	-1.670953000
8	3.184144000	0.194936000	-1.630307000
1	2.222395000	0.170888000	-1.792981000
1	3.334064000	1.097605000	-1.321448000

E(RB+HF-LYP) = -1417.33587737

Zero-point correction=	0.130727
Thermal correction to Energy=	0.148730
Thermal correction to Enthalpy=	0.149674
Thermal correction to Gibbs Free Energy=	0.083300
Sum of electronic and zero-point Energies=	-1417.205150
Sum of electronic and thermal Energies=	-1417.187148
Sum of electronic and thermal Enthalpies=	-1417.186204
Sum of electronic and thermal Free Energies=	-1417.252578

### 36...H<sub>2</sub>O

42	0.093930000	-0.303583000	0.254411000
1	0.238575000	1.124913000	-0.909648000
15	-1.805854000	0.899770000	1.316962000
15	-1.756600000	-1.089964000	-1.206013000
15	1.935676000	0.992875000	1.253849000
15	1.944594000	-1.118926000	-1.164162000
7	0.098488000	-1.703085000	1.426796000
8	0.150089000	-2.611137000	2.202522000
6	-3.402365000	0.192146000	0.652217000
1	-3.489270000	-0.781533000	1.159808000
6	-4.740669000	0.941946000	0.760609000
1	-5.182026000	0.869983000	1.759180000
1	-4.583760000	2.005838000	0.549511000
6	-5.638662000	0.301062000	-0.344761000

1	-6.143716000	1.077786000	-0.926697000
1	-6.422478000	-0.325919000	0.091353000
6	-4.686674000	-0.547971000	-1.243841000
1	-4.794386000	-1.613788000	-1.008262000
1	-4.897153000	-0.428435000	-2.310576000
6	-3.277726000	-0.064465000	-0.865850000
1	-3.068885000	0.898003000	-1.353655000
1	-2.054030000	0.857276000	2.713686000
1	-2.020838000	2.291462000	1.148866000
1	-1.723719000	-1.076735000	-2.623911000
1	-2.265077000	-2.407683000	-1.056445000
6	3.563153000	-0.482708000	-0.475493000
1	3.762803000	-1.142998000	0.383128000
6	4.836021000	-0.367076000	-1.330744000
1	5.334458000	-1.330616000	-1.471432000
1	4.577921000	0.011394000	-2.326745000
6	5.726161000	0.668425000	-0.572726000
1	6.126741000	1.413258000	-1.267155000
1	6.586628000	0.185537000	-0.099744000
6	4.806469000	1.332388000	0.499043000
1	4.950291000	2.414701000	0.567767000
1	5.017371000	0.914357000	1.490502000
6	3.380871000	0.951085000	0.068678000
1	3.064396000	1.594260000	-0.765549000
1	2.573663000	0.581930000	2.456147000
1	1.882935000	2.378788000	1.559627000
1	2.264904000	-2.488821000	-1.356203000
1	2.048327000	-0.725512000	-2.523342000
8	-1.664652000	2.616516000	-1.884680000
1	-0.928767000	2.061410000	-1.545953000
1	-1.539583000	3.464870000	-1.442189000
E(RB3LYP) = -2035.47444958			
Zero-point correction=			0.359263
Thermal correction to Energy=			0.384326
Thermal correction to Enthalpy=			0.385270
Thermal correction to Gibbs Free Energy=			0.302790
Sum of electronic and zero-point Energies=			-2035.115186
Sum of electronic and thermal Energies=			-2035.090123
Sum of electronic and thermal Enthalpies=			-2035.089179
Sum of electronic and thermal Free Energies=			-2035.171660

### 37...H<sub>2</sub>O

74	0.212990000	0.031896000	-0.038524000
1	-0.570811000	0.128851000	-1.673750000
8	-1.602687000	2.591264000	0.631729000
8	1.554778000	-2.567962000	-1.367343000
8	2.384214000	1.884466000	-1.450385000
8	1.709298000	-0.110447000	2.593230000
15	-1.772749000	-1.439315000	0.633335000
6	-0.927084000	1.681985000	0.420385000
6	1.091615000	-1.640446000	-0.868434000
6	1.607616000	1.213842000	-0.926974000
7	1.102205000	-0.064025000	1.583649000
1	-1.474514000	-2.476055000	1.548736000



1	-2.889791000	-0.889501000	1.288345000
1	-2.428324000	-2.197392000	-0.352275000
8	-3.318308000	0.223489000	-1.334236000
1	-3.544858000	1.145020000	-1.156801000
1	-2.428406000	0.267907000	-1.722869000
E(RB3LYP) = -958.009883348			
Zero-point correction=		0.091769	
Thermal correction to Energy=		0.108287	
Thermal correction to Enthalpy=		0.109231	
Thermal correction to Gibbs Free Energy=		0.045673	
Sum of electronic and zero-point Energies=		-957.918115	
Sum of electronic and thermal Energies=		-957.901596	
Sum of electronic and thermal Enthalpies=		-957.900652	
Sum of electronic and thermal Free Energies=		-957.964210	

### 38...H<sub>2</sub>O

74	-0.158311000	-0.011195000	0.001239000
15	1.884903000	-1.362868000	0.538327000
15	-1.937333000	1.374664000	-1.030376000
7	-1.001482000	-0.274918000	1.617482000
8	-1.593411000	-0.423144000	2.634136000
6	0.841308000	1.681517000	0.560843000
8	1.445439000	2.630505000	0.830972000
1	2.533422000	-2.081609000	-0.483307000
1	1.671433000	-2.425104000	1.448805000
1	3.012604000	-0.783629000	1.152756000
1	-2.581368000	0.916194000	-2.202602000
1	-3.095059000	1.699626000	-0.283822000
1	-1.626926000	2.676617000	-1.486368000
1	0.541110000	0.293295000	-1.659513000
8	3.285328000	0.440671000	-1.472610000
1	2.348475000	0.442591000	-1.737013000
1	3.428931000	1.332239000	-1.130841000
6	-0.956957000	-1.670219000	-0.901564000
8	-1.390713000	-2.593292000	-1.443385000
E(RB+HF-LYP) = -1187.82408157			
Zero-point correction=		0.111692	
Thermal correction to Energy=		0.128893	
Thermal correction to Enthalpy=		0.129837	
Thermal correction to Gibbs Free Energy=		0.064514	
Sum of electronic and zero-point Energies=		-1187.712390	
Sum of electronic and thermal Energies=		-1187.695188	
Sum of electronic and thermal Enthalpies=		-1187.694244	
Sum of electronic and thermal Free Energies=		-1187.759568	

### 39...H<sub>2</sub>O

74	0.149993000	0.000335000	0.011767000
15	-1.456119000	1.768829000	0.616125000
15	1.579645000	1.672737000	-1.057738000
15	1.495927000	-1.760866000	-1.020450000
7	1.028122000	-0.004208000	1.608264000
8	1.644808000	-0.007817000	2.635912000
1	-1.765131000	2.803313000	-0.302362000
1	-1.143372000	2.596868000	1.723375000

1	-2.793038000	1.469202000	0.981419000
1	2.592764000	2.319784000	-0.305052000
1	2.393289000	1.327231000	-2.174003000
1	1.028271000	2.844129000	-1.643639000
1	2.325457000	-1.479215000	-2.142924000
1	2.475986000	-2.440748000	-0.253162000
1	0.887823000	-2.915801000	-1.582290000
1	-0.617964000	0.003459000	-1.669891000
8	-3.266664000	0.011626000	-1.533712000
1	-2.298832000	0.013925000	-1.678709000
1	-3.649869000	-0.064520000	-2.415989000
15	-1.536526000	-1.679118000	0.658498000
1	-1.894677000	-2.718480000	-0.235785000
1	-1.250565000	-2.496160000	1.781192000
1	-2.855501000	-1.312553000	1.025121000

E(RB+HF-LYP) = -1647.43889764  
Zero-point correction= 0.150339  
Thermal correction to Energy= 0.168899  
Thermal correction to Enthalpy= 0.169843  
Thermal correction to Gibbs Free Energy= 0.102265  
Sum of electronic and zero-point Energies= -1647.288558  
Sum of electronic and thermal Energies= -1647.269999  
Sum of electronic and thermal Enthalpies= -1647.269055  
Sum of electronic and thermal Free Energies= -1647.336633

#### 40...H<sub>2</sub>O

74	-0.001255000	-0.055544000	-0.081037000
15	-2.435381000	-0.060887000	-0.452533000
15	0.009983000	2.445527000	-0.275301000
15	2.431845000	-0.076541000	-0.456394000
7	0.001257000	-0.114910000	1.754690000
8	0.006368000	-0.118824000	2.946097000
6	-0.005964000	-2.045542000	-0.318279000
8	-0.007442000	-3.196697000	-0.475954000
1	-3.100105000	1.086184000	-0.962792000
1	-3.321146000	-0.312418000	0.624098000
1	-2.980274000	-0.991564000	-1.367412000
1	0.052168000	3.276253000	0.872770000
1	1.051974000	3.086948000	-0.991829000
1	-1.063496000	3.105683000	-0.925870000
1	3.097088000	1.053849000	-1.001445000
1	3.319562000	-0.297910000	0.625381000
1	2.973514000	-1.034502000	-1.344745000
1	0.002426000	0.118055000	-1.902262000

E(RB+HF-LYP) = -1341.20361298  
Zero-point correction= 0.106518  
Thermal correction to Energy= 0.121181  
Thermal correction to Enthalpy= 0.122125  
Thermal correction to Gibbs Free Energy= 0.063254  
Sum of electronic and zero-point Energies= -1341.097095  
Sum of electronic and thermal Energies= -1341.082432  
Sum of electronic and thermal Enthalpies= -1341.081488  
Sum of electronic and thermal Free Energies= -1341.140359

**41...H<sub>2</sub>O**

74	0.113611000	-0.183546000	0.007504000
15	1.930089000	0.221533000	-1.573633000
15	1.886729000	0.408420000	1.571179000
15	-1.782926000	-0.093691000	1.567593000
15	-1.757899000	-0.151124000	-1.579338000
6	3.569477000	0.532822000	-0.683104000
1	4.018695000	-0.454702000	-0.525837000
1	4.252576000	1.111139000	-1.312251000
6	3.328342000	1.223230000	0.665311000
1	3.037269000	2.268486000	0.514040000
1	4.229770000	1.211519000	1.285417000
6	-3.416550000	-0.410216000	0.679960000
1	-3.520967000	-1.499622000	0.616429000
1	-4.254232000	-0.026715000	1.269847000
6	-3.393010000	0.217945000	-0.719251000
1	-3.433413000	1.309144000	-0.637459000
1	-4.233716000	-0.129186000	-1.327408000
8	0.510764000	-3.179936000	0.100815000
7	0.326899000	-1.993847000	0.067683000
1	0.039218000	1.660743000	-0.066979000
1	-1.856870000	0.738748000	-2.678485000
1	2.567186000	-0.604391000	2.297031000
1	2.357796000	-0.737634000	-2.526977000
1	-2.077800000	1.098713000	2.271510000
1	-1.913179000	-0.989593000	2.658216000
1	-2.066258000	-1.341275000	-2.286821000
1	1.889288000	1.335290000	-2.450463000
1	1.739012000	1.326410000	2.641999000
8	-2.120005000	3.144172000	-0.033346000
1	-1.296557000	2.612384000	-0.008409000
1	-1.968835000	3.776258000	-0.746753000

E(RB3LYP) = -1802.31228426

Zero-point correction=	0.230691
Thermal correction to Energy=	0.250311
Thermal correction to Enthalpy=	0.251255
Thermal correction to Gibbs Free Energy=	0.181445
Sum of electronic and zero-point Energies=	-1802.081593
Sum of electronic and thermal Energies=	-1802.061973
Sum of electronic and thermal Enthalpies=	-1802.061029
Sum of electronic and thermal Free Energies=	-1802.130839

**42...H<sub>2</sub>O**

74	0.125375000	-0.014618000	-0.324635000
15	1.948793000	1.570776000	0.044675000
15	1.903923000	-1.576603000	0.265808000
15	-1.770487000	-1.575847000	-0.168220000
15	-1.753621000	1.573202000	-0.186179000
6	3.599684000	0.677853000	0.281066000
1	3.999241000	0.509012000	-0.725542000
1	4.311729000	1.310240000	0.820070000
6	3.386020000	-0.661337000	0.997241000
1	3.144212000	-0.493910000	2.052492000

1	4.284012000	-1.285187000	0.953228000
6	-3.405460000	-0.692627000	-0.486975000
1	-3.502244000	-0.614769000	-1.575798000
1	-4.243868000	-1.289325000	-0.114938000
6	-3.387603000	0.697591000	0.160903000
1	-3.428188000	0.601025000	1.250767000
1	-4.230178000	1.308323000	-0.177170000
6	0.306900000	-0.084388000	-2.134113000
1	0.168932000	0.038925000	1.581185000
1	-1.847164000	2.623178000	0.762497000
1	2.544391000	-2.367916000	-0.720516000
1	2.344585000	2.546456000	-0.903137000
1	-2.070043000	-2.248641000	1.042497000
1	-1.909169000	-2.686938000	-1.033453000
1	-2.073599000	2.342801000	-1.329401000
1	1.958811000	2.421399000	1.180730000
1	1.769326000	-2.594456000	1.244529000
1	0.493506000	-0.134965000	-3.212210000
8	-1.991237000	0.092996000	3.060664000
1	-1.168016000	0.031000000	2.527080000
1	-1.820479000	0.826032000	3.664753000

E(RB3LYP) = -1710.99727790

Zero-point correction=	0.236084
Thermal correction to Energy=	0.254998
Thermal correction to Enthalpy=	0.255943
Thermal correction to Gibbs Free Energy=	0.188492
Sum of electronic and zero-point Energies=	-1710.761194
Sum of electronic and thermal Energies=	-1710.742279
Sum of electronic and thermal Enthalpies=	-1710.741335
Sum of electronic and thermal Free Energies=	-1710.808786

### TS31

42	0.023698000	-0.011494000	-0.012623000
15	-2.408763000	0.682700000	0.013319000
15	2.430674000	-0.565757000	-0.461553000
7	0.174660000	-0.098565000	1.773139000
8	0.248213000	-0.152983000	2.955078000
6	-0.515092000	-1.999831000	-0.065197000
8	-0.826497000	-3.110461000	-0.053154000
1	-2.805788000	1.819758000	-0.723663000
1	-3.024023000	1.015516000	1.243479000
1	-3.393573000	-0.209506000	-0.465900000
1	3.342536000	0.485179000	-0.681577000
1	3.174625000	-1.278659000	0.523609000
1	2.762158000	-1.377710000	-1.565845000
1	1.212277000	0.817587000	-2.136861000
8	-0.838561000	-0.006140000	-2.273054000
1	0.151951000	0.434012000	-2.427496000
1	-0.816349000	-0.873551000	-2.704913000
6	0.609149000	1.997770000	-0.069756000
8	0.952500000	3.094370000	-0.055046000

E(RB+HF-LYP) = -1187.475552

Zero-point correction=	0.106576 (Hartree/Particle)
Thermal correction to Energy=	0.122622

Thermal correction to Enthalpy= 0.123567  
 Thermal correction to Gibbs Free Energy= 0.062559  
 Sum of electronic and zero-point Energies= -1187.368977  
 Sum of electronic and thermal Energies= -1187.352930  
 Sum of electronic and thermal Enthalpies= -1187.351986  
 Sum of electronic and thermal Free Energies= -1187.412994

### TS32

42	-0.569669000	0.016240000	-0.095642000
1	-0.946644000	0.778352000	-2.198543000
15	1.471811000	-1.568784000	0.249176000
15	1.369443000	1.680118000	0.051226000
6	-1.880869000	-1.476817000	-0.514460000
6	-2.006334000	1.443331000	-0.335313000
7	-0.927547000	-0.075775000	1.661029000
8	-1.171080000	-0.114047000	2.822413000
6	3.017119000	-0.538326000	0.541832000
1	3.054311000	-0.361953000	1.622801000
1	3.909430000	-1.113578000	0.278446000
1	3.828534000	1.431435000	0.075807000
6	2.990145000	0.793155000	-0.219102000
1	3.028609000	0.611232000	-1.295194000
1	1.552431000	-2.400174000	1.398184000
1	1.902182000	-2.535535000	-0.684059000
1	1.475493000	2.755794000	-0.856275000
1	1.600758000	2.400091000	1.247820000
8	-2.826638000	2.248174000	-0.417859000
8	-2.619212000	-2.331352000	-0.747395000
8	0.989506000	-0.299327000	-2.110438000
1	0.818074000	-1.120552000	-2.595652000
1	-0.124024000	0.377562000	-2.321112000

E(RB3LYP) = -1264.912216

Zero-point correction= 0.146514 (Hartree/Particle)  
 Thermal correction to Energy= 0.163413  
 Thermal correction to Enthalpy= 0.164357  
 Thermal correction to Gibbs Free Energy= 0.101227  
 Sum of electronic and zero-point Energies= -1264.765703  
 Sum of electronic and thermal Energies= -1264.748804  
 Sum of electronic and thermal Enthalpies= -1264.747859  
 Sum of electronic and thermal Free Energies= -1264.810989

### TS33

42	0.008010000	0.087431000	-0.003448000
15	2.300211000	-0.969961000	0.096149000
15	-2.265565000	0.990799000	-0.474696000
7	-0.110634000	0.336994000	1.761996000
8	-0.180420000	0.488258000	2.939715000
6	0.844061000	1.902254000	-0.214536000
8	1.339244000	2.946345000	-0.307567000
1	2.538913000	-2.257002000	-0.444891000
1	2.902274000	-1.188381000	1.358958000
1	3.390224000	-0.318032000	-0.524209000
1	-3.360697000	0.107005000	-0.596109000

1	-2.853084000	1.902491000	0.452233000
1	-2.484275000	1.756841000	-1.638699000
1	-1.360846000	-0.723859000	-2.005735000
8	0.822174000	-0.292246000	-2.294571000
1	-0.206189000	-0.545493000	-2.395592000
1	0.945295000	0.530040000	-2.791840000
15	-1.089025000	-2.236449000	0.037195000
1	-1.057547000	-3.062017000	1.200473000
1	-0.639130000	-3.213808000	-0.876697000
1	-2.473577000	-2.337051000	-0.220199000

E(RB3LYP) = -957.957777

Zero-point correction=	0.127558 (Hartree/Particle)
Thermal correction to Energy=	0.143881
Thermal correction to Enthalpy=	0.144826
Thermal correction to Gibbs Free Energy=	0.083811
Sum of electronic and zero-point Energies=	-1417.167889
Sum of electronic and thermal Energies=	-1417.151566
Sum of electronic and thermal Enthalpies=	-1417.150622
Sum of electronic and thermal Free Energies=	-1417.211636

#### TS34

42	-0.033425000	0.004907000	0.046630000
15	-1.928020000	1.589582000	-0.131921000
15	-1.920380000	-1.577367000	-0.202976000
15	1.824744000	-1.619487000	-0.158532000
15	1.921504000	1.556258000	0.111568000
6	-3.568285000	0.685888000	0.055865000
1	-3.714829000	0.578957000	1.137179000
1	-4.391744000	1.295074000	-0.329109000
6	-3.532599000	-0.695196000	-0.610844000
1	-3.563424000	-0.599865000	-1.698127000
1	-4.383067000	-1.302697000	-0.286345000
6	3.488738000	-0.786578000	0.135545000
1	3.635858000	-0.779466000	1.221968000
1	4.300311000	-1.374408000	-0.303539000
6	3.486020000	0.647791000	-0.409450000
1	3.468892000	0.635995000	-1.503424000
1	4.377144000	1.192932000	-0.083941000
8	-0.124153000	-0.097486000	3.019759000
7	-0.094351000	-0.062124000	1.820031000
1	-1.249570000	-0.470418000	-2.174906000
1	2.121727000	2.769899000	-0.601144000
1	-2.346877000	-2.271906000	0.974253000
1	-2.137707000	2.650293000	0.786966000
1	2.041500000	-2.252233000	-1.404696000
1	1.971659000	-2.760785000	0.667568000
1	2.308525000	2.051476000	1.383490000
1	-2.140011000	2.341931000	-1.313797000
1	-1.976258000	-2.681639000	-1.081539000
8	0.817200000	0.315283000	-2.315821000
1	0.689465000	1.232306000	-2.600805000
1	-0.202619000	-0.115285000	-2.419023000

E(RB3LYP) = -1801.973206

Zero-point correction=	0.225555 (Hartree/Particle)
Thermal correction to Energy=	0.244190
Thermal correction to Enthalpy=	0.245134
Thermal correction to Gibbs Free Energy=	0.179278
Sum of electronic and zero-point Energies=	-1801.747651
Sum of electronic and thermal Energies=	-1801.729017
Sum of electronic and thermal Enthalpies=	-1801.728073
Sum of electronic and thermal Free Energies=	-1801.793929

### TS35

42	0.019858000	-0.012476000	0.010883000
15	-1.794923000	1.697907000	0.089656000
15	1.878328000	-1.594765000	-0.445857000
7	0.110369000	-0.196039000	1.774858000
8	0.158366000	-0.326274000	2.964321000
1	-1.685876000	2.902893000	-0.648144000
1	-2.143952000	2.281045000	1.333290000
1	-3.112998000	1.377356000	-0.329742000
1	3.180589000	-1.095970000	-0.685510000
1	2.232297000	-2.565436000	0.538521000
1	1.818203000	-2.490256000	-1.539830000
1	1.453273000	0.276424000	-2.117588000
8	-0.772330000	0.393912000	-2.315203000
1	0.302388000	0.378187000	-2.426667000
1	-1.090745000	-0.376057000	-2.808927000
15	1.734018000	1.782385000	-0.096114000
1	2.001501000	2.564587000	1.066664000
1	1.571963000	2.862723000	-0.993588000
1	3.074879000	1.463693000	-0.415640000
15	-1.671561000	-1.827814000	-0.125436000
1	-3.052923000	-1.558673000	-0.338619000
1	-1.597914000	-2.892931000	-1.065981000
1	-1.833528000	-2.638126000	1.023968000

E(RB+HF-LYP) = -1647.102982

Zero-point correction=	0.146169 (Hartree/Particle)
Thermal correction to Energy=	0.163341
Thermal correction to Enthalpy=	0.164285
Thermal correction to Gibbs Free Energy=	0.101680
Sum of electronic and zero-point Energies=	-1646.956814
Sum of electronic and thermal Energies=	-1646.939642
Sum of electronic and thermal Enthalpies=	-1646.938698
Sum of electronic and thermal Free Energies=	-1647.001303

### TS36

42	-0.027291000	-0.020491000	0.032471000
1	-1.316830000	0.028835000	-2.169424000
15	1.884921000	-1.627064000	-0.029979000
15	1.870092000	1.615431000	0.010401000
15	-1.941270000	-1.604571000	-0.241724000
15	-1.915649000	1.617593000	-0.014698000
7	-0.083488000	-0.108198000	1.803744000
8	-0.111301000	-0.168423000	3.004680000
6	3.454207000	-0.673199000	0.316139000
1	3.408309000	-0.475800000	1.398437000

6	4.841563000	-1.235727000	-0.037702000
1	5.186923000	-1.981475000	0.684305000
1	4.801177000	-1.728749000	-1.016168000
6	5.769686000	0.018155000	-0.103005000
1	6.382949000	-0.004797000	-1.008951000
1	6.461657000	0.047642000	0.744019000
6	4.826431000	1.260517000	-0.091127000
1	4.818538000	1.719556000	0.904537000
1	5.136105000	2.033157000	-0.800795000
6	3.435357000	0.690082000	-0.412320000
1	3.346996000	0.509277000	-1.491909000
1	2.015209000	-2.704038000	0.883005000
1	2.264658000	-2.350174000	-1.194681000
1	1.974580000	2.750166000	-0.830606000
1	2.253439000	2.245304000	1.224244000
6	-3.497483000	0.664886000	0.258143000
1	-3.443659000	0.397516000	1.325443000
6	-4.882220000	1.264920000	-0.035793000
1	-5.200722000	1.979291000	0.729157000
1	-4.856525000	1.801705000	-0.991088000
6	-5.827425000	0.025274000	-0.135290000
1	-6.469835000	0.101472000	-1.017778000
1	-6.491078000	-0.040795000	0.732235000
6	-4.899283000	-1.227212000	-0.219044000
1	-5.239629000	-1.954773000	-0.961931000
1	-4.869479000	-1.741871000	0.748557000
6	-3.514910000	-0.648146000	-0.553010000
1	-3.464847000	-0.392604000	-1.617859000
1	-2.336976000	-2.387988000	0.879991000
1	-2.035500000	-2.631592000	-1.213489000
1	-2.056862000	2.613137000	0.990107000
1	-2.218342000	2.433486000	-1.129872000
8	0.869469000	0.275613000	-2.313182000
1	-0.270255000	0.189788000	-2.395205000
1	1.178362000	-0.553345000	-2.708214000

E(RB3LYP) = -2035.430935

Zero-point correction= 0.354456 (Hartree/Particle)

Thermal correction to Energy= 0.378275

Thermal correction to Enthalpy= 0.379220

Thermal correction to Gibbs Free Energy= 0.301322

Sum of electronic and zero-point Energies= -2035.076480

Sum of electronic and thermal Energies= -2035.052660

Sum of electronic and thermal Enthalpies= -2035.051716

Sum of electronic and thermal Free Energies= -2035.129614

### TS37

74	-0.050746000	0.028429000	-0.042953000
7	-0.099000000	0.046075000	1.760817000
8	-0.139543000	0.050485000	2.945012000
6	-1.055569000	-1.774468000	-0.053386000
8	-1.631277000	-2.771711000	0.001771000
1	1.560576000	0.572371000	-1.908616000
8	-0.508043000	-0.082503000	-2.353409000
1	0.495975000	0.235729000	-2.450212000



1	-0.574976000	-0.968798000	-2.740400000
6	1.035503000	1.815369000	-0.150366000
8	1.624438000	2.802625000	-0.131866000
6	-1.826533000	1.032291000	-0.142370000
8	-2.832795000	1.590066000	-0.161000000
15	2.228460000	-1.138887000	-0.127166000
1	3.375832000	-0.325669000	-0.196425000
1	2.634005000	-1.999136000	0.930075000
1	2.507269000	-2.008332000	-1.201431000

E(RB3LYP) = -957.95778

Zero-point correction= 0.087910 (Hartree/Particle)

Thermal correction to Energy= 0.103113

Thermal correction to Enthalpy= 0.104058

Thermal correction to Gibbs Free Energy= 0.044228

Sum of electronic and zero-point Energies= -957.869867

Sum of electronic and thermal Energies= -957.854664

Sum of electronic and thermal Enthalpies= -957.853720

Sum of electronic and thermal Free Energies= -957.913549

### TS38

74	0.028049000	-0.003677000	-0.030157000
15	-2.461228000	0.394379000	0.112269000
15	2.471505000	-0.307459000	-0.455603000
7	0.226970000	-0.030927000	1.755659000
8	0.324952000	-0.050664000	2.943920000
6	-0.258337000	-2.030819000	-0.043277000
8	-0.425445000	-3.174736000	-0.023285000
1	-3.037676000	1.484560000	-0.575860000
1	-3.023839000	0.633497000	1.388007000
1	-3.359338000	-0.605952000	-0.322620000
1	3.238116000	0.810829000	-0.839167000
1	3.294468000	-0.767903000	0.613041000
1	2.903701000	-1.219760000	-1.440434000
1	1.094261000	0.590478000	-2.203312000
8	-0.985521000	-0.084286000	-2.214364000
1	0.051140000	0.283940000	-2.440969000
1	-1.042214000	-0.977021000	-2.588268000
6	0.338982000	2.038205000	-0.120615000
8	0.533385000	3.173163000	-0.145654000

E(RB+HF-LYP) = -1187.77474

Zero-point correction= 0.106729 (Hartree/Particle)

Thermal correction to Energy= 0.122558

Thermal correction to Enthalpy= 0.123502

Thermal correction to Gibbs Free Energy= 0.062452

Sum of electronic and zero-point Energies= -1187.668015

Sum of electronic and thermal Energies= -1187.652186

Sum of electronic and thermal Enthalpies= -1187.651242

Sum of electronic and thermal Free Energies= -1187.712292

### TS39

74	0.020814000	-0.007411000	-0.006797000
15	-1.799648000	1.670380000	0.112791000
15	1.711917000	1.788674000	-0.096096000

15	1.870318000	-1.577924000	-0.442488000
7	0.118619000	-0.194117000	1.758328000
8	0.169338000	-0.329883000	2.954913000
1	-1.733154000	2.892256000	-0.604782000
1	-2.114316000	2.217439000	1.380517000
1	-3.124529000	1.334262000	-0.277502000
1	1.980427000	2.538474000	1.085147000
1	3.051925000	1.480241000	-0.437900000
1	1.543711000	2.888849000	-0.970073000
1	3.169657000	-1.075744000	-0.703915000
1	2.227446000	-2.516738000	0.568068000
1	1.815606000	-2.499470000	-1.516869000
1	1.393145000	0.285240000	-2.106608000
8	-0.815481000	0.378999000	-2.304080000
1	0.260310000	0.373753000	-2.440285000
1	-1.146594000	-0.395726000	-2.782418000
15	-1.655178000	-1.812755000	-0.104228000
1	-1.592707000	-2.910851000	-1.010026000
1	-1.805220000	-2.577779000	1.076751000
1	-3.038289000	-1.545503000	-0.321798000

E(RB3LYP) = -1647.39206

Zero-point correction= 0.146564 (Hartree/Particle)

Thermal correction to Energy= 0.163485

Thermal correction to Enthalpy= 0.164429

Thermal correction to Gibbs Free Energy= 0.101916

Sum of electronic and zero-point Energies= -1647.245502

Sum of electronic and thermal Energies= -1647.228582

Sum of electronic and thermal Enthalpies= -1647.227637

Sum of electronic and thermal Free Energies= -1647.290151

#### TS42

74	-0.028759000	0.018730000	-0.168343000
15	-1.905405000	-1.582673000	-0.046299000
15	-1.925368000	1.568113000	0.159682000
15	1.868482000	1.582418000	-0.081483000
15	1.844858000	-1.588404000	-0.021196000
6	-3.565504000	-0.701750000	-0.207756000
1	-3.722126000	-0.595509000	-1.287054000
1	-4.372861000	-1.328960000	0.182230000
6	-3.561526000	0.676960000	0.461098000
1	-3.657177000	0.577864000	1.543738000
1	-4.387632000	1.292916000	0.091652000
6	3.502594000	0.670198000	-0.339117000
1	3.613075000	0.544225000	-1.422197000
1	4.344752000	1.273547000	0.013681000
6	3.465616000	-0.698201000	0.353951000
1	3.491031000	-0.579175000	1.441849000
1	4.320612000	-1.314607000	0.060672000
6	-0.039527000	0.088765000	-1.950506000
1	-1.412862000	-0.053993000	2.044067000
1	1.931204000	-2.645382000	0.917321000
1	-2.287801000	2.416928000	-0.922018000
1	-2.079273000	-2.555982000	-1.065211000
1	2.202769000	2.335583000	1.081025000

1	2.020927000	2.637940000	-1.010692000
1	2.204530000	-2.328563000	-1.173327000
1	-2.116990000	-2.438073000	1.059865000
1	-1.998563000	2.551101000	1.177596000
1	-0.011188000	0.135994000	-3.038739000
8	0.784332000	-0.209913000	2.222608000
1	-0.349598000	-0.164995000	2.294518000
1	1.072247000	0.624801000	2.620984000

E(RB3LYP) = -1710.960852

Zero-point correction=	0.231567 (Hartree/Particle)
Thermal correction to Energy=	0.249260
Thermal correction to Enthalpy=	0.250205
Thermal correction to Gibbs Free Energy=	0.186646
Sum of electronic and zero-point Energies=	-1710.729285
Sum of electronic and thermal Energies=	-1710.711592
Sum of electronic and thermal Enthalpies=	-1710.710648
Sum of electronic and thermal Free Energies=	-1710.774206

### 39'

74	0.007930000	-0.003219000	-0.045977000
15	-1.481894000	1.972787000	-0.114096000
15	1.981588000	1.485351000	-0.160520000
15	1.467815000	-1.968418000	-0.240458000
7	0.027640000	-0.074734000	1.765134000
8	0.033199000	-0.121223000	2.972103000
1	-1.283686000	2.959088000	-1.113330000
1	-1.555951000	2.834057000	1.007496000
1	-2.885579000	1.832741000	-0.311772000
1	2.327881000	2.290420000	0.952022000
1	3.288336000	0.968202000	-0.398532000
1	2.029352000	2.491186000	-1.159690000
1	2.885341000	-1.853735000	-0.351710000
1	1.465267000	-2.939602000	0.790276000
1	1.318664000	-2.869110000	-1.333124000
8	-0.085692000	0.199324000	-2.101724000
1	0.087897000	-0.557338000	-2.671194000
15	-1.988741000	-1.450501000	-0.194924000
1	-2.079878000	-2.502672000	-1.147334000
1	-2.364793000	-2.201749000	0.944419000
1	-3.274730000	-0.903227000	-0.474216000

E(RB+HF-LYP) = -1646.262018

Zero-point correction=	0.130809 (Hartree/Particle)
Thermal correction to Energy=	0.147764
Thermal correction to Enthalpy=	0.148709
Thermal correction to Gibbs Free Energy=	0.084243
Sum of electronic and zero-point Energies=	-1646.131210
Sum of electronic and thermal Energies=	-1646.114255
Sum of electronic and thermal Enthalpies=	-1646.113310
Sum of electronic and thermal Free Energies=	-1646.177776

### 42'

74	-0.007655000	0.009167000	0.104387000
15	-1.888867000	1.565806000	-0.044770000
15	-1.864740000	-1.598389000	-0.112842000

15	1.872084000	-1.590075000	0.034398000
15	1.889030000	1.581511000	-0.044823000
6	-3.504858000	0.670680000	0.338785000
1	-3.539973000	0.558305000	1.427859000
1	-4.366272000	1.273282000	0.034158000
6	-3.516958000	-0.701811000	-0.346987000
1	-3.641508000	-0.577716000	-1.429031000
1	-4.347711000	-1.317915000	0.009374000
6	3.511114000	-0.707677000	0.339520000
1	3.598176000	-0.581902000	1.424544000
1	4.353330000	-1.321548000	0.005592000
6	3.508652000	0.656821000	-0.362091000
1	3.566556000	0.519758000	-1.447738000
1	4.366898000	1.263670000	-0.058466000
6	-0.113521000	0.056521000	1.923068000
1	2.015516000	2.574394000	-1.054622000
1	-2.181679000	-2.479187000	0.947824000
1	-2.049072000	2.719652000	0.761315000
1	2.154404000	-2.236070000	-1.197051000
1	2.026331000	-2.704455000	0.893653000
1	2.247012000	2.391642000	1.058631000
1	-2.243298000	2.166889000	-1.289196000
1	-1.966432000	-2.530790000	-1.178800000
1	-0.187598000	0.137172000	3.012118000
8	0.170414000	-0.063008000	-1.997898000
1	-0.020691000	0.740561000	-2.494830000

E(RB3LYP) = -1709.824718

Zero-point correction=	0.217789 (Hartree/Particle)
Thermal correction to Energy=	0.235264
Thermal correction to Enthalpy=	0.236208
Thermal correction to Gibbs Free Energy=	0.172642
Sum of electronic and zero-point Energies=	-1709.606930
Sum of electronic and thermal Energies=	-1709.589455
Sum of electronic and thermal Enthalpies=	-1709.588511
Sum of electronic and thermal Free Energies=	-1709.652077