Mechanistic Divergence in Rh(III)-Catalyzed Cascades: How Substrate Identity Switches Between Cyclization and Migratory Insertion

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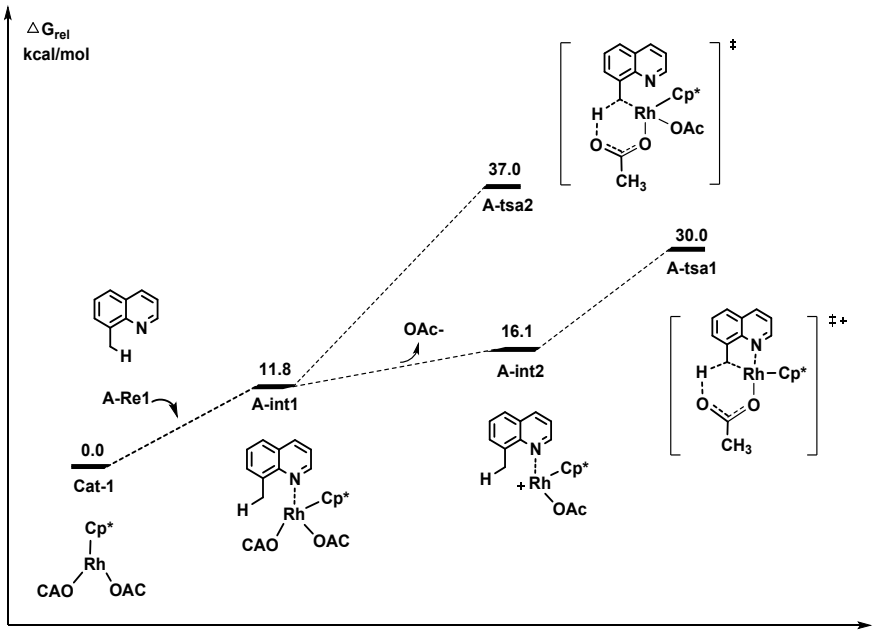

Figure S1. Free energy profile for the pathways to the conditions of $Cp^*Rh(OAc)_2$ (series A). The values are given in kcal mol^{-1}.

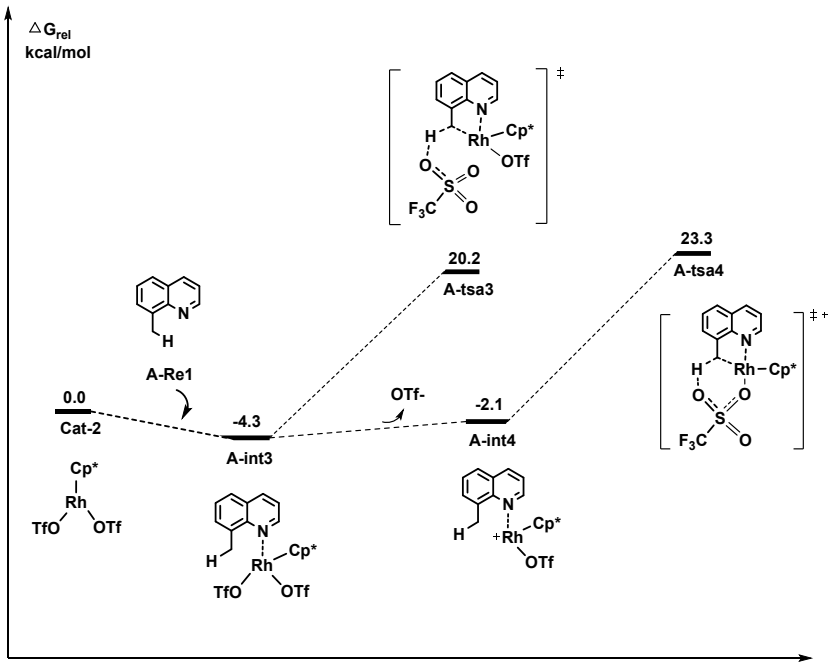

Figure S2. Free energy profile for the pathways to the conditions of $Cp^*Rh(OTf)_2$ (series A). The values are given in kcal mol^{-1}.

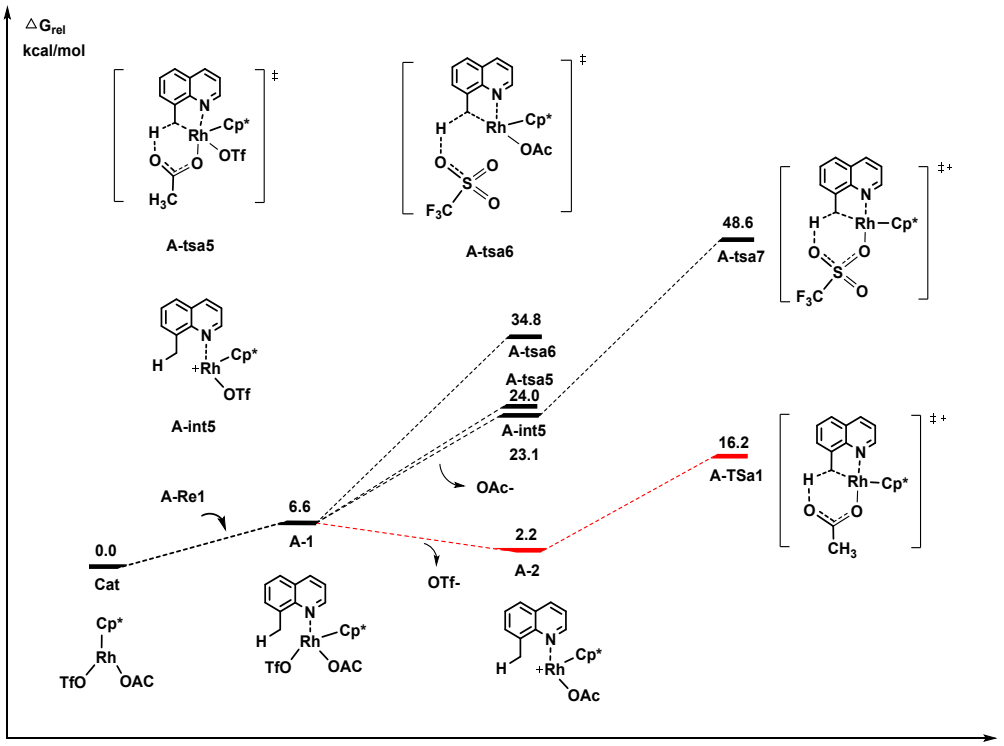

Figure S3. Free energy profile for the pathways to the conditions of $[Cp^*RhOAc]^+OTf^-$ (series A). The values are given in kcal mol^{-1}.

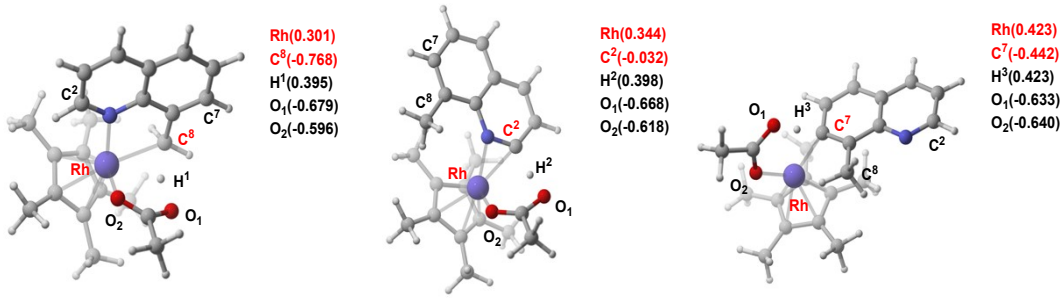

Figure S4. The regioselective transition state structure of C-H activation and the corresponding NPA charge value.

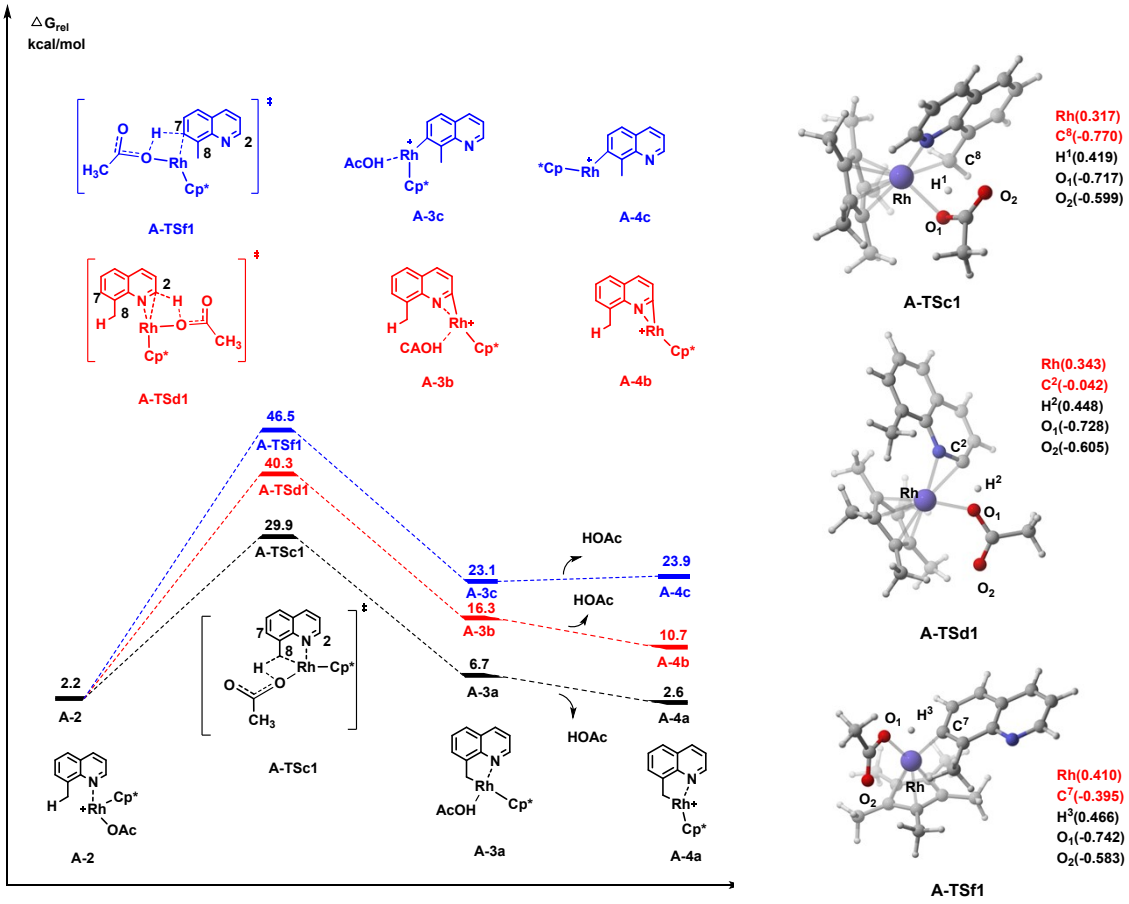

Figure S5. Free energy profile for the A-series C-H activation (σ bond metathesis mechanism). The relative free energies are reported in kcal mol^{-1}.

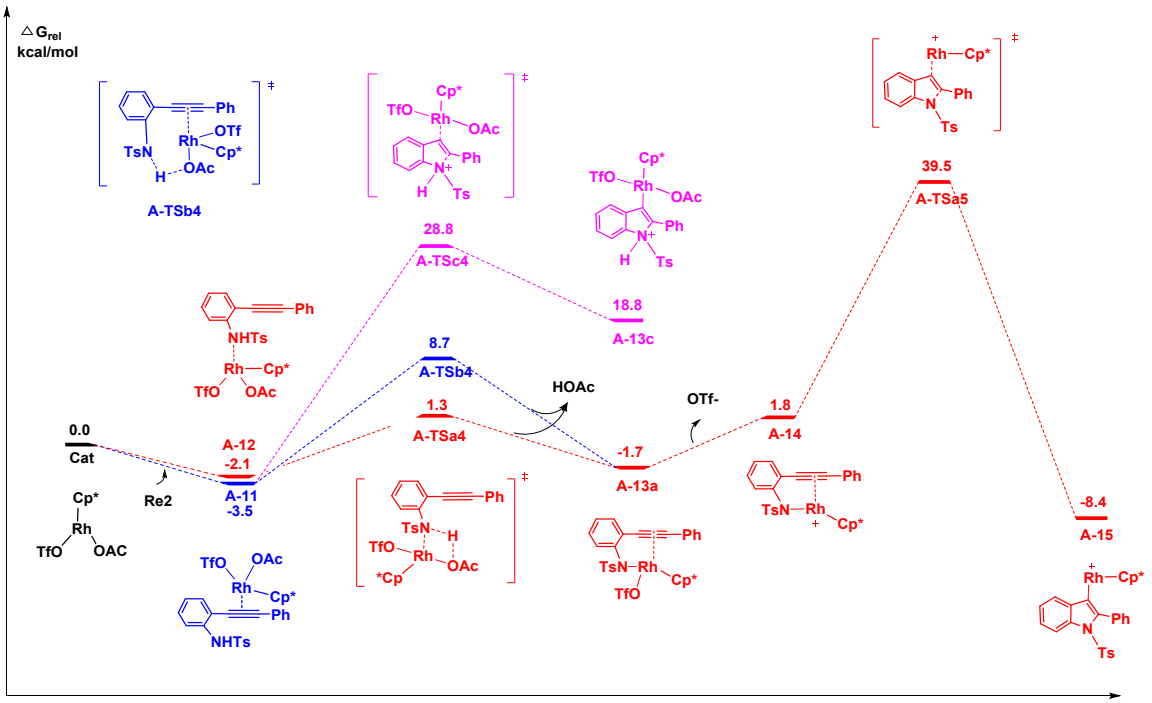

Figure S6. Calculate the free energy distribution of the activation and cyclization sequence of the reaction C-H. The relative free energies are reported in kcal mol^{-1}.

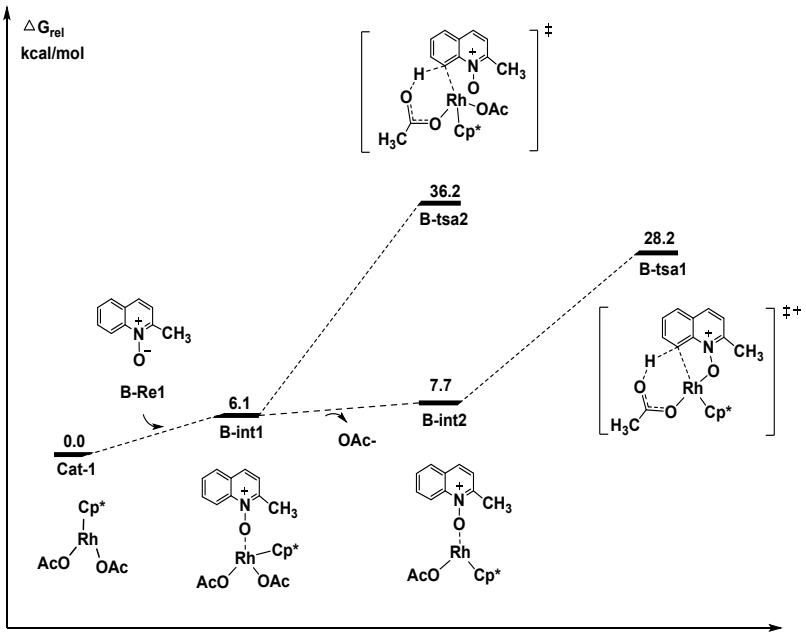

Figure S7. Free energy profile for the pathways to the conditions of $Cp^*Rh(OAc)_2$ (series B). The values are given in kcal mol^{-1}.

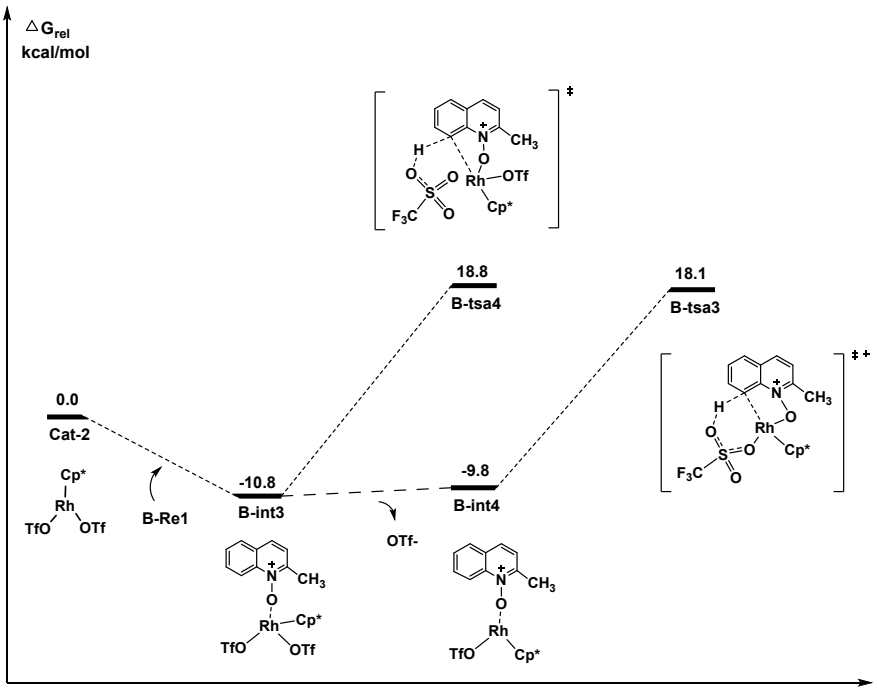

Figure S8. Free energy profile for the pathways to the conditions of $Cp^*Rh(OTf)_2$ (series B). The values are given in kcal mol^{-1}.

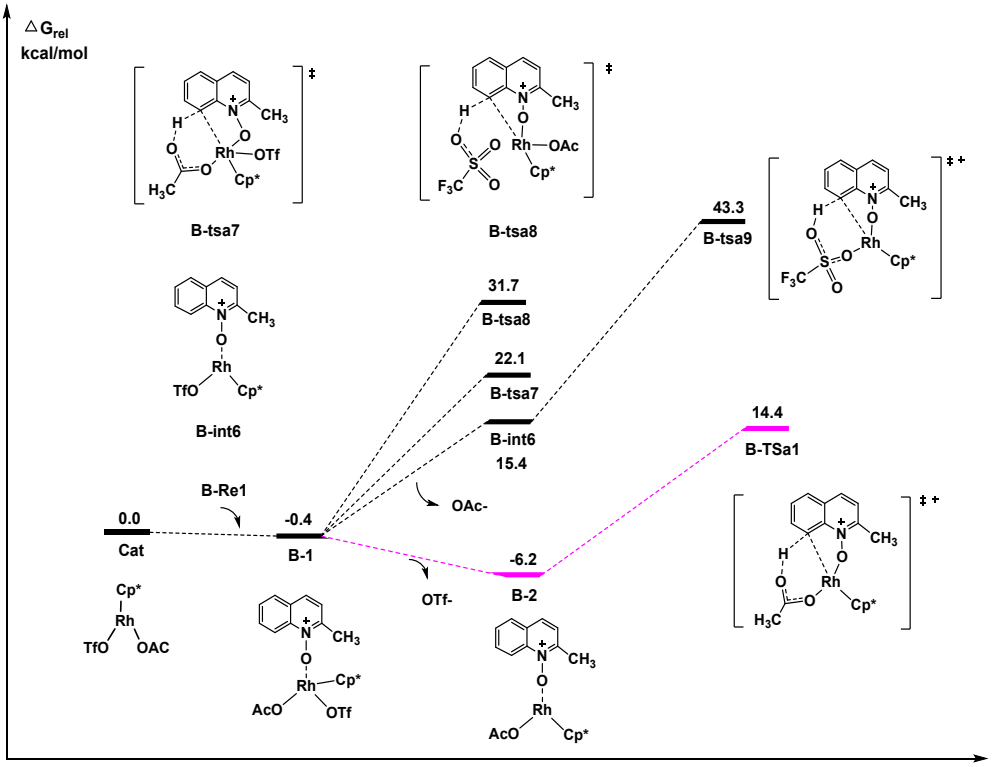

Figure S9. Free energy profile for the pathways to the conditions of [Cp*RhOAc]$^{+}$OTf^{-}(series B). The values are given in kcal mol^{-1}.

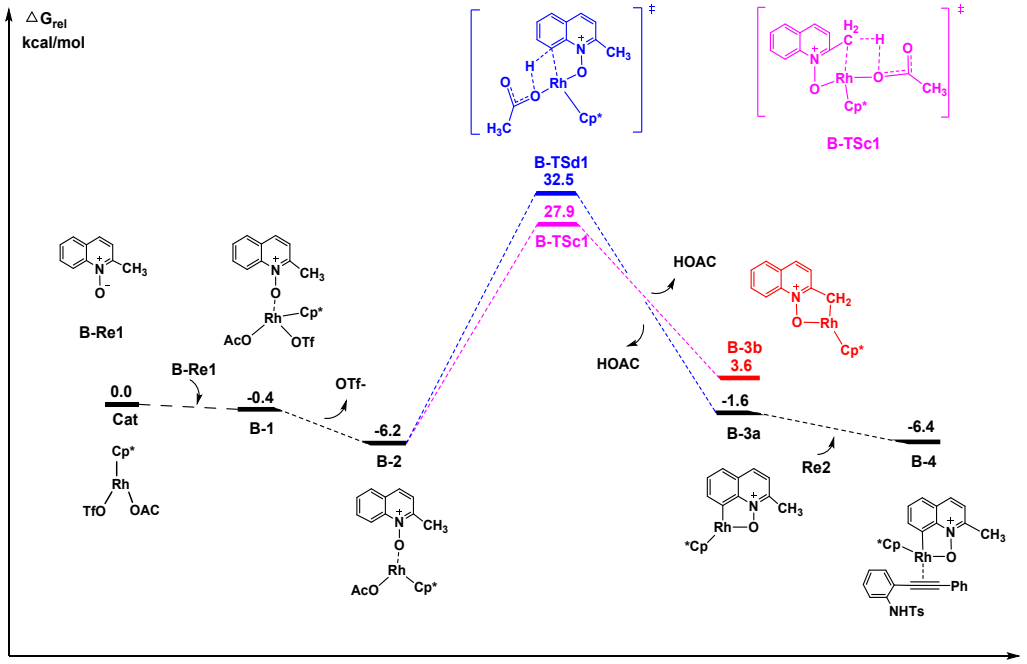

Figure S10. Free energy profile for the B-series C-H activation (σ bond metathesis mechanism). The relative free energies are reported in kcal mol^{-1}.

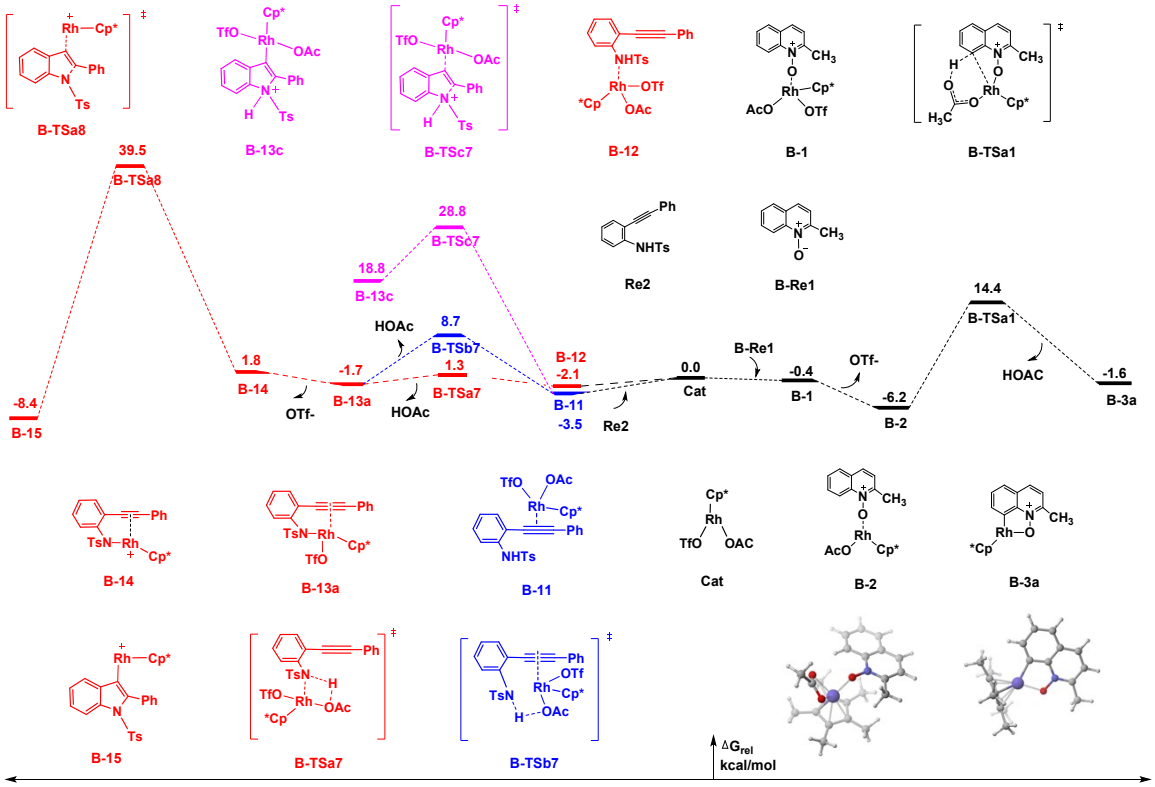

Figure S11. Calculate the free energy distribution of the activation and cyclization sequence of the reaction C-H (B-series). The relative free energies are reported in kcal mol^{-1}.

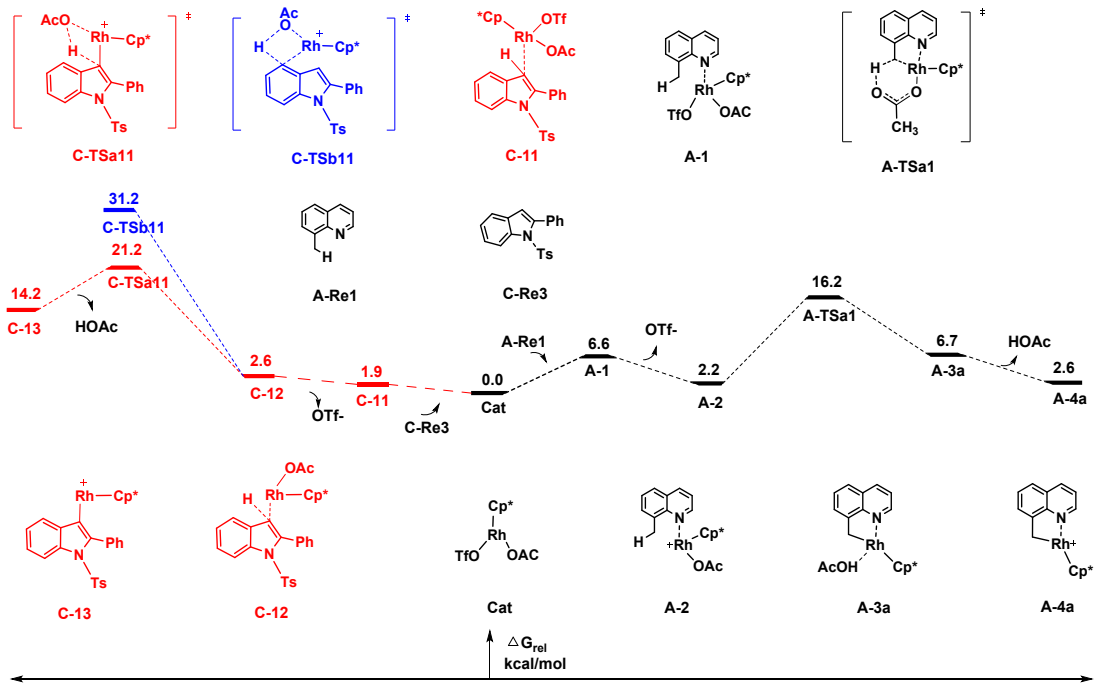

Figure S12. Calculate the free energy profile of C-H activation and cyclization order based on **C-Re3** as the coupled partner (series C). Free energies are given in kcal mol^{-1}.

The Cartesian coordinates of the stationary points

Cat

0 1

Number of imaginary frequencies: 0

C	2.77036900	-0.45395600	0.80558900
C	1.64183400	-1.21371800	1.32577100
C	1.05080500	-1.92870100	0.23272300
C	1.77663000	-1.59987400	-0.97284200
C	2.85922700	-0.71024400	-0.60461000
C	3.86166000	-0.13518200	-1.55368200
H	4.29752800	0.78663200	-1.16549300
H	4.67202400	-0.85426800	-1.72401300
H	3.40201500	0.09244400	-2.51793900
C	3.67234000	0.41295700	1.62695800
H	3.09051300	1.03164700	2.31436900
H	4.35907400	-0.20394800	2.21850200
H	4.26713600	1.07886800	0.99955200
C	1.17028600	-1.24485200	2.74523500
H	0.08397800	-1.13670900	2.78432400
H	1.45187600	-2.19375200	3.21743200
H	1.61096400	-0.43161900	3.32440800
C	-0.15799600	-2.80243900	0.31636900
H	-0.73702300	-2.76270000	-0.60675600
H	0.14804500	-3.84081600	0.49314400
H	-0.81482100	-2.47830600	1.12396400
C	1.50067600	-2.14185400	-2.34019600

H	2.02297200	-3.09468700	-2.49099100
H	0.43181200	-2.31455700	-2.48121700
H	1.83195500	-1.44790800	-3.11573900
C	0.48609100	2.69473500	-0.26658900
O	0.93310500	2.07710600	-1.28895100
O	0.51114800	2.08209300	0.85495300
C	-0.14612600	4.04665800	-0.37115300
H	-1.22951000	3.88332300	-0.34280500
H	0.12549800	4.65957200	0.49104100
H	0.13138800	4.53779700	-1.30450000
Rh	0.94425300	0.22974600	-0.14355700
S	-2.18172500	0.39481700	0.42163600
O	-1.83299000	-0.29612400	1.67604600
O	-2.70811400	1.76007300	0.49095100
C	-3.53986200	-0.63679500	-0.32587200
O	-1.12493500	0.20347800	-0.67461800
F	-4.61032800	-0.62378900	0.47491800
F	-3.12910700	-1.91131000	-0.46742500
F	-3.88618000	-0.16490500	-1.52712100

Zero-point correction= 0.303997 (Hartree/Particle)

Thermal correction to Energy= 0.331333

Thermal correction to Enthalpy= 0.332277

Thermal correction to Gibbs Free Energy= 0.245671

Sum of electronic and zero-point Energies= -1689.340728

Sum of electronic and thermal Energies= -1689.313392

Sum of electronic and thermal Enthalpies= -1689.312448

Sum of electronic and thermal Free Energies= -1689.399054

E(RB3LYP) = -1689.644725 A.U.

Cat-1

0 1

Number of imaginary frequencies: 0

C	1.93104100	0.14399200	1.00255800
C	1.23669500	-1.13437600	1.11762100
C	1.12868300	-1.69807800	-0.19775700
C	1.66735000	-0.74918200	-1.13394400
C	2.20034100	0.37738500	-0.37391500
C	2.85541900	1.57470000	-0.98921100
H	3.00338600	2.37148400	-0.25856200
H	3.83295300	1.30362200	-1.40488800
H	2.23997100	1.97641600	-1.79894300
C	2.24112300	1.04186500	2.16005700
H	1.34460000	1.21227600	2.76252400
H	3.00299400	0.58678500	2.80326600
H	2.61002300	2.01371300	1.82783500
C	0.78893900	-1.78500100	2.38741700
H	-0.22869700	-2.16056100	2.26274700
H	1.45633300	-2.61629300	2.64688000
H	0.79438600	-1.07386900	3.21608900
C	0.53331500	-3.02992000	-0.52601800
H	0.17073300	-3.05802000	-1.55561300
H	1.29464900	-3.81175400	-0.41216600
H	-0.30654400	-3.24316100	0.13549700
C	1.77874600	-0.91634900	-2.61700300
H	2.74197700	-1.36964900	-2.88357800

H	0.98349600	-1.55727700	-3.00256000
H	1.70772000	0.04810900	-3.12568800
C	-2.48447500	-1.31553300	-0.02152700
O	-1.83244100	-0.42902100	-0.72147100
O	-2.06180300	-1.93927300	0.95490300
C	-1.24946000	2.39871700	0.05791900
O	-0.63066000	2.09596200	-1.01243300
O	-1.11454600	1.65329600	1.08148200
C	-3.90794900	-1.52140900	-0.53150300
H	-4.34761200	-2.40480300	-0.06620400
H	-4.50776300	-0.64181200	-0.27561100
H	-3.91651700	-1.61699700	-1.62049500
C	-2.16463000	3.59273200	0.10020600
H	-3.16596100	3.27016000	-0.20436700
H	-2.22450800	3.99089700	1.11477900
H	-1.82307800	4.35913400	-0.59806400
Rh	0.02493800	0.21103600	-0.10204700

Zero-point correction= 0.326171 (Hartree/Particle)

Thermal correction to Energy= 0.350428

Thermal correction to Enthalpy= 0.351372

Thermal correction to Gibbs Free Energy= 0.271840

Sum of electronic and zero-point Energies= -956.376230

Sum of electronic and thermal Energies= -956.351973

Sum of electronic and thermal Enthalpies= -956.351029

Sum of electronic and thermal Free Energies= -956.430561

E(RB3LYP) = -956.702401 A.U.

Cat-2

0 1

Number of imaginary frequencies: 0

C	-1.01694000	2.32236200	0.69936800
C	0.38187900	2.28083200	1.11395500
C	1.19389000	2.26715700	-0.07637800
C	0.31533800	2.15631300	-1.20607900
C	-1.05721800	2.25222300	-0.72780700
C	-2.25853700	2.25275000	-1.61965500
H	-3.18222900	2.36065400	-1.05366500
H	-2.18567900	3.08258800	-2.33091500
H	-2.31741100	1.31905700	-2.18614300
C	-2.18726500	2.37439700	1.62632600
H	-1.98829200	1.79673500	2.53118000
H	-2.38557300	3.41288500	1.91723200
H	-3.08030600	1.95912000	1.16146700
C	0.90573200	2.35876200	2.51062900
H	1.77378500	1.70574100	2.62157400
H	1.20451500	3.38915200	2.74155400
H	0.14916800	2.05418000	3.23588000
C	2.67509400	2.42778300	-0.11145300
H	3.08563800	2.21016100	-1.09584800
H	2.90411400	3.47161400	0.13870300
H	3.15708700	1.77987000	0.62099800
C	0.72478800	2.04860100	-2.63925600
H	0.89628200	3.04709900	-3.06034700
H	1.64369700	1.46862900	-2.73772900
H	-0.05251800	1.55872700	-3.22921500

Rh	-0.11668700	0.46047400	0.06475800
S	2.53439400	-1.30324100	0.83890100
O	2.92332400	-0.10209000	1.59940000
O	2.82507200	-2.61634000	1.39829600
C	3.50344200	-1.20641000	-0.75353700
O	1.10638000	-1.21540600	0.28451700
F	4.79744400	-0.99252500	-0.49923800
F	3.04877900	-0.17543800	-1.50948800
F	3.36786500	-2.32768800	-1.45652600
S	-2.02458000	-1.65001300	0.03432700
O	-1.36130800	-1.00896300	-1.16973600
O	-2.03680000	-3.10044600	0.11830700
C	-3.81550300	-1.15741500	-0.13622200
O	-1.55705700	-0.86296100	1.24169700
F	-4.32244800	-1.65889500	-1.26242900
F	-3.92528400	0.18899000	-0.18314900
F	-4.51229700	-1.60110700	0.90864300

Zero-point correction= 0.281510 (Hartree/Particle)

Thermal correction to Energy= 0.312071

Thermal correction to Enthalpy= 0.313015

Thermal correction to Gibbs Free Energy= 0.218614

Sum of electronic and zero-point Energies= -2422.287103

Sum of electronic and thermal Energies= -2422.256543

Sum of electronic and thermal Enthalpies= -2422.255599

Sum of electronic and thermal Free Energies= -2422.349999

E(RB3LYP) = -2422.568614 A.U.

Cat-3

0 1

Number of imaginary frequencies: 0

C	0.93382200	1.71157900	0.00089700
C	1.29355000	0.93438500	1.16445500
C	1.85109900	-0.31503500	0.72484200
C	1.85026100	-0.31393200	-0.72703800
C	1.29234900	0.93625700	-1.16415200
C	1.06070800	1.36178000	-2.57938000
H	0.08982900	1.85281600	-2.68174700
H	1.83771200	2.06861600	-2.89454200
H	1.07634500	0.50866800	-3.25914600
C	0.36161300	3.09502900	0.00232100
H	-0.26027400	3.26160700	0.88482500
H	1.15936900	3.84826700	0.00353000
H	-0.25959100	3.26371500	-0.88025600
C	1.06347800	1.35787900	2.58053100
H	1.07957600	0.50376700	3.25904100
H	1.84100800	2.06402600	2.89596500
H	0.09286200	1.84906400	2.68462700
C	2.37377600	-1.43326900	1.56983300
H	1.97688000	-2.38769000	1.21482300
H	3.46898500	-1.46565600	1.52209800
H	2.08037500	-1.31814400	2.61462000
C	2.37182000	-1.43103800	-1.57423400
H	3.46709300	-1.46355800	-1.52800600
H	1.97535500	-2.38589600	-1.21993400
H	2.07703200	-1.31451600	-2.61847200

C	-2.70149000	0.20489400	0.00015500
O	-2.04987100	0.17582100	-1.09415900
O	-2.04996700	0.17588300	1.09450100
C	-4.20372700	0.21684100	0.00004400
H	-4.55206300	-0.82141600	-0.00110100
H	-4.58077200	0.70720500	0.89945000
H	-4.58059100	0.70900600	-0.89846600
Rh	-0.20222300	-0.16320700	0.00011400
Cl	-0.66905800	-2.52361200	0.00030400

Zero-point correction= 0.275649 (Hartree/Particle)

Thermal correction to Energy= 0.296493

Thermal correction to Enthalpy= 0.297437

Thermal correction to Gibbs Free Energy= 0.225126

Sum of electronic and zero-point Energies= -1188.152825

Sum of electronic and thermal Energies= -1188.131980

Sum of electronic and thermal Enthalpies= -1188.131036

Sum of electronic and thermal Free Energies= -1188.203347

E(RB3LYP) = -1188.428473 A.U.

A-Re1

0 1

Number of imaginary frequencies: 0

C	-2.19006100	1.18130800	-0.00002900
C	-0.02305000	0.40511300	0.00004500
C	-0.46301100	-0.95840500	-0.00015800
C	-1.86062700	-1.19499500	-0.00029200
C	-2.72869400	-0.12889200	-0.00023000
H	-2.86301600	2.03823600	0.00002200

C	1.37809500	0.69907700	0.00018200
C	0.49588200	-2.00463500	-0.00021700
H	-2.22706100	-2.21860400	-0.00045200
H	-3.80435500	-0.27326800	-0.00033600
C	1.83695400	-1.70331200	-0.00006400
C	2.27041300	-0.35477300	0.00013000
H	0.15372300	-3.03621400	-0.00036900
H	2.57549400	-2.49957400	-0.00009700
H	3.33684500	-0.14491800	0.00025100
N	-0.89960500	1.45154900	0.00011400
C	1.83457700	2.13328900	0.00042200
H	1.44851900	2.66588200	-0.87429900
H	1.44833200	2.66565400	0.87520000
H	2.92588800	2.19931800	0.00054600

Zero-point correction= 0.163601 (Hartree/Particle)

Thermal correction to Energy= 0.171928

Thermal correction to Enthalpy= 0.172872

Thermal correction to Gibbs Free Energy= 0.130493

Sum of electronic and zero-point Energies= -441.113451

Sum of electronic and thermal Energies= -441.105124

Sum of electronic and thermal Enthalpies= -441.104180

Sum of electronic and thermal Free Energies= -441.146559

E(RB3LYP) = -441.277052 A.U.

Re2

0 1

Number of imaginary frequencies: 0

C	2.48482800	-0.73039000	0.74873100

C	3.83489500	-0.82018900	0.40099600
C	4.30879500	-1.93983200	-0.27876500
C	3.44400400	-2.99233100	-0.59594400
C	2.09830300	-2.91338000	-0.25555900
C	1.59155600	-1.77574800	0.40070900
H	4.48981000	0.00140100	0.66383700
H	5.35898200	-1.99805900	-0.54716400
H	3.81939000	-3.87136700	-1.11043600
H	1.41496000	-3.71719800	-0.50840800
C	-2.80902300	-0.10428300	1.83666800
C	-4.15569800	0.24394600	1.88941100
C	-5.08166900	-0.39228100	1.05830100
C	-4.65357600	-1.38792900	0.17586100
C	-3.30857000	-1.74320500	0.11614300
C	-2.36680600	-1.09947500	0.94332000
H	-2.08651100	0.39615100	2.47306400
H	-4.48380900	1.01550300	2.57940500
H	-6.13088300	-0.11640900	1.10046600
H	-5.37026700	-1.88857000	-0.46841500
H	-2.96970900	-2.50932100	-0.57345100
N	2.02214600	0.41190400	1.45517500
H	1.14487200	0.24742700	1.94598600
S	1.87555900	1.90253900	0.61494600
O	3.13683900	2.10334800	-0.09749500
O	1.37215500	2.84199000	1.61738500
C	-0.73599500	1.94409000	-0.24550400
C	-1.76750400	1.55601100	-1.09191800

C	-1.50837500	0.81950100	-2.25742400
C	-0.17939400	0.51462400	-2.57824600
C	0.87044600	0.90084200	-1.74652800
C	0.57735400	1.60261100	-0.57678700
H	-0.93400300	2.49423600	0.66745000
H	-2.79339100	1.79697900	-0.82857600
H	0.03753100	-0.04363400	-3.48457000
H	1.89831700	0.65683000	-1.98992700
C	-0.98205500	-1.40677100	0.83137400
C	0.20091100	-1.63339600	0.66129800
C	-2.65415700	0.35107100	-3.11906400
H	-3.30688400	-0.31945000	-2.54802800
H	-3.26984300	1.19330000	-3.45339500
H	-2.30411400	-0.18539300	-4.00474600

Zero-point correction= 0.327431 (Hartree/Particle)

Thermal correction to Energy= 0.349224

Thermal correction to Enthalpy= 0.350169

Thermal correction to Gibbs Free Energy= 0.274619

Sum of electronic and zero-point Energies= -1413.501837

Sum of electronic and thermal Energies= -1413.480043

Sum of electronic and thermal Enthalpies= -1413.479099

Sum of electronic and thermal Free Energies= -1413.554649

E(RB3LYP) = -1413.829268 A.U.

OAc-

-1 1

Number of imaginary frequencies: 0

C	-0.22050600	0.00180900	-0.00016400

O	-0.69409500	1.16719000	-0.00003700
O	-0.80936300	-1.10821700	0.00009200
C	1.35417500	-0.05658100	-0.00002000
H	1.74705000	0.46841600	0.88171600
H	1.73097400	-1.08635500	-0.00340900
H	1.74763400	0.47478400	-0.87764500

Zero-point correction= 0.048054 (Hartree/Particle)

Thermal correction to Energy= 0.052518

Thermal correction to Enthalpy= 0.053462

Thermal correction to Gibbs Free Energy= 0.020425

Sum of electronic and zero-point Energies= -228.456647

Sum of electronic and thermal Energies= -228.452182

Sum of electronic and thermal Enthalpies= -228.451238

Sum of electronic and thermal Free Energies= -228.484275

E(RB3LYP) = -228.504700 A.U.

OTf-

-1 1

Number of imaginary frequencies: 0

S	0.92741200	-0.00005600	-0.00004800
O	1.24362300	-0.13152600	-1.44110000
O	1.24381100	-1.18241500	0.83435100
C	-0.94225500	0.00019600	0.00015800
O	1.24378000	1.31387900	0.60650800
F	-1.44600500	-1.14003600	-0.52536300
F	-1.44574200	1.02497900	-0.72458600
F	-1.44545000	0.11508100	1.25014400

Zero-point correction= 0.027216 (Hartree/Particle)

Thermal correction to Energy= 0.034401

Thermal correction to Enthalpy= 0.035345

Thermal correction to Gibbs Free Energy= -0.005343

Sum of electronic and zero-point Energies= -961.476232

Sum of electronic and thermal Energies= -961.469048

Sum of electronic and thermal Enthalpies= -961.468104

Sum of electronic and thermal Free Energies= -961.508792

E(RB3LYP) = -961.503449 A.U.

HOAc

0 1

Number of imaginary frequencies: 0

H	1.72009100	-0.80755100	0.00027700
C	0.09293400	0.12624300	-0.00011400
O	0.77777500	-1.04696500	-0.00001800
O	0.64294200	1.20428200	0.00001800
C	-1.39527900	-0.11109400	-0.00003800
H	-1.67844800	-0.69064200	0.88341100
H	-1.91536400	0.84577600	-0.00338600
H	-1.67794900	-0.69701200	-0.87938300

Zero-point correction= 0.061998 (Hartree/Particle)

Thermal correction to Energy= 0.066534

Thermal correction to Enthalpy= 0.067478

Thermal correction to Gibbs Free Energy= 0.034932

Sum of electronic and zero-point Energies= -229.032482

Sum of electronic and thermal Energies= -229.027946

Sum of electronic and thermal Enthalpies= -229.027002

Sum of electronic and thermal Free Energies= -229.059548

E(RB3LYP) = -229.094480 A.U.

Cu(OAC)2

-1 1

Number of imaginary frequencies: 0

O	-1.92669300	-1.11616800	-0.01281700
O	1.92680900	-1.11635000	-0.01301700
C	-2.51944000	0.00011000	-0.00850600
O	-1.92730900	1.11666800	-0.01322900
C	2.51943700	-0.00003000	-0.00846100
O	1.92719500	1.11648800	-0.01323300
C	-4.05144600	-0.00079200	0.04819700
H	-4.45701900	0.90137800	-0.41727400
H	-4.45584900	-0.89437100	-0.43471100
H	-4.36890200	-0.01188700	1.09797400
C	4.05144600	-0.00060800	0.04818100
H	4.45679600	0.90031500	-0.41991700
H	4.36893700	-0.00837600	1.09797700
H	4.45604200	-0.89547900	-0.43214400
Cu	0.00000000	0.00038700	-0.01896600

Zero-point correction= 0.099561 (Hartree/Particle)

Thermal correction to Energy= 0.107878

Thermal correction to Enthalpy= 0.108822

Thermal correction to Gibbs Free Energy= 0.063754

Sum of electronic and zero-point Energies= -653.151203

Sum of electronic and thermal Energies= -653.142886

Sum of electronic and thermal Enthalpies= -653.141941

Sum of electronic and thermal Free Energies= -653.187009

E(RB3LYP) = -653.250764 A.U.

CuOAC

0 1

Number of imaginary frequencies: 0

C	-2.57681600	-0.00165100	0.00052900
H	-2.93025400	-0.53859900	0.88532400
H	-2.93192700	-0.55090700	-0.87591100
H	-2.97388900	1.01299600	-0.00568300
C	-1.06221200	0.00953200	-0.00076100
O	-0.44746400	-1.10685300	-0.00056700
O	-0.44434000	1.12197500	-0.00054700
Cu	1.30360900	-0.00316400	0.00022700

Zero-point correction= 0.050583 (Hartree/Particle)

Thermal correction to Energy= 0.056687

Thermal correction to Enthalpy= 0.057631

Thermal correction to Gibbs Free Energy= 0.018557

Sum of electronic and zero-point Energies= -424.596627

Sum of electronic and thermal Energies= -424.590524

Sum of electronic and thermal Enthalpies= -424.589580

Sum of electronic and thermal Free Energies= -424.628654

E(RB3LYP) = -424.647211 A.U.

A-int1

0 1

Number of imaginary frequencies: 0

Rh	-0.84523100	-0.13421000	-0.08817400
C	-2.94188200	0.34021400	0.10037200
C	-2.72274800	-0.11039500	-1.27005100

C	-2.26199600	-1.45372900	-1.21653600
C	-2.22893600	-1.87658800	0.17584800
C	-2.67447800	-0.77085400	0.97468300
O	0.29042400	0.17477900	1.60056100
O	-0.89798700	1.94554900	2.36144500
C	0.10835900	1.23360400	2.34390000
C	1.33264500	1.55012700	3.18850600
H	2.04309200	2.04992300	2.52225500
H	1.06819700	2.21304100	4.01421000
H	1.80533000	0.63660200	3.55772100
O	-0.47452300	1.81655700	-0.78193200
C	0.53691100	2.57489000	-0.43363600
O	1.64437000	2.19360900	-0.06646700
C	0.18654800	4.05861400	-0.49530000
H	-0.43350300	4.28659900	-1.36646200
H	-0.39550100	4.29011400	0.40329800
H	1.09503500	4.66346800	-0.50212100
C	1.11003000	-0.07103000	-2.27270300
C	2.32092200	-0.84622600	-0.43908100
C	3.49939600	-0.20197500	-0.93834100
C	3.42716100	0.47435000	-2.17792200
C	2.24776700	0.48727800	-2.88070500
H	0.14180000	0.03706300	-2.74867800
C	2.42757800	-1.69778000	0.70318600
C	4.71534300	-0.28368400	-0.21441900
H	4.31656200	0.96425500	-2.56517200
H	2.15733700	0.97144400	-3.84668000

C	4.77720000	-1.02920500	0.93705200
C	3.64299200	-1.75560100	1.36221600
H	5.58883300	0.23737400	-0.59609000
H	5.70248700	-1.09902000	1.50100700
H	3.73190000	-2.40486600	2.22947700
N	1.11852000	-0.67704300	-1.09084400
C	1.29525500	-2.58327800	1.14637400
H	0.58731700	-2.01730400	1.75453600
H	0.75538600	-2.98070800	0.28480900
H	1.67656400	-3.42427500	1.73305500
C	-3.41892400	1.70497500	0.47521000
H	-2.89784200	2.44848600	-0.13295300
H	-4.49920400	1.79493500	0.30359300
H	-3.18541400	1.92457500	1.51549200
C	-2.89344300	0.76836700	-2.46854200
H	-2.61627000	0.25577900	-3.39261100
H	-3.93546900	1.09387600	-2.56050900
H	-2.26358400	1.65784300	-2.35626900
C	-1.87530300	-2.32177100	-2.37433600
H	-2.66917300	-3.04634100	-2.59186900
H	-1.70043700	-1.73384000	-3.27759600
H	-0.96096100	-2.87916300	-2.15523000
C	-1.99284100	-3.27454100	0.65693700
H	-1.52839800	-3.28703200	1.64484500
H	-2.94460200	-3.81700500	0.72701800
H	-1.34609100	-3.83120500	-0.02449400
C	-2.79924200	-0.75280900	2.46507800

H	-3.83110200	-0.98186400	2.75897600
H	-2.14159200	-1.49476700	2.92277000
H	-2.52307200	0.22910500	2.85179600

Zero-point correction= 0.492335 (Hartree/Particle)

Thermal correction to Energy= 0.525757

Thermal correction to Enthalpy= 0.526701

Thermal correction to Gibbs Free Energy= 0.429063

Sum of electronic and zero-point Energies= -1397.491001

Sum of electronic and thermal Energies= -1397.457580

Sum of electronic and thermal Enthalpies= -1397.456636

Sum of electronic and thermal Free Energies= -1397.554273

E(RB3LYP) = -1397.983336 A.U.

A-int2

1 1

Number of imaginary frequencies: 0

Rh	-0.66608600	-0.04832700	0.02682900
C	-2.84153200	-0.02835400	-0.28029000
C	-2.22022300	-1.23562500	-0.80546900
C	-1.69979600	-2.00317600	0.32702200
C	-1.89878700	-1.23323600	1.49809000
C	-2.59831000	0.00292700	1.11800100
O	-0.27330500	1.39634000	-1.40218500
O	-1.08623300	2.86615500	0.08932100
C	-0.62297100	2.60219700	-1.02654400
C	-0.40078900	3.66024300	-2.08904900
H	-0.93446600	3.38894100	-3.00437600
H	-0.74433100	4.62896800	-1.72654300

H	0.66307000	3.71256500	-2.33829300
C	1.44656600	-1.41591500	-1.56975000
C	2.45544400	-0.16808400	0.13771100
C	3.75026300	-0.49022100	-0.39171800
C	3.83202700	-1.31555900	-1.53796000
C	2.68171600	-1.78074900	-2.13021700
H	0.52542200	-1.73650100	-2.04075900
C	2.35911400	0.66874800	1.29077600
C	4.91568200	0.02893300	0.22894300
H	4.80873100	-1.56373300	-1.94313600
H	2.70311500	-2.40344200	-3.01706800
C	4.80437800	0.84388100	1.32814600
C	3.52790700	1.15551500	1.84793100
H	5.88650200	-0.22406700	-0.18604100
H	5.68981300	1.25230900	1.80382200
H	3.46179600	1.79937100	2.72013000
N	1.32501700	-0.66199200	-0.48141400
C	1.03560600	1.00084200	1.92772900
H	0.30200200	1.45289100	1.22655000
H	0.60819200	0.13009300	2.43388100
H	1.14780000	1.78335700	2.68318200
C	-3.56050900	1.00568100	-1.08347600
H	-3.18053300	1.04122200	-2.10607900
H	-4.62974400	0.76652900	-1.12373900
H	-3.43739300	1.99413400	-0.63980900
C	-2.30405700	-1.69384900	-2.22511400
H	-1.62304400	-2.52242300	-2.42837400

H	-3.32115100	-2.04424300	-2.43906100
H	-2.07985500	-0.87651500	-2.91486100
C	-1.07175600	-3.35604700	0.23424200
H	-1.85368500	-4.12110200	0.16113000
H	-0.43926300	-3.44749400	-0.65180300
H	-0.46120700	-3.57935300	1.11026100
C	-1.54468900	-1.62681700	2.89690300
H	-1.30869700	-0.75715300	3.51355200
H	-2.39556800	-2.13632700	3.36476600
H	-0.69163400	-2.30778100	2.92269800
C	-3.00658700	1.10100800	2.04459300
H	-4.07702600	1.01746900	2.26772700
H	-2.46273700	1.05487100	2.98943000
H	-2.81324200	2.07205600	1.58530700

Zero-point correction= 0.440432 (Hartree/Particle)

Thermal correction to Energy= 0.468974

Thermal correction to Enthalpy= 0.469918

Thermal correction to Gibbs Free Energy= 0.380713

Sum of electronic and zero-point Energies= -1168.846369

Sum of electronic and thermal Energies= -1168.817827

Sum of electronic and thermal Enthalpies= -1168.816882

Sum of electronic and thermal Free Energies= -1168.906088

E(RB3LYP) = -1169.286801 A.U.

A-int3

0 1

Number of imaginary frequencies: 0

Rh	0.29424100	1.06474100	0.44531700

C	2.33774400	1.78347300	0.77094900
C	1.44705100	2.89134900	0.45540900
C	0.46912200	2.97667700	1.50364800
C	0.72103900	1.91309500	2.44758900
C	1.90255000	1.19994800	1.99866200
C	-1.55234300	2.07116100	-1.64412300
C	-2.78948100	0.52037900	-0.41835600
C	-3.44974000	0.09356700	-1.61604500
C	-3.14758300	0.75738400	-2.82683700
C	-2.25919100	1.80631600	-2.82838800
H	-0.74091600	2.78696500	-1.66531100
C	-3.24595600	0.03563300	0.83940400
C	-4.41986900	-0.93772100	-1.55502000
H	-3.63572800	0.43712500	-3.74285700
H	-2.01540100	2.35552000	-3.72985500
C	-4.76844600	-1.47765800	-0.34090200
C	-4.20716300	-0.95881000	0.84539900
H	-4.88630500	-1.27320600	-2.47666400
H	-5.50236300	-2.27501500	-0.28183500
H	-4.54179300	-1.35073800	1.80083400
N	-1.75227400	1.42977400	-0.49477500
C	-2.76250500	0.63134400	2.13257900
H	-1.75868900	0.29561400	2.38810600
H	-2.74193800	1.72378200	2.06842400
H	-3.42086300	0.34395900	2.95599100
C	3.49547500	1.36080800	-0.07039000
H	3.22911600	1.39567000	-1.12800600

H	4.34501100	2.03295600	0.10267100
H	3.80260600	0.34043900	0.15854200
C	1.60966700	3.78933900	-0.72908200
H	0.77253300	4.48326500	-0.82902300
H	2.52631500	4.38184700	-0.62865300
H	1.68759000	3.19281600	-1.64311900
C	-0.61967000	3.99730500	1.59227000
H	-0.22127800	4.92604600	2.01804300
H	-1.03169300	4.22352000	0.60661400
H	-1.43653700	3.65398500	2.22761200
C	0.05811900	1.70052400	3.77013400
H	-0.06003000	0.63469700	3.97153900
H	0.68121000	2.13839400	4.56055000
H	-0.92287600	2.17512300	3.81420600
C	2.58399600	0.10890200	2.75246800
H	3.16320000	0.56023900	3.56859700
H	1.85767600	-0.58366100	3.17701000
H	3.26655200	-0.45358200	2.11656500
S	0.66885200	-0.26877600	-2.69635400
O	-0.48319800	-1.12559100	-2.42521200
O	0.85706400	0.27426500	-4.04524300
C	2.18768900	-1.29526200	-2.36247200
O	0.88908000	0.83662600	-1.64983000
F	2.13141700	-2.46037800	-3.00866700
F	2.31418300	-1.53252900	-1.04472700
F	3.28507800	-0.62670300	-2.76251200
S	-0.47394400	-1.99081600	1.63278500

O	-0.13699300	-1.43303700	2.96084000
O	-1.69633000	-2.78404900	1.51943400
C	0.91388100	-3.17213700	1.25285100
O	-0.32974500	-0.97334300	0.50681400
F	0.86766800	-4.20289600	2.10473200
F	2.10202400	-2.55466900	1.40330800
F	0.81805200	-3.62801600	0.00546400

Zero-point correction= 0.447878 (Hartree/Particle)

Thermal correction to Energy= 0.487929

Thermal correction to Enthalpy= 0.488873

Thermal correction to Gibbs Free Energy= 0.374984

Sum of electronic and zero-point Energies= -2863.422200

Sum of electronic and thermal Energies= -2863.382149

Sum of electronic and thermal Enthalpies= -2863.381204

Sum of electronic and thermal Free Energies= -2863.495094

E(RB3LYP) = -2863.870078 A.U.

A-int4

1 1

Number of imaginary frequencies: 0

Rh	0.74862100	-0.55331100	0.05169100
C	2.75754200	-0.43467500	-0.84336400
C	2.87372000	-0.46750700	0.57739100
C	2.27511500	-1.71210200	1.05002600
C	1.83351700	-2.45768600	-0.10344700
C	2.10589000	-1.66591900	-1.27133000
C	-1.30145000	-1.35587100	1.95197200
C	-2.44322200	-0.93576000	-0.05320400

C	-3.62216400	-0.60335000	0.69853400
C	-3.59004300	-0.71654200	2.10700800
C	-2.44439700	-1.14588000	2.73577100
H	-0.36191800	-1.59033400	2.43769900
C	-2.51871700	-0.97987500	-1.47710900
C	-4.80281400	-0.19879700	0.02612500
H	-4.48124600	-0.47138700	2.67745400
H	-2.38829200	-1.27106700	3.81069600
C	-4.83277100	-0.16821800	-1.34592100
C	-3.70227400	-0.58796300	-2.07939800
H	-5.67553700	0.06711100	0.61440000
H	-5.72974700	0.14069300	-1.87227000
H	-3.76775800	-0.62280400	-3.16315300
N	-1.27033800	-1.23053000	0.62366300
C	-1.39007700	-1.49133100	-2.33073300
H	-0.64382200	-0.71339700	-2.50809400
H	-0.89759000	-2.34402100	-1.85760800
H	-1.76731700	-1.81737700	-3.30312400
C	3.21371300	0.63937000	-1.77686200
H	3.56633700	1.51998300	-1.24316600
H	4.03139200	0.26012200	-2.40029600
H	2.40002000	0.94807300	-2.43898100
C	3.45742600	0.58857100	1.45566000
H	2.92638300	0.64452400	2.40791200
H	4.50791000	0.35266000	1.66462800
H	3.40703500	1.57048500	0.98680300
C	2.27657000	-2.18372000	2.46844400

H	3.26774700	-2.57827200	2.72291300
H	2.05977700	-1.36802000	3.16286000
H	1.55298600	-2.98479900	2.63040900
C	1.21118100	-3.81563400	-0.07418500
H	0.63669000	-4.01571100	-0.97949500
H	1.99656100	-4.57663100	0.00422100
H	0.54411200	-3.92941800	0.78278400
C	1.91837500	-2.05957000	-2.69881600
H	2.87683300	-2.41907700	-3.09400600
H	1.18610300	-2.85749500	-2.81783700
H	1.60906400	-1.20890600	-3.30963600
S	-0.49611300	1.97889000	0.16462900
O	-0.23780300	1.13158200	-1.07200100
O	-1.84307100	2.48633500	0.35812500
C	0.62745800	3.45330700	-0.05174800
O	0.13014600	1.20177600	1.31387800
F	0.25062700	4.14546900	-1.11910100
F	1.88971200	3.01633300	-0.23188100
F	0.57930900	4.21073900	1.03655600

Zero-point correction= 0.418580 (Hartree/Particle)

Thermal correction to Energy= 0.450179

Thermal correction to Enthalpy= 0.451123

Thermal correction to Gibbs Free Energy= 0.355996

Sum of electronic and zero-point Energies= -1901.805061

Sum of electronic and thermal Energies= -1901.773462

Sum of electronic and thermal Enthalpies= -1901.772518

Sum of electronic and thermal Free Energies= -1901.867646

E(RB3LYP) = -1902.223641 A.U.

A-int5

1 1

Number of imaginary frequencies: 0

Rh	0.74862100	-0.55331100	0.05169100
C	2.75754200	-0.43467500	-0.84336400
C	2.87372000	-0.46750700	0.57739100
C	2.27511500	-1.71210200	1.05002600
C	1.83351700	-2.45768600	-0.10344700
C	2.10589000	-1.66591900	-1.27133000
C	-1.30145000	-1.35587100	1.95197200
C	-2.44322200	-0.93576000	-0.05320400
C	-3.62216400	-0.60335000	0.69853400
C	-3.59004300	-0.71654200	2.10700800
C	-2.44439700	-1.14588000	2.73577100
H	-0.36191800	-1.59033400	2.43769900
C	-2.51871700	-0.97987500	-1.47710900
C	-4.80281400	-0.19879700	0.02612500
H	-4.48124600	-0.47138700	2.67745400
H	-2.38829200	-1.27106700	3.81069600
C	-4.83277100	-0.16821800	-1.34592100
C	-3.70227400	-0.58796300	-2.07939800
H	-5.67553700	0.06711100	0.61440000
H	-5.72974700	0.14069300	-1.87227000
H	-3.76775800	-0.62280400	-3.16315300
N	-1.27033800	-1.23053000	0.62366300
C	-1.39007700	-1.49133100	-2.33073300

H	-0.64382200	-0.71339700	-2.50809400
H	-0.89759000	-2.34402100	-1.85760800
H	-1.76731700	-1.81737700	-3.30312400
C	3.21371300	0.63937000	-1.77686200
H	3.56633700	1.51998300	-1.24316600
H	4.03139200	0.26012200	-2.40029600
H	2.40002000	0.94807300	-2.43898100
C	3.45742600	0.58857100	1.45566000
H	2.92638300	0.64452400	2.40791200
H	4.50791000	0.35266000	1.66462800
H	3.40703500	1.57048500	0.98680300
C	2.27657000	-2.18372000	2.46844400
H	3.26774700	-2.57827200	2.72291300
H	2.05977700	-1.36802000	3.16286000
H	1.55298600	-2.98479900	2.63040900
C	1.21118100	-3.81563400	-0.07418500
H	0.63669000	-4.01571100	-0.97949500
H	1.99656100	-4.57663100	0.00422100
H	0.54411200	-3.92941800	0.78278400
C	1.91837500	-2.05957000	-2.69881600
H	2.87683300	-2.41907700	-3.09400600
H	1.18610300	-2.85749500	-2.81783700
H	1.60906400	-1.20890600	-3.30963600
S	-0.49611300	1.97889000	0.16462900
O	-0.23780300	1.13158200	-1.07200100
O	-1.84307100	2.48633500	0.35812500
C	0.62745800	3.45330700	-0.05174800

O	0.13014600	1.20177600	1.31387800
F	0.25062700	4.14546900	-1.11910100
F	1.88971200	3.01633300	-0.23188100
F	0.57930900	4.21073900	1.03655600

Zero-point correction= 0.418580 (Hartree/Particle)

Thermal correction to Energy= 0.450179

Thermal correction to Enthalpy= 0.451123

Thermal correction to Gibbs Free Energy= 0.355996

Sum of electronic and zero-point Energies= -1901.805061

Sum of electronic and thermal Energies= -1901.773462

Sum of electronic and thermal Enthalpies= -1901.772518

Sum of electronic and thermal Free Energies= -1901.867646

E(RB3LYP) = -1902.223641 A.U.

A-int6

0 1

Number of imaginary frequencies: 0

Rh	-0.78585900	-0.10277900	-0.08797000
C	-2.90606200	0.22616200	-0.28724700
C	-2.72346300	-1.20996200	-0.09624100
C	-2.10462700	-1.40258300	1.16531700
C	-1.97119200	-0.10469500	1.81652700
C	-2.50112400	0.88443100	0.93437400
O	0.41963800	1.52617800	-0.43835500
O	-1.08839600	2.86674100	-1.47823900
C	0.05612400	2.56165000	-1.14439800
C	1.25477700	3.40836800	-1.56085900
H	1.68159300	2.96561000	-2.46717900

H	0.93608200	4.42850700	-1.78252700
H	2.02944100	3.39951900	-0.79020200
C	1.23411200	-2.30473900	-0.27061500
C	2.48167500	-0.47790500	0.45252400
C	3.61708700	-0.95138000	-0.28383900
C	3.50868900	-2.18359400	-0.97426100
C	2.33591500	-2.89376500	-0.92008800
H	0.26697300	-2.79096600	-0.32105300
C	2.63830000	0.65371000	1.31297600
C	4.82944000	-0.21476000	-0.27567400
H	4.36623900	-2.55616200	-1.52849700
H	2.21650400	-3.84958300	-1.41740800
C	4.93194600	0.92517800	0.48305600
C	3.84733800	1.32650600	1.29470000
H	5.66905100	-0.57967200	-0.86073100
H	5.85436600	1.49782300	0.49742400
H	3.97314000	2.18496600	1.94928800
N	1.27362200	-1.13698600	0.35984700
C	1.56736500	1.06127600	2.28593300
H	0.75556300	1.57435300	1.76764600
H	1.14902700	0.18351600	2.78270400
H	1.97813500	1.72704700	3.05033400
C	-3.55971400	0.86893600	-1.46689200
H	-3.43925200	0.24544100	-2.35436400
H	-4.63185000	1.01168300	-1.27770000
H	-3.08665500	1.83023800	-1.66949200
C	-3.12398600	-2.25262700	-1.09029900

H	-2.78135100	-3.24656500	-0.79514800
H	-4.21631400	-2.28026900	-1.17822200
H	-2.69873600	-2.02307000	-2.07086400
C	-1.68867500	-2.69979700	1.78809100
H	-2.36144500	-2.96090400	2.61367300
H	-1.71021100	-3.51901000	1.06693300
H	-0.67455100	-2.62971800	2.19153100
C	-1.55939000	0.09939300	3.24025500
H	-1.12182800	1.08629700	3.39881700
H	-2.43464000	0.01136000	3.89701000
H	-0.83227000	-0.65050900	3.55920300
C	-2.62444500	2.34727000	1.21746900
H	-3.63425700	2.56569300	1.58791800
H	-1.91000900	2.66508000	1.98055100
H	-2.43732100	2.92256000	0.31070600
Cl	-0.37338800	-0.69265200	-2.41721900

Zero-point correction= 0.441785 (Hartree/Particle)

Thermal correction to Energy= 0.472049

Thermal correction to Enthalpy= 0.472993

Thermal correction to Gibbs Free Energy= 0.381584

Sum of electronic and zero-point Energies= -1629.270386

Sum of electronic and thermal Energies= -1629.240121

Sum of electronic and thermal Enthalpies= -1629.239177

Sum of electronic and thermal Free Energies= -1629.330587

E(RB3LYP) = -1629.712171 A.U.

A-tsa1

1 1

Number of imaginary frequencies: 1

Rh	-0.65501400	-0.03393500	0.05577500
C	-2.49960400	-0.79061600	-0.89635300
C	-2.01424000	-1.82550400	-0.03254000
C	-1.95612800	-1.30785400	1.31318600
C	-2.49844800	0.03966900	1.28770800
C	-2.80607600	0.36986400	-0.06646000
O	-0.18067000	1.34684600	-1.50623600
C	-0.00238000	2.55100000	-1.12101000
O	0.04764200	2.88528200	0.10001000
C	0.16444600	3.61695700	-2.17416200
H	-0.02390700	3.21762900	-3.17023200
H	-0.51315400	4.44703400	-1.95862200
H	1.18493400	4.00792400	-2.11976600
C	1.37262100	-1.74635600	-1.44121700
C	2.33765600	-0.36308000	0.17942100
C	3.64965600	-0.74412000	-0.23960800
C	3.76575600	-1.68645500	-1.29025200
C	2.63183600	-2.18870800	-1.88882200
H	0.46463800	-2.09763400	-1.91689400
C	2.15406100	0.57845400	1.22889800
C	4.77092300	-0.14367700	0.38953000
H	4.75312200	-1.99447400	-1.62198500
H	2.68562100	-2.90124900	-2.70390300
C	4.58288000	0.79520500	1.37783100
C	3.27816700	1.15189000	1.79454600
H	5.76882100	-0.42437900	0.06709100

H	5.43820900	1.26690700	1.85065100
H	3.15675400	1.88629200	2.58552700
N	1.22596800	-0.88110800	-0.44548900
C	0.75867600	0.88947900	1.67659000
H	0.16544900	1.73742500	0.79771700
H	0.35185800	0.07726900	2.28416200
H	0.73479200	1.76618000	2.33579300
C	-2.71826600	-0.85557900	-2.37465600
H	-2.30218300	0.03085500	-2.86100700
H	-2.24755100	-1.73558400	-2.81657500
H	-3.78982300	-0.89727800	-2.60101100
C	-1.63531100	-3.21835800	-0.42235800
H	-1.53468400	-3.33073600	-1.50294300
H	-0.69930000	-3.52691600	0.04979100
H	-2.41655600	-3.91215800	-0.09038400
C	-1.58575100	-2.09098500	2.53442700
H	-1.21720300	-1.44370000	3.33346700
H	-2.46044600	-2.62584700	2.92348200
H	-0.81259300	-2.83052500	2.31416900
C	-2.69173000	0.92660900	2.47656700
H	-1.96719600	0.70938000	3.26381300
H	-2.59913300	1.98072800	2.20821400
H	-3.69357500	0.77039500	2.89372500
C	-3.37405600	1.65791200	-0.57220700
H	-2.98611600	1.88604800	-1.56710900
H	-4.46592300	1.58940200	-0.64122500
H	-3.12489600	2.49035300	0.08807600

Zero-point correction= 0.436343 (Hartree/Particle)

Thermal correction to Energy= 0.463771

Thermal correction to Enthalpy= 0.464715

Thermal correction to Gibbs Free Energy= 0.378328

Sum of electronic and zero-point Energies= -1168.831937

Sum of electronic and thermal Energies= -1168.804509

Sum of electronic and thermal Enthalpies= -1168.803565

Sum of electronic and thermal Free Energies= -1168.889952

E(RB3LYP) = -1169.268280 A.U.

A-tsa2

0 1

Number of imaginary frequencies: 1

H	0.06489300	0.76368800	1.69431200
C	0.12814100	-0.95063600	-1.84824700
C	-0.97058100	-1.74964800	-1.32805800
C	-2.19091200	-1.02831400	-1.57765400
C	-1.84861600	0.25264900	-2.13031800
O	-0.02320200	1.97583100	2.13284300
O	-0.77988100	2.25439500	0.04968400
C	-0.37645200	2.70546900	1.16318800
C	-0.28587600	4.20529500	1.33517200
H	-0.80316700	4.49857200	2.25227700
H	0.76712200	4.48164800	1.44886000
H	-0.71485900	4.72430500	0.47757400
Rh	-0.95432800	0.12835500	-0.15241700
O	-2.45021000	0.33346900	1.27709800
O	-2.59480000	-1.88396500	1.72489200

C	-2.91706600	-0.70403800	1.90772600
C	-3.95276900	-0.32413000	2.96219400
H	-3.47662600	0.29223100	3.73101500
H	-4.74637800	0.27787100	2.50996300
H	-4.37356000	-1.22237900	3.41609100
C	-0.40340200	0.28528500	-2.30280800
C	3.10780900	1.99483700	-0.21292900
C	2.68746300	-0.09069100	0.68337500
C	4.00662500	-0.54329400	0.34216200
C	4.87712800	0.38046600	-0.29170500
C	4.43463700	1.65125700	-0.57373900
H	2.72531600	2.98976900	-0.44040300
C	1.75527100	-0.99772300	1.28993400
C	4.38460000	-1.88464300	0.60414000
H	5.88310200	0.06413700	-0.55691000
H	5.07223900	2.37944000	-1.06522700
C	3.47527800	-2.74868100	1.16973400
C	2.17466000	-2.30338200	1.50310800
H	5.38655300	-2.21480300	0.34267000
H	3.75051500	-3.78133000	1.36515200
H	1.47598200	-3.00613000	1.94960300
N	2.27170700	1.17435300	0.38804100
C	0.36482000	-0.59043000	1.67585100
H	-0.31308100	-1.44650900	1.66451500
H	0.36169200	-0.31494100	2.74365500
C	1.54258200	-1.41011900	-1.99741100
H	1.84238400	-2.08316400	-1.19435500

H	1.64154200	-1.95431500	-2.94540200
H	2.24241200	-0.57409700	-2.01478200
C	-0.86481100	-3.13175400	-0.76389700
H	-1.05314100	-3.88846200	-1.53580400
H	0.13419500	-3.30584600	-0.35667700
H	-1.58343600	-3.25467300	0.04841200
C	-3.57313300	-1.51748500	-1.28483100
H	-4.24289100	-0.68615400	-1.05474500
H	-3.97099400	-2.04345000	-2.16175700
H	-3.57093200	-2.19309300	-0.43007000
C	-2.77979100	1.35359800	-2.53232000
H	-2.37989200	2.32072700	-2.21608100
H	-2.91555200	1.37507700	-3.62088900
H	-3.76086600	1.23106700	-2.06945200
C	0.35174300	1.45500000	-2.85086300
H	1.42792000	1.33274000	-2.71991000
H	0.14163400	1.58350700	-3.91936000
H	0.05134500	2.36696300	-2.32674800

Zero-point correction= 0.487156 (Hartree/Particle)

Thermal correction to Energy= 0.519962

Thermal correction to Enthalpy= 0.520906

Thermal correction to Gibbs Free Energy= 0.423186

Sum of electronic and zero-point Energies= -1397.454377

Sum of electronic and thermal Energies= -1397.421572

Sum of electronic and thermal Enthalpies= -1397.420628

Sum of electronic and thermal Free Energies= -1397.518347

E(RB3LYP) = -1397.941534 A.U.

A-tsa3

0 1

Number of imaginary frequencies: 1

Rh	0.23738500	1.16307300	-0.38204300
C	0.78324200	3.33191200	-0.56733400
C	-0.46637800	3.03203600	-1.23201400
C	-1.41723900	2.63143200	-0.21075100
C	-0.72396700	2.56126200	1.03577200
C	0.64203400	3.03162200	0.81893800
C	3.07029200	0.57415500	-1.46665800
C	1.49642100	-1.09383200	-1.89351200
C	2.52017400	-2.01755500	-2.25404900
C	3.85803200	-1.55508500	-2.24438700
C	4.13144700	-0.26006900	-1.86957100
H	3.26927100	1.56323200	-1.08009400
C	0.12890300	-1.47539500	-1.90320800
C	2.15297700	-3.35430900	-2.55700800
H	4.65860500	-2.23784900	-2.51556400
H	5.14578000	0.11990500	-1.82895200
C	0.83103900	-3.73268000	-2.49229200
C	-0.18097000	-2.79553300	-2.17361300
H	2.93013600	-4.06912000	-2.81117800
H	0.55077200	-4.76186400	-2.69475200
H	-1.21640800	-3.11214200	-2.12239700
N	1.80560500	0.18183100	-1.48624300
C	-0.89010700	-0.41668800	-1.65407700
H	-1.37002300	-0.29408600	-0.34236700

H	-0.83774700	0.36450100	-2.41864600
H	-1.90037800	-0.82474700	-1.75686100
C	1.99355300	3.90638600	-1.23075500
H	2.88946200	3.76862600	-0.62241900
H	2.16282400	3.46227500	-2.21491800
H	1.85384200	4.98477900	-1.37487100
C	-0.78621600	3.30173500	-2.66978400
H	0.08269700	3.12849900	-3.30952100
H	-1.59904000	2.66138500	-3.02017400
H	-1.10251600	4.34346500	-2.80547700
C	-2.86821800	2.36662200	-0.44785900
H	-3.38622800	3.32469600	-0.58141400
H	-3.03412900	1.77031100	-1.34697400
H	-3.32115100	1.83577600	0.38517700
C	-1.27819200	2.14017000	2.35939100
H	-2.15961500	1.51323600	2.23282100
H	-0.53964500	1.55651800	2.91398600
H	-1.54183600	3.02553500	2.95132000
C	1.65703500	3.27071000	1.89017100
H	1.48709500	2.62437100	2.75151700
H	2.66897800	3.07059900	1.53756600
H	1.59218600	4.31587900	2.21950300
S	-3.10399900	-1.62878800	0.70901000
O	-2.71192700	-2.64970800	-0.27039200
O	-3.48420500	-2.00989900	2.06291200
C	-4.62116200	-0.85447300	-0.04224400
O	-2.15505800	-0.41492200	0.68634600

F	-5.60950400	-1.74227500	-0.14846500
F	-4.32823100	-0.38915100	-1.27904400
F	-5.04752000	0.18318600	0.69735500
S	1.92526400	-0.20573300	1.96523400
O	0.74927600	-0.40334400	1.01183000
O	3.04777800	0.54277900	1.36652800
C	2.51860200	-1.96606300	2.06759100
O	1.50816500	0.18923900	3.31815100
F	2.88609000	-2.38077000	0.84343400
F	1.55550000	-2.76422200	2.52628800
F	3.57869000	-2.03830800	2.88075600

Zero-point correction= 0.442970 (Hartree/Particle)

Thermal correction to Energy= 0.481910

Thermal correction to Enthalpy= 0.482854

Thermal correction to Gibbs Free Energy= 0.371825

Sum of electronic and zero-point Energies= -2863.386516

Sum of electronic and thermal Energies= -2863.347577

Sum of electronic and thermal Enthalpies= -2863.346633

Sum of electronic and thermal Free Energies= -2863.457661

E(RB3LYP) = -2863.829486 A.U.

A-tsa4

1 1

Number of imaginary frequencies: 1

Rh	-0.51540800	-0.82426300	0.11847000
C	-1.86867700	-2.23028400	-0.99737200
C	-1.48035600	-2.77141600	0.29803700
C	-2.02495800	-1.90634600	1.31875400

C	-2.63862700	-0.78157700	0.66994900
C	-2.57066900	-1.01129600	-0.76434200
C	1.68516900	-1.58110300	-1.90156400
C	2.49323400	-0.66517400	0.08936800
C	3.80888200	-0.56445300	-0.45437500
C	4.01897300	-1.03620200	-1.77236000
C	2.96284600	-1.55089300	-2.49161100
H	0.83090300	-1.93794000	-2.46366000
C	2.21617700	-0.21826500	1.40883600
C	4.82829700	0.03257400	0.33208500
H	5.01176500	-0.97474600	-2.20857600
H	3.08713600	-1.91067600	-3.50652500
C	4.53799200	0.50623700	1.59102300
C	3.23476800	0.37711700	2.12816200
H	5.82672800	0.12658800	-0.08345300
H	5.31157500	0.98094700	2.18557800
H	3.03336600	0.74754000	3.12903900
N	1.45407600	-1.16220600	-0.66347000
C	0.83064500	-0.42463600	1.93481800
H	0.05025100	0.72647700	1.51201000
H	0.65220900	-1.47637700	2.16905900
H	0.67370400	0.09589800	2.88856800
C	-1.65561600	-2.89567400	-2.32008700
H	-1.52344300	-2.16891100	-3.12498700
H	-0.78962400	-3.56064100	-2.30347700
H	-2.52973200	-3.50861200	-2.57055100
C	-0.78631500	-4.07787500	0.51897800

H	-0.03642400	-4.26400900	-0.25283500
H	-0.28695100	-4.11003500	1.48894900
H	-1.51292700	-4.89864000	0.48736500
C	-1.98020300	-2.14306900	2.79378300
H	-2.91498900	-2.62395700	3.10584800
H	-1.15877300	-2.80148700	3.08100100
H	-1.88636000	-1.20835500	3.35003100
C	-3.36218100	0.34402200	1.34073800
H	-2.97677900	0.52224800	2.34616100
H	-3.26233900	1.27160000	0.77818100
H	-4.42991100	0.10853100	1.42448100
C	-3.12289100	-0.08159700	-1.79296600
H	-2.86831100	0.95288600	-1.55492700
H	-2.74616500	-0.30746900	-2.79114600
H	-4.21623700	-0.16459200	-1.81152500
S	0.17781800	2.31115900	-0.06214700
O	1.48856300	2.90123100	-0.26745200
O	-0.19205400	1.13257600	-0.92952300
C	-1.10831900	3.60566400	-0.46660200
O	-0.17916900	1.94621000	1.39011100
F	-0.88485100	4.04686500	-1.69719500
F	-1.03066400	4.59609900	0.40852500
F	-2.33078100	3.05012300	-0.41040900

Zero-point correction= 0.413122 (Hartree/Particle)

Thermal correction to Energy= 0.443777

Thermal correction to Enthalpy= 0.444722

Thermal correction to Gibbs Free Energy= 0.351866

Sum of electronic and zero-point Energies= -1901.769318

Sum of electronic and thermal Energies= -1901.738663

Sum of electronic and thermal Enthalpies= -1901.737719

Sum of electronic and thermal Free Energies= -1901.830574

E(RB3LYP) = -1902.182440 A.U.

A-tsa5

0 1

Number of imaginary frequencies: 1

Rh	1.29243500	-0.78518800	0.10627200
C	0.31340600	-2.70088900	-0.50719600
C	0.75010100	-2.00533900	-1.68062300
C	2.19623000	-1.86102000	-1.61536600
C	2.63794600	-2.50490200	-0.40932700
C	1.48127000	-2.95949600	0.31303300
O	-0.22737300	-0.52757800	1.49995100
C	-0.04815400	0.22737600	2.51275300
O	1.07316600	0.75033400	2.78380700
C	-1.25642500	0.50761200	3.36039400
H	-1.91104900	-0.36435000	3.37557000
H	-0.96250600	0.83273900	4.35885500
H	-1.81878800	1.29346400	2.84502100
C	-0.30062600	1.43905400	-1.19871900
C	1.71184400	2.21020800	-0.27939800
C	1.44881300	3.53490300	-0.73707200
C	0.24103100	3.76779000	-1.44743200
C	-0.63565500	2.73381000	-1.65479900
H	-0.99403000	0.61796800	-1.33858100

C	2.85215700	1.93325700	0.52034200
C	2.37190800	4.56346500	-0.42140100
H	0.01484000	4.77372500	-1.79087800
H	-1.59434000	2.87356900	-2.13966200
C	3.48263900	4.28449000	0.34364500
C	3.70979800	2.97503700	0.82490600
H	2.17298200	5.57264300	-0.77056200
H	4.18176200	5.07507500	0.59877900
H	4.57122300	2.78187300	1.45842900
N	0.83475500	1.18452900	-0.56558000
C	3.02619600	0.53787700	1.04933800
H	1.93611200	0.36766700	1.81044000
H	3.59475700	-0.07976400	0.35198700
H	3.61442100	0.52887800	1.97523000
C	-1.07860000	-3.08262000	-0.12915900
H	-1.41545000	-2.51670400	0.74616600
H	-1.79192700	-2.86108800	-0.91994200
H	-1.10763000	-4.15144200	0.11271000
C	-0.11603100	-1.57331300	-2.81934300
H	-1.13504800	-1.37375300	-2.48450500
H	0.27691800	-0.67177900	-3.29583700
H	-0.14006300	-2.36586000	-3.57806900
C	4.05571000	-2.68279700	0.03591700
H	4.73186100	-1.97807200	-0.45245400
H	4.15329800	-2.56105500	1.11738300
H	4.39216300	-3.69517900	-0.21751400
C	1.45098700	-3.69217300	1.61859500

H	0.57162800	-3.39486100	2.19485500
H	1.39805000	-4.77559000	1.45476300
H	2.33961900	-3.48371900	2.21873300
S	-3.17431700	-0.03530800	0.18462900
O	-3.31074600	-1.02823800	1.26900100
O	-2.61055000	1.28358400	0.56509100
C	-4.92886400	0.36890700	-0.28168500
O	-2.62326200	-0.57295900	-1.09739200
F	-5.59260800	0.88223300	0.76593700
F	-5.57875600	-0.73054500	-0.69708000
F	-4.95346900	1.27293400	-1.27901200
C	3.06122500	-1.27614000	-2.68986700
H	4.00947900	-0.91096200	-2.28798500
H	3.28839100	-2.02387000	-3.45963400
H	2.56170000	-0.43616800	-3.17802500

Zero-point correction= 0.465827 (Hartree/Particle)

Thermal correction to Energy= 0.501550

Thermal correction to Enthalpy= 0.502495

Thermal correction to Gibbs Free Energy= 0.398479

Sum of electronic and zero-point Energies= -2130.428218

Sum of electronic and thermal Energies= -2130.392495

Sum of electronic and thermal Enthalpies= -2130.391551

Sum of electronic and thermal Free Energies= -2130.495566

E(RB3LYP) = -2130.894045 A.U.

A-tsa6

0 1

Number of imaginary frequencies: 1

Rh	-1.60763900	-0.18617000	0.26043600
C	-2.93157500	1.15449100	1.43823300
C	-3.02325500	1.50422500	0.05982500
C	-3.53577000	0.35040900	-0.66755700
C	-3.76901500	-0.69722600	0.28349900
C	-3.35637200	-0.23190000	1.58240500
C	-0.24649500	0.52191700	-2.43913800
C	0.69841600	1.44725500	-0.51112900
C	1.40821700	2.42195200	-1.26602200
C	1.30008900	2.35323200	-2.67817300
C	0.50784600	1.38874900	-3.26050100
H	-0.91988700	-0.22770300	-2.84049500
C	0.82811200	1.36194700	0.90756200
C	2.14363300	3.41541000	-0.56835900
H	1.84940900	3.06573900	-3.28776900
H	0.42533700	1.29869200	-4.33800600
C	2.16801200	3.40199800	0.80948200
C	1.53640600	2.37073700	1.54362100
H	2.67258700	4.17803800	-1.13196200
H	2.72039700	4.16717900	1.34680900
H	1.65793500	2.33201400	2.62235200
N	-0.16910700	0.57795400	-1.11837500
C	0.31955900	0.16214000	1.59970000
H	1.51018300	-0.45851800	1.82329500
H	-0.07462800	0.26163800	2.60659200
H	0.20619400	-0.79479400	1.07165100
C	-2.47211200	2.06081400	2.53926600

H	-2.19752700	1.49594300	3.43184400
H	-1.60106500	2.64626200	2.23212400
H	-3.27148800	2.75853200	2.81612200
C	-2.66413800	2.82628700	-0.54665300
H	-1.95867000	3.37195200	0.08332600
H	-2.20042300	2.69502300	-1.52753900
H	-3.55791100	3.44771500	-0.67706700
C	-3.82398700	0.27480800	-2.13378900
H	-4.90053300	0.36659400	-2.32250000
H	-3.32044200	1.07779700	-2.67681800
H	-3.47022100	-0.67907500	-2.53139500
C	-4.28446900	-2.06091800	-0.05211800
H	-3.87290700	-2.39417800	-1.00653800
H	-4.00269300	-2.78909700	0.71014400
H	-5.37906400	-2.04274700	-0.12123100
C	-3.46952500	-0.99035800	2.86957300
H	-2.71231500	-0.66905100	3.58835900
H	-4.45506200	-0.83911000	3.32745600
H	-3.33279200	-2.06110200	2.70529000
S	3.14859100	-1.54401500	0.58194400
O	2.14222100	-1.35908200	-0.47690700
O	2.64910200	-1.00079400	1.93702700
C	4.47899700	-0.30834600	0.17822600
O	3.82678300	-2.83034800	0.70826100
F	3.95056700	0.92396000	0.08289400
F	5.04368300	-0.61977100	-0.99501200
F	5.42220000	-0.29633200	1.12548900

O	-0.91363400	-2.12882300	-0.00000500
C	-0.96713800	-2.64346900	-1.19811300
O	-1.64069000	-2.19854100	-2.13786600
C	-0.07684500	-3.86253200	-1.34859600
H	-0.21328700	-4.54513600	-0.50574900
H	-0.28205700	-4.37124700	-2.29144900
H	0.96114100	-3.51488900	-1.32082300

Zero-point correction= 0.464073 (Hartree/Particle)

Thermal correction to Energy= 0.500265

Thermal correction to Enthalpy= 0.501209

Thermal correction to Gibbs Free Energy= 0.395250

Sum of electronic and zero-point Energies= -2130.413979

Sum of electronic and thermal Energies= -2130.377788

Sum of electronic and thermal Enthalpies= -2130.376844

Sum of electronic and thermal Free Energies= -2130.482802

E(RB3LYP) = -2130.878052 A.U.

A-tsa7

1 1

Number of imaginary frequencies: 1

Rh	-0.51540800	-0.82426300	0.11847000
C	-1.86867700	-2.23028400	-0.99737200
C	-1.48035600	-2.77141600	0.29803700
C	-2.02495800	-1.90634600	1.31875400
C	-2.63862700	-0.78157700	0.66994900
C	-2.57066900	-1.01129600	-0.76434200
C	1.68516900	-1.58110300	-1.90156400
C	2.49323400	-0.66517400	0.08936800

C	3.80888200	-0.56445300	-0.45437500
C	4.01897300	-1.03620200	-1.77236000
C	2.96284600	-1.55089300	-2.49161100
H	0.83090300	-1.93794000	-2.46366000
C	2.21617700	-0.21826500	1.40883600
C	4.82829700	0.03257400	0.33208500
H	5.01176500	-0.97474600	-2.20857600
H	3.08713600	-1.91067600	-3.50652500
C	4.53799200	0.50623700	1.59102300
C	3.23476800	0.37711700	2.12816200
H	5.82672800	0.12658800	-0.08345300
H	5.31157500	0.98094700	2.18557800
H	3.03336600	0.74754000	3.12903900
N	1.45407600	-1.16220600	-0.66347000
C	0.83064500	-0.42463600	1.93481800
H	0.05025100	0.72647700	1.51201000
H	0.65220900	-1.47637700	2.16905900
H	0.67370400	0.09589800	2.88856800
C	-1.65561600	-2.89567400	-2.32008700
H	-1.52344300	-2.16891100	-3.12498700
H	-0.78962400	-3.56064100	-2.30347700
H	-2.52973200	-3.50861200	-2.57055100
C	-0.78631500	-4.07787500	0.51897800
H	-0.03642400	-4.26400900	-0.25283500
H	-0.28695100	-4.11003500	1.48894900
H	-1.51292700	-4.89864000	0.48736500
C	-1.98020300	-2.14306900	2.79378300

H	-2.91498900	-2.62395700	3.10584800
H	-1.15877300	-2.80148700	3.08100100
H	-1.88636000	-1.20835500	3.35003100
C	-3.36218100	0.34402200	1.34073800
H	-2.97677900	0.52224800	2.34616100
H	-3.26233900	1.27160000	0.77818100
H	-4.42991100	0.10853100	1.42448100
C	-3.12289100	-0.08159700	-1.79296600
H	-2.86831100	0.95288600	-1.55492700
H	-2.74616500	-0.30746900	-2.79114600
H	-4.21623700	-0.16459200	-1.81152500
S	0.17781800	2.31115900	-0.06214700
O	1.48856300	2.90123100	-0.26745200
O	-0.19205400	1.13257600	-0.92952300
C	-1.10831900	3.60566400	-0.46660200
O	-0.17916900	1.94621000	1.39011100
F	-0.88485100	4.04686500	-1.69719500
F	-1.03066400	4.59609900	0.40852500
F	-2.33078100	3.05012300	-0.41040900

Zero-point correction= 0.413122 (Hartree/Particle)

Thermal correction to Energy= 0.443777

Thermal correction to Enthalpy= 0.444722

Thermal correction to Gibbs Free Energy= 0.351866

Sum of electronic and zero-point Energies= -1901.769318

Sum of electronic and thermal Energies= -1901.738663

Sum of electronic and thermal Enthalpies= -1901.737719

Sum of electronic and thermal Free Energies= -1901.830574

E(RB3LYP) = -1902.182440 A.U.

A-tsa8

0 1

Number of imaginary frequencies: 1

Rh	0.65256600	0.19157900	0.04409400
C	2.44546100	1.11041800	-0.89243800
C	1.91303100	2.07208400	0.02417300
C	1.93724300	1.50221400	1.34678500
C	2.55648300	0.19634300	1.24774200
C	2.84602400	-0.06015000	-0.12665500
O	0.40851200	-0.95918700	-1.67219900
C	-0.60785600	-1.75893600	-1.90565400
O	-1.70502500	-1.71179400	-1.36245500
C	-0.26525700	-2.82463400	-2.93750800
H	0.28893400	-3.60732300	-2.40879400
H	-1.17878800	-3.24901900	-3.35737100
H	0.37480900	-2.42630600	-3.72914500
C	-1.47936500	1.86226300	-1.29958200
C	-2.31667700	0.44076900	0.35179300
C	-3.65768300	0.80535000	0.02775800
C	-3.85585300	1.76302300	-0.99450400
C	-2.77144900	2.29005900	-1.65940000
H	-0.60664900	2.22498700	-1.82958300
C	-2.04044700	-0.54241400	1.33952600
C	-4.72477200	0.15855700	0.70326500
H	-4.86831000	2.05519200	-1.25980200
H	-2.88912200	3.00824000	-2.46327800

C	-4.45100200	-0.81678600	1.63365600
C	-3.11550100	-1.16428700	1.94677000
H	-5.74722100	0.42590400	0.45285200
H	-5.26402200	-1.33170700	2.13674700
H	-2.92811100	-1.94187600	2.68152700
N	-1.26042200	0.99218600	-0.32438800
C	-0.62558200	-0.85106100	1.69989600
H	0.17851800	-1.70808800	0.90583600
H	-0.20592600	-0.06405900	2.33415900
H	-0.59135100	-1.74983200	2.32094100
C	2.59026400	1.21479200	-2.37681000
H	2.08538200	0.36291700	-2.84502200
H	2.15245700	2.13610600	-2.76807400
H	3.64749900	1.19077000	-2.66463800
C	1.42406500	3.44989000	-0.29966300
H	1.31586800	3.60068700	-1.37545100
H	0.45948100	3.65340000	0.17344000
H	2.13866500	4.19493700	0.06975100
C	1.54959100	2.21228900	2.60827300
H	2.39905800	2.76890700	3.02391700
H	0.73978600	2.92433700	2.42829900
H	1.21188700	1.51145900	3.37587700
C	2.84086500	-0.73820900	2.38001000
H	2.30554100	-0.44672800	3.28611700
H	2.54421900	-1.75764500	2.11549200
H	3.91410000	-0.73247700	2.60508000
C	3.45542300	-1.28482300	-0.72835600

H	2.79750300	-1.66197000	-1.51730000
H	4.43550000	-1.04866300	-1.16106100
H	3.56245900	-2.07976800	0.00813500
Cl	0.92207900	-3.21596500	0.67592000

Zero-point correction= 0.435234 (Hartree/Particle)

Thermal correction to Energy= 0.464597

Thermal correction to Enthalpy= 0.465541

Thermal correction to Gibbs Free Energy= 0.376811

Sum of electronic and zero-point Energies= -1629.215647

Sum of electronic and thermal Energies= -1629.186284

Sum of electronic and thermal Enthalpies= -1629.185340

Sum of electronic and thermal Free Energies= -1629.274070

E(RB3LYP) = -1629.650881 A.U.

A-tsa9

0 1

Number of imaginary frequencies: 1

C	1.10650200	0.88144000	1.58937300
H	1.12112400	1.75700800	2.24890400
H	0.65056000	1.72172900	0.62320800
H	0.66381500	0.07663400	2.17380800
C	-2.96764500	-1.12510300	1.01989800
C	-1.99322800	-0.19479900	1.56021300
C	-2.13051400	1.02909500	0.78325400
C	-3.19844100	0.77083500	-0.18307300
C	-3.74778700	-0.50006600	0.02861900
C	-1.92816000	2.42865300	1.32390600
H	-1.60496200	3.12189400	0.54487600

H	-2.85873300	2.80923600	1.76651600
H	-1.16294600	2.45072400	2.10148300
C	-3.52092300	1.66291000	-1.32886200
H	-3.21412000	2.69597000	-1.14948300
H	-2.97232400	1.28995200	-2.20507500
H	-4.58664300	1.64038000	-1.57573400
C	-4.77082100	-1.17998400	-0.83193700
H	-5.35475100	-1.90864600	-0.26051600
H	-5.47310000	-0.46141300	-1.26457400
H	-4.28175400	-1.70990900	-1.65645200
C	-3.05042200	-2.57157700	1.36164400
H	-4.08882300	-2.89504000	1.49215800
H	-2.63696800	-3.14439000	0.52045200
H	-2.48265700	-2.82231100	2.26004700
C	-1.62799900	-0.26783600	3.02838700
H	-2.53192200	-0.23432300	3.65062500
H	-1.09288400	-1.19026700	3.27683600
H	-1.00127200	0.57125300	3.33368900
O	0.64000100	1.06118000	-1.59503300
O	0.82886400	2.78587700	-0.17998500
C	0.92034300	2.26668900	-1.34025800
C	1.40292800	3.14631800	-2.47216400
H	0.76205300	4.03012900	-2.53834300
H	2.41630600	3.49251700	-2.24824000
H	1.39264200	2.60214400	-3.41622300
Rh	-0.36024700	0.01054100	0.01526200
C	1.55430700	-2.33186100	-0.90757000

C	2.61052100	-0.65338100	0.31356100
C	3.90043600	-1.16214400	-0.02349500
C	3.95876900	-2.33504400	-0.81743800
C	2.79206300	-2.92690900	-1.23953200
H	0.61656400	-2.72692900	-1.28252800
C	2.48163500	0.48396600	1.16212900
C	5.05311600	-0.47027600	0.43231400
H	4.92752100	-2.74892800	-1.08503800
H	2.79845300	-3.82595200	-1.84630200
C	4.91512100	0.66664400	1.19606100
C	3.63219900	1.13488200	1.56689600
H	6.03526000	-0.84699300	0.16085600
H	5.79555300	1.20476900	1.53484100
H	3.54678600	2.01460200	2.19866100
N	1.46470300	-1.23585800	-0.17102100
Cl	-1.38397000	-1.29872600	-1.76350000

Zero-point correction= 0.436265 (Hartree/Particle)

Thermal correction to Energy= 0.465627

Thermal correction to Enthalpy= 0.466572

Thermal correction to Gibbs Free Energy= 0.376295

Sum of electronic and zero-point Energies= -1629.203530

Sum of electronic and thermal Energies= -1629.174167

Sum of electronic and thermal Enthalpies= -1629.173223

Sum of electronic and thermal Free Energies= -1629.263499

E(RB3LYP) = -1629.639795 A.U.

A-1

0 1

Number of imaginary frequencies: 0

Rh	0.69984800	-0.76183700	0.16061000
C	2.77536700	-0.81234500	-0.42575600
C	2.74515500	-0.74784300	1.02921800
C	2.05300200	-1.88996600	1.51555300
C	1.69859600	-2.71371200	0.36755200
C	2.18521500	-2.07428700	-0.81847700
O	-0.52416000	-0.17792200	-1.35565400
O	0.87502700	0.03071100	-3.12919900
C	-0.20922200	0.19129200	-2.56792200
C	-1.37613700	0.89984400	-3.23767900
H	-1.54904400	1.83520500	-2.69759800
H	-1.15176700	1.09553100	-4.28709100
H	-2.28565900	0.30055300	-3.13952600
C	-1.29354500	-0.37302500	2.35440100
C	-2.57118200	-0.94635600	0.49484000
C	-3.58160700	-0.01331800	0.89097200
C	-3.39905000	0.71053200	2.09341800
C	-2.28551400	0.48431300	2.86418600
H	-0.35257400	-0.46437900	2.88408000
C	-2.81089500	-1.79784500	-0.62663300
C	-4.74768600	0.14882400	0.10055400
H	-4.15095200	1.43419800	2.39511300
H	-2.11242100	1.01029400	3.79557000
C	-4.93011500	-0.62670400	-1.01775100
C	-3.97424500	-1.61263900	-1.35193700
H	-5.48931300	0.88165100	0.40493800

H	-5.81895900	-0.51143300	-1.63045300
H	-4.16530600	-2.26046000	-2.20351100
N	-1.39135700	-1.03224600	1.20451400
C	-1.86867900	-2.91447600	-0.98300500
H	-0.94954300	-2.51979500	-1.42124700
H	-1.59607500	-3.48765100	-0.09342500
H	-2.33241200	-3.59491600	-1.70254400
C	3.45319100	0.17351300	-1.32192300
H	3.46129900	1.16629000	-0.86889300
H	4.49154800	-0.13388900	-1.50253700
H	2.91832300	0.24025600	-2.26971400
C	3.29380800	0.38959100	1.82549700
H	3.03675400	0.30790200	2.88232500
H	4.38582000	0.40721100	1.73242200
H	2.89781600	1.33752100	1.45531100
C	1.77725600	-2.25108100	2.94242200
H	2.49259900	-3.00452900	3.29382200
H	1.85802300	-1.38223900	3.59872500
H	0.77321200	-2.66915900	3.05498700
C	1.08325400	-4.07247100	0.46411000
H	0.63604500	-4.38381000	-0.47994700
H	1.85638400	-4.80422800	0.73089100
H	0.31254600	-4.10474600	1.23733900
C	2.13822900	-2.62743400	-2.20591200
H	3.09547600	-3.11341500	-2.43452500
H	1.34860400	-3.37493100	-2.31027900
H	1.95068900	-1.82629400	-2.92042300

S	-0.20636700	2.52767900	0.66802300
O	-1.42471500	2.35606900	-0.12739600
O	-0.23742900	3.43232000	1.82139800
C	1.04763800	3.26397100	-0.49478200
O	0.51358600	1.22866100	1.03434400
F	0.71006600	4.51132100	-0.83282900
F	1.15291300	2.52623100	-1.60989000
F	2.26497700	3.29531400	0.09329300

Zero-point correction= 0.469984 (Hartree/Particle)

Thermal correction to Energy= 0.506867

Thermal correction to Enthalpy= 0.507811

Thermal correction to Gibbs Free Energy= 0.401851

Sum of electronic and zero-point Energies= -2130.461974

Sum of electronic and thermal Energies= -2130.425091

Sum of electronic and thermal Enthalpies= -2130.424147

Sum of electronic and thermal Free Energies= -2130.530107

E(RB3LYP) = -2130.931958 A.U.

A-2

1 1

Number of imaginary frequencies: 0

Rh	-0.66608600	-0.04832700	0.02682900
C	-2.84153200	-0.02835400	-0.28029000
C	-2.22022300	-1.23562500	-0.80546900
C	-1.69979600	-2.00317600	0.32702200
C	-1.89878700	-1.23323600	1.49809000
C	-2.59831000	0.00292700	1.11800100
O	-0.27330500	1.39634000	-1.40218500

O	-1.08623300	2.86615500	0.08932100
C	-0.62297100	2.60219700	-1.02654400
C	-0.40078900	3.66024300	-2.08904900
H	-0.93446600	3.38894100	-3.00437600
H	-0.74433100	4.62896800	-1.72654300
H	0.66307000	3.71256500	-2.33829300
C	1.44656600	-1.41591500	-1.56975000
C	2.45544400	-0.16808400	0.13771100
C	3.75026300	-0.49022100	-0.39171800
C	3.83202700	-1.31555900	-1.53796000
C	2.68171600	-1.78074900	-2.13021700
H	0.52542200	-1.73650100	-2.04075900
C	2.35911400	0.66874800	1.29077600
C	4.91568200	0.02893300	0.22894300
H	4.80873100	-1.56373300	-1.94313600
H	2.70311500	-2.40344200	-3.01706800
C	4.80437800	0.84388100	1.32814600
C	3.52790700	1.15551500	1.84793100
H	5.88650200	-0.22406700	-0.18604100
H	5.68981300	1.25230900	1.80382200
H	3.46179600	1.79937100	2.72013000
N	1.32501700	-0.66199200	-0.48141400
C	1.03560600	1.00084200	1.92772900
H	0.30200200	1.45289100	1.22655000
H	0.60819200	0.13009300	2.43388100
H	1.14780000	1.78335700	2.68318200
C	-3.56050900	1.00568100	-1.08347600

H	-3.18053300	1.04122200	-2.10607900
H	-4.62974400	0.76652900	-1.12373900
H	-3.43739300	1.99413400	-0.63980900
C	-2.30405700	-1.69384900	-2.22511400
H	-1.62304400	-2.52242300	-2.42837400
H	-3.32115100	-2.04424300	-2.43906100
H	-2.07985500	-0.87651500	-2.91486100
C	-1.07175600	-3.35604700	0.23424200
H	-1.85368500	-4.12110200	0.16113000
H	-0.43926300	-3.44749400	-0.65180300
H	-0.46120700	-3.57935300	1.11026100
C	-1.54468900	-1.62681700	2.89690300
H	-1.30869700	-0.75715300	3.51355200
H	-2.39556800	-2.13632700	3.36476600
H	-0.69163400	-2.30778100	2.92269800
C	-3.00658700	1.10100800	2.04459300
H	-4.07702600	1.01746900	2.26772700
H	-2.46273700	1.05487100	2.98943000
H	-2.81324200	2.07205600	1.58530700

Zero-point correction= 0.440432 (Hartree/Particle)

Thermal correction to Energy= 0.468974

Thermal correction to Enthalpy= 0.469918

Thermal correction to Gibbs Free Energy= 0.380713

Sum of electronic and zero-point Energies= -1168.846369

Sum of electronic and thermal Energies= -1168.817827

Sum of electronic and thermal Enthalpies= -1168.816882

Sum of electronic and thermal Free Energies= -1168.906088

E(RB3LYP) = -1169.286801 A.U.

A-3a

1 1

Number of imaginary frequencies: 0

Rh	-0.69597900	-0.01373300	0.13715800
C	-2.81504200	-0.01886600	-0.86315200
C	-2.31695200	-1.32491300	-0.91396900
C	-1.96249900	-1.72929700	0.45732500
C	-2.41960200	-0.68950900	1.35436200
C	-2.82092200	0.41104300	0.54456400
O	-0.26148000	2.09649200	-0.56326500
C	0.64042500	2.93585300	-0.54332200
O	1.83830500	2.73164100	-0.01099000
C	0.48627400	4.30918300	-1.12675600
H	-0.50440800	4.42003700	-1.56435800
H	0.63937100	5.05627500	-0.34221900
H	1.25727300	4.47324300	-1.88510500
C	1.27502600	-1.08797200	-2.00165800
C	2.22020900	-0.57102400	0.06611400
C	3.52794500	-0.89228500	-0.40287100
C	3.65292000	-1.35211300	-1.73847800
C	2.53184300	-1.45018900	-2.53274900
H	0.38035600	-1.13429300	-2.61270900
C	1.99507900	-0.09299000	1.38366300
C	4.62177500	-0.71345000	0.48133700
H	4.63383600	-1.61433400	-2.12430500
H	2.59392200	-1.78891300	-3.56069600

C	4.40751100	-0.22419800	1.75284100
C	3.10108500	0.08583100	2.20198200
H	5.62390100	-0.95220600	0.13857000
H	5.24720600	-0.07575500	2.42417500
H	2.96009900	0.46195300	3.21138600
N	1.11875000	-0.67026500	-0.75284400
C	0.56612500	0.17398800	1.79188100
H	1.90881100	1.83504400	0.36946600
H	0.25455500	-0.54602500	2.55422200
H	0.44818300	1.17634100	2.22236500
C	-3.23238000	0.86552500	-1.99562300
H	-2.68338500	1.81217500	-1.96079000
H	-3.04997900	0.40011500	-2.96592000
H	-4.30082900	1.09992600	-1.92886700
C	-2.15420100	-2.19773400	-2.11919200
H	-2.12344400	-1.61703300	-3.04401900
H	-1.24481400	-2.80137600	-2.05848000
H	-2.99644500	-2.89579900	-2.19469000
C	-1.50903400	-3.10075800	0.85393300
H	-0.99802200	-3.08786800	1.81880300
H	-2.36615400	-3.78048100	0.93509300
H	-0.82053000	-3.51927900	0.11612700
C	-2.47094900	-0.76185900	2.84850900
H	-1.76888200	-1.49823500	3.24405500
H	-2.24796300	0.20309100	3.30924000
H	-3.47633800	-1.06104300	3.16698200
C	-3.33579100	1.73745800	1.00941200

H	-2.93608000	2.54464600	0.38995000
H	-4.42959700	1.76973100	0.93743400
H	-3.06050600	1.93447300	2.04718800

Zero-point correction= 0.441215 (Hartree/Particle)

Thermal correction to Energy= 0.469396

Thermal correction to Enthalpy= 0.470340

Thermal correction to Gibbs Free Energy= 0.382356

Sum of electronic and zero-point Energies= -1168.855220

Sum of electronic and thermal Energies= -1168.827040

Sum of electronic and thermal Enthalpies= -1168.826095

Sum of electronic and thermal Free Energies= -1168.914079

E(RB3LYP) = -1169.296436 A.U.

A-3b

1 1

Number of imaginary frequencies: 0

Rh	0.78076500	0.08332000	0.00996000
C	2.91397900	0.26916200	0.41329300
C	2.75304100	0.91272700	-0.90363200
C	1.86934700	1.98633100	-0.75396500
C	1.43549100	2.02120400	0.65325800
C	2.19740500	1.03465700	1.38473000
O	1.16749900	-3.17799600	0.61325000
O	0.70136400	-1.88466700	-1.12253100
C	0.84805800	-3.01456500	-0.67662500
C	0.68435500	-4.25064400	-1.52152400
H	-0.13805400	-4.86065800	-1.13172900
H	0.46533800	-3.96472000	-2.54888800

H	1.59681000	-4.85588600	-1.49443600
C	-0.80372900	-0.48720100	1.07760800
C	-2.73966600	0.08857900	-0.12085200
C	-3.53560600	-0.25881500	1.01898600
C	-2.87625700	-0.72548800	2.19160400
C	-1.49990800	-0.83794600	2.25154000
H	1.24493600	-4.11720500	0.83982200
C	-3.32523200	0.57618900	-1.31889400
C	-4.94372800	-0.11526200	0.92844100
H	-3.48228800	-0.98462400	3.05652400
H	-0.98443600	-1.16726800	3.14578800
C	-5.51001600	0.35839700	-0.23419000
C	-4.70289400	0.70214800	-1.34568500
H	-5.56063700	-0.37865500	1.78252200
H	-6.58682300	0.47277300	-0.30665500
H	-5.18115000	1.07396800	-2.24753200
N	-1.39021600	-0.08585300	-0.01034300
C	-2.44769300	0.93001600	-2.48989800
H	-1.84808600	0.06913200	-2.80484700
H	-3.04266700	1.27036200	-3.34020300
H	-1.73969600	1.72362700	-2.22539200
C	3.84176500	-0.87312900	0.68729500
H	4.86359200	-0.50319500	0.83690700
H	3.54375800	-1.42350600	1.58133600
H	3.86363800	-1.57241700	-0.15170100
C	3.42020300	0.43123700	-2.15409100
H	4.49852300	0.62466900	-2.11278300

H	3.28367700	-0.64691200	-2.28050700
H	3.02214600	0.92554800	-3.04166100
C	1.38385400	2.93307300	-1.80644800
H	1.89287200	3.89959800	-1.70943700
H	1.57004400	2.55342100	-2.81243200
H	0.31109400	3.11958800	-1.70782900
C	0.55599600	3.07747000	1.24738300
H	1.13738400	3.98437900	1.45315700
H	-0.25328300	3.34796500	0.56512700
H	0.10945900	2.74273300	2.18576600
C	2.21278600	0.84465800	2.87006100
H	2.98569800	1.47805800	3.32155100
H	1.25468300	1.11663400	3.31782000
H	2.43034200	-0.19131600	3.13780000

Zero-point correction= 0.439643 (Hartree/Particle)

Thermal correction to Energy= 0.469045

Thermal correction to Enthalpy= 0.469990

Thermal correction to Gibbs Free Energy= 0.377912

Sum of electronic and zero-point Energies= -1168.824508

Sum of electronic and thermal Energies= -1168.795105

Sum of electronic and thermal Enthalpies= -1168.794161

Sum of electronic and thermal Free Energies= -1168.886238

E(RB3LYP) = -1169.264151 A.U.

A-3c

1 1

Number of imaginary frequencies: 0

Rh	-1.13568400	0.10543700	-0.20238000

C	-3.28567500	-0.85339800	-0.44018300
C	-2.13941700	-1.78038500	-0.61290600
C	-1.43380300	-1.87383400	0.62314100
C	-2.01323000	-0.86550400	1.49046600
C	-3.21573500	-0.31263600	0.83969800
O	0.99984300	2.82050100	-0.89799900
C	-0.26104200	3.10052500	-0.67675900
O	-1.12212600	2.25282000	-0.37176900
C	-0.60197900	4.55218500	-0.81224200
H	-0.27312000	4.91418100	-1.79038600
H	-1.67293300	4.70239600	-0.68793200
H	-0.05071000	5.11936800	-0.05555000
C	5.35546600	-0.00886500	1.17183400
C	3.19988000	-0.08516500	0.37429100
C	3.61312000	-0.76885000	-0.81023500
C	4.99316500	-1.06122100	-0.95553100
C	5.86826300	-0.68279700	0.03539000
H	6.03373200	0.29926900	1.96584000
C	1.81106700	0.23357700	0.57583000
C	2.64099200	-1.12261800	-1.78189200
H	5.33983100	-1.57865300	-1.84602400
H	6.93099200	-0.88770800	-0.03836400
C	1.31523200	-0.82208100	-1.57484100
C	0.88435200	-0.14071400	-0.39309400
H	2.95639500	-1.63459500	-2.68751100
H	0.58915300	-1.10358500	-2.33309900
H	1.17896200	1.85760600	-0.75043000

N	4.08013300	0.28337700	1.34584000
C	-4.27954800	-0.56585700	-1.51780700
H	-4.93882600	0.26219700	-1.25501700
H	-3.77928700	-0.31817700	-2.45942700
H	-4.89926200	-1.45082300	-1.70532800
C	-1.91452700	-2.61408800	-1.83119800
H	-2.10298800	-2.04545800	-2.74566200
H	-0.89752500	-3.00707600	-1.86716300
H	-2.60641700	-3.46594300	-1.82622200
C	-0.33489900	-2.82712900	0.97471100
H	0.34805000	-2.39143700	1.70594100
H	-0.75856100	-3.74337600	1.40148000
H	0.25465000	-3.09517600	0.09650700
C	-1.63085400	-0.60122900	2.90730000
H	-0.58312900	-0.83673000	3.09536700
H	-1.81151300	0.44017400	3.18274700
H	-2.24484400	-1.23016400	3.56573500
C	-4.10264200	0.71238800	1.47184100
H	-4.85916400	1.07805400	0.77646600
H	-4.61579000	0.28929000	2.34267000
H	-3.52021200	1.57179800	1.81923100
C	1.43806700	0.96755900	1.84279500
H	1.62017900	0.34159600	2.72275300
H	2.06180200	1.85561200	1.97501400
H	0.38612000	1.26331100	1.83905600

Zero-point correction= 0.439623 (Hartree/Particle)

Thermal correction to Energy= 0.468602

Thermal correction to Enthalpy= 0.469546

Thermal correction to Gibbs Free Energy= 0.378721

Sum of electronic and zero-point Energies= -1168.814738

Sum of electronic and thermal Energies= -1168.785760

Sum of electronic and thermal Enthalpies= -1168.784815

Sum of electronic and thermal Free Energies= -1168.875640

E(RB3LYP) = -1169.254362 A.U.

A-4a

1 1

Number of imaginary frequencies: 0

Rh	-0.61310800	-0.16326500	-0.37383900
C	-2.74939700	0.86178300	-0.41509200
C	-2.78830000	-0.61558700	-0.48765200
C	-2.24742400	-1.14532900	0.71052000
C	-1.69170400	-0.01613100	1.44513700
C	-2.11009800	1.22504000	0.76969000
C	-1.83835600	2.60042300	1.29418600
H	-1.97038100	3.36289900	0.52380600
H	-2.52316000	2.83643500	2.11697900
H	-0.82110600	2.68327200	1.68755000
C	-3.30866900	1.75555300	-1.47536700
H	-3.01536700	2.79648600	-1.33017200
H	-2.98014600	1.44328100	-2.47131500
H	-4.40431000	1.70998200	-1.46900600
C	-3.45265700	-1.37890600	-1.58915600
H	-3.14860700	-2.42695600	-1.59492700
H	-4.54213200	-1.34392700	-1.46426800

H	-3.22249700	-0.94891800	-2.56756000
C	-2.25091000	-2.57353000	1.15827700
H	-1.38199100	-2.80160700	1.77895800
H	-3.14907900	-2.77543800	1.75358500
H	-2.25075600	-3.26132100	0.31022200
C	-1.05933500	-0.07867600	2.79697400
H	-1.83388600	0.00245100	3.57076800
H	-0.53007300	-1.02121200	2.94821600
H	-0.35326000	0.74112000	2.94521100
C	1.42739000	2.15727500	-0.34286700
C	2.32582700	0.00090000	-0.25541500
C	3.64503000	0.50977600	-0.08409900
C	3.80626700	1.91529600	-0.07136500
C	2.70297600	2.73545600	-0.21100500
H	0.54014800	2.77539800	-0.43133000
C	2.05737000	-1.38802700	-0.29786600
C	4.70257900	-0.42098200	0.09534100
H	4.79842900	2.33939300	0.05466900
H	2.79821100	3.81526600	-0.20871500
C	4.43211800	-1.77229700	0.10291200
C	3.11419200	-2.25726200	-0.09668300
H	5.71395400	-0.05339600	0.23829700
H	5.23849400	-2.48312300	0.25256300
H	2.93788200	-3.32904200	-0.11232900
N	1.23887400	0.83891100	-0.35982300
C	0.64397800	-1.77763800	-0.60754300
H	0.52075900	-1.90404600	-1.70061100

H	0.33133100	-2.70526900	-0.12264600

Zero-point correction= 0.377143 (Hartree/Particle)

Thermal correction to Energy= 0.399379

Thermal correction to Enthalpy= 0.400323

Thermal correction to Gibbs Free Energy= 0.326770

Sum of electronic and zero-point Energies= -939.791548

Sum of electronic and thermal Energies= -939.769313

Sum of electronic and thermal Enthalpies= -939.768368

Sum of electronic and thermal Free Energies= -939.841922

E(RB3LYP) = -940.168691 A.U.

A-4b

1 1

Number of imaginary frequencies: 0

Rh	-0.74255900	-0.21777700	0.00008100
C	-2.58255100	-0.11654600	1.14873100
C	-2.34620600	1.26585300	0.70034400
C	-2.34635000	1.26556500	-0.70045900
C	-2.58279300	-0.11701800	-1.14822700
C	-2.82419600	-0.94247700	0.00044600
C	0.81487700	-1.45268000	0.00017000
C	2.64061800	0.06314400	-0.00022400
C	3.53925400	-1.05148500	-0.00009900
C	2.99594100	-2.37307000	0.00016700
C	1.63606200	-2.60180500	0.00030900
C	3.10068700	1.40363200	-0.00049500
C	4.92908600	-0.79128800	-0.00024100
H	3.68801000	-3.21152700	0.00026700

H	1.21750600	-3.60069500	0.00051900
C	5.38013700	0.51378700	-0.00050000
C	4.47312800	1.59743300	-0.00062600
H	5.62815800	-1.62184000	-0.00014700
H	6.44615700	0.71710100	-0.00061200
H	4.86345900	2.61095200	-0.00083000
N	1.30609100	-0.23321600	-0.00007700
C	2.11412300	2.54018700	-0.00062700
H	1.46263300	2.49361100	0.87927100
H	2.62553200	3.50488600	-0.00082400
H	1.46252100	2.49331100	-0.88042600
C	-2.70150500	-0.53312900	2.57751200
H	-3.71050600	-0.30181600	2.94288500
H	-2.53681600	-1.60481000	2.70007000
H	-1.99119100	0.00216000	3.21172300
C	-2.13644900	2.42944700	1.61692400
H	-3.09859400	2.77547800	2.01359700
H	-1.51012600	2.15774400	2.47048600
H	-1.66481200	3.26853300	1.10267500
C	-2.13677600	2.42878200	-1.61756100
H	-3.09900000	2.77465500	-2.01418000
H	-1.66502900	3.26807700	-1.10375500
H	-1.51063000	2.15672600	-2.47114000
C	-2.70205500	-0.53418800	-2.57681100
H	-3.71114800	-0.30306300	-2.94204700
H	-1.99190500	0.00086700	-3.21140200
H	-2.53735500	-1.60591300	-2.69896500

C	-3.25788800	-2.37645800	0.00078500
H	-4.35251200	-2.43881700	0.00088500
H	-2.89242800	-2.90483100	-0.88181600
H	-2.89228800	-2.90445800	0.88355100

Zero-point correction= 0.376379 (Hartree/Particle)

Thermal correction to Energy= 0.399612

Thermal correction to Enthalpy= 0.400556

Thermal correction to Gibbs Free Energy= 0.323054

Sum of electronic and zero-point Energies= -939.773244

Sum of electronic and thermal Energies= -939.750011

Sum of electronic and thermal Enthalpies= -939.749067

Sum of electronic and thermal Free Energies= -939.826569

E(RB3LYP) = -940.149623 A.U.

A-4c

1 1

Number of imaginary frequencies: 0

Rh	0.86916300	-0.26375700	0.00045700
C	3.07612200	-0.70486800	-0.69997600
C	2.49937300	0.56487000	-1.15667000
C	2.23208500	1.39029300	-0.00114900
C	2.49994400	0.56650600	1.15537500
C	3.07639400	-0.70391200	0.70008000
C	-5.28856000	-1.44130400	-0.00008600
C	-3.20502200	-0.48280500	0.00027100
C	-3.74328900	0.84078600	0.00005200
C	-5.15345200	0.96428900	-0.00025600
C	-5.92748700	-0.17568900	-0.00032900

H	-5.88874900	-2.34903700	-0.00012800
C	-1.78661400	-0.64802100	0.00058900
C	-2.86154500	1.96349300	0.00018500
H	-5.60782200	1.95111700	-0.00043000
H	-7.01093400	-0.12015900	-0.00057200
C	-1.50075700	1.78656000	0.00044000
C	-0.95617200	0.47124600	0.00058000
H	-3.28885300	2.96287900	0.00009200
H	-0.84452000	2.64964300	0.00060700
N	-3.97800900	-1.60125800	0.00020400
C	3.52597900	-1.79576100	-1.61963000
H	3.68231200	-2.73680000	-1.09039400
H	2.79752000	-1.97011900	-2.41687200
H	4.47186300	-1.51817200	-2.09980400
C	2.39526900	0.99013700	-2.58361900
H	2.14472300	0.15028500	-3.23524800
H	1.64387800	1.77003600	-2.71771300
H	3.36235800	1.39008700	-2.91620900
C	1.89545000	2.84661800	-0.00230400
H	1.32371800	3.12791200	0.88412700
H	2.81979600	3.43687000	-0.00453500
H	1.32081000	3.12582600	-0.88752100
C	2.39693400	0.99370400	2.58183200
H	1.64623100	1.77435500	2.71535900
H	2.14603700	0.15487600	3.23464800
H	3.36453300	1.39325200	2.91340500
C	3.52659100	-1.79358000	1.62104300

H	3.68255000	-2.73537500	1.09304500
H	4.47274400	-1.51543300	2.10036500
H	2.79849700	-1.96673100	2.41887800
C	-1.21912900	-2.05815800	0.00089200
H	-1.54676600	-2.61238100	0.88378500
H	-1.54649900	-2.61266200	-0.88192000
H	-0.10237300	-2.11881200	0.00111400

Zero-point correction= 0.375282 (Hartree/Particle)

Thermal correction to Energy= 0.398494

Thermal correction to Enthalpy= 0.399439

Thermal correction to Gibbs Free Energy= 0.320964

Sum of electronic and zero-point Energies= -939.741053

Sum of electronic and thermal Energies= -939.717841

Sum of electronic and thermal Enthalpies= -939.716897

Sum of electronic and thermal Free Energies= -939.795371

E(RB3LYP) = -940.116335 A.U.

A-5

1 1

Number of imaginary frequencies: 0

Rh	-1.23565900	-0.73453900	0.32940900
C	-0.64904000	-2.41094100	1.72560100
C	-0.00060700	-1.23409700	2.31530100
C	-0.99374900	-0.30719400	2.66645300
C	-2.28599400	-0.88987700	2.28434700
C	-2.06584300	-2.22344700	1.81088500
C	-2.31243700	2.20686600	0.24957700
C	-3.60160000	0.58828200	-0.82599500

C	-4.69857200	1.48442300	-0.96441700
C	-4.52418800	2.80893800	-0.49034000
C	-3.33261000	3.17050400	0.09986000
H	-1.38489800	2.45696300	0.74969700
C	-3.66534400	-0.75014900	-1.28939800
C	-5.90220800	0.98599800	-1.52937100
H	-5.33616300	3.52385600	-0.58851100
H	-3.16533600	4.17482100	0.47213900
C	-5.98379500	-0.33383400	-1.91784200
C	-4.86748600	-1.20121900	-1.80352800
H	-6.75417700	1.65106800	-1.63201700
H	-6.91049700	-0.71813700	-2.33229000
H	-4.95100200	-2.22708100	-2.15106300
N	-2.44308800	0.96267900	-0.19149200
C	0.04770500	-3.70339700	1.43478000
H	-0.45612500	-4.26981900	0.64965400
H	1.07911100	-3.54502400	1.11854900
H	0.06343800	-4.32239900	2.34049600
C	1.47738800	-1.12435700	2.51558200
H	1.81664800	-1.89528500	3.21733000
H	2.01434200	-1.29227300	1.57699400
H	1.76940500	-0.15199100	2.91223600
C	-0.82749600	1.00021900	3.37999300
H	-1.07604900	0.87809900	4.44135800
H	0.19075700	1.38737200	3.31609700
H	-1.50414500	1.76147500	2.98254200
C	-3.62242300	-0.27423900	2.56228000

H	-4.38458100	-0.65165200	1.87712000
H	-3.93897700	-0.51179000	3.58495900
H	-3.58998400	0.81326900	2.46961300
C	-3.12725200	-3.23347000	1.50344200
H	-3.48545800	-3.69399800	2.43147200
H	-3.98625000	-2.77579300	1.00537000
H	-2.74686800	-4.03220100	0.86348300
C	0.60398900	-3.44087800	-1.84748800
C	1.31875500	-4.61927300	-2.04871500
C	2.67066900	-4.69359900	-1.69976200
C	3.31377500	-3.57591800	-1.16074500
C	2.61131600	-2.38851000	-0.96660000
C	1.24605700	-2.31569100	-1.30307000
H	0.82015700	-5.48400600	-2.47546300
H	3.22018600	-5.61739600	-1.85100800
H	4.36463600	-3.62547100	-0.89202400
H	3.10915200	-1.51508200	-0.56209500
C	0.81160000	2.53017900	-0.59871600
C	0.83005500	3.86895100	-1.00866600
C	0.43898600	4.20259500	-2.30359600
C	-0.00875700	3.21857200	-3.19275400
C	-0.04749400	1.88955400	-2.78762500
C	0.38144500	1.52701100	-1.49745700
H	-0.44692300	-3.38483300	-2.10734400
H	1.15732500	4.62819200	-0.30978700
H	0.46601100	5.24232700	-2.61405100
H	-0.32659000	3.48881400	-4.19435300

H	-0.39347800	1.11229500	-3.46089600
N	1.13686200	2.17008300	0.73243700
H	0.90065400	1.20435200	0.95517600
S	2.66556800	2.53284300	1.42132900
O	2.54717000	2.04393500	2.79838000
O	2.94645300	3.92873600	1.10522000
C	4.05936200	1.70630800	-0.81157600
C	4.91551900	0.84662300	-1.49261300
C	5.54706800	-0.22388800	-0.83731200
C	5.30446600	-0.40787000	0.53135500
C	4.43505000	0.43055600	1.22965800
C	3.81434000	1.47774200	0.54748400
H	3.59743200	2.54425900	-1.32171900
H	5.10699200	1.01341400	-2.54878200
H	5.80194700	-1.21613500	1.05991500
H	4.24912100	0.29106200	2.28831600
C	0.36114300	0.15355900	-1.09313800
C	0.55299300	-1.07587500	-1.07952900
C	6.43923400	-1.16745100	-1.60408100
H	7.08065300	-0.62793600	-2.30706900
H	7.07891600	-1.75100100	-0.93691900
H	5.83560400	-1.87088600	-2.19089300
C	-2.39103100	-1.53417300	-1.23056300
H	-1.81230500	-1.37324500	-2.14548200
H	-2.56047000	-2.60530900	-1.10104300

Zero-point correction= 0.708795 (Hartree/Particle)

Thermal correction to Energy= 0.753427

Thermal correction to Enthalpy= 0.754371

Thermal correction to Gibbs Free Energy= 0.632279

Sum of electronic and zero-point Energies= -2353.325273

Sum of electronic and thermal Energies= -2353.280641

Sum of electronic and thermal Enthalpies= -2353.279697

Sum of electronic and thermal Free Energies= -2353.401789

E(RB3LYP) = -2354.034068 A.U.

A-6a

1 1

Number of imaginary frequencies: 0

Rh	-1.88526600	-0.02050100	0.05381300
C	-2.76121900	-1.43617500	1.68295400
C	-3.35509000	-0.17850800	1.92128600
C	-4.11709400	0.18702500	0.73085500
C	-4.01979300	-0.86954100	-0.20645700
C	-3.09298800	-1.84647700	0.32576600
C	-1.46103100	3.02599000	0.68963500
C	-0.75086600	2.31566400	-1.40690400
C	-0.23475600	3.60662500	-1.72048100
C	-0.39487800	4.63089600	-0.75293900
C	-1.02127200	4.34407700	0.43972400
H	-1.93960200	2.77527800	1.63011800
C	-0.73374800	1.25510500	-2.35218900
C	0.39902300	3.79077500	-2.97755800
H	-0.03079500	5.63183900	-0.96635300
H	-1.17690000	5.10602500	1.19559700
C	0.50110100	2.73111400	-3.85589500

C	-0.06957800	1.47033200	-3.54926600
H	0.79776100	4.76822200	-3.23282000
H	0.99288600	2.87046400	-4.81402200
H	-0.03828000	0.67677800	-4.29072800
N	-1.31769300	2.03931100	-0.18519700
C	-1.55108100	0.05260200	-2.00773900
H	-2.56183200	0.21614500	-2.40157800
H	-1.16795200	-0.86842800	-2.44264100
C	-1.95798100	-2.25233100	2.64925400
H	-1.51415300	-1.63607900	3.43345600
H	-2.59250600	-3.00755300	3.12788500
H	-1.14747800	-2.77785000	2.13773800
C	-3.34201800	0.60019400	3.20273800
H	-4.23750000	0.38595100	3.79932500
H	-2.47147600	0.35754800	3.81626800
H	-3.33953700	1.68010100	3.02202600
C	-4.94325600	1.43193700	0.60859900
H	-5.85220200	1.35734000	1.21760400
H	-4.39189200	2.31201500	0.95552600
H	-5.24720900	1.61577500	-0.42384000
C	-4.74894900	-0.99362000	-1.50879000
H	-5.67259500	-1.56875800	-1.37298200
H	-5.02478500	-0.01871000	-1.91857600
H	-4.14659300	-1.51544600	-2.25689800
C	-2.81615500	-3.19221700	-0.27488400
H	-3.63488000	-3.89144500	-0.06280000
H	-2.70081000	-3.12898400	-1.35961200

H	-1.89628300	-3.62275000	0.12226500
C	1.64817000	-1.13299800	2.13618000
C	2.33126400	-1.13170800	3.34084300
C	1.93781800	-0.16924600	4.27962600
C	0.90903700	0.73248800	3.98293200
C	0.23103200	0.68813800	2.75924300
C	0.59781100	-0.26600400	1.80949700
H	3.13773700	-1.82808500	3.54019500
H	2.43576700	-0.12739400	5.24255900
H	0.62233400	1.47255500	4.72399800
H	-0.58179200	1.36996300	2.55598700
C	0.62212100	-3.92937500	-0.99267200
C	0.62267100	-4.78971100	-2.08933200
C	0.76135100	-4.27407700	-3.37976800
C	0.90762900	-2.89763800	-3.56416400
C	0.91351300	-2.03969600	-2.46560800
C	0.75498800	-2.54128400	-1.16588100
H	0.49050100	-4.34099500	0.00636700
H	0.50964500	-5.85865100	-1.93765000
H	0.76295100	-4.94215900	-4.23528700
H	1.03178700	-2.49320200	-4.56424400
H	1.04721900	-0.97368900	-2.60670700
N	1.89877900	-1.95893600	0.97493800
S	3.75161100	-1.54308300	0.27307800
O	4.57097200	-1.96001500	1.40568800
O	3.76847900	-2.20304800	-1.02231000
C	3.09230800	0.73986000	-1.03436600

C	2.93266200	2.11862500	-1.10964200
C	3.28828400	2.94876100	-0.03567900
C	3.82786000	2.36929000	1.12682500
C	4.00124100	0.99640400	1.23026500
C	3.63091500	0.20018400	0.13769600
H	2.82951700	0.09763100	-1.86547700
H	2.52166500	2.55331200	-2.01301800
H	4.11947700	3.00534500	1.95718900
H	4.41577600	0.54536600	2.12325400
C	0.79461000	-1.65554800	0.01238700
C	0.01842200	-0.63865000	0.49206600
C	3.08272700	4.43864400	-0.11229500
H	3.92917900	4.98015000	0.31989700
H	2.94600700	4.77272100	-1.14325600
H	2.18671000	4.72349600	0.45137300
H	2.00928500	-2.95965200	1.16867200

Zero-point correction= 0.709142 (Hartree/Particle)

Thermal correction to Energy= 0.753225

Thermal correction to Enthalpy= 0.754169

Thermal correction to Gibbs Free Energy= 0.633274

Sum of electronic and zero-point Energies= -2353.310443

Sum of electronic and thermal Energies= -2353.266359

Sum of electronic and thermal Enthalpies= -2353.265415

Sum of electronic and thermal Free Energies= -2353.386310

E(RB3LYP) = -2354.019585 A.U.

A-6c

1 1

Number of imaginary frequencies: 0

Rh	-1.80138200	-0.83986700	-0.27514900
C	-2.73413100	-1.47156000	-2.15334900
C	-1.87358300	-2.51703600	-1.73092800
C	-2.43604400	-3.12057000	-0.49660100
C	-3.57379500	-2.40279200	-0.13469700
C	-3.72193800	-1.30174300	-1.09788500
C	-1.54616800	-1.05979300	2.57893200
C	-1.58877700	1.25537400	2.24830700
C	-1.16053600	1.44980700	3.60485200
C	-0.93600700	0.31808300	4.42262100
C	-1.14576200	-0.94078100	3.91765300
H	-1.69263500	-2.04749800	2.15762300
C	-1.87326700	2.40328400	1.44913800
C	-0.97850100	2.76016600	4.11409900
H	-0.60369100	0.46228500	5.44664600
H	-0.98147900	-1.83568300	4.50511700
C	-1.22744100	3.85131400	3.31767000
C	-1.67775300	3.66104200	1.99509100
H	-0.64615900	2.87943600	5.14091600
H	-1.08891400	4.85757700	3.69927400
H	-1.87362700	4.53028200	1.37452500
N	-1.74020600	-0.02687500	1.75424800
C	-2.66065300	-0.70577000	-3.43660100
H	-3.07127900	0.29928500	-3.32292900
H	-1.62860400	-0.60601000	-3.77800400
H	-3.23291100	-1.22285900	-4.21572100

C	-0.72844300	-3.09448500	-2.50222300
H	-1.08752400	-3.92600200	-3.12154100
H	-0.27085100	-2.35229600	-3.15744200
H	0.04941500	-3.48753300	-1.84323700
C	-1.80048100	-4.27688600	0.20808400
H	-1.79863200	-5.16232400	-0.43786700
H	-0.75568000	-4.06210700	0.46091600
H	-2.32482600	-4.53245500	1.13025300
C	-4.46808600	-2.60340000	1.04957400
H	-5.47185000	-2.90318400	0.72826700
H	-4.08735000	-3.37657400	1.71923200
H	-4.57035800	-1.67893800	1.62657600
C	-4.87771000	-0.35593300	-1.12081400
H	-5.74472000	-0.85054800	-1.57814200
H	-5.16452100	-0.05295700	-0.11100800
H	-4.65657800	0.53899400	-1.70481800
C	-0.68792000	4.21861200	-1.86912100
C	0.12274200	5.31553500	-2.16214500
C	1.44538600	5.34702400	-1.71434400
C	1.95130900	4.27668300	-0.97222600
C	1.14675400	3.17486200	-0.68709600
C	-0.18169100	3.13017800	-1.14074100
H	-0.27747300	6.14434800	-2.73865900
H	2.07496000	6.20321900	-1.93718200
H	2.97464100	4.30460000	-0.60864600
H	1.52396300	2.34729500	-0.09567500
C	1.38852300	-0.69162000	-1.49336800

C	2.51233600	-0.97061400	-2.27651300
C	2.70537200	-0.32143700	-3.49413200
C	1.75224700	0.59755900	-3.93983700
C	0.63973800	0.88754400	-3.15454800
C	0.44447100	0.28314700	-1.89541200
H	-1.71463900	4.19809700	-2.22631900
H	3.21601900	-1.71538000	-1.92019100
H	3.57762500	-0.54838100	-4.09863600
H	1.87768200	1.09438900	-4.89702600
H	-0.08217700	1.62346800	-3.49043700
N	1.22942500	-1.47497100	-0.30266900
H	0.29700300	-1.86364100	-0.15497000
S	1.79328600	-0.91953800	1.21124400
O	1.29216200	-1.94738800	2.13630700
O	1.45919300	0.49487300	1.42824100
C	4.29607000	0.09476300	0.72140800
C	5.66710000	-0.03194500	0.50667900
C	6.29910400	-1.28192300	0.57136600
C	5.52106700	-2.41656100	0.85861400
C	4.15100100	-2.31319700	1.07487100
C	3.55340800	-1.05203900	1.00277200
H	3.80562200	1.06041900	0.67561700
H	6.25550900	0.85383600	0.28540600
H	5.99883600	-3.39053800	0.91584200
H	3.55109300	-3.18771100	1.30262700
C	-1.04502300	1.96095900	-0.81252200
C	-0.70508900	0.67892600	-1.05585500

C	7.78841700	-1.40675400	0.36995200
H	8.04871500	-2.34904000	-0.12072300
H	8.18407500	-0.58416800	-0.23164700
H	8.30826600	-1.38812000	1.33542700
C	-2.28997400	2.27908800	0.00475400
H	-3.04549500	1.50097000	-0.11902100
H	-2.73482500	3.22247800	-0.32293100

Zero-point correction= 0.709132 (Hartree/Particle)

Thermal correction to Energy= 0.753801

Thermal correction to Enthalpy= 0.754745

Thermal correction to Gibbs Free Energy= 0.629302

Sum of electronic and zero-point Energies= -2353.334345

Sum of electronic and thermal Energies= -2353.289676

Sum of electronic and thermal Enthalpies= -2353.288732

Sum of electronic and thermal Free Energies= -2353.414175

E(RB3LYP) = -2354.043477 A.U.

A-6d

1 1

Number of imaginary frequencies: 0

Rh	1.98307000	0.28536300	-0.11678400
C	3.51044400	1.18578700	1.18824400
C	3.61832800	-0.22403600	1.29561900
C	4.11346800	-0.75615800	0.00086900
C	4.21151300	0.29939400	-0.90071000
C	3.73807100	1.51147600	-0.21084400
C	1.26425600	-0.93705200	-2.62284300
C	-0.22827100	0.86739500	-2.49664300

C	-0.92487800	0.35692400	-3.65043400
C	-0.45535300	-0.82272800	-4.26952000
C	0.65043200	-1.46938800	-3.76528400
H	2.13095700	-1.43557200	-2.20103700
C	-0.67174200	2.10154700	-1.92540000
C	-2.06264300	1.03250400	-4.15877000
H	-0.97694200	-1.20489800	-5.14228600
H	1.04813000	-2.37031400	-4.21820500
C	-2.50091400	2.18586300	-3.56085400
C	-1.79533700	2.71071400	-2.45896600
H	-2.57899300	0.61282700	-5.01618000
H	-3.38181700	2.69995200	-3.92950200
H	-2.14422200	3.63317300	-2.00465400
N	0.85318100	0.16732500	-1.98888600
C	3.23138000	2.15973000	2.28837400
H	2.65991700	3.01707900	1.92685700
H	2.66163700	1.69166800	3.09213400
H	4.17419900	2.52954700	2.70818800
C	3.47112400	-1.04127500	2.53917000
H	4.45086800	-1.17241100	3.01561000
H	2.79851100	-0.56646300	3.25478500
H	3.07000000	-2.03242800	2.31842400
C	4.40976800	-2.20349900	-0.22902900
H	5.28992900	-2.50707400	0.35017800
H	3.57746300	-2.83249400	0.10302600
H	4.60931300	-2.42061100	-1.27999700
C	4.63772600	0.26917900	-2.33574700

H	5.57975200	0.81303500	-2.46893600
H	4.79002700	-0.75081200	-2.69360600
H	3.89146900	0.74577000	-2.97929100
C	3.80539400	2.88470600	-0.79484700
H	4.84414800	3.23937600	-0.76961000
H	3.47999600	2.89136300	-1.83797000
H	3.19723600	3.59534400	-0.23291400
C	0.08112400	-1.29878000	2.01313400
C	-0.01524700	-2.09951300	3.14898000
C	-0.00931000	-1.51785100	4.41896400
C	0.07255000	-0.12709900	4.54507200
C	0.16635600	0.67813100	3.41082300
C	0.18528500	0.10440800	2.12497300
H	-0.11401300	-3.17475200	3.03801800
H	-0.08607000	-2.14036500	5.30500500
H	0.05434100	0.33055800	5.52965300
H	0.21045600	1.75829600	3.50452800
C	-2.78059200	1.46937700	1.16944100
C	-4.02451300	1.88544300	1.66291100
C	-4.19334000	3.19327800	2.10780300
C	-3.12768500	4.09742900	2.08031800
C	-1.89339100	3.68317300	1.58840100
C	-1.69064500	2.37265000	1.12783900
H	0.03635300	-1.76190300	1.02940400
H	-4.84433400	1.17788300	1.69107400
H	-5.16197300	3.50425300	2.48666100
H	-3.25819700	5.11318500	2.43935600

H	-1.06057200	4.38143500	1.56265800
N	-2.57150300	0.13151200	0.75620700
H	-1.62680100	-0.00020600	0.40510400
S	-3.61175800	-0.71046400	-0.30205100
O	-3.50715100	-0.18595100	-1.67159800
O	-4.91562000	-0.83201200	0.34918500
C	-2.90453300	-3.10506200	0.86844600
C	-2.10834400	-4.24151600	0.98261200
C	-1.11873500	-4.53601900	0.02970900
C	-0.95354400	-3.66442900	-1.05685400
C	-1.74863200	-2.52653800	-1.19306200
C	-2.71182000	-2.25669000	-0.22245800
H	-3.65827600	-2.86787100	1.61141200
H	-2.25321000	-4.91179800	1.82546000
H	-0.20432200	-3.88459900	-1.81289600
H	-1.63295200	-1.85703400	-2.03639200
C	-0.38141700	1.98385000	0.52816600
C	0.37160600	0.93916700	0.92458100
C	-0.28109200	-5.78442600	0.15872300
H	-0.02254700	-5.98779000	1.20238700
H	-0.83062100	-6.65730400	-0.21293700
H	0.64570800	-5.71151200	-0.41744700
C	0.01044900	2.73735900	-0.73689500
H	1.09334100	2.72417900	-0.86580900
H	-0.30125500	3.78266400	-0.66816800

Zero-point correction= 0.709844 (Hartree/Particle)

Thermal correction to Energy= 0.754386

Thermal correction to Enthalpy= 0.755330

Thermal correction to Gibbs Free Energy= 0.631809

Sum of electronic and zero-point Energies= -2353.328141

Sum of electronic and thermal Energies= -2353.283600

Sum of electronic and thermal Enthalpies= -2353.282656

Sum of electronic and thermal Free Energies= -2353.406177

E(RB3LYP) = -2354.037986 A.U.

A-6e

1 1

Number of imaginary frequencies: 0

Rh	-2.02384400	-0.47322000	-0.28470200
C	-2.26273300	-2.47737700	-1.07991300
C	-1.73067500	-2.69673300	0.26542700
C	-2.66899700	-2.17698800	1.17678000
C	-3.85062600	-1.73884800	0.43167100
C	-3.62170000	-1.96358500	-0.94005700
C	0.25989100	2.88481600	1.45562700
C	-1.92438800	2.25565800	0.71891900
C	-2.44568800	2.81767700	1.94178100
C	-1.56674300	3.40837900	2.88439400
C	-0.22136300	3.47162800	2.62730900
H	1.32350100	2.82804100	1.26757500
C	-2.85754500	1.77480900	-0.28105000
C	-3.83306400	2.84225800	2.19448800
H	-1.98168400	3.82088000	3.79920000
H	0.48765500	3.92004000	3.31216900
C	-4.72006200	2.35498200	1.25302900

C	-4.23104900	1.84838400	0.05320400
H	-4.18572700	3.27538400	3.12485800
H	-5.78977600	2.38810100	1.43122400
H	-4.93348400	1.49167700	-0.69298600
N	-0.53144500	2.28336900	0.55433900
C	-1.66954600	-2.99760200	-2.34963500
H	-0.57997300	-2.99625100	-2.31730600
H	-2.00601500	-4.02838000	-2.52142500
H	-1.97830200	-2.39624800	-3.20692300
C	-0.49998300	-3.47492600	0.61951600
H	-0.79096200	-4.46456000	0.99262900
H	0.14441300	-3.62574700	-0.24523400
H	0.08944500	-2.98612400	1.39900300
C	-2.55531400	-2.16022500	2.66922100
H	-3.12876700	-2.98609000	3.10942400
H	-1.51717100	-2.26432600	2.99171700
H	-2.95225000	-1.23113300	3.08901100
C	-5.10459500	-1.24090000	1.08138300
H	-5.79288800	-0.80222500	0.35672800
H	-5.62564300	-2.06842800	1.57757300
H	-4.88922400	-0.48557500	1.84276200
C	-4.57846500	-1.73670800	-2.06973000
H	-5.12208800	-2.65980000	-2.30373600
H	-5.31941600	-0.97136000	-1.82547500
H	-4.05592500	-1.42286900	-2.97626800
C	-2.51632600	1.13637400	-1.55673300
H	-3.38860100	0.93134700	-2.17584200

H	-1.70190900	1.55370300	-2.13456700
C	2.65652800	2.10415900	-1.07179200
C	3.57797700	3.01336600	-1.60614500
C	3.14178700	4.19245300	-2.20223300
C	1.77304900	4.46120400	-2.29128800
C	0.85620000	3.56116000	-1.75607300
C	1.27268300	2.37730600	-1.12022300
H	4.63265400	2.77017100	-1.53935700
H	3.86527100	4.89122400	-2.60972300
H	1.42206100	5.36748800	-2.77462600
H	-0.20730200	3.77961200	-1.81291400
C	0.56897800	-0.28775700	-3.10971400
C	1.30098200	-1.07210900	-4.00024100
C	2.11693700	-2.10585500	-3.53088900
C	2.19623300	-2.34894300	-2.15890800
C	1.44939600	-1.57737500	-1.26642300
C	0.62609700	-0.53386700	-1.72760100
H	-0.04871200	0.52261600	-3.48291700
H	1.24350900	-0.86826100	-5.06535500
H	2.69177600	-2.70694800	-4.22822300
H	2.84066500	-3.13305000	-1.77329600
H	1.51244800	-1.77567100	-0.20138000
N	3.16515000	0.91033400	-0.49034400
H	2.51524700	0.13139300	-0.52992100
S	3.83974700	0.99824900	1.07580100
O	2.92058400	1.69907900	1.99885900
O	5.21410400	1.47813800	0.94909300

C	4.59665300	-1.62210500	0.72931400
C	4.44472800	-2.99350800	0.92116800
C	3.48889300	-3.50048400	1.81607000
C	2.68743300	-2.59406500	2.52771400
C	2.81610700	-1.21848100	2.34270400
C	3.77066100	-0.74882700	1.43972900
H	5.33255100	-1.23245600	0.03416600
H	5.07943700	-3.68238500	0.37080900
H	1.95679400	-2.97209900	3.23791100
H	2.19226700	-0.51273500	2.87986700
C	-0.16635200	0.26506100	-0.76438900
C	0.21275800	1.53049900	-0.48797200
C	3.34949700	-4.98643800	2.03374700
H	4.02127900	-5.32233100	2.83261500
H	2.33125900	-5.25564800	2.32912700
H	3.60766200	-5.55051700	1.13315600

Zero-point correction= 0.708893 (Hartree/Particle)

Thermal correction to Energy= 0.753284

Thermal correction to Enthalpy= 0.754228

Thermal correction to Gibbs Free Energy= 0.630307

Sum of electronic and zero-point Energies= -2353.287189

Sum of electronic and thermal Energies= -2353.242798

Sum of electronic and thermal Enthalpies= -2353.241854

Sum of electronic and thermal Free Energies= -2353.365775

E(RB3LYP) = -2353.996082 A.U.

A-6f

1 1

Number of imaginary frequencies: 0

Rh	-1.91310000	0.71824900	0.03358000
C	-1.61474500	2.63985700	-0.98139800
C	-2.81530100	2.08995200	-1.59051400
C	-3.77763500	1.96210100	-0.56447200
C	-3.23799800	2.53545100	0.66846400
C	-1.92106500	2.96549400	0.41188900
C	-1.86239800	-3.86104700	-0.07322800
C	-2.35806000	-1.97483900	1.29550000
C	-3.56061400	-2.65259600	1.71316500
C	-3.84752700	-3.94980300	1.23169900
C	-2.96929700	-4.57458000	0.37660000
H	-1.19604400	-4.27385900	-0.81828100
C	-1.98975800	-0.73733500	1.94491000
C	-4.43116100	-2.06239700	2.65784600
H	-4.75385700	-4.44722800	1.56313900
H	-3.13432800	-5.57853600	0.00521300
C	-4.11231600	-0.84632000	3.22820600
C	-2.91301900	-0.22384300	2.88417600
H	-5.32972600	-2.59884800	2.94476000
H	-4.76478800	-0.39275100	3.96700900
H	-2.64034100	0.70437700	3.37332100
N	-1.57351000	-2.60521400	0.31949800
C	-0.41246000	3.13085200	-1.71511100
H	-0.20649500	2.53911400	-2.60645600
H	-0.59938600	4.16524700	-2.03525900
H	0.48230900	3.13422200	-1.09241200

C	-3.03104800	1.84087500	-3.05169600
H	-3.53542300	2.70219700	-3.50663900
H	-2.08609700	1.69838500	-3.57462400
H	-3.65484600	0.96058800	-3.22795500
C	-5.16336300	1.41243700	-0.69549000
H	-5.89701700	2.22799300	-0.72303200
H	-5.27954000	0.82648900	-1.60920000
H	-5.41894000	0.77556800	0.15725000
C	-4.03977100	2.74728700	1.91658600
H	-3.40251900	2.94114800	2.78197400
H	-4.69925400	3.61525000	1.79523800
H	-4.67458300	1.88642100	2.14229000
C	-0.98437900	3.67129300	1.34135100
H	-0.92961500	4.73571000	1.08255600
H	-1.31741400	3.59815600	2.37915300
H	0.02389100	3.25581100	1.28176100
C	-0.78796700	0.05268400	1.68259800
H	-0.60625300	0.84930300	2.39876300
H	0.12366100	-0.48404800	1.46584000
C	1.49668800	0.33008600	-1.72458400
C	2.26114500	0.86098400	-2.77113800
C	1.75182300	0.91400700	-4.06445500
C	0.48127200	0.39557300	-4.33248000
C	-0.28102900	-0.12872400	-3.29157300
C	0.19154600	-0.14261400	-1.96795600
H	3.25217200	1.24151300	-2.55427000
H	2.35366400	1.33499100	-4.86330000

H	0.08792200	0.39950200	-5.34438900
H	-1.27040700	-0.53015900	-3.48750700
C	0.99132100	-3.13116600	-2.14761700
C	2.13264500	-3.89750200	-2.38874600
C	2.90257800	-4.37217100	-1.32550500
C	2.52557800	-4.08049700	-0.01206600
C	1.38883200	-3.31196300	0.23209800
C	0.61143900	-2.81969800	-0.83339600
H	0.40203000	-2.75875900	-2.97734400
H	2.41740300	-4.12539000	-3.41135400
H	3.78970500	-4.96750600	-1.51791800
H	3.11918200	-4.44498000	0.82079200
H	1.10087400	-3.08202400	1.25557400
N	2.07470200	0.20181600	-0.43212200
H	1.67757400	-0.52303200	0.15359800
S	2.59326500	1.52504600	0.49305500
O	1.77367100	1.61995500	1.71235400
O	2.66901000	2.67091300	-0.41843000
C	5.08400500	0.39878200	0.07209200
C	6.37652300	0.07305300	0.47057900
C	6.82917700	0.35327700	1.77008900
C	5.94348900	0.96112100	2.67070500
C	4.64421000	1.29401600	2.29218100
C	4.22691400	1.00899000	0.99126500
H	4.73634800	0.15965700	-0.92702800
H	7.04593900	-0.41001700	-0.23571500
H	6.27352200	1.17524300	3.68325600

H	3.95707300	1.75624300	2.99201300
C	-0.55134800	-1.93850200	-0.51483900
C	-0.71439400	-0.65081000	-0.90466400
C	8.24459900	0.02759300	2.17701500
H	8.91907200	0.85015300	1.90994900
H	8.32806500	-0.12685400	3.25618300
H	8.61112500	-0.87051500	1.67153700

Zero-point correction= 0.709075 (Hartree/Particle)

Thermal correction to Energy= 0.753380

Thermal correction to Enthalpy= 0.754324

Thermal correction to Gibbs Free Energy= 0.630687

Sum of electronic and zero-point Energies= -2353.288928

Sum of electronic and thermal Energies= -2353.244623

Sum of electronic and thermal Enthalpies= -2353.243679

Sum of electronic and thermal Free Energies= -2353.367316

E(RB3LYP) = -2353.998003 A.U.

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0 1

Number of imaginary frequencies: 0

Rh	-2.02295000	0.16938900	-0.28198000
C	-3.24575700	-1.51115700	0.72540400
C	-3.91780100	-0.31692300	1.08588500
C	-4.39146300	0.31219000	-0.13636700
C	-4.03744100	-0.50780000	-1.23216200
C	-3.25115300	-1.61389300	-0.72146600
C	-1.68831200	3.02298100	0.95504500
C	-0.34434200	2.53211000	-0.87622400

C	0.39869700	3.73644700	-0.71416000
C	0.01968300	4.60380200	0.34120800
C	-1.03939800	4.26084400	1.15150700
H	-2.49825800	2.71476400	1.60689600
C	-0.11142000	1.64675900	-1.96232700
C	1.45984900	3.99593700	-1.61944600
H	0.56166000	5.53352600	0.49209000
H	-1.36947500	4.90778600	1.95710200
C	1.73124500	3.09997500	-2.63122900
C	0.94178600	1.93921300	-2.81334000
H	2.04576300	4.90294600	-1.50333300
H	2.54790000	3.29719600	-3.31950400
H	1.14436500	1.28209800	-3.65428000
N	-1.33730100	2.16955100	0.00295300
C	-1.09284100	0.53202700	-2.11535400
H	-1.92947100	0.89256900	-2.73021700
H	-0.66753300	-0.34726400	-2.59627400
C	-2.64922700	-2.51803500	1.66290100
H	-2.31441400	-2.05056900	2.59139500
H	-3.38193300	-3.29580900	1.91188700
H	-1.77949800	-3.00111500	1.21322800
C	-4.23220300	0.16080400	2.47272100
H	-5.25145000	-0.12251100	2.76748300
H	-3.54368500	-0.25877700	3.20906800
H	-4.17544300	1.25272200	2.54881200
C	-5.18159500	1.58640700	-0.17619500
H	-6.20766300	1.42664900	0.17860200

H	-4.73402900	2.35204800	0.46706500
H	-5.23775000	1.99571100	-1.18749100
C	-4.40548500	-0.31067100	-2.67147100
H	-5.29632500	-0.89659500	-2.93084200
H	-4.62096800	0.73733200	-2.89725100
H	-3.59865700	-0.63456900	-3.33502600
C	-2.81252500	-2.79847500	-1.52958900
H	-3.65098000	-3.48464900	-1.70992200
H	-2.41526400	-2.49220300	-2.50120700
H	-2.02173200	-3.35397700	-1.02633500
C	1.03831500	-1.02116800	2.46651300
C	1.46405300	-1.02002000	3.79834800
C	0.76972500	-0.21487100	4.69967900
C	-0.33782000	0.54360500	4.28699500
C	-0.75805400	0.51938300	2.96083400
C	-0.06061600	-0.25278900	2.01876100
H	2.30020600	-1.62877500	4.11328600
H	1.08029800	-0.19539400	5.74028700
H	-0.87869000	1.14492000	5.01289200
H	-1.63081400	1.07721100	2.65525400
C	0.59006600	-3.58769500	-1.01545600
C	0.75571000	-4.34315500	-2.17384500
C	1.20085700	-3.73405300	-3.35041800
C	1.49393000	-2.36953200	-3.35185400
C	1.32601100	-1.61548400	-2.18906200
C	0.84866800	-2.20831300	-1.01471500
H	0.27000800	-4.06241000	-0.09278700

H	0.54494300	-5.40872600	-2.15822700
H	1.33244700	-4.32282900	-4.25387800
H	1.86372200	-1.89211400	-4.25566100
H	1.58775000	-0.56495400	-2.17216300
N	1.49430200	-1.78860600	1.36821000
S	3.19922300	-1.99501600	1.13782600
O	3.78099200	-2.15723400	2.47089200
O	3.39061100	-3.01602200	0.11275100
C	4.12419500	-0.33942100	-0.86050100
C	4.50630900	0.89768700	-1.37782000
C	4.47365000	2.05401100	-0.58831400
C	4.03507600	1.94874200	0.74041700
C	3.65953400	0.72233200	1.28034900
C	3.70900600	-0.41426000	0.46811900
H	4.13636900	-1.23678100	-1.46814900
H	4.83593700	0.96421900	-2.41128200
H	3.99471100	2.83913300	1.36213600
H	3.33207100	0.64544400	2.31103400
C	0.66311400	-1.43057400	0.23016400
C	-0.29086200	-0.51505000	0.59684200
C	4.93864200	3.38073700	-1.13575900
H	5.98469400	3.56755900	-0.86352900
H	4.87253000	3.41131500	-2.22689200
H	4.34316500	4.20612100	-0.73538900

Zero-point correction= 0.696706 (Hartree/Particle)

Thermal correction to Energy= 0.739372

Thermal correction to Enthalpy= 0.740316

Thermal correction to Gibbs Free Energy= 0.623500

Sum of electronic and zero-point Energies= -2352.932719

Sum of electronic and thermal Energies= -2352.890054

Sum of electronic and thermal Enthalpies= -2352.889110

Sum of electronic and thermal Free Energies= -2353.005926

E(RB3LYP) = -2353.629426 A.U.

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Number of imaginary frequencies: 0

Rh	-1.78589600	-0.40315200	-0.14645600
C	-3.82345400	0.35022500	0.68627200
C	-3.65507200	0.94835200	-0.65133200
C	-3.64228300	-0.08614000	-1.59709400
C	-3.69744100	-1.33926700	-0.86246600
C	-3.93662200	-1.04304600	0.53764900
C	-3.91613100	-2.67871400	-1.49433500
H	-4.98352500	-2.82508700	-1.70964100
H	-3.36518600	-2.77535400	-2.43153400
H	-3.58890100	-3.48845500	-0.83976200
C	-4.19690400	-2.07510400	1.59293400
H	-5.22034300	-2.46832800	1.52698500
H	-3.51140400	-2.92218800	1.48300700
H	-4.06470100	-1.66567600	2.59852100
C	-3.54374600	0.02748800	-3.08879000
H	-4.51265700	-0.15521500	-3.57252800
H	-3.20597100	1.02156300	-3.39552400
H	-2.83434100	-0.70355600	-3.49038800

C	-3.64119700	2.42460000	-0.91816600
H	-3.14256900	2.66191100	-1.86157600
H	-4.66273600	2.82427300	-0.97301700
H	-3.12054700	2.97249700	-0.12861600
C	-3.97495200	1.15177000	1.94524100
H	-3.24286900	1.96406900	1.99251000
H	-4.97114400	1.60927800	2.01063200
H	-3.83489600	0.53135900	2.83459500
C	5.12464500	1.56627100	-2.47873900
C	4.65100900	0.34044900	-2.01403500
C	3.27259800	0.21600700	-1.80531900
C	2.38911000	1.28775800	-2.06731400
C	2.88925400	2.50759400	-2.54577100
C	4.25830500	2.64087400	-2.74416000
H	6.19103200	1.68442300	-2.64716400
H	5.32222700	-0.48393800	-1.82425700
H	2.21275500	3.33143700	-2.74887000
H	4.66360300	3.57936700	-3.11131800
C	1.09879300	-0.45049300	-1.33354400
C	-0.01192600	-1.39917300	-1.02817700
C	-0.32284800	-2.31977600	-2.10626700
C	-0.28957700	-1.86042600	0.32813700
C	-0.81819800	-3.57095700	-1.86832400
H	-0.09390300	-2.00447200	-3.12104700
C	-0.75995200	-3.20657700	0.52724500
H	0.28257300	-1.42981700	1.14128300
C	-1.02959900	-4.02991400	-0.53022200

H	-1.02526400	-4.23839600	-2.70015100
H	-0.86258000	-3.56992500	1.54720300
H	-1.37782900	-5.04545900	-0.36265300
N	2.47705800	-0.87628200	-1.37416800
S	3.10920000	-2.14153600	-0.39409300
O	4.54026500	-2.21183600	-0.68694000
O	2.26906300	-3.32042400	-0.55668000
C	2.87460500	-1.50223900	1.26784900
C	3.08189600	-0.14985000	1.54376500
C	2.45693500	-2.38803300	2.26171200
C	2.84732000	0.31721200	2.83461500
H	3.39244100	0.53456200	0.76188200
C	2.23681600	-1.90306400	3.54934800
H	2.26454200	-3.42502800	2.00981500
C	2.42350500	-0.54700500	3.85431300
H	2.97970700	1.37395600	3.04870900
H	1.89942600	-2.58528300	4.32518300
C	2.18913500	-0.02954000	5.25262000
H	3.09878300	-0.11757600	5.85909300
H	1.90428300	1.02668000	5.24356300
H	1.40280100	-0.59392000	5.76336200
C	1.04963600	0.84151000	-1.77786800
C	-0.17509300	1.69468800	-1.94472100
H	-0.14903700	2.18912000	-2.92263000
H	-1.06002500	1.05148900	-1.91186500
C	-0.41239200	1.82569100	3.23661200
C	-0.32735500	3.14462600	2.86649100

C	-0.30819500	3.48238400	1.49039900
C	-0.38832300	2.42675700	0.51945100
C	-0.54946100	0.85071700	2.22850400
H	-0.15862100	5.61474900	1.82346700
H	-0.40965800	1.51825000	4.27641700
H	-0.26559700	3.93715000	3.60763300
C	-0.20429000	4.83377900	1.06948300
C	-0.26688700	2.75791500	-0.87050700
H	-0.67489700	-0.18985900	2.50178300
C	-0.16865800	4.09192500	-1.22162600
C	-0.15476300	5.13480800	-0.26901600
H	-0.08474200	4.34453200	-2.27522100
H	-0.07943000	6.16567400	-0.60126600
N	-0.58230800	1.12073900	0.92692200

Zero-point correction= 0.697573 (Hartree/Particle)

Thermal correction to Energy= 0.740886

Thermal correction to Enthalpy= 0.741830

Thermal correction to Gibbs Free Energy= 0.621955

Sum of electronic and zero-point Energies= -2352.922629

Sum of electronic and thermal Energies= -2352.879316

Sum of electronic and thermal Enthalpies= -2352.878372

Sum of electronic and thermal Free Energies= -2352.998246

E(RB3LYP) = -2353.620202 A.U.

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Number of imaginary frequencies: 0

Rh	2.03031500	-0.37166500	-0.12206100

C	1.63994500	-2.16989900	-1.66227500
C	2.32440700	-1.14988100	-2.34119700
C	3.55295000	-0.86911700	-1.59811100
C	3.65444900	-1.83136100	-0.52565100
C	2.42162400	-2.54876900	-0.48053400
C	1.67178900	2.47205700	-1.33908700
C	2.23300900	2.40707700	0.91902300
C	2.07911500	3.81770000	1.04502300
C	1.73959200	4.54667300	-0.12235600
C	1.55646300	3.87789800	-1.31156600
H	1.47249900	1.92132800	-2.24869000
C	2.63279500	1.59973400	2.01264100
C	2.26657600	4.40062500	2.32471100
H	1.62604400	5.62554800	-0.06562400
H	1.29199300	4.40167600	-2.22247500
C	2.59460200	3.60449000	3.40153100
C	2.78636200	2.20929800	3.24571500
H	2.14323000	5.47310700	2.44136900
H	2.72777800	4.05041300	4.38227800
H	3.08190300	1.61252100	4.10414200
N	1.97978600	1.75711700	-0.26677900
C	2.90559900	0.15387800	1.71334400
H	3.98311100	0.00844400	1.59603300
H	2.55980400	-0.51339500	2.50731100
C	0.38272800	-2.84746100	-2.09871100
H	-0.27880900	-2.19126600	-2.66551000
H	0.63954500	-3.69928300	-2.74137600

H	-0.17798200	-3.24483800	-1.25242800
C	1.94321700	-0.52239200	-3.64686700
H	2.44342700	-1.03627300	-4.47702800
H	0.86797700	-0.58162500	-3.82786800
H	2.24521400	0.52708900	-3.70006700
C	4.62239900	0.08030200	-2.04123600
H	5.24292000	-0.37941700	-2.82018900
H	4.19176000	0.99492600	-2.45652300
H	5.27494800	0.36301300	-1.21283100
C	4.85234000	-2.08786000	0.33306600
H	5.42971800	-2.91841200	-0.09020300
H	5.51453400	-1.22121800	0.38576800
H	4.56867400	-2.36694500	1.35039200
C	2.11539100	-3.69423800	0.43407700
H	2.52153900	-4.62782600	0.02488600
H	2.55447200	-3.54086300	1.42182800
H	1.04260300	-3.82697300	0.57072200
C	-1.16424800	-2.22140700	1.08609900
C	-1.52083100	-3.53898900	1.40125200
C	-0.98222000	-4.08830100	2.56385400
C	-0.10332500	-3.36336100	3.38655900
C	0.26912600	-2.06649700	3.05294100
C	-0.25699100	-1.49106700	1.88909700
H	-2.19468700	-4.10764300	0.77872000
H	-1.25468700	-5.10300600	2.83586600
H	0.28701700	-3.82231600	4.28934800
H	0.94363000	-1.50032800	3.68689100

C	-1.60436000	2.22044300	0.12845700
C	-1.93685200	3.40759800	-0.52160600
C	-1.90028800	3.47642900	-1.91584600
C	-1.50729000	2.35760200	-2.65499500
C	-1.16672800	1.17135800	-2.00744900
C	-1.23243400	1.08287400	-0.60847900
H	-1.66244500	2.15882500	1.21020900
H	-2.23543700	4.27338800	0.06111400
H	-2.17115000	4.39720100	-2.42363400
H	-1.46216400	2.40753800	-3.73875300
H	-0.85729400	0.31012900	-2.58120700
N	-1.53631000	-1.38075700	-0.00098300
S	-2.94533400	-1.67156300	-1.03124600
O	-2.57816000	-1.25069400	-2.37870000
O	-3.32304400	-3.05040000	-0.75191500
C	-4.70567900	-0.86559300	0.89603600
C	-5.62274500	0.02138200	1.44769800
C	-5.98880800	1.20093100	0.77603800
C	-5.40675600	1.47504000	-0.46969900
C	-4.48222000	0.60472500	-1.04215700
C	-4.14267200	-0.55588300	-0.34661500
H	-4.43420000	-1.78078400	1.41172300
H	-6.06877600	-0.20508400	2.41180300
H	-5.67787300	2.38293900	-1.00024100
H	-4.02357700	0.82155500	-1.99929600
C	-0.90104500	-0.14205500	0.14610800
C	-0.06531400	-0.20182500	1.26294700

C	-7.01179100	2.13290000	1.37421100
H	-8.02587500	1.78237000	1.14768700
H	-6.92128200	2.18097700	2.46326800
H	-6.91762400	3.14590600	0.97434500
H	0.32471300	0.68239700	1.74421500

Zero-point correction= 0.709544 (Hartree/Particle)

Thermal correction to Energy= 0.753654

Thermal correction to Enthalpy= 0.754598

Thermal correction to Gibbs Free Energy= 0.631917

Sum of electronic and zero-point Energies= -2353.365026

Sum of electronic and thermal Energies= -2353.320916

Sum of electronic and thermal Enthalpies= -2353.319972

Sum of electronic and thermal Free Energies= -2353.442652

E(RB3LYP) = -2354.074570 A.U.

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0 1

Number of imaginary frequencies: 0

C	-1.84459400	-1.35049600	0.01366200
C	-3.06218700	-1.36046700	0.69813000
C	-4.22454000	-1.49181100	-0.06033700
C	-4.17983800	-1.63168200	-1.45823600
C	-2.96415700	-1.64146400	-2.13218100
C	-1.78291300	-1.48921800	-1.39292800
H	-3.09853600	-1.27044900	1.77444500
H	-5.18430000	-1.50070800	0.44719400
H	-5.10583800	-1.74368900	-2.01428500
H	-2.92300600	-1.76443800	-3.21030300

C	2.52840000	-2.08861300	0.38688200
C	3.92019100	-2.10706200	0.38102000
C	4.63300000	-1.36748200	-0.56638000
C	3.94400700	-0.60501300	-1.51131000
C	2.55039800	-0.58098200	-1.50617500
C	1.82661100	-1.32327800	-0.55803200
H	1.97491700	-2.65459700	1.12612600
H	4.45081600	-2.70120700	1.11882900
H	5.71891500	-1.38317800	-0.56516200
H	4.49061400	-0.02171800	-2.24660500
H	2.00863300	0.02996300	-2.22157600
N	-0.51045000	-1.27442800	0.50506700
S	-0.15353400	-0.15472300	1.80105800
O	-1.31152800	-0.18806300	2.69096200
O	1.18309300	-0.47024100	2.29057700
C	1.12459400	1.92560200	0.53592100
C	1.14236200	3.11418100	-0.18992200
C	-0.04518400	3.78682800	-0.51041500
C	-1.26507900	3.23930200	-0.08535100
C	-1.30753300	2.05439400	0.64334300
C	-0.10558000	1.41175100	0.94712400
H	2.03953200	1.39730100	0.77708200
H	2.09460700	3.52416200	-0.51466800
H	-2.19349600	3.74822300	-0.32892300
H	-2.24952600	1.63072200	0.97251700
C	0.35937500	-1.33032000	-0.63231300
C	-0.39473400	-1.47126200	-1.76102800

C	-0.01290700	5.08949200	-1.27120300
H	0.00658400	5.94109400	-0.58021500
H	0.87524000	5.16235400	-1.90513100
H	-0.89692900	5.20485500	-1.90509200
H	0.01080400	-1.63010400	-2.75057100

Zero-point correction= 0.329299 (Hartree/Particle)

Thermal correction to Energy= 0.349959

Thermal correction to Enthalpy= 0.350903

Thermal correction to Gibbs Free Energy= 0.277367

Sum of electronic and zero-point Energies= -1413.548615

Sum of electronic and thermal Energies= -1413.527955

Sum of electronic and thermal Enthalpies= -1413.527011

Sum of electronic and thermal Free Energies= -1413.600547

E(RB3LYP) = -1413.877914 A.U.

A-11

0 1

Number of imaginary frequencies: 0

C	0.93537000	-3.08863800	-0.42056300
C	1.07560100	-4.47693600	-0.54055500
C	0.52914500	-5.15811300	-1.62398700
C	-0.19004300	-4.46963800	-2.60730300
C	-0.32836300	-3.09184700	-2.51305700
C	0.25115000	-2.38337000	-1.44228500
H	1.61616200	-5.00295300	0.23617700
H	0.64474900	-6.23564900	-1.68992900
H	-0.63633200	-5.00569900	-3.43888700
H	-0.87057500	-2.53765500	-3.27299800

C	1.04533600	2.59993400	-1.10322600
C	1.39152700	3.85686900	-1.59246100
C	1.43180400	4.10152800	-2.96780300
C	1.14272700	3.06895800	-3.86468300
C	0.79512800	1.80669500	-3.38729300
C	0.72535300	1.56487900	-2.00012600
H	1.00531600	2.40677800	-0.04134900
H	1.63448300	4.65018100	-0.89181500
H	1.69889000	5.08628100	-3.33962200
H	1.19042300	3.24467900	-4.93527100
H	0.57708300	0.99830700	-4.07768700
N	1.44542300	-2.43892700	0.72038100
H	0.90166000	-1.67067300	1.12135700
S	3.10472900	-2.33777500	1.03222300
O	3.72643400	-3.45868500	0.31997000
O	3.25185300	-2.15713400	2.47227000
C	3.48021000	0.39016200	0.91098000
C	3.85463900	1.56696800	0.26400000
C	4.34181600	1.55228000	-1.04954200
C	4.44440200	0.32078000	-1.71395500
C	4.08166400	-0.86746400	-1.08556600
C	3.60589000	-0.81912400	0.22672200
H	3.08639700	0.40407900	1.92019200
H	3.75578900	2.51206400	0.79030100
H	4.82250400	0.29374800	-2.73294400
H	4.17989800	-1.82470100	-1.58601500
C	0.32502300	0.25929900	-1.55592600

C	0.18765900	-0.96088100	-1.44805100
C	4.73834300	2.82650800	-1.75388600
H	4.65233000	3.69419300	-1.09453400
H	5.77250900	2.77404100	-2.11231200
H	4.09628100	3.00517900	-2.62290400
Rh	-1.74381000	0.11141700	-0.27210700
C	-3.92291400	0.12287800	0.03943600
C	-3.41749200	1.46399600	0.13581400
C	-2.83447300	1.83115600	-1.13984000
C	-2.98485400	0.70747100	-2.01603000
C	-3.62471400	-0.36866600	-1.29280000
O	-2.80837800	-2.97402900	0.63949200
C	-1.86302700	-2.51767900	1.27856800
O	-1.19513100	-1.42674400	0.98519500
C	-1.32978400	-3.17801400	2.53876000
C	-4.05154000	-1.68107400	-1.86784200
H	-3.88245300	-2.47125200	-1.13650000
H	-5.11417000	-1.64325000	-2.13922600
H	-3.48191600	-1.91907300	-2.76880200
C	-4.66098600	-0.59166200	1.12474400
H	-4.19255400	-0.40074000	2.09371200
H	-5.69351200	-0.22236900	1.16604400
H	-4.66025700	-1.66670800	0.95839000
C	-3.46187700	2.34051500	1.34365500
H	-2.57483600	2.97368500	1.39569500
H	-4.35029300	2.98313000	1.30081900
H	-3.48767600	1.74942500	2.25891800

C	-2.26743300	3.17666500	-1.46621000
H	-1.63412100	3.14869900	-2.35353900
H	-3.07825100	3.89396400	-1.64225700
H	-1.65804200	3.54935700	-0.64043400
C	-2.56950000	0.64441000	-3.44997400
H	-3.44541900	0.79691700	-4.09188400
H	-1.83252700	1.41092900	-3.68850000
H	-2.14263100	-0.33093600	-3.69402600
H	-0.26905800	-3.41352300	2.41948600
H	-1.40569000	-2.46603900	3.36588900
H	-1.89886100	-4.08283200	2.75472200
S	-0.24909900	0.80480600	2.52925200
O	-0.46361800	1.23094300	1.07368300
O	-1.49957300	0.60083600	3.27273300
C	0.43738500	2.43067900	3.12692400
O	0.85133600	-0.15169900	2.70911100
F	-0.45514300	3.41690700	2.93220600
F	1.55589400	2.73691700	2.43620500
F	0.73877200	2.37057500	4.42367900

Zero-point correction= 0.633101 (Hartree/Particle)

Thermal correction to Energy= 0.683652

Thermal correction to Enthalpy= 0.684596

Thermal correction to Gibbs Free Energy= 0.545882

Sum of electronic and zero-point Energies= -3102.854698

Sum of electronic and thermal Energies= -3102.804147

Sum of electronic and thermal Enthalpies= -3102.803203

Sum of electronic and thermal Free Energies= -3102.941918

E(RB3LYP) = -3103.487799 A.U.

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0 1

Number of imaginary frequencies: 0

C	0.24996400	-2.41190600	0.63993000
C	1.23973000	-3.38783000	0.73216700
C	1.16207900	-4.38016900	1.70281200
C	0.08978000	-4.39636900	2.59971900
C	-0.90730200	-3.43304200	2.50907900
C	-0.85653100	-2.42980800	1.52022100
H	2.06716800	-3.35610800	0.03789600
H	1.94326100	-5.13071000	1.76845600
H	0.03356100	-5.15909900	3.37008300
H	-1.74475300	-3.43685800	3.19856400
C	-3.84835200	1.40479800	0.54260500
C	-4.95598900	2.24314700	0.45108600
C	-6.15375900	1.90926800	1.09027200
C	-6.24122200	0.72522100	1.82909800
C	-5.14063300	-0.12353800	1.92516900
C	-3.93207200	0.20794800	1.27945100
H	-2.92896000	1.66580900	0.03669700
H	-4.87575400	3.16093600	-0.12380600
H	-7.01430900	2.56774900	1.01533200
H	-7.16876800	0.46163200	2.32906700
H	-5.20410400	-1.04705200	2.49208900
N	0.37538900	-1.36380000	-0.33273700
H	-0.34037000	-0.64608700	-0.15628100

S	0.08111000	-1.87967500	-2.04537800
O	0.46385900	-3.29143600	-2.11167200
O	0.74192900	-0.88106700	-2.88307800
C	-2.18517100	-0.39869400	-2.36609600
C	-3.55786700	-0.20930400	-2.27856600
C	-4.42063200	-1.26910000	-1.95588800
C	-3.87769100	-2.54654400	-1.75821600
C	-2.50416400	-2.76683400	-1.84216600
C	-1.67830200	-1.68334500	-2.14339800
H	-1.52338000	0.43669100	-2.55598600
H	-3.95831800	0.78909300	-2.42145000
H	-4.53596300	-3.37622400	-1.51676600
H	-2.07574000	-3.74829000	-1.67166300
C	-2.81881300	-0.67631500	1.35649300
C	-1.89798900	-1.46754600	1.42817700
C	-5.89252500	-1.00653200	-1.76807800
H	-6.05616700	-0.46884700	-0.82676000
H	-6.29084400	-0.38110100	-2.57330200
H	-6.47037700	-1.93406400	-1.73375700
Rh	2.00834300	0.20388600	-0.04961100
C	3.66587600	1.58355200	-0.36518800
C	4.02384500	0.66630900	0.67665400
C	3.99068100	-0.66542800	0.12807900
C	3.69837500	-0.55157900	-1.29702800
C	3.47220800	0.81794600	-1.59679400
O	0.93595200	0.41584700	1.69358800
C	1.22628500	-0.18809200	2.81355300

O	2.15136400	-0.98212800	2.99626600
C	0.24505400	0.17907200	3.91897400
C	3.09411000	1.40827800	-2.91700000
H	2.39407700	2.23489100	-2.77794800
H	3.98775700	1.79059100	-3.42618700
H	2.61334600	0.66505100	-3.55292800
C	3.63917000	3.07313000	-0.26368200
H	3.51639400	3.39916000	0.76960700
H	4.58911500	3.47420100	-0.64027100
H	2.82471600	3.49465700	-0.85371800
C	4.38025300	1.02096200	2.08355900
H	4.10065800	0.21757500	2.76404400
H	5.46093100	1.20078200	2.15001000
H	3.86592100	1.93049800	2.40045600
C	4.37644600	-1.90586400	0.86995000
H	4.29386300	-2.79183100	0.23800900
H	5.41765700	-1.82898400	1.20538000
H	3.73418400	-2.02030100	1.74692400
C	3.68319300	-1.69564100	-2.26032300
H	4.71578200	-1.98973400	-2.48555400
H	3.16936400	-2.56835500	-1.85174000
H	3.17966400	-1.42915200	-3.18759400
H	-0.73102000	-0.25464100	3.68153300
H	0.59660800	-0.20215400	4.87855500
H	0.11312700	1.26350600	3.95559500
S	-0.23654700	2.68174300	-0.98500600
O	0.18705800	1.23295000	-0.85358200

O	0.77001700	3.53784100	-1.63413000
C	-0.27919700	3.27205600	0.78449000
O	-1.62691400	2.77903600	-1.45649400
F	0.95773300	3.25754000	1.31025400
F	-1.07680100	2.49790200	1.52689700
F	-0.74022400	4.52875900	0.82322300

Zero-point correction= 0.634682 (Hartree/Particle)

Thermal correction to Energy= 0.684683

Thermal correction to Enthalpy= 0.685627

Thermal correction to Gibbs Free Energy= 0.550934

Sum of electronic and zero-point Energies= -3102.869860

Sum of electronic and thermal Energies= -3102.819858

Sum of electronic and thermal Enthalpies= -3102.818914

Sum of electronic and thermal Free Energies= -3102.953608

E(RB3LYP) = -3103.504542 A.U.

A-13a

0 1

Number of imaginary frequencies: 0

C	-1.98269100	-1.78302700	0.64833600
C	-3.25797800	-2.38748200	0.66072500
C	-3.58962400	-3.30514800	1.65420800
C	-2.68105600	-3.66838500	2.65537900
C	-1.41626400	-3.09162100	2.65685500
C	-1.06800900	-2.15420800	1.67150400
H	-3.96665600	-2.15851700	-0.12255700
H	-4.57670600	-3.75908800	1.63441900
H	-2.95500400	-4.39209400	3.41594900

H	-0.68569700	-3.34865800	3.41793000
C	2.81953500	0.83510900	2.32536100
C	4.05043100	1.34460800	2.72602200
C	5.02462200	0.49417700	3.25672400
C	4.76550200	-0.87489100	3.38513400
C	3.54620300	-1.39880800	2.96542100
C	2.56379900	-0.54456100	2.42263100
H	2.04914800	1.47532900	1.92315800
H	4.24012300	2.40781000	2.62054500
H	5.98253800	0.89539300	3.57441900
H	5.51856200	-1.53437900	3.80617000
H	3.34193800	-2.46181100	3.05215000
N	-1.50841100	-0.85477000	-0.27176900
S	-2.54238000	-0.04523900	-1.29479400
O	-3.40528100	-0.98707600	-2.04300700
O	-1.70672200	0.88450800	-2.06093200
C	-2.99416700	1.87412600	0.61380700
C	-3.80069600	2.60614200	1.47789100
C	-5.18322600	2.37107500	1.56213800
C	-5.74674500	1.38337200	0.74574700
C	-4.95610300	0.63740300	-0.12983300
C	-3.58724300	0.88848300	-0.18094200
H	-1.93176700	2.07388200	0.54300600
H	-3.35001300	3.38166100	2.09163300
H	-6.81635700	1.19585700	0.79108000
H	-5.38784900	-0.11978100	-0.77479900
C	1.31789800	-1.06601900	1.97677100

C	0.21685700	-1.52908800	1.66957200
C	-6.03188600	3.16516800	2.52569300
H	-5.84025500	2.85740100	3.56090300
H	-5.80773100	4.23516200	2.46167200
H	-7.09939500	3.02920100	2.33106900
Rh	0.60281200	-0.78598200	-0.55830400
C	2.22131500	-0.80957700	-2.19227100
C	2.53589800	-1.75636300	-1.18427900
C	1.43069100	-2.71046300	-1.10501400
C	0.45530600	-2.34013700	-2.08775200
C	0.90599500	-1.11673400	-2.72189100
C	0.26222100	-0.40856700	-3.86686000
H	0.31008800	0.67018800	-3.71613900
H	0.78925100	-0.67123000	-4.79403900
H	-0.78773700	-0.67964400	-3.96515300
C	3.11951200	0.27177500	-2.69000800
H	3.88431100	0.53065300	-1.95785100
H	3.62045200	-0.08652800	-3.59915900
H	2.55194200	1.16919100	-2.93201700
C	3.82438700	-1.82018700	-0.42763900
H	3.75038500	-2.47233500	0.44200500
H	4.61944900	-2.20756300	-1.07634000
H	4.12498500	-0.83143500	-0.07320600
C	1.38727700	-3.92702900	-0.23588100
H	0.35953100	-4.19112000	0.02031700
H	1.84460900	-4.77749300	-0.75578700
H	1.92887800	-3.76230600	0.69723700

C	-0.79556800	-3.09453800	-2.40510600
H	-0.57334400	-3.85614800	-3.16303500
H	-1.18873800	-3.59750100	-1.51934300
H	-1.58236200	-2.44058400	-2.78097400
S	0.67591200	2.56331500	-0.76398100
O	0.59009600	1.28587000	0.07202300
O	0.88649900	2.34213800	-2.20036900
C	2.32741400	3.23643800	-0.20492700
O	-0.29490800	3.56735800	-0.32747900
F	3.28904900	2.29581300	-0.33118900
F	2.29144800	3.61482600	1.08677600
F	2.67174000	4.29171800	-0.94600600

Zero-point correction= 0.569784 (Hartree/Particle)

Thermal correction to Energy= 0.614322

Thermal correction to Enthalpy= 0.615266

Thermal correction to Gibbs Free Energy= 0.490893

Sum of electronic and zero-point Energies= -2873.801906

Sum of electronic and thermal Energies= -2873.757369

Sum of electronic and thermal Enthalpies= -2873.756424

Sum of electronic and thermal Free Energies= -2873.880798

E(RB3LYP) = -2874.371691 A.U.

A-13c

0 1

Number of imaginary frequencies: 0

Rh	0.61620900	-1.24164600	-0.37620500
C	0.11719200	-2.26470800	-2.25082100
C	1.48426400	-1.84863000	-2.32742100

C	2.24722900	-2.64722700	-1.36072200
C	1.34913300	-3.45654600	-0.65198600
C	-0.00407800	-3.18258400	-1.14504000
C	-0.98263000	-1.87066800	-3.18841300
H	-0.83725700	-0.85829700	-3.57133600
H	-1.00003900	-2.55866200	-4.04246700
H	-1.95575900	-1.91332000	-2.69643400
C	2.08061200	-0.98958800	-3.39876300
H	2.43855800	-1.62197200	-4.22183500
H	1.34353800	-0.29417100	-3.80561700
H	2.91939200	-0.41111500	-3.01253500
C	3.73493900	-2.63462800	-1.18279100
H	4.15255200	-3.59438100	-1.51086900
H	4.20037100	-1.83003400	-1.74913200
H	4.00695700	-2.48350300	-0.13486100
C	1.71158400	-4.46882100	0.38786300
H	1.85742000	-5.44865100	-0.08632700
H	2.64581400	-4.19950000	0.88705700
H	0.92739100	-4.55839500	1.13938300
C	-1.22020800	-3.96968600	-0.77631500
H	-1.16182700	-4.96614700	-1.23455700
H	-1.27741200	-4.07082100	0.30725900
H	-2.13420400	-3.48580800	-1.12404500
C	-1.59559900	2.10741600	-1.88984700
C	-1.64253300	3.27534700	-2.63274200
C	-0.41625800	3.76916100	-3.09408000
C	0.77402100	3.09303000	-2.80125000

C	0.78781600	1.91451100	-2.04663400
C	-0.42201100	1.40842600	-1.56465600
H	-2.57684100	3.78792500	-2.83003500
H	-0.39438000	4.68058200	-3.68270800
H	1.71648000	3.48983300	-3.16637200
H	1.71912100	1.41033700	-1.84106600
C	-4.30626300	-1.08221700	-0.88282600
C	-5.18538000	-2.05478900	-0.41087100
C	-4.87012900	-2.78816700	0.73700900
C	-3.67277000	-2.53787400	1.41001300
C	-2.80205700	-1.55394400	0.94929200
C	-3.10042000	-0.81874200	-0.20584600
H	-4.55981700	-0.54806700	-1.79669400
H	-6.11139200	-2.24699900	-0.94480200
H	-5.55212300	-3.55313600	1.09656200
H	-3.38872400	-3.11489600	2.28389900
H	-1.87025900	-1.35926900	1.45611200
N	-2.69713700	1.42577800	-1.25807700
S	-3.44784800	2.61123000	0.25875600
O	-3.46637900	3.92924000	-0.37004600
O	-4.66350100	1.88882300	0.61580200
C	-2.28156000	1.40345700	2.37612400
C	-1.16986600	1.09764500	3.14319400
C	0.06522200	1.73108200	2.92568000
C	0.15055000	2.74185600	1.95261700
C	-0.94842700	3.08767100	1.18087400
C	-2.15540600	2.40571700	1.40410300

H	-3.21693500	0.87041400	2.49628900
H	-1.24439600	0.31963800	3.89467600
H	1.10077600	3.22740200	1.76916400
H	-0.87605600	3.84446900	0.40846100
C	-2.13887800	0.16665300	-0.70931600
C	-0.77603300	0.18539500	-0.80469100
C	1.29125300	1.27441100	3.65625100
H	1.98877500	2.09327600	3.83704400
H	1.04162500	0.79802700	4.60680700
H	1.78901700	0.53280500	3.02130100
H	-3.53602300	1.31632900	-1.83259600
O	-0.56515900	-3.28405000	2.21180500
C	0.11026800	-2.28708200	2.50186800
O	0.33658700	-1.25472000	1.75034500
C	0.73647800	-2.18294400	3.89380700
H	1.76218700	-1.81322200	3.82468500
H	0.17086800	-1.47220800	4.50529600
H	0.71140000	-3.15772200	4.38335700
S	3.37062800	0.56807900	0.21441800
O	1.86931300	0.51583500	0.37536100
O	4.11390600	-0.25507100	1.17670200
C	3.70489700	2.34136200	0.68929700
O	3.80755000	0.53329800	-1.19744200
F	3.47576600	2.55640400	1.99774600
F	2.90403000	3.16987000	-0.00997100
F	4.97564900	2.65609700	0.42710500

Zero-point correction= 0.636777 (Hartree/Particle)

Thermal correction to Energy= 0.685300

Thermal correction to Enthalpy= 0.686244

Thermal correction to Gibbs Free Energy= 0.557038

Sum of electronic and zero-point Energies= -3102.846720

Sum of electronic and thermal Energies= -3102.798197

Sum of electronic and thermal Enthalpies= -3102.797253

Sum of electronic and thermal Free Energies= -3102.926459

E(RB3LYP) = -3103.483497 A.U.

A-14

1 1

Number of imaginary frequencies: 0

C	-1.42979500	0.41373200	1.59182800
C	-2.65118800	0.38608200	2.28727000
C	-2.88570500	1.32374400	3.28924000
C	-1.93591400	2.29989300	3.62451700
C	-0.71555000	2.33073100	2.95990200
C	-0.45747700	1.38021300	1.96167000
H	-3.38858200	-0.37446700	2.07123800
H	-3.82588400	1.28545300	3.83076900
H	-2.14373200	3.01539400	4.41266800
H	0.04304800	3.06433500	3.21198400
C	2.80899500	2.37834600	-1.60973000
C	3.88570800	2.99735600	-2.23551500
C	4.97824400	3.43656300	-1.47988900
C	4.98792600	3.26970900	-0.09114400
C	3.91147700	2.66012200	0.54744700
C	2.81480400	2.20002100	-0.21143500

H	1.95613700	2.03072100	-2.18393700
H	3.87572700	3.14020700	-3.31131900
H	5.81827400	3.91641300	-1.97213600
H	5.83173500	3.62167100	0.49358700
H	3.90441200	2.53641000	1.62539600
N	-1.03562100	-0.40140300	0.52503400
S	-2.18233100	-1.36562600	-0.28677900
O	-2.77690700	-2.33964100	0.64092700
O	-1.48248600	-1.83955800	-1.48917300
C	-3.07214500	0.89461100	-1.57983000
C	-4.05948400	1.78530700	-1.98627100
C	-5.40375100	1.59577600	-1.62328100
C	-5.73494600	0.48610100	-0.83336400
C	-4.75947900	-0.41426900	-0.40834900
C	-3.43471700	-0.19591200	-0.78476300
H	-2.03655500	1.04399200	-1.86673600
H	-3.78783100	2.64162800	-2.59714100
H	-6.76953500	0.32381900	-0.54519900
H	-5.01360200	-1.27274300	0.20383100
C	1.69755100	1.59223400	0.43784100
C	0.74657400	1.31983100	1.20380300
C	-6.46795200	2.55166500	-2.10041700
H	-6.08919700	3.57615200	-2.15894200
H	-6.81119200	2.27289600	-3.10403900
H	-7.34032600	2.54442000	-1.44175000
Rh	0.95635400	-0.56724500	0.10130600
C	1.75212400	-2.27174800	-1.29452000

C	2.84773800	-1.40546100	-0.89313900
C	2.94710700	-1.43996900	0.53070000
C	1.86831500	-2.27633500	1.02727400
C	1.16585100	-2.82404000	-0.12040700
C	0.13294100	-3.90100000	-0.04594800
H	-0.40831600	-4.00492000	-0.98352600
H	0.63951800	-4.84700300	0.18409600
H	-0.60243700	-3.71205100	0.73825400
C	1.34220600	-2.56197500	-2.69801700
H	1.67259200	-1.77866800	-3.38279200
H	1.79695300	-3.50566500	-3.02616300
H	0.25845200	-2.65700800	-2.76832600
C	3.80509100	-0.74895100	-1.83498800
H	4.38996800	0.03029600	-1.34738400
H	4.49956600	-1.50264400	-2.22604000
H	3.29039000	-0.30089900	-2.68723300
C	4.00732000	-0.80994400	1.37408300
H	3.61617700	-0.51204100	2.34932500
H	4.81348100	-1.53369900	1.54443900
H	4.44003900	0.06786400	0.89346300
C	1.62207100	-2.65316800	2.45030700
H	2.19716000	-3.55500400	2.69784700
H	1.92966000	-1.86060600	3.13521900
H	0.56611400	-2.87035300	2.62173700

Zero-point correction= 0.540182 (Hartree/Particle)

Thermal correction to Energy= 0.576278

Thermal correction to Enthalpy= 0.577222

Thermal correction to Gibbs Free Energy= 0.471017

Sum of electronic and zero-point Energies= -1912.177155

Sum of electronic and thermal Energies= -1912.141060

Sum of electronic and thermal Enthalpies= -1912.140115

Sum of electronic and thermal Free Energies= -1912.246320

E(RB3LYP) = -1912.717337 A.U.

A-15

1 1

Number of imaginary frequencies: 0

Rh	1.95849800	-0.07064500	-0.29696800
C	3.41680900	-1.57715400	0.28259500
C	3.32642000	-1.51922600	-1.14635800
C	3.77690200	-0.19159900	-1.56252700
C	4.19953000	0.53205500	-0.40098200
C	3.93704500	-0.28843900	0.73557400
C	3.13043300	-2.76612600	1.14448600
H	2.28490900	-3.34138700	0.76038600
H	4.00592900	-3.42552000	1.18219600
H	2.89185200	-2.46806800	2.16713800
C	2.98932000	-2.64271100	-2.07480000
H	3.90936700	-3.04027100	-2.52064200
H	2.49414400	-3.45918800	-1.54833200
H	2.33988500	-2.31249000	-2.88850400
C	3.86704000	0.26579500	-2.98205900
H	4.82882400	-0.04228500	-3.41160200
H	3.07575500	-0.17535100	-3.59210900
H	3.79946300	1.35236900	-3.06236200

C	4.76608900	1.91826500	-0.36040800
H	5.83827800	1.88585100	-0.13669400
H	4.64015000	2.43128000	-1.31516000
H	4.27985800	2.52574200	0.40800700
C	4.17865700	0.09223000	2.15979800
H	5.18458100	-0.22275700	2.46499900
H	4.11071800	1.17302400	2.30021700
H	3.46388200	-0.38905800	2.83095200
C	-1.67211000	-1.61785200	1.03272000
C	-2.57780000	-2.55276000	1.53014300
C	-2.42343700	-3.87545200	1.10925800
C	-1.39705000	-4.25740700	0.22931400
C	-0.49048400	-3.31753700	-0.25183700
C	-0.62558900	-1.98082500	0.14621800
H	-3.35343500	-2.26992300	2.22962200
H	-3.11154700	-4.62724300	1.48267000
H	-1.31157000	-5.29634700	-0.07260700
H	0.29693300	-3.60230900	-0.94158300
C	0.34798200	2.35741100	1.70714700
C	1.12825700	3.49753100	1.63867400
C	1.71467900	3.90942700	0.42259800
C	1.49343800	3.18083500	-0.73310300
C	0.70264900	2.01085200	-0.69342500
C	0.13192400	1.58093700	0.54274100
H	-0.09766700	2.04281300	2.64178900
H	1.29491100	4.08255200	2.53793200
H	2.31306800	4.81454900	0.39243700

H	1.90036800	3.51277600	-1.68307200
H	0.36045000	1.56187500	-1.62055300
N	-1.56677100	-0.21977100	1.30266600
S	-2.99240000	0.75060500	1.68557500
O	-3.70288000	-0.00737500	2.70652800
O	-2.47402400	2.09358000	1.91771000
C	-3.58257500	1.65992500	-0.82845400
C	-4.26344300	1.60552300	-2.04071500
C	-5.23996600	0.62547500	-2.28321600
C	-5.52899000	-0.30193500	-1.27049100
C	-4.86097600	-0.26913500	-0.04943100
C	-3.89119600	0.71508200	0.15456800
H	-2.84753600	2.43306100	-0.63167400
H	-4.04579000	2.34362600	-2.80732900
H	-6.29408100	-1.05451400	-1.43706100
H	-5.09711500	-0.97535900	0.73777300
C	-0.50327100	0.25874700	0.54325100
C	0.13066600	-0.78695300	-0.14092000
C	-5.95232600	0.56035300	-3.61044400
H	-6.96991600	0.17602500	-3.50017400
H	-6.00570200	1.54297300	-4.08670200
H	-5.42213600	-0.11034600	-4.29765300

Zero-point correction= 0.541629 (Hartree/Particle)

Thermal correction to Energy= 0.577390

Thermal correction to Enthalpy= 0.578334

Thermal correction to Gibbs Free Energy= 0.470129

Sum of electronic and zero-point Energies= -1912.190395

Sum of electronic and thermal Energies= -1912.154633

Sum of electronic and thermal Enthalpies= -1912.153689

Sum of electronic and thermal Free Energies= -1912.261895

E(RB3LYP) = -1912.732024 A.U.

A-TSa1

1 1

Number of imaginary frequencies: 1

Rh	-0.65501400	-0.03393500	0.05577500
C	-2.49960400	-0.79061600	-0.89635300
C	-2.01424000	-1.82550400	-0.03254000
C	-1.95612800	-1.30785400	1.31318600
C	-2.49844800	0.03966900	1.28770800
C	-2.80607600	0.36986400	-0.06646000
O	-0.18067000	1.34684600	-1.50623600
C	-0.00238000	2.55100000	-1.12101000
O	0.04764200	2.88528200	0.10001000
C	0.16444600	3.61695700	-2.17416200
H	-0.02390700	3.21762900	-3.17023200
H	-0.51315400	4.44703400	-1.95862200
H	1.18493400	4.00792400	-2.11976600
C	1.37262100	-1.74635600	-1.44121700
C	2.33765600	-0.36308000	0.17942100
C	3.64965600	-0.74412000	-0.23960800
C	3.76575600	-1.68645500	-1.29025200
C	2.63183600	-2.18870800	-1.88882200
H	0.46463800	-2.09763400	-1.91689400
C	2.15406100	0.57845400	1.22889800

C	4.77092300	-0.14367700	0.38953000
H	4.75312200	-1.99447400	-1.62198500
H	2.68562100	-2.90124900	-2.70390300
C	4.58288000	0.79520500	1.37783100
C	3.27816700	1.15189000	1.79454600
H	5.76882100	-0.42437900	0.06709100
H	5.43820900	1.26690700	1.85065100
H	3.15675400	1.88629200	2.58552700
N	1.22596800	-0.88110800	-0.44548900
C	0.75867600	0.88947900	1.67659000
H	0.16544900	1.73742500	0.79771700
H	0.35185800	0.07726900	2.28416200
H	0.73479200	1.76618000	2.33579300
C	-2.71826600	-0.85557900	-2.37465600
H	-2.30218300	0.03085500	-2.86100700
H	-2.24755100	-1.73558400	-2.81657500
H	-3.78982300	-0.89727800	-2.60101100
C	-1.63531100	-3.21835800	-0.42235800
H	-1.53468400	-3.33073600	-1.50294300
H	-0.69930000	-3.52691600	0.04979100
H	-2.41655600	-3.91215800	-0.09038400
C	-1.58575100	-2.09098500	2.53442700
H	-1.21720300	-1.44370000	3.33346700
H	-2.46044600	-2.62584700	2.92348200
H	-0.81259300	-2.83052500	2.31416900
C	-2.69173000	0.92660900	2.47656700
H	-1.96719600	0.70938000	3.26381300

H	-2.59913300	1.98072800	2.20821400
H	-3.69357500	0.77039500	2.89372500
C	-3.37405600	1.65791200	-0.57220700
H	-2.98611600	1.88604800	-1.56710900
H	-4.46592300	1.58940200	-0.64122500
H	-3.12489600	2.49035300	0.08807600

Zero-point correction= 0.436343 (Hartree/Particle)

Thermal correction to Energy= 0.463771

Thermal correction to Enthalpy= 0.464715

Thermal correction to Gibbs Free Energy= 0.378328

Sum of electronic and zero-point Energies= -1168.831937

Sum of electronic and thermal Energies= -1168.804509

Sum of electronic and thermal Enthalpies= -1168.803565

Sum of electronic and thermal Free Energies= -1168.889952

E(RB3LYP) = -1169.268280 A.U.

A-TSb1

1 1

Number of imaginary frequencies: 1

Rh	-0.78176600	-0.02827800	0.00527000
C	-2.62161900	-1.23128000	0.05719200
C	-1.64876500	-1.87118600	-0.80595500
C	-0.50871500	-2.23216300	0.00530300
C	-0.74358400	-1.76075800	1.34034700
C	-2.07110500	-1.16374800	1.37809500
O	-1.67350600	1.49666700	-1.19341800
C	-1.85716000	2.67108700	-0.73234000
O	-1.33888500	3.09867100	0.34843400

C	-2.72735700	3.61746200	-1.51870700
H	-3.24655100	3.09444600	-2.32132000
H	-3.44036800	4.10099800	-0.84637000
H	-2.09431200	4.40361500	-1.94197200
C	0.62664100	1.47823200	0.89995700
C	2.42959400	0.49510500	-0.28479600
C	3.31566800	0.78473200	0.80293000
C	2.78487100	1.44123900	1.94710600
C	1.45322500	1.79027800	2.00924000
H	-0.49877900	2.21243600	0.72177200
C	2.89420900	-0.15013600	-1.46536100
C	4.67302800	0.38974300	0.70211500
H	3.45078300	1.65816200	2.77867200
H	1.03743400	2.29970400	2.87135200
C	5.11220200	-0.26107600	-0.42934500
C	4.22735500	-0.52178800	-1.50316300
H	5.35247900	0.61019200	1.51985800
H	6.15004900	-0.56729600	-0.51230600
H	4.61241800	-1.01213700	-2.39268300
N	1.11891700	0.86490900	-0.16731600
C	1.97194700	-0.35119500	-2.63854700
H	1.63454100	0.61352500	-3.03229800
H	2.47327600	-0.89581700	-3.44154000
H	1.06866700	-0.89801600	-2.35688200
C	-3.94709700	-0.71273100	-0.40230000
H	-4.58093600	-1.54197300	-0.73434100
H	-4.47104500	-0.18169200	0.39334900

H	-3.81390300	-0.02538600	-1.24289700
C	-1.85393400	-2.17345700	-2.25503100
H	-2.38322400	-3.12769900	-2.36849300
H	-2.45364000	-1.39680000	-2.73406600
H	-0.90647700	-2.25000500	-2.79195200
C	0.71014000	-2.97659000	-0.44057900
H	0.70914900	-3.97654400	0.00832100
H	0.74004800	-3.09605300	-1.52369100
H	1.62773900	-2.47188500	-0.12681800
C	0.17634400	-1.94630500	2.50609900
H	-0.04684000	-2.88989000	3.01797800
H	1.21953500	-1.97675300	2.18395100
H	0.06988700	-1.13741400	3.23144900
C	-2.73457100	-0.59966800	2.59317300
H	-3.44306500	0.18945700	2.33516700
H	-3.28510800	-1.39093200	3.11664500
H	-2.00350200	-0.18559700	3.29042700

Zero-point correction= 0.434851 (Hartree/Particle)

Thermal correction to Energy= 0.463291

Thermal correction to Enthalpy= 0.464235

Thermal correction to Gibbs Free Energy= 0.375345

Sum of electronic and zero-point Energies= -1168.818579

Sum of electronic and thermal Energies= -1168.790139

Sum of electronic and thermal Enthalpies= -1168.789195

Sum of electronic and thermal Free Energies= -1168.878085

E(RB3LYP) = -1169.253429 A.U.

A-TSc1

1 1

Number of imaginary frequencies: 1

Rh	-0.74041300	-0.04093100	0.16513800
C	-2.59449800	0.14721600	-1.04672000
C	-2.01080600	-1.12704200	-1.31375900
C	-1.92166700	-1.85636000	-0.06473600
C	-2.56080000	-1.04780200	0.96207600
C	-2.93779600	0.19236700	0.37120700
O	1.81301200	2.48073300	0.32839900
C	0.64713200	2.79516500	0.43671100
O	-0.29944100	1.98512100	0.97343200
C	0.07501000	4.12972400	0.01165500
H	0.86882700	4.76831200	-0.37520100
H	-0.68753700	3.97405600	-0.75900000
H	-0.41560000	4.61334600	0.86108200
C	1.28801500	0.04633500	-2.10365700
C	2.23109500	-0.42492600	-0.01485300
C	3.52606000	-0.55474700	-0.60242200
C	3.64653900	-0.36973700	-1.99980200
C	2.53345100	-0.05624800	-2.74849000
H	0.39635600	0.29553600	-2.66671800
C	2.05761600	-0.52714500	1.38854700
C	4.63503100	-0.82580700	0.23979200
H	4.62309700	-0.46026800	-2.46655900
H	2.59446100	0.11609400	-3.81682200
C	4.45608500	-0.93076100	1.59971700
C	3.17059400	-0.76951800	2.17013100

H	5.62067100	-0.92708100	-0.20379400
H	5.30428000	-1.12514900	2.24798200
H	3.05887600	-0.82807700	3.24912700
N	1.13299400	-0.14976600	-0.79940700
C	0.68272900	-0.31505200	1.95883500
H	0.20168200	0.90169700	1.53292900
H	0.15991900	-1.25811300	2.14503400
H	0.71929200	0.17172000	2.94413100
C	-2.88535500	1.24345500	-2.02153100
H	-2.73040900	2.22273800	-1.56163800
H	-2.25311200	1.17842800	-2.90936700
H	-3.93036700	1.19266700	-2.35039700
C	-1.58888000	-1.66471000	-2.64355000
H	-1.52973500	-0.88322800	-3.40275600
H	-0.62214200	-2.17035000	-2.58684300
H	-2.32774000	-2.39947000	-2.98421700
C	-1.44317800	-3.26526100	0.09135700
H	-1.04444400	-3.44547500	1.09206200
H	-2.27161900	-3.96641700	-0.06742200
H	-0.66037700	-3.50130400	-0.63235700
C	-2.78249800	-1.46071100	2.38297300
H	-2.02304100	-2.16818400	2.72198100
H	-2.77705400	-0.60355000	3.05859900
H	-3.75647300	-1.95616400	2.47302700
C	-3.56633500	1.37160000	1.04287000
H	-2.90801000	2.24307000	0.96840800
H	-4.51874400	1.61680200	0.56099600

H	-3.75723500	1.18160200	2.09963600

Zero-point correction= 0.435350 (Hartree/Particle)

Thermal correction to Energy= 0.463028

Thermal correction to Enthalpy= 0.463973

Thermal correction to Gibbs Free Energy= 0.377013

Sum of electronic and zero-point Energies= -1168.804986

Sum of electronic and thermal Energies= -1168.777308

Sum of electronic and thermal Enthalpies= -1168.776364

Sum of electronic and thermal Free Energies= -1168.863323

E(RB3LYP) = -1169.240336 A.U.

A-TSd1

1 1

Number of imaginary frequencies: 1

Rh	-0.68104500	-0.07299500	-0.05438000
C	-2.28797100	-1.60988000	-0.16434400
C	-1.01318200	-2.26322600	-0.31120500
C	-0.22857800	-1.98080900	0.86810700
C	-1.05405200	-1.20114600	1.76719200
C	-2.32462600	-0.96228000	1.12284700
O	-3.66638100	1.59139300	-0.99546000
C	-2.67175600	2.28484100	-1.05036600
O	-1.43145300	1.74719800	-1.11288000
C	-2.67890700	3.79450200	-1.08382000
H	-3.70293700	4.16130400	-1.02407100
H	-2.09215800	4.19103800	-0.24758300
H	-2.20800200	4.14548100	-2.00665300
C	0.62589000	1.76551800	0.33162900

C	2.52341900	0.52391600	-0.39326500
C	3.33932000	1.19785800	0.57229600
C	2.72986500	2.16918700	1.41680300
C	1.39062500	2.46419900	1.30328400
H	-0.59311300	2.12189700	-0.38277500
C	3.08278000	-0.42446700	-1.29428000
C	4.71289900	0.86598000	0.65854300
H	3.34836000	2.67841500	2.15195700
H	0.92221300	3.21646700	1.92819400
C	5.24163100	-0.08421300	-0.18820800
C	4.43116000	-0.71326500	-1.16083700
H	5.33637900	1.37179100	1.38954700
H	6.29376400	-0.34301500	-0.12628100
H	4.88526700	-1.43038400	-1.83871400
N	1.18694700	0.82941500	-0.43006200
C	2.25198600	-1.01639900	-2.40132900
H	2.03419800	-0.25685100	-3.16085000
H	2.77615200	-1.84194100	-2.88815700
H	1.28741300	-1.37495100	-2.04149600
C	-3.40921400	-1.64684200	-1.14930000
H	-4.15588200	-2.37876000	-0.81636100
H	-3.88436000	-0.66817400	-1.22531000
H	-3.06259600	-1.94584000	-2.13988800
C	-0.62502400	-3.14201900	-1.45593000
H	-1.19513400	-4.07742300	-1.39970700
H	-0.85344700	-2.67738400	-2.41848700
H	0.43482600	-3.39670400	-1.43499600

C	1.15036200	-2.48769800	1.15252000
H	1.09938500	-3.49286600	1.58675500
H	1.75196000	-2.54016100	0.24299100
H	1.67414900	-1.84150400	1.85938400
C	-0.66164700	-0.74226700	3.13313000
H	-0.90665800	-1.52323400	3.86370200
H	0.41038000	-0.54648100	3.19937600
H	-1.19695500	0.16415800	3.42031100
C	-3.50122800	-0.24666800	1.70350400
H	-4.04856800	0.29097000	0.92871700
H	-4.17760800	-0.97278800	2.17146700
H	-3.19846900	0.46815400	2.47137300

Zero-point correction= 0.434674 (Hartree/Particle)

Thermal correction to Energy= 0.463077

Thermal correction to Enthalpy= 0.464021

Thermal correction to Gibbs Free Energy= 0.376040

Sum of electronic and zero-point Energies= -1168.789731

Sum of electronic and thermal Energies= -1168.761328

Sum of electronic and thermal Enthalpies= -1168.760384

Sum of electronic and thermal Free Energies= -1168.848364

E(RB3LYP) = -1169.224405 A.U.

A-TSe1

1 1

Number of imaginary frequencies: 1

Rh	1.16453600	0.07448600	0.07794900
C	2.66172300	-1.53400300	0.49750800
C	1.29755000	-1.95148500	0.87299400

C	0.49548000	-1.99541300	-0.30547100
C	1.32070100	-1.50891000	-1.38927800
C	2.67784900	-1.28487800	-0.89214200
O	0.36996000	3.15190300	0.64675700
C	1.59006800	3.02128600	0.34858300
O	2.14430300	1.89426900	0.07408400
C	2.47229000	4.24080600	0.30569600
H	1.89882800	5.13947500	0.52811700
H	3.28177800	4.12016800	1.03145000
H	2.93040800	4.31664900	-0.68440900
C	-5.14408200	0.02030700	-1.25792000
C	-3.07585000	0.41817000	-0.33372700
C	-3.49721700	-0.06200300	0.94568600
C	-4.83814100	-0.50608300	1.06942600
C	-5.66374000	-0.46500700	-0.02985200
H	-5.78426100	0.05374700	-2.13769700
C	-1.72998000	0.87137300	-0.51430000
C	-2.57867100	-0.06666300	2.03446400
H	-5.19633300	-0.86944900	2.02873600
H	-6.69606700	-0.79407300	0.02657900
C	-1.29066300	0.36170500	1.84241200
C	-0.83123100	0.82428300	0.56162800
H	-2.92074400	-0.39555300	3.01245700
H	-0.60343100	0.38118400	2.68439000
H	-0.17378900	2.00080700	0.61916700
N	-3.90661100	0.44705200	-1.41495400
C	3.80072700	-1.41351500	1.45481300

H	4.60506600	-0.79756200	1.05100400
H	3.47755500	-0.97763600	2.40358300
H	4.20801300	-2.40877100	1.67182600
C	0.88156400	-2.36868500	2.24378300
H	1.38079400	-1.77475000	3.01292900
H	-0.19652500	-2.27514100	2.37798000
H	1.15948100	-3.41823100	2.40417200
C	-0.92029200	-2.46865500	-0.40323600
H	-1.42921300	-2.03791000	-1.26620800
H	-0.94077600	-3.55970200	-0.50440700
H	-1.49043100	-2.19484400	0.48616300
C	0.90906300	-1.37305000	-2.81485500
H	-0.17181100	-1.27863400	-2.91829000
H	1.38406900	-0.51106200	-3.28864300
H	1.22588000	-2.26908800	-3.36465900
C	3.83380100	-0.83498600	-1.72654300
H	4.61830600	-0.38551100	-1.11632600
H	4.26537200	-1.68802800	-2.26339200
H	3.52232200	-0.09735200	-2.47002600
C	-1.33421700	1.43143200	-1.85460900
H	-1.45792100	0.68846900	-2.64811500
H	-1.99011500	2.26426800	-2.12524000
H	-0.29879100	1.78178300	-1.85126300

Zero-point correction= 0.433880 (Hartree/Particle)

Thermal correction to Energy= 0.462580

Thermal correction to Enthalpy= 0.463525

Thermal correction to Gibbs Free Energy= 0.372751

Sum of electronic and zero-point Energies= -1168.802838

Sum of electronic and thermal Energies= -1168.774137

Sum of electronic and thermal Enthalpies= -1168.773193

Sum of electronic and thermal Free Energies= -1168.863967

E(RB3LYP) = -1169.236718 A.U.

A-TSf1

1 1

Number of imaginary frequencies: 1

Rh	-1.10050800	-0.11934800	-0.40679500
C	-2.88139100	-1.51804100	-0.22712200
C	-1.59342400	-2.18099900	0.05545000
C	-1.01900600	-1.57253700	1.20771600
C	-1.88453800	-0.45765300	1.57007900
C	-3.06504500	-0.48209500	0.70746600
O	-0.93483100	1.81032500	-1.34786300
C	-1.31952800	2.94218600	-0.67199600
O	-1.91082600	2.87707200	0.38331800
C	-0.93083900	4.20766000	-1.38448400
H	0.15918500	4.24990800	-1.48184500
H	-1.34416700	4.20344600	-2.39703400
H	-1.28986000	5.07394800	-0.83014400
C	5.33173000	0.35288600	1.20587100
C	3.24773200	0.28926700	0.23574000
C	3.70958600	-0.55117000	-0.82480300
C	5.07757600	-0.92637200	-0.81518900
C	5.89022000	-0.47637000	0.19845700
H	5.96282200	0.71665200	2.01477000

C	1.87029200	0.68269500	0.28648500
C	2.80614400	-0.96451400	-1.84349700
H	5.46508900	-1.56005100	-1.60810000
H	6.94186500	-0.74012200	0.23865900
C	1.49481900	-0.56620000	-1.79487600
C	1.00187100	0.25214000	-0.72322200
H	3.17417100	-1.57935800	-2.66054700
H	0.82255400	-0.86136100	-2.59824200
H	0.15291900	1.36034000	-1.13761800
N	4.06826300	0.72722500	1.23272300
C	-3.79053700	-1.90501100	-1.34632300
H	-4.55033600	-1.14579300	-1.53428400
H	-3.23306600	-2.07133900	-2.27275100
H	-4.29922400	-2.84561000	-1.10152600
C	-1.05981200	-3.36354400	-0.68582300
H	-1.32389800	-3.32448900	-1.74514600
H	0.02667700	-3.42737100	-0.60451500
H	-1.48769500	-4.28528000	-0.27220400
C	0.22255400	-1.99824500	1.92422200
H	0.72046800	-1.15188400	2.39853900
H	-0.03370200	-2.72366400	2.70533600
H	0.93412100	-2.46778200	1.24305900
C	-1.71892800	0.46652700	2.72491300
H	-0.71409800	0.42456000	3.14372000
H	-1.93989900	1.49337300	2.42467300
H	-2.43138400	0.18175800	3.51038200
C	-4.21476100	0.46587800	0.82844800

H	-4.85518100	0.43920600	-0.05437700
H	-4.82670800	0.19678600	1.69775300
H	-3.85638600	1.48782000	0.96389300
C	1.42915400	1.58321200	1.40919000
H	1.60329100	1.11066600	2.38144500
H	2.03385900	2.49504800	1.42234100
H	0.37564700	1.85330000	1.32660500

Zero-point correction= 0.433968 (Hartree/Particle)

Thermal correction to Energy= 0.462334

Thermal correction to Enthalpy= 0.463278

Thermal correction to Gibbs Free Energy= 0.375117

Sum of electronic and zero-point Energies= -1168.775394

Sum of electronic and thermal Energies= -1168.747028

Sum of electronic and thermal Enthalpies= -1168.746084

Sum of electronic and thermal Free Energies= -1168.834245

E(RB3LYP) = -1169.209362 A.U.

A-TSa2

1 1

Number of imaginary frequencies: 1

C	-0.76446600	2.54576500	1.75895400
C	-0.96389600	3.72527900	2.46590000
C	0.10489700	4.62071500	2.57616200
C	1.32769500	4.33339200	1.96645800
C	1.51016100	3.14536100	1.25391200
C	0.46411000	2.22831800	1.14614100
H	-1.93326000	3.94933000	2.89745400
H	-0.02575400	5.54527200	3.12864000

H	2.14788400	5.03997900	2.04655200
H	2.45719800	2.92924700	0.77902800
C	-1.71612300	-1.59340900	-0.71414900
C	-2.36541500	-2.82396000	-0.76296000
C	-2.63925800	-3.52016200	0.41747900
C	-2.25157500	-2.98805900	1.65080500
C	-1.58696100	-1.76624600	1.70406300
C	-1.31384100	-1.05421200	0.52013700
H	-1.51138900	-1.03758800	-1.61984100
H	-2.67237000	-3.23315800	-1.72055400
H	-3.15163600	-4.47674900	0.37689800
H	-2.45476200	-3.53293200	2.56739400
H	-1.25357900	-1.36247300	2.65517500
N	-1.79232900	1.56736300	1.50011200
S	-3.05145200	2.28885400	0.41515600
O	-3.89735100	3.08088800	1.30728900
O	-2.29459000	2.88121500	-0.68400000
C	-3.98993300	0.64365000	-1.54540100
C	-4.73637800	-0.43475900	-2.01618100
C	-5.41243700	-1.28819400	-1.13474000
C	-5.35189700	-1.02078200	0.24382600
C	-4.63692400	0.06428900	0.73446300
C	-3.94473800	0.87455600	-0.17040800
H	-3.45660900	1.29975000	-2.22354300
H	-4.78901400	-0.61789200	-3.08538200
H	-5.88168900	-1.66726000	0.93707800
H	-4.62986200	0.28089200	1.79783200

C	-0.60418000	0.19417400	0.59039200
C	0.47827200	0.90807100	0.50548800
C	-6.17176000	-2.48842100	-1.63788100
H	-5.62699800	-3.40966200	-1.39743400
H	-7.15578400	-2.56357200	-1.16525100
H	-6.31376800	-2.45541100	-2.72063500
H	-2.26929600	1.24134800	2.34305700
C	3.34614100	1.03631100	-2.17433000
C	3.18587700	-0.32945400	-2.56972500
C	1.79836600	-0.51070200	-2.99059000
C	1.10999100	0.69776000	-2.78335700
C	2.05108100	1.65730700	-2.21483500
C	4.63193200	1.71250300	-1.80925300
H	5.34742200	1.01451600	-1.36879200
H	5.09845000	2.14528400	-2.70201600
H	4.46961200	2.52204600	-1.09368700
C	4.27440000	-1.35053900	-2.71343200
H	4.65802200	-1.37648500	-3.74088900
H	5.11515900	-1.13088600	-2.05139200
H	3.91569700	-2.35422100	-2.46893500
C	1.24631600	-1.76050600	-3.60744800
H	1.34666600	-1.72470200	-4.69891400
H	1.78386000	-2.64949900	-3.26855100
H	0.18490500	-1.89334600	-3.37998000
C	-0.31639200	1.02411700	-3.10585800
H	-0.83243200	1.45799800	-2.24323700
H	-0.36476800	1.76277600	-3.91503800

H	-0.86807100	0.14142500	-3.43908000
C	1.74026200	3.11580500	-2.05794000
H	1.70436300	3.59338100	-3.04518500
H	0.77110200	3.27120900	-1.57825700
H	2.49696300	3.63633400	-1.46923400
Rh	1.96554100	0.02987400	-0.69139300
C	1.19426400	-2.96590600	-0.20459300
C	2.21015100	-1.86761100	1.57562100
C	1.93513200	-2.94696400	2.46261000
C	1.30057500	-4.09218600	1.92019400
C	0.95481900	-4.10862100	0.58714500
H	0.86229500	-2.93076200	-1.23397900
C	2.91606800	-0.71299600	1.99715600
C	2.29847100	-2.79890100	3.82702800
H	1.09022700	-4.94307000	2.56206900
H	0.46652400	-4.96632500	0.13924200
C	2.90949400	-1.63821600	4.25206700
C	3.22985700	-0.60146500	3.33972900
H	2.08378400	-3.60407500	4.52334300
H	3.17574400	-1.52167000	5.29823300
H	3.75607800	0.27979500	3.69546100
N	1.78574100	-1.87787900	0.26956000
C	3.30416900	0.24470600	0.91796400
H	3.41767300	1.25973200	1.29771000
H	4.25897000	-0.06657900	0.47710600

Zero-point correction= 0.706744 (Hartree/Particle)

Thermal correction to Energy= 0.750934

Thermal correction to Enthalpy= 0.751878

Thermal correction to Gibbs Free Energy= 0.628744

Sum of electronic and zero-point Energies= -2353.293905

Sum of electronic and thermal Energies= -2353.249714

Sum of electronic and thermal Enthalpies= -2353.248770

Sum of electronic and thermal Free Energies= -2353.371905

E(RB3LYP) = -2354.000649 A.U.

A-TSb2

1 1

Number of imaginary frequencies: 1

C	-1.52818500	2.82834100	1.54763900
C	-2.01040700	3.96152400	2.16803600
C	-1.01494600	4.88028100	2.53853300
C	0.34306400	4.63496900	2.27780400
C	0.79162900	3.47245800	1.63534200
C	-0.19315700	2.56123300	1.26123600
H	-3.06430300	4.14160000	2.33935800
H	-1.30223400	5.80237300	3.03247300
H	1.07347700	5.37784700	2.58318800
H	1.84256900	3.30522000	1.44289500
C	-0.77272600	-1.74341400	-1.31955900
C	-1.47822400	-2.93380400	-1.47231400
C	-2.18818300	-3.47741100	-0.39717500
C	-2.19242000	-2.81292900	0.82985400
C	-1.49227200	-1.61519300	0.98201700
C	-0.77084700	-1.05860900	-0.09057800
H	-0.19933900	-1.33718400	-2.14393600

H	-1.46658800	-3.44605700	-2.43040100
H	-2.72401200	-4.41463100	-0.51336600
H	-2.72884800	-3.23265700	1.67571400
H	-1.44643100	-1.13464600	1.95569700
N	-2.09139000	1.60964800	0.96275200
S	-3.20395700	1.96171300	-0.48741400
O	-4.02129100	3.07024300	-0.00576100
O	-2.29961900	2.07994400	-1.62355100
C	-5.18167000	0.29298600	0.37244600
C	-5.92575800	-0.88083300	0.31311700
C	-5.67271200	-1.84968400	-0.67127800
C	-4.65585000	-1.61233100	-1.60895800
C	-3.88492100	-0.45690700	-1.56269700
C	-4.15839400	0.47899700	-0.56374800
H	-5.40550800	1.05876000	1.10815600
H	-6.72396400	-1.04201800	1.03127400
H	-4.45623400	-2.35042000	-2.37894300
H	-3.08858400	-0.28065600	-2.27451600
C	0.05225400	0.14331200	0.12290300
C	-0.41150600	1.25375800	0.65418700
C	-6.45497600	-3.13639400	-0.71409200
H	-6.73231300	-3.39860000	-1.73941600
H	-5.84702100	-3.96086900	-0.32174900
H	-7.36649800	-3.07971200	-0.11463600
H	-2.58482000	0.97477900	1.59763700
C	3.53209600	1.62435800	-1.27011000
C	3.89823900	0.33498300	-1.75625000

C	2.83506200	-0.12128100	-2.64926800
C	1.81158900	0.84376000	-2.65220200
C	2.20285400	1.91288300	-1.74407700
C	4.39127800	2.53463300	-0.44684000
H	5.03363900	1.97845900	0.24035900
H	5.04249500	3.13097100	-1.09677400
H	3.79112500	3.23047000	0.14366300
C	5.20975000	-0.36220300	-1.54744100
H	5.90046100	-0.16231100	-2.37607000
H	5.69404900	-0.03117600	-0.62572700
H	5.07996500	-1.44609900	-1.48063600
C	2.89498600	-1.36476100	-3.48387500
H	3.36826500	-1.15300200	-4.45036200
H	3.49036600	-2.14570500	-3.00410000
H	1.89926400	-1.76754400	-3.69059800
C	0.56522200	0.87578000	-3.48534800
H	-0.31209200	1.13730300	-2.88697300
H	0.65787300	1.63492900	-4.27190300
H	0.37892300	-0.08052500	-3.98041800
C	1.47303900	3.22095100	-1.67095800
H	1.61009900	3.77198200	-2.61009900
H	0.39914800	3.07454300	-1.53142900
H	1.83889500	3.85520700	-0.86365400
Rh	2.05884700	0.10647800	-0.42188200
C	2.00468900	-3.01382300	-0.41651900
C	2.09300100	-1.99747400	1.67322200
C	1.86481900	-3.23610400	2.33791300

C	1.74818100	-4.39870900	1.53517100
C	1.83475200	-4.28824500	0.16586400
H	2.01111800	-2.89784300	-1.49274700
C	2.25278800	-0.78420100	2.38707400
C	1.73885500	-3.22540300	3.75094100
H	1.58420000	-5.36263800	2.00859700
H	1.74633200	-5.15515600	-0.47929900
C	1.83458900	-2.03448200	4.43926300
C	2.09579500	-0.81787100	3.76180500
H	1.55563200	-4.15943100	4.27367100
H	1.72568400	-2.02569900	5.51961400
H	2.19858000	0.10040200	4.33356300
N	2.12433500	-1.90769800	0.30269200
C	2.61278800	0.42401800	1.58055500
H	2.20960800	1.32851600	2.03469500
H	3.70390000	0.52422000	1.52707800

Zero-point correction= 0.706205 (Hartree/Particle)

Thermal correction to Energy= 0.750571

Thermal correction to Enthalpy= 0.751516

Thermal correction to Gibbs Free Energy= 0.627394

Sum of electronic and zero-point Energies= -2353.269001

Sum of electronic and thermal Energies= -2353.224635

Sum of electronic and thermal Enthalpies= -2353.223691

Sum of electronic and thermal Free Energies= -2353.347813

E(RB3LYP) = -2353.975206 A.U.

A-TSc2

1 1

Number of imaginary frequencies: 1

Rh	1.60394300	-1.10214300	-0.00596500
C	2.30451400	-2.21062600	1.74672300
C	0.91363800	-2.55220300	1.58819500
C	0.77455800	-3.17365800	0.31025700
C	2.10867800	-3.33580800	-0.27551500
C	3.04424300	-2.78045600	0.62155900
C	-0.19316200	-1.06632800	-2.57763100
C	1.47877300	0.55169800	-2.62083400
C	0.93754600	1.13561000	-3.80334000
C	-0.21286400	0.53166600	-4.37133600
C	-0.76388200	-0.57614800	-3.77036600
H	-0.65908100	-1.89279000	-2.06225700
C	2.66721200	1.07110200	-2.03859700
C	1.56189500	2.29319500	-4.33936200
H	-0.64841100	0.95522400	-5.27190400
H	-1.65142600	-1.06181000	-4.15770000
C	2.67271600	2.82782800	-3.72473300
C	3.23038300	2.21535200	-2.57781500
H	1.14594500	2.74898000	-5.23276900
H	3.14118700	3.71903300	-4.13003900
H	4.12415800	2.63302900	-2.12542500
N	0.86959900	-0.51473300	-2.00143700
C	2.90863300	-1.59165100	2.97010300
H	2.25283900	-0.82291500	3.38527600
H	3.06928700	-2.35113800	3.74463900
H	3.87560900	-1.13416200	2.74976800

C	-0.16964800	-2.34149600	2.59777000
H	-0.20900500	-3.20799600	3.26965200
H	0.01443800	-1.45481100	3.20687500
H	-1.14959100	-2.23449800	2.13026500
C	-0.46911800	-3.81003600	-0.22481100
H	-0.53000200	-4.83911100	0.15252100
H	-1.37423700	-3.29144400	0.09107400
H	-0.45979400	-3.87432800	-1.31485800
C	2.37699600	-4.02175700	-1.57956200
H	3.38990300	-3.82999900	-1.93895900
H	2.25714600	-5.10659600	-1.47646700
H	1.67720000	-3.68638100	-2.35075200
C	4.53254200	-2.73193600	0.46646800
H	5.00163800	-3.51333900	1.07556600
H	4.83983300	-2.89053900	-0.56944000
H	4.93869300	-1.77212400	0.79752000
C	0.04310400	1.40947600	3.01932500
C	-0.93881500	1.63489100	3.97611000
C	-2.27525700	1.38003800	3.65657800
C	-2.62231800	0.91498200	2.39231600
C	-1.63433800	0.66659100	1.43007800
C	-0.27926800	0.91130100	1.74045400
H	-0.66733900	2.00820300	4.95810500
H	-3.05568200	1.55470200	4.39044200
H	-3.66469500	0.74976600	2.15169200
H	1.08564200	1.60735400	3.24694500
C	2.44049400	3.56326500	0.47739600

C	3.17476100	4.68979500	0.84903100
C	4.26715900	4.56468300	1.70936900
C	4.62589700	3.30724800	2.20624600
C	3.89479100	2.17885600	1.84465600
C	2.78972000	2.29891700	0.98254300
H	1.59420800	3.64988600	-0.19538200
H	2.89516000	5.66482500	0.46198200
H	4.83882200	5.44279700	1.99310100
H	5.47264600	3.20905600	2.87857900
H	4.16561900	1.20083200	2.23075300
N	-1.98145700	0.22994500	0.12915500
H	-1.19178700	0.06507900	-0.48922400
S	-3.16803100	-0.96008600	-0.14727100
O	-3.20445400	-1.91770800	0.96640000
O	-2.87313900	-1.43068200	-1.50783000
C	-5.73655800	-0.46711100	0.67527600
C	-6.94163100	0.23308700	0.64104600
C	-7.11428300	1.34036200	-0.20089100
C	-6.04092100	1.74035900	-1.01550300
C	-4.83111400	1.05591500	-0.99944400
C	-4.69166100	-0.04195400	-0.14578800
H	-5.59830200	-1.32094700	1.32921500
H	-7.75998500	-0.08676400	1.27945800
H	-6.15830500	2.60123700	-1.66757200
H	-4.00304600	1.37330500	-1.62411900
C	1.97900600	1.14711400	0.62591100
C	0.81555600	0.62900000	0.81880200

C	-8.42960600	2.07577700	-0.25443100
H	-8.28156100	3.15023200	-0.39677200
H	-9.03518100	1.71628700	-1.09512500
H	-9.01242800	1.92660900	0.65813000
C	3.23773300	0.33070200	-0.89718500
H	3.55931600	-0.67011900	-1.19515300
H	4.06875300	0.81793500	-0.39990800

Zero-point correction= 0.707000 (Hartree/Particle)

Thermal correction to Energy= 0.751601

Thermal correction to Enthalpy= 0.752546

Thermal correction to Gibbs Free Energy= 0.627369

Sum of electronic and zero-point Energies= -2353.289762

Sum of electronic and thermal Energies= -2353.245161

Sum of electronic and thermal Enthalpies= -2353.244217

Sum of electronic and thermal Free Energies= -2353.369393

E(RB3LYP) = -2353.996762 A.U.

A-TSd2

1 1

Number of imaginary frequencies: 1

Rh	-1.76861200	-0.69827000	-0.67723500
C	-0.52717600	-2.22040400	-1.75757300
C	-1.01971600	-2.83159100	-0.55306400
C	-2.44912400	-2.81535000	-0.62253700
C	-2.83197800	-2.29463700	-1.94199800
C	-1.65752700	-1.95359800	-2.63900100
C	-4.56852300	0.09270400	0.35805500
C	-3.37872500	1.89795300	-0.51193200

C	-4.43605800	2.79726700	-0.17291400
C	-5.59949800	2.25828700	0.42864700
C	-5.66878000	0.90790800	0.68667200
H	-4.58330900	-0.96585400	0.58715700
C	-2.19030400	2.38242300	-1.13006500
C	-4.27005500	4.18284100	-0.43332000
H	-6.42109800	2.91953300	0.68836100
H	-6.53934900	0.46139400	1.15369900
C	-3.10056200	4.64368900	-0.99492100
C	-2.06357500	3.74604600	-1.33990100
H	-5.07193300	4.86682900	-0.17288200
H	-2.96880700	5.70431100	-1.18373400
H	-1.15150100	4.12906900	-1.78690100
N	-3.46652000	0.55776600	-0.22007300
C	0.90501300	-2.10476300	-2.18506200
H	1.59755800	-2.28530000	-1.36265000
H	1.11009100	-2.85014700	-2.96340100
H	1.12086100	-1.12208600	-2.61492200
C	-0.19920500	-3.40810600	0.55899900
H	-0.03725300	-4.47757700	0.37723800
H	0.77995600	-2.93303800	0.63913700
H	-0.70488600	-3.30293700	1.52065600
C	-3.37500900	-3.48648000	0.34537300
H	-3.43314300	-4.55967400	0.12491400
H	-3.02704400	-3.37775700	1.37439700
H	-4.39300600	-3.09446200	0.27742400
C	-4.23992600	-2.21218900	-2.44170700

H	-4.31931400	-1.58323000	-3.33010600
H	-4.60708000	-3.21225500	-2.70077200
H	-4.91255200	-1.80612500	-1.68112200
C	-1.53781400	-1.41542500	-4.03137500
H	-1.26145800	-2.21417200	-4.72989000
H	-2.47468100	-0.97719300	-4.38229400
H	-0.75867700	-0.64943600	-4.09896800
C	0.25992200	-0.63413400	3.13621500
C	0.29236300	-1.25850100	4.38177600
C	-0.85839200	-1.85450500	4.90378400
C	-2.05136200	-1.82291600	4.17523000
C	-2.08684500	-1.21284200	2.92315500
C	-0.93264900	-0.61350600	2.39126600
H	1.22294800	-1.28091400	4.94016800
H	-0.82744800	-2.34039400	5.87414500
H	-2.95072400	-2.27523700	4.58250500
H	-3.00678900	-1.18626100	2.35047900
C	0.35918700	3.28121100	0.93510200
C	1.36610900	4.22967600	1.08509400
C	2.69348900	3.87676100	0.82344500
C	3.01948500	2.58478400	0.41670200
C	2.01733700	1.61973300	0.28444300
C	0.67004400	1.96449400	0.55006200
H	-0.67450100	3.53384500	1.13954900
H	1.11998300	5.23648300	1.40594900
H	3.48242000	4.61456800	0.93124300
H	4.04841900	2.31940500	0.20225600

H	1.16007900	-0.17771900	2.74078600
N	2.32423600	0.30368300	-0.13536600
H	1.49172300	-0.27029000	-0.25436900
S	3.43010400	-0.65392200	0.77387900
O	2.99330800	-2.02402200	0.46295500
O	3.49324000	-0.17542800	2.15732900
C	5.99647000	0.31548200	0.71854200
C	7.22266000	0.55500500	0.09939400
C	7.45907100	0.15323900	-1.22250200
C	6.42944300	-0.49952400	-1.92228400
C	5.19940100	-0.74900200	-1.32477800
C	4.99558800	-0.33141300	-0.00673400
H	5.81160800	0.61922000	1.74294900
H	8.00886800	1.05820200	0.65466300
H	6.59934200	-0.81685100	-2.94726200
H	4.41005300	-1.25852000	-1.86689400
C	-0.36046400	0.95412900	0.44993800
C	-0.95040000	-0.01240000	1.06374900
C	8.79845100	0.38538800	-1.87523200
H	9.34244700	1.20516300	-1.39899000
H	9.42244000	-0.51315300	-1.79825600
H	8.69049700	0.61560300	-2.93919200
C	-1.14337900	1.40683200	-1.50483200
H	-1.43358100	0.82291000	-2.38354000
H	-0.17355600	1.84699600	-1.71570900

Zero-point correction= 0.707241 (Hartree/Particle)

Thermal correction to Energy= 0.751613

Thermal correction to Enthalpy= 0.752557

Thermal correction to Gibbs Free Energy= 0.628656

Sum of electronic and zero-point Energies= -2353.288309

Sum of electronic and thermal Energies= -2353.243936

Sum of electronic and thermal Enthalpies= -2353.242992

Sum of electronic and thermal Free Energies= -2353.366894

E(RB3LYP) = -2353.995550 A.U.

A-TSe2

1 1

Number of imaginary frequencies: 1

Rh	2.03173300	-0.66130900	-0.38785500
C	2.74636900	-2.61648600	-0.99803800
C	1.51483400	-2.49838000	-1.76478300
C	1.63288900	-1.36692700	-2.59548100
C	2.98174800	-0.82274000	-2.44831800
C	3.69029200	-1.63573600	-1.53124100
C	0.52299500	2.05727700	-1.12777700
C	2.44518400	2.24349300	0.24783400
C	2.59806600	3.61266500	-0.11723800
C	1.68034900	4.15886100	-1.04999300
C	0.68358400	3.36941900	-1.59205900
H	-0.31279400	1.43354400	-1.42736400
C	3.42734700	1.55285600	0.99655500
C	3.70387000	4.33426200	0.40077400
H	1.78701300	5.19765900	-1.35016600
H	-0.00613000	3.75549700	-2.33354100
C	4.62436800	3.68608800	1.19581000

C	4.49732100	2.30348700	1.46734800
H	3.82810900	5.37922800	0.13407400
H	5.48073700	4.22702300	1.58584900
H	5.27608300	1.80334700	2.03632000
N	1.34504500	1.52396700	-0.20980200
C	3.07532900	-3.73706000	-0.05972400
H	2.21734000	-3.98370900	0.57098600
H	3.36115700	-4.63954900	-0.61436000
H	3.90353400	-3.47102800	0.60046600
C	0.35672400	-3.44808000	-1.74653000
H	0.34592200	-4.02370900	-2.68039100
H	0.43889000	-4.16710700	-0.92960800
H	-0.60421600	-2.93631400	-1.66200900
C	0.58064100	-0.85504000	-3.53186500
H	0.60791500	-1.40965600	-4.47831500
H	-0.41814600	-0.95970300	-3.10270000
H	0.73605100	0.20042900	-3.76930500
C	3.51800100	0.34875600	-3.21478000
H	4.43703800	0.73318300	-2.76725500
H	3.74019200	0.06912100	-4.25157500
H	2.79174100	1.16712400	-3.24730300
C	5.14753700	-1.54997700	-1.19989100
H	5.73034500	-2.12127300	-1.93218200
H	5.50919400	-0.51870400	-1.21685000
H	5.36279000	-1.96840100	-0.21449600
C	3.32217200	0.05688200	1.14297600
H	4.31202700	-0.39166900	1.03068600

H	2.95428200	-0.21651800	2.13630900
C	-2.12933200	1.04921500	1.39788200
C	-3.18278200	1.92161400	1.68144800
C	-2.92969000	3.25169900	2.01234700
C	-1.61249700	3.71640600	2.09432200
C	-0.55577100	2.85577200	1.82318700
C	-0.79079100	1.51922500	1.44717100
H	-4.19537300	1.53504500	1.64557900
H	-3.75754700	3.91972500	2.22800600
H	-1.41345600	4.74476300	2.37832100
H	0.46707300	3.21226600	1.88519100
C	0.48362900	-1.28742100	3.55905700
C	0.15037300	-2.22757700	4.53259400
C	-0.34998000	-3.47862000	4.16216600
C	-0.51380200	-3.78756400	2.80963800
C	-0.15879000	-2.86273700	1.82806600
C	0.34228100	-1.60020900	2.19370800
H	0.86485900	-0.31143800	3.84303500
H	0.27495600	-1.98014200	5.58247000
H	-0.61452700	-4.20601000	4.92321400
H	-0.91597100	-4.75213000	2.51501000
H	-0.30487900	-3.09046600	0.78064600
N	-2.44707000	-0.30118200	1.07590000
H	-1.84744200	-1.01657200	1.48353900
S	-2.72507800	-0.71071400	-0.55083100
O	-2.54056300	-2.16563100	-0.59067000
O	-1.93267900	0.15889200	-1.44080700

C	-4.78007300	0.87578300	-1.45739900
C	-6.12899000	1.19901900	-1.59709900
C	-7.13157800	0.36704400	-1.07954800
C	-6.75168600	-0.80902600	-0.40998300
C	-5.41256200	-1.15030700	-0.25749000
C	-4.43840100	-0.29811000	-0.78593400
H	-4.00317100	1.51284600	-1.86413500
H	-6.40693100	2.10976400	-2.11972300
H	-7.51811300	-1.46475100	-0.00669500
H	-5.12201900	-2.06192600	0.25349500
C	0.70493600	-0.61360400	1.17062300
C	0.29419200	0.62243700	1.12139400
C	-8.59021300	0.70396900	-1.26073300
H	-9.17276000	0.44537500	-0.37155300
H	-8.73655100	1.76653900	-1.47115600
H	-9.01240000	0.13925400	-2.10058600

Zero-point correction= 0.705739 (Hartree/Particle)

Thermal correction to Energy= 0.750420

Thermal correction to Enthalpy= 0.751365

Thermal correction to Gibbs Free Energy= 0.624766

Sum of electronic and zero-point Energies= -2353.266922

Sum of electronic and thermal Energies= -2353.222240

Sum of electronic and thermal Enthalpies= -2353.221296

Sum of electronic and thermal Free Energies= -2353.347895

E(RB3LYP) = -2353.972661 A.U.

A-TSf2

1 1

Number of imaginary frequencies: 1

Rh	2.30462200	-0.20975500	-0.05980700
C	4.23818500	0.63655000	-0.62293800
C	4.35031800	0.53732500	0.82458900
C	4.21918900	-0.82174700	1.17537100
C	4.11962900	-1.60648700	-0.05100200
C	4.20725900	-0.72520300	-1.15294300
C	0.65118800	-2.39069900	1.55840900
C	-0.01361100	-2.01919600	-0.68789600
C	-0.71790800	-3.25864600	-0.69972300
C	-0.65116600	-4.07652500	0.45673500
C	0.08113900	-3.66771500	1.55736500
H	1.11891400	-1.97497900	2.44352600
C	0.17623500	-1.25196100	-1.85413000
C	-1.37630700	-3.64689300	-1.89379600
H	-1.16179600	-5.03524600	0.45951400
H	0.17772500	-4.29185000	2.43802900
C	-1.28107100	-2.84613900	-3.01454500
C	-0.49295600	-1.67278700	-2.99893200
H	-1.91623600	-4.58838700	-1.92024800
H	-1.77848900	-3.13868400	-3.93381000
H	-0.38589400	-1.08968900	-3.90805500
N	0.56827800	-1.56078800	0.50062600
C	4.45489400	1.87225600	-1.44194700
H	4.04391500	2.75771500	-0.95434700
H	5.52610900	2.04164400	-1.60830800
H	3.97336700	1.78695300	-2.41837400

C	4.62938200	1.65438500	1.78709400
H	5.61171000	1.50600600	2.25044600
H	4.65268800	2.62488900	1.28903600
H	3.89189700	1.69972400	2.59386900
C	4.27498700	-1.38215000	2.56496000
H	5.31059700	-1.60453200	2.85191200
H	3.87722900	-0.67554600	3.29850000
H	3.71297800	-2.31623400	2.64687900
C	4.01027200	-3.10035100	-0.09900500
H	3.70125300	-3.44769700	-1.08696000
H	4.97233700	-3.57026300	0.13721900
H	3.28100300	-3.46892100	0.63009400
C	4.31341000	-1.10625700	-2.59697600
H	5.36068000	-1.30098700	-2.85691200
H	3.73988800	-2.00876200	-2.82276600
H	3.95941500	-0.30877600	-3.25340900
C	1.14490500	-0.10074700	-1.83204600
H	1.82977200	-0.19515800	-2.67838800
H	0.61333000	0.84578000	-1.94527900
C	-0.70601800	3.01354100	0.06342900
C	-0.82781900	4.38343500	-0.20746900
C	0.27525500	5.22558100	-0.11829700
C	1.52028900	4.71187500	0.25893000
C	1.65445700	3.35148600	0.50112200
C	0.56433000	2.46729000	0.40116200
H	-1.80411700	4.76735200	-0.47934500
H	0.15945900	6.28421500	-0.32754900

H	2.38028100	5.36758700	0.35212900
H	2.61439900	2.93810400	0.77430200
C	-1.02668200	0.72329200	3.19806400
C	-2.09832800	0.69818700	4.08827400
C	-3.19543500	-0.13001200	3.84052800
C	-3.22715200	-0.93041900	2.69316400
C	-2.16712500	-0.90543800	1.79440300
C	-1.05409500	-0.07345200	2.03644300
H	-0.17215500	1.36787400	3.37637500
H	-2.07483000	1.32154000	4.97646300
H	-4.02785900	-0.14850200	4.53712800
H	-4.08820300	-1.55689800	2.48648700
H	-2.21478200	-1.49707500	0.88806100
N	-1.87823400	2.21793800	-0.00287800
H	-1.77912200	1.30468200	0.42475900
S	-2.63211900	1.98118500	-1.53344000
O	-1.71166500	1.31571400	-2.46951000
O	-3.25831400	3.24907400	-1.90446600
C	-4.88637400	1.19653500	-0.15685400
C	-5.78593800	0.24291100	0.31018200
C	-5.66605600	-1.10950000	-0.05172200
C	-4.61449700	-1.48730600	-0.89890000
C	-3.70122500	-0.54752800	-1.37513100
C	-3.84666800	0.78568000	-0.99415300
H	-4.98090000	2.24032400	0.12247200
H	-6.59739600	0.55021200	0.96390600
H	-4.50835400	-2.52785600	-1.19392100

H	-2.88594800	-0.83561500	-2.02707800
C	0.00257800	0.10506200	1.05455900
C	0.78946900	1.03469300	0.56502300
C	-6.66973000	-2.12354200	0.43910600
H	-7.56972500	-2.10773500	-0.18689200
H	-6.26715300	-3.13984100	0.40726000
H	-6.98781200	-1.91001600	1.46415400

Zero-point correction= 0.705651 (Hartree/Particle)

Thermal correction to Energy= 0.750297

Thermal correction to Enthalpy= 0.751241

Thermal correction to Gibbs Free Energy= 0.627632

Sum of electronic and zero-point Energies= -2353.253109

Sum of electronic and thermal Energies= -2353.208463

Sum of electronic and thermal Enthalpies= -2353.207519

Sum of electronic and thermal Free Energies= -2353.331128

E(RB3LYP) = -2353.958760 A.U.

A-TSa3

0 1

Number of imaginary frequencies: 1

Rh	-1.28828700	1.34735000	0.22853800
C	-0.03531000	3.31308000	0.38573500
C	0.23251600	2.71764100	-0.89356900
C	-0.98841400	2.69018200	-1.60378100
C	-2.00529600	3.38577900	-0.79786000
C	-1.39742600	3.81040000	0.39314000
C	-3.29377600	0.01156700	-1.63972500
C	-3.06696300	-1.09502300	0.39005700

C	-3.93548500	-2.14430000	-0.04058100
C	-4.51432100	-2.03804900	-1.32999600
C	-4.20637700	-0.94845200	-2.11152400
H	-2.99993900	0.83358400	-2.27294900
C	-2.49818900	-1.12035800	1.68863400
C	-4.15610700	-3.24133100	0.82717300
H	-5.18308600	-2.81725500	-1.68374000
H	-4.62538500	-0.82733800	-3.10502800
C	-3.54838900	-3.28165600	2.06708700
C	-2.72499500	-2.22430700	2.49980500
H	-4.79891400	-4.05149900	0.49521600
H	-3.71068700	-4.13261100	2.72220700
H	-2.26577800	-2.26367200	3.48350500
N	-2.71947100	-0.04945400	-0.43465600
C	-1.66311100	0.02432400	2.08838500
H	-2.26489200	0.95522900	2.10384600
H	-1.25398400	-0.07959800	3.08923200
C	1.04500400	3.76048100	1.32581300
H	1.83209100	3.01217100	1.42931000
H	1.50455600	4.68046900	0.93860800
H	0.66315500	3.98450900	2.32380700
C	1.56066400	2.21016100	-1.35780700
H	2.26851900	3.03031500	-1.53884900
H	2.01624600	1.54579900	-0.61761900
H	1.46749300	1.64203400	-2.28568200
C	-1.14243800	2.27233900	-3.04092900
H	-0.46620900	2.84947900	-3.68226500

H	-0.91078300	1.21253300	-3.19619400
H	-2.15719300	2.45137600	-3.40703400
C	-3.40685600	3.65887900	-1.25533400
H	-3.42130100	4.36172800	-2.09863100
H	-3.91290900	2.74559200	-1.58857700
H	-4.01138100	4.09052600	-0.45411400
C	-2.01532500	4.58364400	1.51902700
H	-1.67850200	5.62896100	1.52469400
H	-3.10668800	4.58941100	1.45628100
H	-1.74452200	4.15538600	2.49047900
C	2.05336700	-0.59119600	2.22483300
C	3.12813700	-0.50297400	3.11633500
C	3.10651600	0.52428900	4.05894900
C	2.02390200	1.41421900	4.14297300
C	0.95850900	1.30914200	3.25454800
C	0.98799900	0.33088700	2.25351900
H	3.93421100	-1.22238400	3.08814500
H	3.93139600	0.61263800	4.75991500
H	2.01540900	2.18289800	4.91041800
H	0.10967900	1.98192700	3.31870000
C	-0.50924600	-3.37047700	-0.09214400
C	-1.11071200	-4.16653100	-1.06201700
C	-1.33102800	-3.66340200	-2.34730600
C	-0.94144100	-2.35850000	-2.65534500
C	-0.34507600	-1.55844100	-1.68118000
C	-0.12879700	-2.05105800	-0.38512800
H	-0.33494900	-3.75835200	0.90508100

H	-1.41088100	-5.18055100	-0.81476000
H	-1.80098600	-4.28547600	-3.10391100
H	-1.10517700	-1.96165000	-3.65362500
H	-0.04115500	-0.54220300	-1.90528600
N	1.73281100	-1.57954900	1.26066300
S	2.99328400	-2.36497700	0.36896200
O	4.08404800	-2.57315600	1.32160400
O	2.39422200	-3.48887900	-0.34091600
C	3.02841200	-1.22957400	-2.13825000
C	3.43771600	-0.27320000	-3.06479100
C	4.31102700	0.76229000	-2.70248200
C	4.78420700	0.81202700	-1.38294100
C	4.39391100	-0.13745200	-0.44199900
C	3.51432100	-1.14988500	-0.83260400
H	2.34984800	-2.02929700	-2.41170900
H	3.07072700	-0.33024900	-4.08626600
H	5.46794100	1.60394500	-1.08953900
H	4.76887200	-0.10631600	0.57480700
C	0.48533300	-1.19348300	0.64327100
C	-0.01482400	-0.04487800	1.25021200
C	4.69556700	1.82771500	-3.69900200
H	5.67990200	2.25046700	-3.47807100
H	4.71149800	1.43684300	-4.72063900
H	3.97136700	2.65172100	-3.67413500

Zero-point correction= 0.694745 (Hartree/Particle)

Thermal correction to Energy= 0.738207

Thermal correction to Enthalpy= 0.739151

Thermal correction to Gibbs Free Energy= 0.619606

Sum of electronic and zero-point Energies= -2352.884340

Sum of electronic and thermal Energies= -2352.840878

Sum of electronic and thermal Enthalpies= -2352.839933

Sum of electronic and thermal Free Energies= -2352.959479

E(RB3LYP) = -2353.579085 A.U.

A-TSb3

0 1

Number of imaginary frequencies: 1

Rh	1.58173000	-0.81956900	-0.58532700
C	2.33903600	-2.89175500	0.33148700
C	1.16593100	-3.19420400	-0.37394400
C	1.32750800	-2.75271600	-1.75631500
C	2.66912300	-2.27862800	-1.90569400
C	3.26897800	-2.25733300	-0.60208800
C	2.57168700	0.33286000	2.07749000
C	2.94078200	1.67323800	0.20841300
C	3.63744600	2.64276300	0.98307700
C	3.78135900	2.39385000	2.37164200
C	3.25340900	1.24502000	2.91378100
H	2.13211100	-0.56757100	2.48532700
C	2.74752800	1.82424600	-1.18487200
C	4.15154700	3.78709700	0.32111500
H	4.30726200	3.11472000	2.99209300
H	3.33304400	1.02429500	3.97230200
C	3.97416900	3.92844600	-1.03918100
C	3.27621800	2.95068300	-1.79001500

H	4.68575200	4.53740300	0.89702300
H	4.36864600	4.80389500	-1.54700100
H	3.12943300	3.09902500	-2.85612200
N	2.42021000	0.53714200	0.77879300
C	1.91576800	0.78692500	-1.88134600
H	0.95407200	1.23672900	-2.13502900
H	2.39489400	0.44923400	-2.80451400
C	2.61806700	-3.19054200	1.77538900
H	1.72463600	-3.05910400	2.39294200
H	2.96644900	-4.22311900	1.90442700
H	3.39862000	-2.53727100	2.17375500
C	-0.02980100	-3.93205500	0.13879200
H	-0.04865800	-4.94472300	-0.28391000
H	-0.00828700	-4.02535300	1.22553700
H	-0.96594900	-3.44648600	-0.14275500
C	0.37278100	-3.07096200	-2.86686900
H	0.44542400	-2.34688900	-3.68033400
H	0.58319900	-4.06755700	-3.27798900
H	-0.66177700	-3.06040300	-2.52055100
C	3.34246300	-1.93945600	-3.19945100
H	3.82840100	-2.83143400	-3.61439500
H	2.62495400	-1.57924200	-3.94056100
H	4.11036200	-1.17246700	-3.07093400
C	4.67764200	-1.85711400	-0.27860600
H	4.73751300	-1.38433000	0.70576200
H	5.34525000	-2.72810100	-0.27168900
H	5.06226800	-1.14231400	-1.00990900

C	-2.45158900	-1.37741100	-1.03023300
C	-3.36199600	-1.97514900	-1.90270900
C	-3.25005700	-1.65426000	-3.25613800
C	-2.26211600	-0.76349000	-3.70819200
C	-1.33468400	-0.20960800	-2.82937700
C	-1.40948200	-0.53889900	-1.46990000
H	-4.13808900	-2.63323200	-1.53403900
H	-3.94510300	-2.09407100	-3.96534600
H	-2.21631300	-0.50967100	-4.76355500
H	-0.58145300	0.48245300	-3.18011100
C	-0.89642200	-1.81436400	3.01722800
C	-0.48911900	-1.75903300	4.34696800
C	-0.03882900	-0.55260600	4.89427200
C	0.00493900	0.59174700	4.09680000
C	-0.37260900	0.53674000	2.75370700
C	-0.82737700	-0.67214400	2.19876800
H	-1.28979300	-2.73504500	2.60289000
H	-0.54307100	-2.65145200	4.96380900
H	0.26211000	-0.50603900	5.93710400
H	0.34489600	1.53520700	4.51451500
H	-0.31584600	1.42143700	2.12876100
N	-2.38159600	-1.47643500	0.39690000
S	-3.92321500	-1.05963900	1.20348800
O	-4.93095200	-1.93222300	0.60282200
O	-3.67452900	-1.06925100	2.64118700
C	-3.40572100	1.62421400	1.26961500
C	-3.30041000	2.86728300	0.65462800

C	-3.86958300	3.10494900	-0.60483400
C	-4.61966400	2.08351200	-1.20582700
C	-4.73919800	0.83172600	-0.61076700
C	-4.11286600	0.61043000	0.61849100
H	-2.92761700	1.42867000	2.22234000
H	-2.72895400	3.65225800	1.14020600
H	-5.08189000	2.25854200	-2.17307200
H	-5.27743600	0.02753400	-1.09729500
C	-1.22535400	-0.73870900	0.78707600
C	-0.57686100	-0.18582300	-0.31452900
C	-3.60820300	4.39579600	-1.33464500
H	-2.68622800	4.27784800	-1.91727400
H	-4.42232100	4.64789000	-2.02059100
H	-3.46498000	5.23116300	-0.64260100
H	-0.14632600	1.01962400	-0.13864400
C	-0.24940700	3.15371900	-0.73983400
O	0.06374300	2.29567400	0.18308200
O	-0.65285500	2.87725000	-1.87543400
C	-0.02797400	4.60403600	-0.31255700
H	-0.51199400	4.79758500	0.64948600
H	1.04609600	4.76791300	-0.17412300
H	-0.40562500	5.29259600	-1.06998700

Zero-point correction= 0.756016 (Hartree/Particle)

Thermal correction to Energy= 0.804401

Thermal correction to Enthalpy= 0.805345

Thermal correction to Gibbs Free Energy= 0.676464

Sum of electronic and zero-point Energies= -2581.969708

Sum of electronic and thermal Energies= -2581.921324

Sum of electronic and thermal Enthalpies= -2581.920379

Sum of electronic and thermal Free Energies= -2582.049260

E(RB3LYP) = -2582.725724 A.U.

A-TSa4

0 1

Number of imaginary frequencies: 1

C	-0.24615200	-0.50724700	1.72633200
C	0.63811700	-0.98900100	2.69596900
C	0.60372700	-0.52540300	4.00570700
C	-0.33502700	0.44259100	4.37269400
C	-1.23988300	0.91301500	3.43197300
C	-1.22610200	0.44370800	2.10135600
H	1.35358600	-1.73948600	2.39671000
H	1.31384600	-0.90823000	4.73233800
H	-0.35765700	0.83031200	5.38639500
H	-1.97421100	1.66424400	3.70064800
C	-4.23186700	1.48276200	-1.67061900
C	-5.32262900	1.84929600	-2.45407900
C	-6.44173700	2.45508900	-1.87415800
C	-6.46137300	2.69849800	-0.49812200
C	-5.37473000	2.33578800	0.29564200
C	-4.24582800	1.71845900	-0.28029800
H	-3.36149400	1.00250500	-2.10072200
H	-5.30189600	1.66148700	-3.52429400
H	-7.29039100	2.73825000	-2.49002400
H	-7.32558400	3.17266800	-0.04157400

H	-5.38665100	2.52119200	1.36504500
N	-0.13033600	-0.97444100	0.36524400
H	-0.74101100	-0.25641000	-0.61739300
S	-0.72040300	-2.57134600	0.14609700
O	-0.29505800	-3.43900800	1.25472600
O	-0.37025000	-2.92695500	-1.24008100
C	-3.20867100	-2.03808000	-0.89651100
C	-4.56013500	-1.73793600	-0.77881100
C	-5.19530900	-1.72957900	0.47255100
C	-4.45114900	-2.08019300	1.60630900
C	-3.09705400	-2.39553900	1.51004800
C	-2.48683300	-2.35591100	0.25607700
H	-2.70584500	-2.00980300	-1.85520500
H	-5.12762700	-1.46815500	-1.66448100
H	-4.93269900	-2.09145700	2.58013300
H	-2.51565200	-2.65717000	2.38676300
C	-3.15339100	1.31020800	0.53352400
C	-2.22640800	0.91857100	1.21349600
C	-6.63639700	-1.29969000	0.58261000
H	-6.71238300	-0.21367700	0.44966900
H	-7.25339500	-1.76586500	-0.19259600
H	-7.06217500	-1.55191400	1.55767900
Rh	1.88388800	-0.54762300	-0.54487800
C	3.01226700	-2.45490900	-0.23873000
C	3.00034300	-2.05269400	-1.61616500
C	3.72438600	-0.79028800	-1.71879000
C	4.14244300	-0.41971300	-0.40983400

C	3.63876000	-1.40506100	0.52598100
O	-1.18374500	0.22442900	-1.57461600
C	-0.30402700	0.40772100	-2.48397800
O	0.91280800	0.11323900	-2.37550400
C	-0.79815700	1.02345500	-3.77020500
C	3.96418500	-1.40022200	1.98654600
H	3.51558700	-2.24976800	2.50358000
H	5.05101400	-1.46074200	2.12260600
H	3.61383200	-0.47290500	2.44680800
C	2.55326200	-3.77572200	0.28226200
H	1.75359100	-4.19134300	-0.32916500
H	3.40728700	-4.46552800	0.25997800
H	2.18008600	-3.71481700	1.30333600
C	2.44995200	-2.82447000	-2.77150400
H	2.09109000	-2.14206300	-3.54484300
H	3.23088300	-3.46064500	-3.20678200
H	1.61048900	-3.44461100	-2.45859100
C	3.97147600	-0.04720100	-2.99138900
H	4.33458900	0.96269000	-2.79536000
H	4.71203300	-0.57448500	-3.60417600
H	3.04301600	0.03485500	-3.56190800
C	5.03269500	0.71335300	-0.02728900
H	6.01881000	0.29841100	0.21994900
H	5.15496200	1.43425900	-0.83343000
H	4.64601000	1.22940300	0.85195100
H	-1.24615700	1.99557300	-3.54463700
H	0.01723700	1.14357300	-4.48292700

H	-1.58084200	0.38944700	-4.19740100
S	1.74461400	2.32742200	1.15109500
O	0.70975500	3.07015600	1.86608600
O	2.84161300	1.72543700	1.93157200
C	2.56480900	3.58425100	0.04142300
O	1.17500300	1.38963800	0.09342200
F	3.38807600	4.37039000	0.74453300
F	1.64714200	4.34175300	-0.56487700
F	3.29093700	2.96165800	-0.91469000

Zero-point correction= 0.629896 (Hartree/Particle)

Thermal correction to Energy= 0.679313

Thermal correction to Enthalpy= 0.680257

Thermal correction to Gibbs Free Energy= 0.544770

Sum of electronic and zero-point Energies= -3102.862496

Sum of electronic and thermal Energies= -3102.813079

Sum of electronic and thermal Enthalpies= -3102.812135

Sum of electronic and thermal Free Energies= -3102.947622

E(RB3LYP) = -3103.492392 A.U.

A-TSb4

0 1

Number of imaginary frequencies: 1

C	-2.95876600	1.42345200	-0.29819100
C	-4.30911500	1.70034700	-0.07816300
C	-4.84474300	2.92288100	-0.49192400
C	-4.05290700	3.87600500	-1.13352700
C	-2.70174800	3.61402300	-1.34627400
C	-2.14678600	2.39888700	-0.91904400

H	-4.94595800	0.98670500	0.42288800
H	-5.89527000	3.12519900	-0.30688700
H	-4.48023300	4.82027800	-1.45493900
H	-2.05952200	4.34545000	-1.82588900
C	2.61083800	1.21764700	-2.11664100
C	3.93716600	1.42797800	-2.48608800
C	4.41589200	2.72961200	-2.65611700
C	3.57796200	3.83167900	-2.44290300
C	2.26007300	3.63655900	-2.04597800
C	1.76716000	2.32027400	-1.88337100
H	2.26475400	0.21080600	-1.92355200
H	4.59874900	0.57239200	-2.58254800
H	5.45220100	2.88767300	-2.94004900
H	3.95701900	4.84098700	-2.57365900
H	1.60307300	4.48192900	-1.86398800
N	-2.27100100	0.20477200	0.02147600
S	-3.03263200	-0.99112700	0.98676300
O	-3.59609800	-0.33737500	2.17917700
O	-2.01678500	-2.03802600	1.10987200
C	-5.68025200	-1.58315200	0.55639300
C	-6.73904200	-2.12431800	-0.17113300
C	-6.52934600	-2.70720600	-1.42764300
C	-5.22223900	-2.74641400	-1.93901300
C	-4.14758200	-2.22076700	-1.22850000
C	-4.39499000	-1.62937700	0.01457300
H	-5.83922700	-1.13582800	1.53151500
H	-7.74149100	-2.09567000	0.24671600

H	-5.04187400	-3.20184400	-2.90892800
H	-3.14403900	-2.25605800	-1.63786800
C	0.42902600	2.15234100	-1.44057400
C	-0.74266300	2.13896800	-1.04863000
C	-7.67896900	-3.26574800	-2.22921000
H	-8.56540500	-3.42255300	-1.60889700
H	-7.95625900	-2.57949300	-3.03849900
H	-7.41226700	-4.22057400	-2.69293000
Rh	-0.09799500	0.67109200	0.65334900
C	1.30697000	-0.02979600	2.26088300
C	1.76422800	1.20938800	1.68437500
C	0.75363900	2.22426400	1.95682100
C	-0.34054100	1.60009400	2.62767600
C	0.01119800	0.19539700	2.82936900
C	-0.75098100	-0.79553600	3.64520800
H	-0.71291900	-1.78790500	3.19606400
H	-0.29549600	-0.84361800	4.64280700
H	-1.79802900	-0.51691700	3.75059900
C	2.05291700	-1.31416200	2.18055500
H	2.24320800	-1.57272400	1.13141800
H	3.03598000	-1.20641200	2.64830500
H	1.51184700	-2.12843300	2.66302300
C	3.12057400	1.40132500	1.09341900
H	3.19164900	2.32097700	0.51266300
H	3.85722000	1.44659700	1.90534500
H	3.38872100	0.55395500	0.45673800
C	0.86654300	3.66702600	1.58655100

H	-0.11481200	4.11551500	1.41965400
H	1.36061500	4.21487200	2.39816100
H	1.46470900	3.79510400	0.68260800
C	-1.59368100	2.25919900	3.11298800
H	-1.48499200	2.55322400	4.16408200
H	-1.81675200	3.15635200	2.53135700
H	-2.44468000	1.58061600	3.02975900
H	-1.84435100	-0.35640000	-0.94835800
O	0.52248500	-0.86944300	-0.60337400
C	-0.10810300	-1.39458100	-1.57238900
O	-1.29035800	-1.06256700	-1.91269200
C	0.61112200	-2.48023900	-2.32941300
H	0.41843100	-2.37290800	-3.39960700
H	1.67869900	-2.45465100	-2.10396700
H	0.19978900	-3.44469500	-2.01102200
S	4.74334400	-1.98184600	-0.96272800
O	3.38679600	-1.37928900	-0.76740700
O	4.73187600	-3.36361600	-1.46622100
C	5.32071100	-2.14312600	0.80212200
O	5.73026100	-1.05438300	-1.55826400
F	4.53483900	-2.99624500	1.49221200
F	5.25827200	-0.94514200	1.43974300
F	6.58194600	-2.58270800	0.87985600

Zero-point correction= 0.630378 (Hartree/Particle)

Thermal correction to Energy= 0.679684

Thermal correction to Enthalpy= 0.680628

Thermal correction to Gibbs Free Energy= 0.545956

Sum of electronic and zero-point Energies= -3102.842776

Sum of electronic and thermal Energies= -3102.793470

Sum of electronic and thermal Enthalpies= -3102.792526

Sum of electronic and thermal Free Energies= -3102.927197

E(RB3LYP) = -3103.473154 A.U.

A-TSc4

0 1

Number of imaginary frequencies: 1

C	0.95241000	2.83878900	-0.66890300
C	1.05738700	4.17638600	-1.02805600
C	-0.07359700	4.98493600	-0.87608500
C	-1.26672400	4.44327800	-0.39321000
C	-1.35064500	3.09742100	-0.02982500
C	-0.22506200	2.28068200	-0.14432700
H	1.98931500	4.57261800	-1.41450800
H	-0.02422500	6.03129900	-1.15986300
H	-2.15117300	5.06825600	-0.31916600
H	-2.29248100	2.66307400	0.26934200
C	2.43403600	-1.74828100	0.11300200
C	3.04212300	-2.87387300	-0.43572500
C	2.90389700	-3.14900300	-1.79723800
C	2.12706300	-2.31630400	-2.61124300
C	1.49756500	-1.20176600	-2.06603000
C	1.67160900	-0.89956800	-0.69962600
H	2.52013700	-1.53250300	1.16995800
H	3.61281100	-3.54174500	0.20159400
H	3.38048800	-4.02802500	-2.22254300

H	1.98725500	-2.55611500	-3.66094500
H	0.82306900	-0.58606200	-2.65368200
N	2.00933200	1.85797900	-0.79451700
S	3.46272300	2.32068000	0.14704700
O	4.10251800	3.39389700	-0.61756300
O	2.98961700	2.51667800	1.51348100
C	4.80082700	0.20307600	1.23287000
C	5.61851700	-0.92296300	1.16060000
C	6.07303600	-1.40902500	-0.07155700
C	5.72285500	-0.71688700	-1.24258900
C	4.93374500	0.42481900	-1.19185800
C	4.46305300	0.85926900	0.05043600
H	4.42273300	0.56900000	2.18078900
H	5.89017500	-1.44253300	2.07485900
H	6.07385900	-1.08021400	-2.20379600
H	4.69508900	0.96808000	-2.10043900
C	1.01403200	0.27327400	-0.18660200
C	-0.11890200	0.84277700	0.12151100
C	6.88416000	-2.67613500	-0.15671700
H	6.24423600	-3.50756200	-0.47678000
H	7.69200700	-2.58718400	-0.88936500
H	7.32175700	-2.94419600	0.80827000
H	2.29220800	1.69855300	-1.76442300
C	-2.68076100	0.70747800	2.63237000
C	-3.23892200	-0.63976300	2.51876100
C	-2.21086400	-1.56874100	2.79450600
C	-0.97324600	-0.82268100	2.99320300

C	-1.30520500	0.59155800	2.98010200
C	-3.51036100	1.94566900	2.49824600
H	-4.06794700	1.92818300	1.55643600
H	-4.23835100	1.99884700	3.31689100
H	-2.90269600	2.85121600	2.52806700
C	-4.65952600	-0.90912700	2.12923700
H	-5.35254100	-0.48877600	2.86760000
H	-4.87314100	-0.44604100	1.15953800
H	-4.85782100	-1.97887600	2.04508300
C	-2.34375200	-3.05652800	2.87235400
H	-2.45494500	-3.35848500	3.92194500
H	-3.22285800	-3.40679600	2.32695800
H	-1.46378500	-3.54224300	2.45128500
C	0.34328000	-1.41742900	3.38553100
H	1.14946700	-0.69079500	3.25413100
H	0.33329900	-1.72251400	4.44011400
H	0.54778700	-2.28502900	2.75584000
C	-0.35248400	1.71033800	3.27537200
H	-0.24289500	1.83440200	4.35930700
H	0.63703200	1.51736200	2.85414500
H	-0.70360100	2.65462400	2.85593500
Rh	-1.60407100	-0.31018300	0.97781400
O	-1.28415000	-1.81559000	-0.40420400
C	-0.67959600	-2.94021600	-0.19150700
O	-0.03544800	-3.26297700	0.81543500
C	-0.83763000	-3.92123200	-1.35084300
H	0.10819200	-4.44164300	-1.51504300

H	-1.59071800	-4.66750400	-1.07410600
H	-1.16387000	-3.41252800	-2.25797600
S	-2.82225300	0.67969500	-2.01306200
O	-3.01680900	0.45050400	-0.51416600
O	-3.52623600	1.88991700	-2.45332800
C	-3.81346100	-0.73041500	-2.72217900
O	-1.44664100	0.47040700	-2.49069000
F	-5.04913800	-0.72808400	-2.19547700
F	-3.24822900	-1.91555400	-2.46646100
F	-3.91412800	-0.58561600	-4.05193000

Zero-point correction= 0.633034 (Hartree/Particle)

Thermal correction to Energy= 0.682393

Thermal correction to Enthalpy= 0.683337

Thermal correction to Gibbs Free Energy= 0.547096

Sum of electronic and zero-point Energies= -3102.810324

Sum of electronic and thermal Energies= -3102.760965

Sum of electronic and thermal Enthalpies= -3102.760021

Sum of electronic and thermal Free Energies= -3102.896262

E(RB3LYP) = -3103.443358 A.U.

A-TSa5

1 1

Number of imaginary frequencies: 1

C	2.54930600	3.14208100	-0.71724800
C	2.08594200	2.04516400	0.01994300
C	1.27535400	1.10514600	-0.61760600
C	0.88463700	1.30720800	-1.97736600
C	1.34250600	2.43130600	-2.68253300

C	2.19354300	3.33837500	-2.05728700
H	3.18894400	3.86635600	-0.22169600
H	2.34363600	1.95399100	1.06580000
H	1.02784800	2.56601000	-3.71221500
H	2.56786700	4.20182100	-2.59701400
C	-0.06059600	0.32915700	-2.42267700
C	-0.21831600	-0.63829000	-1.49757000
C	-1.12965800	-1.75874700	-1.34923100
C	-2.00286400	-2.04786100	-2.44344200
C	-1.35325600	-2.40617500	-0.10144500
C	-3.05366200	-2.92186600	-2.27320200
H	-1.82634700	-1.54703400	-3.38762700
C	-2.45070200	-3.28655300	0.04059800
H	-0.59923800	-2.38322600	0.67449700
C	-3.29641000	-3.53798400	-1.02167800
H	-3.70659600	-3.13913100	-3.11324500
H	-2.59260200	-3.79095300	0.99108500
H	-4.12437300	-4.23173500	-0.91408400
N	0.69719500	-0.07799000	-0.06891500
S	1.57156900	-0.76002500	1.30164000
O	1.06298000	-2.11927200	1.49639600
O	1.44786000	0.21242200	2.39937400
C	3.25640400	-0.84483800	0.74155900
C	3.54707000	-1.60551000	-0.39472600
C	4.25232200	-0.18391800	1.45986000
C	4.86797700	-1.68655900	-0.81958500
H	2.75803200	-2.11783900	-0.93546700

C	5.57043400	-0.28834100	1.02010500
H	3.99677800	0.39302600	2.34161900
C	5.89872600	-1.03450600	-0.12072600
H	5.10768100	-2.26739000	-1.70548400
H	6.35597900	0.21929100	1.57202700
C	7.32967400	-1.16319500	-0.57706500
H	7.94845300	-0.34451900	-0.20108000
H	7.76418500	-2.10104800	-0.21071600
H	7.40105200	-1.17681600	-1.66848000
Rh	-1.53652900	0.05776300	0.12685700
C	-1.84087200	1.94424700	1.20202800
C	-2.48438700	2.04740800	-0.07647900
C	-3.48950000	0.99824700	-0.14277600
C	-3.50694100	0.31076500	1.12678600
C	-2.46343100	0.85974900	1.94776100
C	-4.44722100	-0.79125100	1.49070800
H	-5.42605600	-0.36803200	1.74552900
H	-4.58740300	-1.48524100	0.65812400
H	-4.08953600	-1.35954100	2.35028800
C	-2.08020500	0.45462900	3.33490700
H	-2.48446800	1.16976500	4.06179000
H	-2.46474600	-0.53528300	3.58542600
H	-0.99243700	0.43582500	3.44471800
C	-4.40443900	0.72664600	-1.29279100
H	-4.66448900	-0.33263700	-1.34656800
H	-5.33306500	1.29953300	-1.18094900
H	-3.94308100	1.00936100	-2.24087300

C	-2.16575800	3.05052600	-1.13530600
H	-2.52480300	2.72832900	-2.11342800
H	-2.63735300	4.01064000	-0.89331800
H	-1.08763900	3.21453400	-1.21377800
C	-0.75513100	2.82340500	1.72613500
H	-0.02744100	2.24569600	2.30019700
H	-0.22813100	3.33570200	0.92088600
H	-1.19231100	3.58154200	2.38754100

Zero-point correction= 0.538834 (Hartree/Particle)

Thermal correction to Energy= 0.574032

Thermal correction to Enthalpy= 0.574976

Thermal correction to Gibbs Free Energy= 0.471862

Sum of electronic and zero-point Energies= -1912.113885

Sum of electronic and thermal Energies= -1912.078688

Sum of electronic and thermal Enthalpies= -1912.077744

Sum of electronic and thermal Free Energies= -1912.180858

E(RB3LYP) = -1912.652720 A.U.

B-Re1

0 1

Number of imaginary frequencies: 0

C	1.93246700	0.26366300	0.00004200
C	-0.37106000	-0.40368100	0.00004300
C	-0.78293600	0.95683000	-0.00001100
C	0.20378000	1.97461400	-0.00001600
C	1.52979800	1.61267600	-0.00001100
C	-1.31048800	-1.45251500	0.00001900
C	-2.17782200	1.22243700	-0.00006000

H	-0.09541600	3.01748400	-0.00005900
H	2.31117100	2.36543200	-0.00004700
C	-3.09342300	0.19347700	-0.00006800
C	-2.65663500	-1.15203000	-0.00003300
H	-2.50733600	2.25755900	-0.00009800
H	-4.15664500	0.41363500	-0.00010800
H	-3.38735800	-1.95479000	-0.00004200
N	0.99905000	-0.72593500	0.00011300
O	1.36255200	-1.95574000	-0.00002200
H	-0.93708100	-2.46823800	0.00006100
C	3.35173900	-0.19810600	0.00002900
H	3.54499900	-0.82992300	0.87362800
H	3.54492500	-0.83013100	-0.87343800
H	4.03645300	0.65225200	-0.00010700

Zero-point correction= 0.167956 (Hartree/Particle)

Thermal correction to Energy= 0.177046

Thermal correction to Enthalpy= 0.177991

Thermal correction to Gibbs Free Energy= 0.133950

Sum of electronic and zero-point Energies= -516.279889

Sum of electronic and thermal Energies= -516.270798

Sum of electronic and thermal Enthalpies= -516.269854

Sum of electronic and thermal Free Energies= -516.313895

E(RB3LYP) = -516.447845 A.U.

B-int1

0 1

Number of imaginary frequencies: 0

Rh	0.94780500	-0.30147200	-0.13105100

C	1.07140300	0.82153700	-2.05397000
C	2.24867900	0.02156400	-1.86572400
C	1.84172000	-1.35936800	-1.76565700
C	0.40280500	-1.41863600	-1.98241500
C	-0.06006400	-0.08592600	-2.14960200
O	-0.52644200	-3.15701300	2.50459900
O	0.60349500	-2.08955500	0.92745700
C	0.32658400	-2.32619200	2.19301600
C	1.08718100	-1.54257400	3.24840300
H	0.77510400	-0.49595200	3.20311400
H	0.87059800	-1.95706500	4.23434200
H	2.15840000	-1.55361200	3.04040300
C	1.03368900	2.30183600	-2.27154000
H	1.77366300	2.79176000	-1.63835400
H	1.23232300	2.54665800	-3.32298300
H	0.05218300	2.71071900	-2.01628600
C	3.65211800	0.53104900	-1.78258800
H	4.08965600	0.57290900	-2.78776000
H	3.67394900	1.52652100	-1.33932000
H	4.27122700	-0.12685400	-1.16937500
C	2.70425100	-2.56112800	-1.54449800
H	2.81383200	-3.13523800	-2.47276000
H	3.69960300	-2.27876500	-1.19681600
H	2.24731000	-3.20359900	-0.78648700
C	-0.39729700	-2.67982800	-1.92739500
H	-0.02857000	-3.40217400	-2.66390300
H	-0.29692300	-3.11575800	-0.92519400

H	-1.45595100	-2.49751700	-2.12088600
C	-1.46177500	0.33704000	-2.45329300
H	-1.56688900	0.50227200	-3.53269300
H	-2.19019300	-0.41593600	-2.15142900
H	-1.71453200	1.27632000	-1.95665200
C	-1.66947400	2.42924700	0.69445600
C	-2.67942000	0.25061400	0.53411600
C	-3.87732900	0.82744400	0.02356600
C	-3.94249900	2.23346800	-0.13854600
C	-2.85809100	3.00766200	0.19699800
C	-2.55935300	-1.14119400	0.71548900
C	-4.94511500	-0.04149000	-0.31994200
H	-4.85033400	2.68545600	-0.52642100
H	-2.88392600	4.08620200	0.09008700
C	-4.81882500	-1.40394300	-0.15542400
C	-3.62382000	-1.94952000	0.36925300
H	-5.86032900	0.39089200	-0.71401400
H	-5.64053000	-2.06173900	-0.42168100
H	-3.52950900	-3.02085700	0.51452300
N	-1.60368800	1.08850800	0.83526900
O	-0.49022800	0.55708800	1.30836300
H	-1.64928500	-1.56835000	1.10942000
C	-0.46925500	3.20888500	1.10302400
H	-0.26268000	3.03622400	2.16498600
H	0.43434100	2.87245000	0.58194400
H	-0.62956200	4.27477400	0.93064700
O	2.52358000	2.42532700	0.55325400

O	2.34923900	0.28529500	1.28283400
C	2.79789300	1.49954100	1.33107900
C	3.76040200	1.71824000	2.49501700
H	4.61067000	1.03522000	2.40576800
H	4.11227300	2.75072800	2.50691200
H	3.25507600	1.48188600	3.43624400

Zero-point correction= 0.496780 (Hartree/Particle)

Thermal correction to Energy= 0.530900

Thermal correction to Enthalpy= 0.531844

Thermal correction to Gibbs Free Energy= 0.432453

Sum of electronic and zero-point Energies= -1472.666347

Sum of electronic and thermal Energies= -1472.632227

Sum of electronic and thermal Enthalpies= -1472.631283

Sum of electronic and thermal Free Energies= -1472.730673

E(RB3LYP) = -1473.163126 A.U.

B-int2

1 1

Number of imaginary frequencies: 0

Rh	-1.10388800	-0.02048200	-0.14876600
C	-1.22625800	1.76642100	1.12060400
C	-2.53409400	1.16494300	1.00505400
C	-2.46401600	-0.17222200	1.52973400
C	-1.10728800	-0.38565900	2.01044600
C	-0.35643300	0.80785000	1.77107100
O	-1.29732800	-2.01092900	-1.02927600
O	-2.18144500	-0.26564900	-2.00455100
C	-1.90523500	-1.51116100	-2.03647700

C	-2.24753600	-2.34925700	-3.23053000
H	-1.38857200	-2.35251000	-3.91029700
H	-2.44699900	-3.37817300	-2.92586200
H	-3.10417500	-1.92748200	-3.75836800
C	-0.87153700	3.18073000	0.78443900
H	0.19436200	3.28604000	0.57205200
H	-1.43071400	3.54179300	-0.08126000
H	-1.10673400	3.83746000	1.63074400
C	-3.74133800	1.80158400	0.39702100
H	-4.36798300	2.23515800	1.18540400
H	-3.46695300	2.59877000	-0.29568000
H	-4.33904600	1.07101200	-0.15140900
C	-3.58403100	-1.15922600	1.62507900
H	-3.99705000	-1.16656400	2.64047200
H	-4.39137400	-0.91169800	0.93395700
H	-3.23712300	-2.16834000	1.39135500
C	-0.60626200	-1.64285700	2.64431500
H	-0.80464100	-1.62247300	3.72262600
H	-1.10799200	-2.51807100	2.22615800
H	0.46815500	-1.76471800	2.49530900
C	1.06214300	1.05851200	2.17028700
H	1.08260000	1.58822300	3.13007900
H	1.62191800	0.12980500	2.28656100
H	1.58223700	1.68293100	1.44047900
C	2.16066900	1.66630000	-1.39135000
C	2.48737500	-0.49354000	-0.38097200
C	3.76022700	-0.08748600	0.10982000

C	4.21682100	1.22103700	-0.18533900
C	3.43193700	2.07009900	-0.93102400
C	1.99000700	-1.79248100	-0.14977400
C	4.50848300	-1.01767100	0.87773900
H	5.18918200	1.54138100	0.17559500
H	3.76795900	3.06965700	-1.18136800
C	4.01060000	-2.27822500	1.12538200
C	2.75363400	-2.66547000	0.60116500
H	5.47938100	-0.71745300	1.25970000
H	4.58815900	-2.98502400	1.71205500
H	2.38611700	-3.67067600	0.78207800
N	1.72397000	0.42749100	-1.09159000
O	0.52559900	0.05561500	-1.53487600
H	1.03478300	-2.08287500	-0.56974300
C	1.25746000	2.52022000	-2.21874900
H	1.12044900	2.06796000	-3.20658800
H	0.26075700	2.57633200	-1.77391700
H	1.67391900	3.52184500	-2.33254800

Zero-point correction= 0.445534 (Hartree/Particle)

Thermal correction to Energy= 0.474625

Thermal correction to Enthalpy= 0.475569

Thermal correction to Gibbs Free Energy= 0.385889

Sum of electronic and zero-point Energies= -1244.037308

Sum of electronic and thermal Energies= -1244.008217

Sum of electronic and thermal Enthalpies= -1244.007273

Sum of electronic and thermal Free Energies= -1244.096952

E(RB3LYP) = -1244.482841 A.U.

B-int3

0 1

Number of imaginary frequencies: 0

Rh	-0.35387100	0.24185500	-0.75079600
C	-1.38647300	-0.70478900	-2.44914400
C	-1.30055800	0.72886500	-2.66387500
C	0.09488900	1.07278500	-2.74863600
C	0.87354100	-0.11177900	-2.52312900
C	-0.05367600	-1.21919300	-2.34923900
C	-2.65226200	-1.49261400	-2.38679900
H	-2.98938800	-1.70514100	-3.40934400
H	-2.51234400	-2.44386900	-1.87112200
H	-3.43162900	-0.93166600	-1.87023300
C	-2.43531500	1.66682600	-2.91671100
H	-2.65873500	1.68764400	-3.99138100
H	-3.32434500	1.36660700	-2.36523400
H	-2.17445500	2.68037100	-2.60532100
C	0.62305800	2.43851700	-3.03989700
H	0.50017000	2.64220200	-4.11102500
H	0.07657600	3.20390000	-2.48519200
H	1.67484700	2.52751700	-2.77409100
C	2.36315900	-0.19512100	-2.61144500
H	2.67039500	-0.17231700	-3.66450800
H	2.82064400	0.64714900	-2.09121000
H	2.74301900	-1.11646200	-2.16895900
C	0.33312200	-2.65501700	-2.19377700
H	0.43899200	-3.12012600	-3.18137400

H	1.28806400	-2.75922900	-1.67556600
H	-0.42053300	-3.21616700	-1.63867300
C	0.64083900	-2.88602300	1.13989600
C	2.72832500	-1.79002500	0.66820800
C	3.39642100	-3.04547000	0.60665300
C	2.64297300	-4.22692700	0.82027300
C	1.30131600	-4.13420500	1.09727200
C	3.42925100	-0.57899700	0.51814400
C	4.79229500	-3.04721700	0.35181700
H	3.13790700	-5.19244200	0.78034500
H	0.70664500	-5.02006500	1.28909900
C	5.47414500	-1.86032900	0.19149900
C	4.78868800	-0.62637900	0.28306500
H	5.30998500	-4.00044700	0.29808600
H	6.54298800	-1.86989100	0.00182300
H	5.33265800	0.30520500	0.16337300
N	1.34948400	-1.76412200	0.89278400
O	0.75072500	-0.58511800	0.94108300
H	2.89555900	0.35943600	0.57222900
S	1.23990700	2.91100200	0.26219600
O	1.02615100	4.30887100	-0.11791400
O	-0.05200200	2.10316100	0.26667800
C	1.66813700	2.91376400	2.07327300
O	2.37097000	2.20016500	-0.37969300
F	0.66804400	3.42091900	2.79154100
F	2.77097800	3.64980400	2.26928800
F	1.91431400	1.66013000	2.48432900

C	-0.80874200	-2.73754800	1.44196600
H	-0.97305700	-1.93046000	2.15842900
H	-1.36987500	-2.43138000	0.55530300
H	-1.21927600	-3.67656500	1.81618600
S	-3.34739900	0.41943400	0.87730900
O	-3.99202600	0.67849000	-0.42432700
O	-1.88862200	0.00465400	0.76616500
C	-4.06630000	-1.21767800	1.40164800
O	-3.61997800	1.33471800	1.98097100
F	-3.82168300	-2.15608800	0.45518400
F	-5.38727100	-1.12817200	1.56741200
F	-3.51214300	-1.64254800	2.54808300

Zero-point correction= 0.452167 (Hartree/Particle)

Thermal correction to Energy= 0.493004

Thermal correction to Enthalpy= 0.493948

Thermal correction to Gibbs Free Energy= 0.378651

Sum of electronic and zero-point Energies= -2938.600853

Sum of electronic and thermal Energies= -2938.560017

Sum of electronic and thermal Enthalpies= -2938.559072

Sum of electronic and thermal Free Energies= -2938.674370

E(RB3LYP) = -2939.053020 A.U.

B-int4

1 1

Number of imaginary frequencies: 0

Rh	-0.48940800	0.96487100	-0.22850900
C	0.10088100	3.05586000	-0.06518600
C	-1.33066100	2.93178900	0.20978300

C	-1.48890300	2.10315600	1.35873600
C	-0.16158700	1.67697800	1.78140600
C	0.82051600	2.29721500	0.91409000
C	0.68990300	3.88732700	-1.15569400
H	0.69268200	4.93953100	-0.84460800
H	1.71988000	3.60180800	-1.37502200
H	0.10167500	3.82041700	-2.07409100
C	-2.43113800	3.56610600	-0.57571500
H	-2.68147600	4.54153000	-0.14109200
H	-2.14377400	3.72598000	-1.61677100
H	-3.32967300	2.94668600	-0.56112200
C	-2.77772000	1.70997400	2.00287800
H	-3.07327500	2.47995500	2.72561200
H	-3.57655600	1.60409600	1.26675500
H	-2.68504600	0.75640200	2.52209600
C	0.11134300	0.78449600	2.94188900
H	0.00827900	1.36265000	3.86913100
H	-0.60611600	-0.03793500	2.96367400
H	1.11761600	0.36665000	2.90478900
C	2.30696100	2.18676200	1.04405100
H	2.69207800	2.99472300	1.67636900
H	2.59541900	1.23811200	1.49986600
H	2.80120400	2.25754800	0.07255400
C	2.73312900	0.06191300	-1.95098400
C	2.42657800	-1.22042800	0.06884900
C	3.83788200	-1.27294600	0.26149000
C	4.67793100	-0.64591300	-0.69102900

C	4.13106500	-0.00457700	-1.77902600
C	1.53830000	-1.85784600	0.95782200
C	4.33308000	-1.96067100	1.39990200
H	5.75487600	-0.68671800	-0.56002800
H	4.75807300	0.46330800	-2.52888200
C	3.46321200	-2.56703100	2.27966900
C	2.06756800	-2.52012800	2.04947400
H	5.40640000	-2.00533200	1.55638100
H	3.84700000	-3.09537600	3.14613000
H	1.39336300	-3.02107400	2.73686400
N	1.94247400	-0.51518900	-1.02788000
O	0.60982600	-0.45894000	-1.19846600
H	0.47148300	-1.84163900	0.77564200
S	-2.62334400	-1.22970700	0.08591600
O	-4.05319600	-1.11683600	0.35137000
O	-2.12527600	-0.16744100	-0.91783700
C	-2.33930300	-2.79616900	-0.88252600
O	-1.69858200	-1.32608100	1.24343400
F	-2.97171500	-2.73313500	-2.05050400
F	-2.78563300	-3.83419000	-0.17803800
F	-1.02262400	-2.94183600	-1.09620700
C	2.06568600	0.73217200	-3.10704200
H	1.41632200	0.02374900	-3.63018800
H	1.41897800	1.54654300	-2.76441800
H	2.80934600	1.12941200	-3.79852900

Zero-point correction= 0.422401 (Hartree/Particle)

Thermal correction to Energy= 0.455127

Thermal correction to Enthalpy= 0.456071

Thermal correction to Gibbs Free Energy= 0.357037

Sum of electronic and zero-point Energies= -1976.978136

Sum of electronic and thermal Energies= -1976.945410

Sum of electronic and thermal Enthalpies= -1976.944466

Sum of electronic and thermal Free Energies= -1977.043499

E(RB3LYP) = -1977.400537 A.U.

B-int5

0 1

Number of imaginary frequencies: 0

Rh	-0.96021600	-0.35499600	-0.24429900
C	-1.08629400	0.04118800	1.94462200
C	-2.29391400	-0.58779400	1.48542100
C	-1.94875400	-1.87021000	0.92733600
C	-0.51597100	-2.06804600	1.11721600
C	0.00008200	-0.90071200	1.73834200
O	-2.39917000	2.51586300	0.10161200
O	-2.26751000	0.79073900	-1.36756000
C	-2.66060900	1.95944300	-0.97718000
C	-3.51891300	2.66510400	-2.02332400
H	-4.26358600	1.97828800	-2.43323700
H	-4.00229900	3.54030000	-1.58603500
H	-2.87684000	2.97981000	-2.85254200
C	-0.98650800	1.34728300	2.66726300
H	-1.70132500	2.05930400	2.25583900
H	-1.17890500	1.20974000	3.73922800
H	0.01308200	1.77791800	2.56305600

C	-3.67228100	-0.01376600	1.56783700
H	-4.14966000	-0.33156300	2.50320400
H	-3.63881600	1.07456900	1.52937600
H	-4.28844900	-0.36169600	0.73628300
C	-2.88430600	-2.89279500	0.36523800
H	-3.08933200	-3.67105800	1.11128200
H	-3.83351900	-2.44110200	0.07191800
H	-2.44744700	-3.35695600	-0.52153600
C	0.23272300	-3.30478100	0.73444500
H	0.01490400	-4.11542000	1.44065500
H	-0.05950500	-3.62229100	-0.26956300
H	1.31097100	-3.13305600	0.72935300
C	1.40926500	-0.68286100	2.18890300
H	1.49557300	-0.93675200	3.25270000
H	2.11630000	-1.30119300	1.63484300
H	1.70903800	0.36151100	2.08018200
C	1.75593500	2.43551100	0.04125900
C	2.67751000	0.30981400	-0.60194800
C	3.88182900	0.59933100	0.09853500
C	3.99846900	1.84294900	0.76798000
C	2.95482500	2.73569700	0.72585600
C	2.50430100	-0.90532500	-1.29426500
C	4.90176500	-0.38712900	0.10858600
H	4.91158900	2.07801500	1.30627100
H	3.02075600	3.69847900	1.22006100
C	4.72199200	-1.58519400	-0.54811800
C	3.52205800	-1.83801000	-1.25462000

H	5.82273100	-0.17756100	0.64502500
H	5.50580200	-2.33634800	-0.53164200
H	3.39402300	-2.77933400	-1.77998500
N	1.63808500	1.24133000	-0.57817000
O	0.51982000	0.96542200	-1.22020400
H	1.57698400	-1.09256300	-1.82573100
C	0.60190600	3.36817200	-0.07026900
H	0.43450700	3.61868400	-1.12390100
H	-0.33431700	2.90379700	0.25989800
H	0.79321000	4.28199600	0.49544600
Cl	-0.75930200	-1.78843600	-2.23384000

Zero-point correction= 0.446556 (Hartree/Particle)

Thermal correction to Energy= 0.477212

Thermal correction to Enthalpy= 0.478157

Thermal correction to Gibbs Free Energy= 0.386505

Sum of electronic and zero-point Energies= -1704.449623

Sum of electronic and thermal Energies= -1704.418967

Sum of electronic and thermal Enthalpies= -1704.418023

Sum of electronic and thermal Free Energies= -1704.509674

E(RB3LYP) = -1704.896179 A.U.

B-int6

1 1

Number of imaginary frequencies: 0

Rh	-0.48940800	0.96487100	-0.22850900
C	0.10088100	3.05586000	-0.06518600
C	-1.33066100	2.93178900	0.20978300
C	-1.48890300	2.10315600	1.35873600

C	-0.16158700	1.67697800	1.78140600
C	0.82051600	2.29721500	0.91409000
C	0.68990300	3.88732700	-1.15569400
H	0.69268200	4.93953100	-0.84460800
H	1.71988000	3.60180800	-1.37502200
H	0.10167500	3.82041700	-2.07409100
C	-2.43113800	3.56610600	-0.57571500
H	-2.68147600	4.54153000	-0.14109200
H	-2.14377400	3.72598000	-1.61677100
H	-3.32967300	2.94668600	-0.56112200
C	-2.77772000	1.70997400	2.00287800
H	-3.07327500	2.47995500	2.72561200
H	-3.57655600	1.60409600	1.26675500
H	-2.68504600	0.75640200	2.52209600
C	0.11134300	0.78449600	2.94188900
H	0.00827900	1.36265000	3.86913100
H	-0.60611600	-0.03793500	2.96367400
H	1.11761600	0.36665000	2.90478900
C	2.30696100	2.18676200	1.04405100
H	2.69207800	2.99472300	1.67636900
H	2.59541900	1.23811200	1.49986600
H	2.80120400	2.25754800	0.07255400
C	2.73312900	0.06191300	-1.95098400
C	2.42657800	-1.22042800	0.06884900
C	3.83788200	-1.27294600	0.26149000
C	4.67793100	-0.64591300	-0.69102900
C	4.13106500	-0.00457700	-1.77902600

C	1.53830000	-1.85784600	0.95782200
C	4.33308000	-1.96067100	1.39990200
H	5.75487600	-0.68671800	-0.56002800
H	4.75807300	0.46330800	-2.52888200
C	3.46321200	-2.56703100	2.27966900
C	2.06756800	-2.52012800	2.04947400
H	5.40640000	-2.00533200	1.55638100
H	3.84700000	-3.09537600	3.14613000
H	1.39336300	-3.02107400	2.73686400
N	1.94247400	-0.51518900	-1.02788000
O	0.60982600	-0.45894000	-1.19846600
H	0.47148300	-1.84163900	0.77564200
S	-2.62334400	-1.22970700	0.08591600
O	-4.05319600	-1.11683600	0.35137000
O	-2.12527600	-0.16744100	-0.91783700
C	-2.33930300	-2.79616900	-0.88252600
O	-1.69858200	-1.32608100	1.24343400
F	-2.97171500	-2.73313500	-2.05050400
F	-2.78563300	-3.83419000	-0.17803800
F	-1.02262400	-2.94183600	-1.09620700
C	2.06568600	0.73217200	-3.10704200
H	1.41632200	0.02374900	-3.63018800
H	1.41897800	1.54654300	-2.76441800
H	2.80934600	1.12941200	-3.79852900

Zero-point correction= 0.422401 (Hartree/Particle)

Thermal correction to Energy= 0.455127

Thermal correction to Enthalpy= 0.456071

Thermal correction to Gibbs Free Energy= 0.357037

Sum of electronic and zero-point Energies= -1976.978136

Sum of electronic and thermal Energies= -1976.945410

Sum of electronic and thermal Enthalpies= -1976.944466

Sum of electronic and thermal Free Energies= -1977.043499

E(RB3LYP) = -1977.400537 A.U.

B-tsa1

1 1

Number of imaginary frequencies: 1

Rh	-0.82112900	0.05961900	0.05079200
C	-2.27823500	-0.74064500	1.45642700
C	-2.81608500	-0.90353100	0.12541400
C	-1.91539900	-1.73071200	-0.62003600
C	-0.83509200	-2.14443900	0.27227800
C	-1.07605200	-1.54926600	1.54777400
O	-0.05061100	2.52037000	-1.77807900
O	-1.68921200	1.91755300	-0.36811100
C	-1.12111800	2.75217100	-1.16177300
C	-1.79523900	4.09500500	-1.32248300
H	-1.40858700	4.76655500	-0.54847600
H	-1.55605400	4.51993800	-2.29787200
H	-2.87398500	4.00411100	-1.18890300
C	-2.91660700	0.03288800	2.56532100
H	-2.17193700	0.40136200	3.27396500
H	-3.46658000	0.89107800	2.17393900
H	-3.62167400	-0.60214800	3.11570400
C	-4.05653700	-0.23483400	-0.37267300

H	-4.91843900	-0.55679700	0.22108500
H	-3.96017900	0.85131700	-0.27753500
H	-4.25321600	-0.47259300	-1.41871900
C	-2.09789800	-2.19135400	-2.03169600
H	-2.69992800	-3.10780100	-2.04950900
H	-2.61088900	-1.43999100	-2.63532600
H	-1.13976700	-2.41330900	-2.50407400
C	0.26747300	-3.09401800	-0.07910200
H	-0.07309100	-4.12891200	0.04084500
H	0.59172700	-2.96206600	-1.11275100
H	1.13840900	-2.95060500	0.56344000
C	-0.22389600	-1.66468300	2.76964600
H	-0.69736800	-2.33682500	3.49438900
H	0.76595700	-2.06039500	2.53662300
H	-0.10181800	-0.68807400	3.24445800
C	2.92419200	0.89238600	1.65842800
C	2.08046600	0.14169900	-0.45868400
C	3.33702100	-0.42289600	-0.78969700
C	4.40620500	-0.28215600	0.13118400
C	4.19742700	0.38892100	1.31383300
C	0.96536100	0.12476000	-1.34214300
C	3.44210700	-1.09902100	-2.03548700
H	5.38007600	-0.69821500	-0.10635700
H	5.00074700	0.52437400	2.02873800
C	2.36135300	-1.16771500	-2.89135700
C	1.14156200	-0.53897100	-2.55360000
H	4.39289800	-1.54812700	-2.30615000

H	2.45923900	-1.67531700	-3.84576500
H	0.33190700	-0.52902100	-3.27765600
N	1.91212200	0.72829900	0.78523600
O	0.68770100	1.13238000	1.14036800
H	0.33843300	1.20356200	-1.46282000
C	2.60881900	1.57312200	2.94867400
H	2.20129100	2.57167100	2.76210400
H	1.83464600	1.02015600	3.49046900
H	3.50215700	1.65241300	3.56896000

Zero-point correction= 0.439873 (Hartree/Particle)

Thermal correction to Energy= 0.468782

Thermal correction to Enthalpy= 0.469726

Thermal correction to Gibbs Free Energy= 0.380493

Sum of electronic and zero-point Energies= -1244.008261

Sum of electronic and thermal Energies= -1243.979351

Sum of electronic and thermal Enthalpies= -1243.978407

Sum of electronic and thermal Free Energies= -1244.067640

E(RB3LYP) = -1244.448134 A.U.

B-tsa2

0 1

Number of imaginary frequencies: 1

Rh	0.98821400	-0.00450400	-0.07283300
C	0.54722200	-0.72921000	-2.11721100
C	1.68821100	0.15599100	-2.16280400
C	2.71601100	-0.40504300	-1.33569800
C	2.24103500	-1.68777700	-0.83421500
C	0.93885100	-1.90107400	-1.35986200

O	0.42111100	1.00825600	2.90429800
O	2.19063200	0.36154600	1.67413200
C	1.66870400	0.92368200	2.68559400
C	2.59737300	1.55872800	3.69461000
H	2.16190600	1.51633100	4.69421600
H	3.57582200	1.07621200	3.67228500
H	2.72256600	2.61128100	3.41855600
C	-0.73028300	-0.57197600	-2.88121000
H	-1.05053900	0.46903800	-2.84323100
H	-0.59853100	-0.88541500	-3.92507600
H	-1.52344200	-1.18173300	-2.44180600
C	1.79050500	1.42727100	-2.94247200
H	2.27030600	1.22511300	-3.90853800
H	0.80449100	1.85880500	-3.10491600
H	2.39401300	2.16550000	-2.40968200
C	4.06368100	0.17257000	-1.03673700
H	4.85284900	-0.42719400	-1.50606800
H	4.14770500	1.19647000	-1.40445000
H	4.23643600	0.18555700	0.04358600
C	3.03484100	-2.59585300	0.05276400
H	3.82486500	-3.10470700	-0.51282000
H	3.50775500	-2.02076900	0.85395900
H	2.40149300	-3.35682600	0.51328300
C	0.11519500	-3.14008800	-1.24592200
H	0.19046000	-3.70163400	-2.18564600
H	0.44891500	-3.78472700	-0.43337300
H	-0.93703200	-2.90850400	-1.07914900

C	-3.68368900	0.76451900	-0.25120200
C	-2.04399800	-0.63426900	0.80522600
C	-2.86085500	-1.77845100	0.58239800
C	-4.06404800	-1.63552800	-0.15509000
C	-4.41871500	-0.38257400	-0.60365700
C	-0.72705400	-0.72297400	1.33136900
C	-2.41679000	-3.01337600	1.13028300
H	-4.68494600	-2.50334700	-0.35447500
H	-5.31376500	-0.23762300	-1.19990800
C	-1.20940000	-3.09491500	1.79289400
C	-0.35407600	-1.97130000	1.83473200
H	-3.05190200	-3.88843400	1.01923600
H	-0.89251500	-4.03760800	2.23136100
H	0.64102700	-2.08255500	2.26064800
N	-2.58140400	0.63575800	0.53736800
O	-2.03094100	1.66404100	1.05516700
H	-0.16046200	0.35059000	2.04993400
C	-4.05915500	2.16534700	-0.60134200
H	-4.26651400	2.74395400	0.30557500
H	-3.20749700	2.64394800	-1.09769600
H	-4.93546500	2.17832200	-1.25332700
O	-0.85890200	2.24470700	-1.56204400
O	0.63522400	2.02128900	0.13083100
C	-0.23879400	2.67052500	-0.57988000
C	-0.46179100	4.09056800	-0.07958500
H	0.42734300	4.49027700	0.41242000
H	-0.76693700	4.73374600	-0.90799100

H	-1.27309800	4.04083900	0.65202900

Zero-point correction= 0.490958 (Hartree/Particle)

Thermal correction to Energy= 0.524787

Thermal correction to Enthalpy= 0.525732

Thermal correction to Gibbs Free Energy= 0.427667

Sum of electronic and zero-point Energies= -1472.626201

Sum of electronic and thermal Energies= -1472.592372

Sum of electronic and thermal Enthalpies= -1472.591428

Sum of electronic and thermal Free Energies= -1472.689492

E(RB3LYP) = -1473.117159 A.U.

B-tsa3

1 1

Number of imaginary frequencies: 1

Rh	-1.03038600	-0.07430100	0.13226000
C	-2.61342200	-0.68904900	1.56625100
C	-2.92497300	0.61372200	1.08625100
C	-3.08578200	0.53092800	-0.36631100
C	-2.90828200	-0.82917500	-0.75886800
C	-2.52787000	-1.58660500	0.42233000
C	-2.31237500	-1.09245300	2.97377600
H	-3.02084000	-1.85940700	3.30436400
H	-1.30288900	-1.50990900	3.04086500
H	-2.37496600	-0.24709800	3.65929400
C	-3.05250600	1.88025600	1.86832800
H	-4.09588400	2.21622900	1.86997100
H	-2.73124500	1.75353600	2.90276200
H	-2.44335200	2.66775700	1.41633600

C	-3.42462100	1.69538500	-1.23963700
H	-4.47635900	1.97336700	-1.10288300
H	-2.80925500	2.56042900	-0.97979800
H	-3.26770400	1.46919200	-2.29541100
C	-3.12727500	-1.39066600	-2.12671000
H	-4.18635900	-1.65196600	-2.23945000
H	-2.88210900	-0.66686900	-2.90665500
H	-2.54074800	-2.29506300	-2.29207100
C	-2.30759800	-3.06456200	0.49604600
H	-3.26255500	-3.58492200	0.63765100
H	-1.84873600	-3.44441300	-0.41896500
H	-1.65870800	-3.32134500	1.33628400
C	2.55775600	-1.56061200	1.73094800
C	1.42222600	-1.63261200	-0.38025700
C	2.30228400	-2.63994000	-0.84672500
C	3.34702300	-3.07596900	0.00562800
C	3.48228400	-2.51223300	1.25443500
C	0.41601500	-1.03146000	-1.19819800
C	2.08215700	-3.14647000	-2.15672100
H	4.03865600	-3.83895800	-0.33687000
H	4.28914200	-2.80482200	1.91618600
C	1.06676400	-2.64317300	-2.94343200
C	0.26169500	-1.58261600	-2.47295300
H	2.73783000	-3.92702500	-2.53072700
H	0.91468300	-3.02937300	-3.94608700
H	-0.44989500	-1.12654500	-3.15431500
N	1.53959100	-1.20125700	0.92353400

O	0.59481900	-0.39619900	1.42259900
H	0.59023500	0.25721100	-1.43910400
S	0.71618600	2.53236500	-0.90406900
O	0.47881200	3.83840900	-1.48959200
O	-0.31202600	2.03895500	0.08263000
C	2.28047900	2.62786900	0.11489200
O	1.02424700	1.41213800	-1.89383500
F	2.04200000	3.30698700	1.23246200
F	3.23909300	3.21775300	-0.58670700
F	2.67010400	1.37878300	0.43326300
C	2.60691600	-0.93003200	3.08157100
H	2.63665400	0.15923200	2.97491800
H	1.70031300	-1.16369900	3.64903500
H	3.48240700	-1.27234600	3.63389900

Zero-point correction= 0.416545 (Hartree/Particle)

Thermal correction to Energy= 0.448628

Thermal correction to Enthalpy= 0.449572

Thermal correction to Gibbs Free Energy= 0.353108

Sum of electronic and zero-point Energies= -1976.949057

Sum of electronic and thermal Energies= -1976.916973

Sum of electronic and thermal Enthalpies= -1976.916029

Sum of electronic and thermal Free Energies= -1977.012494

E(RB3LYP) = -1977.365602 A.U.

B-tsa4

0 1

Number of imaginary frequencies: 1

Rh	0.63634800	0.25123300	-1.02475700

C	2.09085800	0.01909800	-2.63917700
C	1.36974600	-1.20657300	-2.53479100
C	-0.03661500	-0.93586800	-2.78171400
C	-0.16722000	0.45924500	-3.08958900
C	1.13353800	1.07524100	-2.95155700
C	3.55540500	0.18553500	-2.38299600
H	4.13476500	-0.19141200	-3.23384400
H	3.81327400	1.23462900	-2.23020300
H	3.84047100	-0.37039500	-1.48544500
C	1.91354200	-2.55447700	-2.19994900
H	1.95253600	-3.16554000	-3.11068400
H	2.90644700	-2.49046900	-1.75843600
H	1.26539800	-3.05566300	-1.47874800
C	-1.08996000	-1.99544100	-2.83551900
H	-0.88764000	-2.66257800	-3.68285100
H	-1.09222700	-2.59489100	-1.92168700
H	-2.08641600	-1.57167000	-2.93787100
C	-1.42756900	1.13930900	-3.51528000
H	-1.54480800	1.02614800	-4.60039500
H	-2.29158600	0.69354300	-3.02218300
H	-1.40458400	2.20652800	-3.28833900
C	1.47183500	2.50955800	-3.21359700
H	1.80857200	2.64579600	-4.24845000
H	0.60554600	3.15378300	-3.05072100
H	2.27164700	2.84711300	-2.55020800
C	2.33678700	2.57415000	2.03266000
C	0.20491700	2.47851300	0.92237200

C	-0.21308800	3.65998000	1.58966300
C	0.64878300	4.23348900	2.55681200
C	1.87782500	3.66456000	2.79839600
C	-0.64856600	1.73529300	0.04919300
C	-1.47331600	4.20878800	1.23417300
H	0.32826500	5.11660500	3.10077900
H	2.54698100	4.06912200	3.54880700
C	-2.24996900	3.59427800	0.27686100
C	-1.85273900	2.36063500	-0.28435500
H	-1.80708500	5.11519300	1.73081800
H	-3.20934300	4.01948900	-0.00128700
H	-2.55819400	1.81038800	-0.89669900
N	1.51094200	2.06674500	1.09686500
O	2.02127100	1.17979500	0.24444200
H	-1.04461300	0.52876800	0.34389000
S	-2.94499600	-1.03269000	0.06282100
O	-3.14543800	-0.29113300	-1.20594900
O	-2.82578800	-2.48857900	-0.02745000
C	-4.49926300	-0.69085600	1.02516400
O	-1.91266600	-0.36445000	0.95633900
F	-5.55809800	-1.18317700	0.37070400
F	-4.65784800	0.63700400	1.16048800
F	-4.43978600	-1.24467500	2.23842200
C	3.69811600	1.97540000	2.13579800
H	3.60074200	0.90704300	2.35395100
H	4.22401700	2.05773800	1.17882900
H	4.27354600	2.47427100	2.91720400

S	1.91783200	-1.50662000	1.33519300
O	3.15147000	-1.57620900	0.52793600
O	1.96557200	-0.72188400	2.57889900
C	1.58379200	-3.26167800	1.85855500
O	0.65353300	-1.28116900	0.50742700
F	2.60010000	-3.70112100	2.61256700
F	1.48602400	-4.05169800	0.77474800
F	0.45316000	-3.34158900	2.55770000

Zero-point correction= 0.446108 (Hartree/Particle)

Thermal correction to Energy= 0.486653

Thermal correction to Enthalpy= 0.487597

Thermal correction to Gibbs Free Energy= 0.371416

Sum of electronic and zero-point Energies= -2938.556472

Sum of electronic and thermal Energies= -2938.515927

Sum of electronic and thermal Enthalpies= -2938.514983

Sum of electronic and thermal Free Energies= -2938.631164

E(RB3LYP) = -2939.002580 A.U.

B-tsa5

0 1

Number of imaginary frequencies: 1

Rh	-0.62615800	-0.51292800	0.14195600
C	-0.35140700	-2.24420900	-1.13587600
C	-1.73437300	-2.15639900	-0.71346000
C	-2.27250300	-0.91437600	-1.23071900
C	-1.23838400	-0.27778800	-1.99992100
C	-0.03985400	-1.07995000	-1.92271300
O	-0.98374600	2.58223100	1.66482600

O	-2.26852300	2.38844800	-0.17296600
C	-2.10033200	2.63039100	1.05370500
C	-3.32036900	2.95271400	1.90860700
H	-3.65771400	2.01209400	2.35720000
H	-3.06030200	3.63822700	2.71855000
H	-4.12663900	3.36411800	1.29655500
C	0.58924100	-3.35633300	-0.79670700
H	0.39070100	-3.74214200	0.20524400
H	0.47513200	-4.18070400	-1.51102300
H	1.62743100	-3.01975800	-0.83110900
C	-2.49981500	-3.18069600	0.05898300
H	-3.14396000	-3.75212500	-0.62075300
H	-1.83312400	-3.87823900	0.56907300
H	-3.11936400	-2.69735800	0.81641300
C	-3.65575300	-0.37984400	-1.04217000
H	-4.14431000	-0.86436400	-0.19591200
H	-3.60350300	0.69397500	-0.83494800
H	-4.25720800	-0.55120200	-1.94413900
C	-1.42138500	0.99983700	-2.74410000
H	-2.15225900	0.84368100	-3.54700000
H	-1.81104100	1.75865600	-2.05657400
H	-0.48819200	1.35167000	-3.18562300
C	1.26247700	-0.77925500	-2.59846100
H	1.26466900	-1.15914900	-3.62724500
H	1.44733100	0.29630200	-2.63111300
H	2.09985800	-1.24052300	-2.06938700
C	3.33115900	-0.89127300	1.33775000

C	2.08626100	0.87572100	0.27472300
C	3.27718900	1.34589500	-0.35110200
C	4.50650100	0.70592200	-0.05406700
C	4.52651000	-0.37004900	0.80146500
C	0.82822700	1.50513700	0.09607600
C	3.16535400	2.42688500	-1.26224300
H	5.42210300	1.07088200	-0.50948700
H	5.45400200	-0.87182700	1.05329300
C	1.93465000	3.00193300	-1.50573100
C	0.78939800	2.56261100	-0.80724000
H	4.06305500	2.78912400	-1.75513100
H	1.85207500	3.82834700	-2.20600300
H	-0.16614400	3.06635200	-0.91971900
N	2.16535400	-0.28584500	1.04034200
O	1.04650100	-0.84115900	1.48052700
H	-0.06515500	1.66882600	0.89813500
C	3.25158100	-2.11465600	2.19136800
H	2.77517000	-1.88106800	3.14862600
H	2.61667200	-2.86837100	1.71412200
H	4.24739500	-2.52642500	2.36469800
Cl	-1.93689100	-0.51034000	2.14733900

Zero-point correction= 0.441022 (Hartree/Particle)

Thermal correction to Energy= 0.471617

Thermal correction to Enthalpy= 0.472561

Thermal correction to Gibbs Free Energy= 0.381534

Sum of electronic and zero-point Energies= -1704.391880

Sum of electronic and thermal Energies= -1704.361285

Sum of electronic and thermal Enthalpies= -1704.360341

Sum of electronic and thermal Free Energies= -1704.451368

E(RB3LYP) = -1704.832902 A.U.

B-tsa6

0 1

Number of imaginary frequencies: 1

Rh	-0.72820900	0.01281300	0.14193400
C	-2.15331100	0.58544200	1.70822000
C	-2.79114300	0.76936400	0.43595800
C	-2.85205700	-0.51940700	-0.22118100
C	-2.28051900	-1.49087600	0.66727600
C	-1.82024500	-0.81482200	1.85872600
O	-0.59128800	3.08450700	-0.71343700
O	-0.19937900	1.03037000	-1.60200400
C	-0.20808800	2.33199100	-1.61541300
C	0.36395700	2.88963900	-2.91800500
H	-0.04588500	2.35097400	-3.77555600
H	0.15211700	3.95752000	-2.99401900
H	1.44831900	2.73373000	-2.92745800
C	-1.82406800	1.69847900	2.65276100
H	-1.35031200	2.51705800	2.10250900
H	-2.73565500	2.07984300	3.12701200
H	-1.13953100	1.37024200	3.43640400
C	-3.36414100	2.04776400	-0.08357400
H	-4.41946900	2.12102900	0.21095900
H	-2.81622500	2.90825900	0.29562300
H	-3.30842800	2.08659600	-1.17218800

C	-3.47210200	-0.81398400	-1.54907700
H	-4.45377000	-1.28495600	-1.41090200
H	-3.60966700	0.10065600	-2.12790500
H	-2.82854000	-1.48026900	-2.12949200
C	-2.20466700	-2.95386100	0.36986900
H	-3.20540800	-3.39581200	0.45099400
H	-1.84237500	-3.11050700	-0.65147900
H	-1.54660500	-3.47604600	1.06661900
C	-1.19596200	-1.45814900	3.05923500
H	-1.95956200	-1.77717200	3.77914900
H	-0.61261400	-2.33611900	2.77256800
H	-0.52050700	-0.76605300	3.56766400
C	3.01155600	1.71678400	0.53767800
C	2.22241800	-0.52595500	0.14946500
C	3.55729200	-1.01395400	0.19036500
C	4.61802700	-0.07671400	0.28128100
C	4.33941000	1.26649200	0.39275200
C	1.10043700	-1.35768700	-0.13836800
C	3.74716700	-2.41919900	0.15916000
H	5.64403800	-0.43109100	0.25957100
H	5.13194500	2.00495300	0.43452900
C	2.65450200	-3.25654000	0.09545500
C	1.35782700	-2.72831700	-0.08701700
H	4.75819800	-2.81402800	0.19451000
H	2.79283800	-4.33338200	0.09983200
H	0.55197400	-3.40573600	-0.34527900
N	2.02376200	0.80272100	0.49110000

O	0.82104000	1.18239000	0.90068500
H	0.29162100	-1.29011700	-1.13915300
C	2.60878000	3.12382700	0.84011900
H	1.73546100	3.40599200	0.24316600
H	2.30282600	3.21272800	1.88939900
H	3.44348700	3.80307900	0.65598900
Cl	-0.35227000	-2.07806200	-2.65493400

Zero-point correction= 0.439449 (Hartree/Particle)

Thermal correction to Energy= 0.470186

Thermal correction to Enthalpy= 0.471130

Thermal correction to Gibbs Free Energy= 0.378078

Sum of electronic and zero-point Energies= -1704.383700

Sum of electronic and thermal Energies= -1704.352963

Sum of electronic and thermal Enthalpies= -1704.352019

Sum of electronic and thermal Free Energies= -1704.445071

E(RB3LYP) = -1704.823149 A.U.

B-tsa7

0 1

Number of imaginary frequencies: 1

Rh	-0.95111300	-0.93707200	0.14174900
C	-0.16413200	-1.83200300	-1.71858800
C	-0.23523500	-2.84321800	-0.70255700
C	-1.61570200	-2.95769000	-0.28321900
C	-2.40121500	-2.05448000	-1.10622500
C	-1.50886900	-1.32686400	-1.95034700
O	-0.62131200	0.58306300	2.90413600
O	0.23450900	-1.18540500	1.82049200

C	0.28583600	-0.26794600	2.71945400
C	1.55003200	-0.22359200	3.53651000
H	2.26210300	0.35879200	2.93799300
H	1.37503500	0.27115200	4.49283600
H	1.95800000	-1.22612900	3.67311800
C	1.04934100	-1.37816000	-2.45275300
H	1.22658200	-0.30699600	-2.32061800
H	1.94689700	-1.86995900	-2.08433600
H	0.91841000	-1.58496700	-3.52262500
C	0.94165900	-3.56706900	-0.13594000
H	1.31610300	-4.29403900	-0.86674200
H	1.73719100	-2.85154000	0.09066400
H	0.67801100	-4.09991800	0.77841300
C	-2.14749300	-3.93021300	0.72351200
H	-2.31346700	-4.91314300	0.26583800
H	-1.44296700	-4.05341400	1.54862800
H	-3.09703600	-3.58948100	1.14290900
C	-3.89139600	-1.92957600	-1.09226600
H	-4.31882700	-2.61908000	-1.83060000
H	-4.30876600	-2.18264300	-0.11630200
H	-4.21343200	-0.91771000	-1.34431100
C	-1.85793100	-0.26877900	-2.95035500
H	-1.99986800	-0.70422300	-3.94681700
H	-2.77670600	0.25485300	-2.67524800
H	-1.05163300	0.46565800	-3.01855600
C	-0.55828600	3.16797600	-0.65456300
C	-2.24527600	1.73929000	0.27983800

C	-3.25908700	2.68476300	-0.00325400
C	-2.88248600	3.90880400	-0.61405800
C	-1.55478400	4.14458000	-0.88593600
C	-2.47985900	0.54165000	1.01178000
C	-4.58654100	2.34158700	0.37020500
H	-3.63870800	4.65462900	-0.83836700
H	-1.23293300	5.08473400	-1.31929000
C	-4.84861400	1.15857800	1.03358900
C	-3.79560600	0.28368600	1.38308000
H	-5.38804500	3.03916400	0.14455000
H	-5.86632000	0.91970500	1.32764400
H	-4.00893600	-0.59205900	1.98948500
N	-0.94992300	1.98171700	-0.14464100
O	-0.05766000	1.00714200	-0.04852500
H	-1.61030700	0.32412800	1.84418300
S	3.13660200	0.50166700	-0.15491900
O	2.83737100	1.45260600	0.94317100
O	2.68574800	-0.89261400	0.07533600
C	4.98991100	0.35121800	-0.09844400
O	2.88638800	1.01655200	-1.52677600
F	5.39193500	-0.10638100	1.10027300
F	5.57566500	1.54137000	-0.31125200
F	5.42647400	-0.50501600	-1.04027500
C	0.88740900	3.33184900	-0.95427300
H	1.48585300	3.13641100	-0.05556100
H	1.24401900	2.56730800	-1.65317600
H	1.08661300	4.33146900	-1.34375500

Zero-point correction= 0.469280 (Hartree/Particle)

Thermal correction to Energy= 0.506383

Thermal correction to Enthalpy= 0.507328

Thermal correction to Gibbs Free Energy= 0.400003

Sum of electronic and zero-point Energies= -2205.595247

Sum of electronic and thermal Energies= -2205.558144

Sum of electronic and thermal Enthalpies= -2205.557200

Sum of electronic and thermal Free Energies= -2205.664525

E(RB3LYP) = -2206.064528 A.U.

B-tsa8

0 1

Number of imaginary frequencies: 1

Rh	0.88632200	-0.71366200	-0.20120500
C	2.60710300	-1.97421000	-0.72377700
C	1.40729700	-2.67277800	-1.07582700
C	0.68730700	-1.87647600	-2.03965200
C	1.51510800	-0.72086600	-2.35804600
C	2.66793700	-0.75833100	-1.52959200
O	1.29740900	-2.51967800	2.38814000
O	-0.36102800	-1.54619500	1.19282800
C	0.12222200	-2.18128900	2.22825700
C	-0.95101100	-2.46221900	3.26886500
H	-0.64299800	-3.29306400	3.90640400
H	-1.06822100	-1.56391200	3.88478400
H	-1.91493600	-2.64932800	2.79290800
C	3.63329000	-2.43604500	0.26116900
H	4.16631500	-3.31213800	-0.12738900

H	4.36835900	-1.65387900	0.46176700
H	3.13805900	-2.69707500	1.19975900
C	0.94019700	-3.97043400	-0.49982700
H	1.22658000	-4.79694200	-1.16205300
H	1.37052500	-4.12967200	0.48874800
H	-0.14692100	-3.97201700	-0.39745900
C	-0.58914300	-2.26516300	-2.71436600
H	-0.38301100	-2.93095300	-3.56236100
H	-1.25912200	-2.76867200	-2.01727800
H	-1.12924800	-1.39079500	-3.07867500
C	1.21364800	0.29833000	-3.41063800
H	1.69431800	0.00384700	-4.35165900
H	0.14127000	0.37698500	-3.59184100
H	1.57974500	1.28954600	-3.13602500
C	3.77056100	0.25373200	-1.47145000
H	4.65899500	-0.10290200	-2.00575000
H	3.46376400	1.20205800	-1.91796600
H	4.05817700	0.44505100	-0.43390200
C	2.50754300	2.54859100	1.84684100
C	0.79932100	2.20688500	0.19034900
C	0.88821200	3.56768100	-0.20578300
C	1.78367100	4.42197200	0.48493400
C	2.55091200	3.91648900	1.50923200
C	-0.12283600	1.28205900	-0.37828000
C	0.06685900	3.98997300	-1.28495400
H	1.85321300	5.46780300	0.20200500
H	3.23546700	4.54959400	2.06240200

C	-0.79628500	3.10086700	-1.89099400
C	-0.90301900	1.77161000	-1.42735500
H	0.12297300	5.02506600	-1.60937700
H	-1.43062400	3.43450900	-2.70704000
H	-1.66378100	1.11691900	-1.83964900
N	1.66957600	1.74115800	1.16684300
O	1.70682400	0.44092100	1.42600200
H	-0.95892000	0.64199300	0.41769100
S	-3.03851500	-0.46494100	0.45419500
O	-2.55293400	-0.92194000	-0.86261500
O	-3.59829100	-1.44331600	1.38577500
C	-4.45288500	0.66847700	0.02670300
O	-2.08765100	0.54899300	1.10026300
F	-5.42484600	-0.01738800	-0.58812000
F	-4.02503800	1.63685800	-0.80865800
F	-4.95611500	1.24683100	1.12210000
C	3.36393600	1.90037900	2.88388600
H	2.74189700	1.40188700	3.63411200
H	3.97479600	1.11188900	2.43126600
H	4.00771300	2.63753300	3.36658800

Zero-point correction= 0.467955 (Hartree/Particle)

Thermal correction to Energy= 0.505533

Thermal correction to Enthalpy= 0.506477

Thermal correction to Gibbs Free Energy= 0.397745

Sum of electronic and zero-point Energies= -2205.588027

Sum of electronic and thermal Energies= -2205.550450

Sum of electronic and thermal Enthalpies= -2205.549505

Sum of electronic and thermal Free Energies= -2205.658237

E(RB3LYP) = -2206.055982 A.U.

B-tsa9

1 1

Number of imaginary frequencies: 1

Rh	-1.03038600	-0.07430100	0.13226000
C	-2.61342200	-0.68904900	1.56625100
C	-2.92497300	0.61372200	1.08625100
C	-3.08578200	0.53092800	-0.36631100
C	-2.90828200	-0.82917500	-0.75886800
C	-2.52787000	-1.58660500	0.42233000
C	-2.31237500	-1.09245300	2.97377600
H	-3.02084000	-1.85940700	3.30436400
H	-1.30288900	-1.50990900	3.04086500
H	-2.37496600	-0.24709800	3.65929400
C	-3.05250600	1.88025600	1.86832800
H	-4.09588400	2.21622900	1.86997100
H	-2.73124500	1.75353600	2.90276200
H	-2.44335200	2.66775700	1.41633600
C	-3.42462100	1.69538500	-1.23963700
H	-4.47635900	1.97336700	-1.10288300
H	-2.80925500	2.56042900	-0.97979800
H	-3.26770400	1.46919200	-2.29541100
C	-3.12727500	-1.39066600	-2.12671000
H	-4.18635900	-1.65196600	-2.23945000
H	-2.88210900	-0.66686900	-2.90665500
H	-2.54074800	-2.29506300	-2.29207100

C	-2.30759800	-3.06456200	0.49604600
H	-3.26255500	-3.58492200	0.63765100
H	-1.84873600	-3.44441300	-0.41896500
H	-1.65870800	-3.32134500	1.33628400
C	2.55775600	-1.56061200	1.73094800
C	1.42222600	-1.63261200	-0.38025700
C	2.30228400	-2.63994000	-0.84672500
C	3.34702300	-3.07596900	0.00562800
C	3.48228400	-2.51223300	1.25443500
C	0.41601500	-1.03146000	-1.19819800
C	2.08215700	-3.14647000	-2.15672100
H	4.03865600	-3.83895800	-0.33687000
H	4.28914200	-2.80482200	1.91618600
C	1.06676400	-2.64317300	-2.94343200
C	0.26169500	-1.58261600	-2.47295300
H	2.73783000	-3.92702500	-2.53072700
H	0.91468300	-3.02937300	-3.94608700
H	-0.44989500	-1.12654500	-3.15431500
N	1.53959100	-1.20125700	0.92353400
O	0.59481900	-0.39619900	1.42259900
H	0.59023500	0.25721100	-1.43910400
S	0.71618600	2.53236500	-0.90406900
O	0.47881200	3.83840900	-1.48959200
O	-0.31202600	2.03895500	0.08263000
C	2.28047900	2.62786900	0.11489200
O	1.02424700	1.41213800	-1.89383500
F	2.04200000	3.30698700	1.23246200

F	3.23909300	3.21775300	-0.58670700
F	2.67010400	1.37878300	0.43326300
C	2.60691600	-0.93003200	3.08157100
H	2.63665400	0.15923200	2.97491800
H	1.70031300	-1.16369900	3.64903500
H	3.48240700	-1.27234600	3.63389900

Zero-point correction= 0.416545 (Hartree/Particle)

Thermal correction to Energy= 0.448628

Thermal correction to Enthalpy= 0.449572

Thermal correction to Gibbs Free Energy= 0.353108

Sum of electronic and zero-point Energies= -1976.949057

Sum of electronic and thermal Energies= -1976.916973

Sum of electronic and thermal Enthalpies= -1976.916029

Sum of electronic and thermal Free Energies= -1977.012494

E(RB3LYP) = -1977.365602 A.U.

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0 1

Number of imaginary frequencies: 0

Rh	0.18870900	0.58028400	0.27323000
C	-0.80418100	0.25983700	2.24845000
C	0.60000300	0.11824700	2.40198900
C	1.22676600	1.37483100	2.00241300
C	0.18110600	2.28711600	1.63346000
C	-1.07941200	1.59751300	1.73892700
O	-1.42592600	2.75108800	-1.45452500
O	0.55012600	1.64506300	-1.44735400
C	-0.33317100	2.44341900	-1.95720100

C	0.09718800	2.99567600	-3.30918100
H	0.03380200	2.19335600	-4.05129900
H	-0.55406300	3.81963200	-3.60508800
H	1.14032400	3.31843500	-3.27180500
C	-1.83966000	-0.77306800	2.56437000
H	-1.45740700	-1.78555600	2.41884500
H	-2.15613900	-0.67979400	3.61012900
H	-2.72660500	-0.65285700	1.93984800
C	1.35505200	-1.09113700	2.85476600
H	1.79550000	-0.91536800	3.84323700
H	0.70685200	-1.96730800	2.92529900
H	2.16503600	-1.31494600	2.15693500
C	2.68798900	1.67636700	2.08464400
H	2.92138300	2.09443200	3.07259200
H	3.28647400	0.77917700	1.93103100
H	2.98827400	2.38599000	1.31430100
C	0.36414700	3.69909000	1.17821000
H	0.29595100	4.37800000	2.03735500
H	1.34215900	3.83227700	0.71233800
H	-0.40234900	3.96623200	0.44967600
C	-2.42244500	2.22694200	1.54682300
H	-2.64240600	2.90281000	2.38294500
H	-2.43252200	2.79035300	0.61265600
H	-3.21463200	1.47843000	1.49948900
C	-1.63594700	-2.66451100	-0.36583000
C	-3.25740700	-0.91881000	-0.69964100
C	-4.30707600	-1.78895400	-0.29074400

C	-3.98129500	-3.11662200	0.08449500
C	-2.67358300	-3.53394800	0.03888900
C	-3.51240800	0.41060400	-1.09021100
C	-5.63083300	-1.27870500	-0.27992100
H	-4.77079200	-3.79334200	0.39685000
H	-2.39993900	-4.54759200	0.30921800
C	-5.88019100	0.02185700	-0.66161900
C	-4.81717900	0.86325400	-1.06564000
H	-6.43906200	-1.93451200	0.03050200
H	-6.89609400	0.40470200	-0.65223200
H	-5.02192500	1.88852300	-1.35756800
N	-1.94572100	-1.39694500	-0.70868500
O	-0.99373500	-0.58528600	-1.13279800
H	-2.69064300	1.06201100	-1.37008400
S	3.02806800	-0.33690600	-1.14368800
O	3.52351400	0.99348800	-0.77024100
O	1.76818900	-0.75974800	-0.38289400
C	4.20876900	-1.51862700	-0.31615100
O	3.02202200	-0.73199100	-2.55275400
F	4.26812700	-1.27035000	1.01683100
F	5.44161800	-1.38732900	-0.81381800
F	3.80976400	-2.78954200	-0.47424900
C	-0.20331700	-3.06892100	-0.44433800
H	0.24435200	-2.72149100	-1.37867300
H	0.38641300	-2.57820900	0.33576900
H	-0.10952600	-4.15170500	-0.34388400

Zero-point correction= 0.474254 (Hartree/Particle)

Thermal correction to Energy= 0.511982

Thermal correction to Enthalpy= 0.512926

Thermal correction to Gibbs Free Energy= 0.404209

Sum of electronic and zero-point Energies= -2205.638754

Sum of electronic and thermal Energies= -2205.601026

Sum of electronic and thermal Enthalpies= -2205.600082

Sum of electronic and thermal Free Energies= -2205.708798

E(RB3LYP) = -2206.113007 A.U.

B-2

1 1

Number of imaginary frequencies: 0

Rh	-1.10388800	-0.02048200	-0.14876600
C	-1.22625800	1.76642100	1.12060400
C	-2.53409400	1.16494300	1.00505400
C	-2.46401600	-0.17222200	1.52973400
C	-1.10728800	-0.38565900	2.01044600
C	-0.35643300	0.80785000	1.77107100
O	-1.29732800	-2.01092900	-1.02927600
O	-2.18144500	-0.26564900	-2.00455100
C	-1.90523500	-1.51116100	-2.03647700
C	-2.24753600	-2.34925700	-3.23053000
H	-1.38857200	-2.35251000	-3.91029700
H	-2.44699900	-3.37817300	-2.92586200
H	-3.10417500	-1.92748200	-3.75836800
C	-0.87153700	3.18073000	0.78443900
H	0.19436200	3.28604000	0.57205200
H	-1.43071400	3.54179300	-0.08126000

H	-1.10673400	3.83746000	1.63074400
C	-3.74133800	1.80158400	0.39702100
H	-4.36798300	2.23515800	1.18540400
H	-3.46695300	2.59877000	-0.29568000
H	-4.33904600	1.07101200	-0.15140900
C	-3.58403100	-1.15922600	1.62507900
H	-3.99705000	-1.16656400	2.64047200
H	-4.39137400	-0.91169800	0.93395700
H	-3.23712300	-2.16834000	1.39135500
C	-0.60626200	-1.64285700	2.64431500
H	-0.80464100	-1.62247300	3.72262600
H	-1.10799200	-2.51807100	2.22615800
H	0.46815500	-1.76471800	2.49530900
C	1.06214300	1.05851200	2.17028700
H	1.08260000	1.58822300	3.13007900
H	1.62191800	0.12980500	2.28656100
H	1.58223700	1.68293100	1.44047900
C	2.16066900	1.66630000	-1.39135000
C	2.48737500	-0.49354000	-0.38097200
C	3.76022700	-0.08748600	0.10982000
C	4.21682100	1.22103700	-0.18533900
C	3.43193700	2.07009900	-0.93102400
C	1.99000700	-1.79248100	-0.14977400
C	4.50848300	-1.01767100	0.87773900
H	5.18918200	1.54138100	0.17559500
H	3.76795900	3.06965700	-1.18136800
C	4.01060000	-2.27822500	1.12538200

C	2.75363400	-2.66547000	0.60116500
H	5.47938100	-0.71745300	1.25970000
H	4.58815900	-2.98502400	1.71205500
H	2.38611700	-3.67067600	0.78207800
N	1.72397000	0.42749100	-1.09159000
O	0.52559900	0.05561500	-1.53487600
H	1.03478300	-2.08287500	-0.56974300
C	1.25746000	2.52022000	-2.21874900
H	1.12044900	2.06796000	-3.20658800
H	0.26075700	2.57633200	-1.77391700
H	1.67391900	3.52184500	-2.33254800

Zero-point correction= 0.445534 (Hartree/Particle)

Thermal correction to Energy= 0.474625

Thermal correction to Enthalpy= 0.475569

Thermal correction to Gibbs Free Energy= 0.385889

Sum of electronic and zero-point Energies= -1244.037308

Sum of electronic and thermal Energies= -1244.008217

Sum of electronic and thermal Enthalpies= -1244.007273

Sum of electronic and thermal Free Energies= -1244.096952

E(RB3LYP) = -1244.482841 A.U.

B-3a

1 1

Number of imaginary frequencies: 0

Rh	-0.64477700	-0.09338100	-0.04016800
C	-2.67193300	-0.89238400	-0.76204200
C	-2.61998800	-1.05751500	0.62941700
C	-2.36546000	0.25979000	1.22467300

C	-2.37147500	1.24819100	0.17687600
C	-2.46548200	0.53583200	-1.05927700
C	-2.87375200	-1.94458900	-1.80515700
H	-2.17806400	-1.81407300	-2.63855100
H	-2.73418300	-2.94813100	-1.40079300
H	-3.88987500	-1.88094500	-2.21277600
C	-2.75182600	-2.32627700	1.41159500
H	-3.73442600	-2.37278600	1.89576700
H	-2.64779500	-3.20597200	0.77471800
H	-1.99414900	-2.38689700	2.19741000
C	-2.29377300	0.53193300	2.69068700
H	-3.30984200	0.62436100	3.09623000
H	-1.79763100	-0.28193300	3.22379900
H	-1.76064300	1.46041600	2.90165900
C	-2.37094800	2.73311100	0.36305200
H	-3.39514700	3.08552500	0.53184600
H	-1.77153100	3.03240100	1.22556900
H	-1.98781500	3.24992800	-0.51920200
C	-2.51550300	1.12980300	-2.42895100
H	-3.56069400	1.26783200	-2.73425200
H	-2.02143100	2.10205800	-2.46457700
H	-2.04019900	0.47605300	-3.16370500
C	3.11450500	-1.85006000	-0.02016800
C	2.18685000	0.36694800	-0.01623000
C	3.48407500	0.94268600	-0.00857900
C	4.60187500	0.07269700	-0.00465000
C	4.41053600	-1.29259700	-0.00950400

C	0.98037000	1.11367700	-0.02002600
C	3.56418600	2.35814400	-0.00785700
H	5.60515900	0.48753800	0.00093300
H	5.25234400	-1.97498600	-0.00695500
C	2.40765000	3.11243000	-0.01579400
C	1.13269200	2.49603300	-0.01988700
H	4.54054000	2.83261300	-0.00184100
H	2.47293300	4.19612700	-0.01756000
H	0.25752100	3.13659300	-0.02348100
N	2.06906100	-1.00525200	-0.02382300
O	0.82123800	-1.51599900	-0.03914600
C	2.82479800	-3.31497300	-0.03071700
H	2.21635500	-3.58826700	0.83694600
H	2.24288800	-3.58070300	-0.91883200
H	3.75294700	-3.88710500	-0.01963800

Zero-point correction= 0.381346 (Hartree/Particle)

Thermal correction to Energy= 0.405022

Thermal correction to Enthalpy= 0.405966

Thermal correction to Gibbs Free Energy= 0.328223

Sum of electronic and zero-point Energies= -1014.971159

Sum of electronic and thermal Energies= -1014.947483

Sum of electronic and thermal Enthalpies= -1014.946538

Sum of electronic and thermal Free Energies= -1015.024281

E(RB3LYP) = -1015.352504 A.U.

B-3b

1 1

Number of imaginary frequencies: 0

Rh	1.03272500	-0.11645900	-0.28539400
C	3.20554400	-0.27263800	-0.62904800
C	2.96128000	1.17877900	-0.52826000
C	2.40415100	1.44257800	0.72775600
C	2.26366300	0.15737100	1.42882800
C	2.86981400	-0.87919700	0.61307200
C	3.85075300	-0.93552600	-1.80412900
H	3.48359000	-0.52243500	-2.74695900
H	4.93540100	-0.77306700	-1.77409100
H	3.67287100	-2.01228700	-1.80838200
C	3.25580800	2.14930800	-1.62705500
H	4.33877800	2.29311900	-1.72221100
H	2.89227800	1.77971800	-2.59027100
H	2.79984700	3.12310200	-1.44343000
C	1.95554900	2.75526800	1.28907700
H	2.60947800	3.06064600	2.11388400
H	1.97115900	3.54377000	0.53539200
H	0.93722700	2.68462000	1.68252000
C	1.78968800	0.00607000	2.83665800
H	2.62023500	0.20819200	3.52568300
H	0.98897000	0.71273500	3.06471900
H	1.42895900	-1.00501100	3.03367700
C	3.10451900	-2.30061700	1.02103800
H	4.07771300	-2.39308500	1.51702500
H	2.34014200	-2.64798700	1.71939700
H	3.10417400	-2.97078000	0.15893600
C	-1.52666100	-1.50352700	-0.24115600

C	-3.12416800	0.30072000	-0.16815100
C	-4.18305800	-0.63617500	0.00232200
C	-3.86964800	-2.01943600	0.07338000
C	-2.56750900	-2.43946900	-0.04736200
C	-3.37122300	1.68545500	-0.22545500
C	-5.50506500	-0.13440300	0.10535500
H	-4.67083600	-2.73786800	0.21621400
H	-2.30420900	-3.49047500	-0.01745000
C	-5.74611300	1.22108300	0.04151800
C	-4.67519500	2.12972500	-0.12399400
H	-6.32106600	-0.83881600	0.23380200
H	-6.76095900	1.59676200	0.11924800
H	-4.88035600	3.19429800	-0.17221900
N	-1.83175900	-0.19563500	-0.25937600
O	-0.82502000	0.70492200	-0.33326100
H	-2.54148700	2.36765600	-0.35148600
C	-0.09805100	-1.82266200	-0.48033900
H	0.21274100	-2.74355900	0.01615300
H	0.05073300	-1.95475200	-1.57002700

Zero-point correction= 0.380692 (Hartree/Particle)

Thermal correction to Energy= 0.404057

Thermal correction to Enthalpy= 0.405002

Thermal correction to Gibbs Free Energy= 0.328208

Sum of electronic and zero-point Energies= -1014.962116

Sum of electronic and thermal Energies= -1014.938751

Sum of electronic and thermal Enthalpies= -1014.937807

Sum of electronic and thermal Free Energies= -1015.014601

E(RB3LYP) = -1015.342809 A.U.

B-4

1 1

Number of imaginary frequencies: 0

Rh	1.73266600	-0.41032600	0.09800800
C	3.47453400	0.38392100	-1.19067800
C	3.75012100	0.73852400	0.15049100
C	3.80521200	-0.49238600	0.92401600
C	3.63945700	-1.60380900	0.03112900
C	3.34353000	-1.06687500	-1.27246200
C	-0.78292200	-0.37324300	3.47364100
C	-0.16000600	-1.88302400	1.71904800
C	-1.05408700	-2.87047900	2.20994800
C	-1.82374100	-2.56515500	3.35824900
C	-1.68350100	-1.33899500	3.96750800
C	0.59734800	-2.03471100	0.53371900
C	-1.15050000	-4.08299400	1.47626800
H	-2.53587500	-3.29136300	3.73542200
H	-2.27299200	-1.07875000	4.83884400
C	-0.40390000	-4.25232600	0.32765200
C	0.45822300	-3.22897600	-0.14751900
H	-1.82406400	-4.85842900	1.82643600
H	-0.48775400	-5.17626200	-0.23706000
H	0.98275300	-3.38567100	-1.08438600
N	-0.05701700	-0.68116100	2.38523000
C	3.35008100	1.30704000	-2.35891500
H	2.55944300	0.97636600	-3.03681200

H	3.12572900	2.32809700	-2.04913300
H	4.28893500	1.31707900	-2.92530000
C	3.99494200	2.10768600	0.70459600
H	5.07114200	2.28899200	0.81200200
H	3.58095800	2.88530900	0.06157200
H	3.53900700	2.21898600	1.69149400
C	4.06806300	-0.54672600	2.39528300
H	5.09392900	-0.22734900	2.61145600
H	3.38548400	0.12432900	2.92519800
H	3.93287800	-1.55332400	2.79361200
C	3.80698400	-3.04842700	0.38220400
H	3.20330200	-3.69395500	-0.25659300
H	4.85714500	-3.33682700	0.25580100
H	3.52280800	-3.24755900	1.41691700
C	3.18902700	-1.84643400	-2.54224000
H	4.13422200	-1.86746700	-3.09799100
H	2.90061800	-2.88046200	-2.34349300
H	2.42751800	-1.40882300	-3.19126800
C	0.59381800	3.43232300	-1.64419900
C	0.82630800	4.79285300	-1.45376300
C	1.02436900	5.29749700	-0.16534100
C	0.97576800	4.43543300	0.93371300
C	0.74467500	3.07354200	0.75454400
C	0.55900000	2.55833300	-0.53936400
H	0.85572000	5.45816400	-2.31120700
H	1.20926100	6.35716600	-0.01932000
H	1.12283200	4.82661000	1.93603300

H	0.71690800	2.39325700	1.59518900
C	-1.79188300	-1.57814400	-1.92332400
C	-2.40570400	-2.38629700	-2.88399000
C	-1.95870000	-2.38354300	-4.20470000
C	-0.89773400	-1.55493300	-4.58095300
C	-0.28453000	-0.73880900	-3.63552600
C	-0.71690100	-0.74173500	-2.29410700
H	0.43987200	3.03435500	-2.64184600
H	-3.25302800	-2.99358400	-2.58542400
H	-2.44568800	-3.01538300	-4.94047600
H	-0.55469900	-1.53953000	-5.61059400
H	0.52698800	-0.07912900	-3.92531500
N	-2.22302100	-1.58064800	-0.56118300
H	-2.24010600	-2.51173300	-0.14674300
S	-3.72904300	-0.87040500	-0.15716000
O	-3.99589300	-1.40592400	1.18315500
O	-4.67910100	-1.03806100	-1.26015800
C	-3.35296200	1.65287900	-1.18370900
C	-3.05906500	3.00941600	-1.06956700
C	-2.76670200	3.58716500	0.17485500
C	-2.75081500	2.76309500	1.30973100
C	-3.02453800	1.40065100	1.21545300
C	-3.32770000	0.86090900	-0.03438000
H	-3.61948000	1.21498400	-2.13942300
H	-3.07683600	3.63597000	-1.95682600
H	-2.53978200	3.20190600	2.28121200
H	-3.03501000	0.76160300	2.09131400

C	-0.06552300	0.13439900	-1.36606700
C	0.34927300	1.15690400	-0.79556700
C	-2.52028300	5.06973500	0.29031500
H	-3.47101200	5.61354600	0.34131300
H	-1.94756500	5.31278300	1.18846300
H	-1.96755000	5.44702300	-0.57370800
O	0.81572300	0.22170100	1.91248700
C	-0.58459400	0.98211000	4.06935400
H	0.46353900	1.13196900	4.34736000
H	-0.83217400	1.75300400	3.33265200
H	-1.21491300	1.10783400	4.95056000

Zero-point correction= 0.710854 (Hartree/Particle)

Thermal correction to Energy= 0.757442

Thermal correction to Enthalpy= 0.758386

Thermal correction to Gibbs Free Energy= 0.631305

Sum of electronic and zero-point Energies= -2428.498784

Sum of electronic and thermal Energies= -2428.452195

Sum of electronic and thermal Enthalpies= -2428.451251

Sum of electronic and thermal Free Energies= -2428.578333

E(RB3LYP) = -2429.209638 A.U.

B-5a

1 1

Number of imaginary frequencies: 0

C	1.57863800	2.46413100	2.45420600
C	1.78139600	2.33766700	0.06237200
C	2.44525600	3.59758900	0.04311300
C	2.56473000	4.32273500	1.25691300

C	2.06602500	3.78776800	2.41847700
C	1.39045000	1.69770800	-1.15850900
C	2.93582200	4.09188100	-1.19229700
H	3.03667600	5.29987900	1.24927700
H	2.10654000	4.33492500	3.35302400
C	2.73977300	3.37680400	-2.35322500
C	1.93428900	2.22121000	-2.33229500
H	3.46181700	5.04154300	-1.20157500
H	3.13108800	3.74221000	-3.29692700
H	1.63230500	1.77063300	-3.27296400
N	1.54093800	1.75876700	1.30610800
O	1.33367900	0.45295100	1.39957500
Rh	2.04470800	-0.79878600	-0.18405700
C	3.69308200	-1.80850300	1.10574500
C	2.45904700	-2.58566200	0.88703000
C	2.39773800	-2.95786200	-0.51282400
C	3.42036500	-2.21520500	-1.16882500
C	4.26325400	-1.56590500	-0.14313200
C	4.11156100	-1.29580800	2.44637300
H	3.29895700	-0.70974600	2.88804000
H	4.33424600	-2.12476300	3.12707900
H	4.99675800	-0.66074700	2.38222700
C	1.57502200	-3.09085200	1.98018900
H	2.05525100	-3.93147700	2.49680700
H	1.38060700	-2.30320900	2.71193700
H	0.61793400	-3.43209800	1.58275700
C	1.47092000	-3.96163400	-1.11518500

H	1.90693700	-4.96324700	-1.01616400
H	0.49836700	-3.96476800	-0.62088000
H	1.30137900	-3.77141200	-2.17575000
C	3.74655200	-2.24206600	-2.62942100
H	4.11579400	-1.27131500	-2.97004000
H	4.53047600	-2.98282300	-2.83074100
H	2.87262000	-2.50434200	-3.22878200
C	5.47593100	-0.75005800	-0.46460100
H	6.27857000	-1.39089500	-0.84802300
H	5.25656900	-0.00814500	-1.23923900
H	5.85418800	-0.22179600	0.41211300
C	-1.36292400	2.78131200	-1.43691100
C	-2.49116500	3.44015000	-1.91650100
C	-3.27962100	2.85505500	-2.91227500
C	-2.92024200	1.60963400	-3.42798500
C	-1.78968900	0.94711800	-2.94519300
C	-1.00454600	1.51149000	-1.92805600
H	-2.76202200	4.40821700	-1.50610900
H	-4.15829100	3.37090800	-3.28738500
H	-3.51252000	1.15260100	-4.21526400
H	-1.51739900	-0.01126800	-3.36536500
C	-1.09928000	-2.22092500	-2.16816800
C	-2.04211100	-3.24538100	-2.20913400
C	-2.74719100	-3.58510400	-1.05306900
C	-2.49851500	-2.89285200	0.13032200
C	-1.54218800	-1.87032200	0.17890200
C	-0.83415700	-1.50487100	-0.98730900

H	-0.52940600	-1.97541500	-3.05903700
H	-2.22242300	-3.77796100	-3.13767900
H	-3.48897000	-4.37700200	-1.07186600
H	-3.05812700	-3.13146000	1.03056200
H	-0.77976500	3.23136300	-0.64176700
N	-1.24457400	-1.24613000	1.43062200
H	-1.40786700	-1.86799500	2.21819100
S	-1.98164500	0.24280300	1.90056200
O	-1.37414400	1.35069500	1.16647600
O	-1.90347600	0.18759700	3.36739500
C	-4.61004600	-0.50368800	2.21546800
C	-5.91307400	-0.67956200	1.75684600
C	-6.29255300	-0.26294500	0.47063100
C	-5.33018800	0.34271800	-0.35050800
C	-4.02256600	0.53303200	0.08825500
C	-3.67823900	0.10672800	1.37267200
H	-4.31974100	-0.81278200	3.21436200
H	-6.64970600	-1.14276900	2.40740700
H	-5.60355200	0.67373900	-1.34840100
H	-3.28739500	1.00885200	-0.54820700
C	0.16648900	0.80228100	-1.32983800
C	0.21333500	-0.48260300	-0.94759400
C	-7.71462900	-0.43207800	-0.00309100
H	-8.31956200	0.43855200	0.27787100
H	-7.76651500	-0.52844000	-1.09117800
H	-8.18516200	-1.31270500	0.44330100
C	1.20195500	1.75383600	3.71028900

H	0.18693100	1.35169200	3.63525800
H	1.86663700	0.90023000	3.87990700
H	1.26696700	2.43358800	4.56097100

Zero-point correction= 0.712166 (Hartree/Particle)

Thermal correction to Energy= 0.758110

Thermal correction to Enthalpy= 0.759054

Thermal correction to Gibbs Free Energy= 0.632075

Sum of electronic and zero-point Energies= -2428.491518

Sum of electronic and thermal Energies= -2428.445575

Sum of electronic and thermal Enthalpies= -2428.444631

Sum of electronic and thermal Free Energies= -2428.571609

E(RB3LYP) = -2429.203684 A.U.

B-5b

1 1

Number of imaginary frequencies: 0

C	0.31473400	-2.94543700	-1.68058200
C	0.64506500	-2.19439000	0.57525300
C	0.59482200	-3.53801700	1.03996300
C	0.31724400	-4.57125800	0.10742300
C	0.09902300	-4.25641600	-1.20970900
C	0.62154600	-1.09785900	1.49597700
C	0.76560800	-3.78722200	2.42547000
H	0.24506700	-5.59651200	0.45578100
H	-0.18494000	-5.01150900	-1.93265300
C	0.92462400	-2.73917000	3.30493600
C	0.80682500	-1.41362500	2.84135600
H	0.75461600	-4.81498600	2.77533700

H	1.06687200	-2.92715400	4.36414700
H	0.76613100	-0.60225000	3.56176200
N	0.68348900	-1.99520400	-0.80164000
O	1.13439100	-0.84378600	-1.29397000
Rh	2.51312500	0.20105800	-0.04012300
C	3.79896400	1.17250300	-1.41995800
C	4.05798100	1.79497900	-0.13809600
C	4.51530600	0.75901400	0.72423000
C	4.77564700	-0.45115200	-0.08028000
C	4.35691200	-0.19692400	-1.38501800
C	3.28930600	1.86451700	-2.64242000
H	2.54235200	2.61851800	-2.38231800
H	4.11306200	2.36132700	-3.17087400
H	2.82622000	1.15272000	-3.32919100
C	3.93002000	3.24960500	0.17120100
H	4.84840200	3.76615100	-0.13422200
H	3.09365100	3.70455300	-0.36066000
H	3.78673000	3.42678300	1.23880100
C	4.88003300	0.89662300	2.16912800
H	5.95815300	1.07216300	2.27272400
H	4.35527000	1.73190400	2.63655700
H	4.64040700	-0.01323500	2.72568700
C	5.33650400	-1.71913500	0.48476500
H	6.38376500	-1.58060200	0.77793000
H	4.78793700	-2.02845100	1.38035500
H	5.29357200	-2.53769500	-0.23574900
C	4.32016300	-1.12694500	-2.55478500

H	3.29145000	-1.22679200	-2.91629400
H	4.92801400	-0.73720900	-3.37864200
H	4.69055400	-2.12062100	-2.29708700
C	-0.23557800	2.52914400	-1.27916300
C	-0.60585900	3.75867800	-1.82324300
C	-0.31766000	4.94844200	-1.14740100
C	0.34331200	4.90253800	0.08199400
C	0.71974100	3.67549000	0.63003200
C	0.43060500	2.47496600	-0.03896300
H	-1.12507800	3.78796600	-2.77703700
H	-0.60890700	5.90355000	-1.57377900
H	0.56553100	5.82183400	0.61599300
H	1.23911100	3.64302800	1.58330100
C	-1.34716200	1.76880300	2.62065400
C	-2.53702500	2.08917500	3.27071500
C	-3.64635400	1.25196800	3.14744600
C	-3.55461200	0.11065200	2.35478800
C	-2.36152700	-0.21114100	1.69785300
C	-1.22560000	0.61795300	1.82382700
H	-0.48079700	2.40698500	2.74280800
H	-2.59158600	2.98354200	3.88360400
H	-4.57673700	1.48798300	3.65387000
H	-4.41913900	-0.53304200	2.21842000
H	-0.46920100	1.59955800	-1.78554500
N	-2.30203000	-1.39433300	0.88684700
H	-2.84600200	-2.16702700	1.26427000
S	-2.70055200	-1.27132900	-0.77746900

O	-2.81169000	-2.66744400	-1.21466900
O	-1.72046800	-0.36443400	-1.37730800
C	-4.36316500	0.90975200	-0.85383100
C	-5.61516100	1.51853900	-0.83868600
C	-6.79411600	0.75742700	-0.82926000
C	-6.69144700	-0.64272900	-0.83556400
C	-5.45000900	-1.27351300	-0.84806500
C	-4.29623400	-0.48627400	-0.86002200
H	-3.45258500	1.49915600	-0.86399000
H	-5.67925500	2.60295700	-0.83302900
H	-7.59573200	-1.24477000	-0.83583800
H	-5.36955800	-2.35535600	-0.86718200
C	0.08393600	0.29128800	1.18570700
C	0.82323400	1.16138000	0.48025900
C	-8.14443100	1.42914000	-0.84665300
H	-8.48167700	1.58585600	-1.87841900
H	-8.90232800	0.82102400	-0.34499100
H	-8.11211700	2.40863000	-0.36148100
C	0.22486300	-2.54377400	-3.11308900
H	-0.41850500	-1.66314400	-3.19368800
H	1.20930900	-2.26446100	-3.50262800
H	-0.18236700	-3.36123400	-3.70900500

Zero-point correction= 0.711899 (Hartree/Particle)

Thermal correction to Energy= 0.758103

Thermal correction to Enthalpy= 0.759047

Thermal correction to Gibbs Free Energy= 0.629784

Sum of electronic and zero-point Energies= -2428.493995

Sum of electronic and thermal Energies= -2428.447792

Sum of electronic and thermal Enthalpies= -2428.446847

Sum of electronic and thermal Free Energies= -2428.576111

E(RB3LYP) = -2429.205895 A.U.

B-5c

1 1

Number of imaginary frequencies: 0

C	-3.33176900	2.64446600	-1.40601100
C	-3.55688900	0.89712200	0.27458100
C	-4.72869700	1.53602300	0.78624300
C	-5.19069200	2.71053000	0.14543500
C	-4.52877800	3.22958000	-0.94456300
C	-3.06880000	-0.34994200	0.74940300
C	-5.38348200	0.94547500	1.89303600
H	-6.09126800	3.19276900	0.51485400
H	-4.89356100	4.11042600	-1.45925100
C	-4.87788700	-0.21897300	2.42889800
C	-3.74924300	-0.85143300	1.85608800
H	-6.27221800	1.41836800	2.29800200
H	-5.35970500	-0.67192500	3.29023600
H	-3.40861200	-1.77853900	2.30595400
N	-2.89936600	1.55442600	-0.75850900
O	-1.64462300	1.02442500	-1.13029200
Rh	-1.58148100	-1.26459700	-0.30496000
C	-2.57074300	-3.30130000	-0.63611800
C	-2.07273800	-2.88636500	-1.88261900
C	-0.60587500	-2.77853900	-1.80099300

C	-0.21474100	-3.11454100	-0.49595400
C	-1.43598900	-3.32202400	0.28424200
C	-3.97840900	-3.66176600	-0.27844900
H	-4.68656100	-3.32944000	-1.04001500
H	-4.07727000	-4.74921100	-0.17883200
H	-4.28036100	-3.21578500	0.67270300
C	-2.85034700	-2.64100600	-3.13796000
H	-2.68160100	-3.45241200	-3.85614100
H	-3.92317400	-2.57644700	-2.94719200
H	-2.53162000	-1.71279800	-3.62198000
C	0.27189100	-2.45503100	-2.96952200
H	1.25542100	-2.11569000	-2.64937700
H	0.38648600	-3.33723200	-3.61198900
H	-0.16748300	-1.66265800	-3.58243500
C	1.16507100	-3.28035700	0.05621600
H	1.29346300	-2.70561100	0.97717300
H	1.33675200	-4.33727200	0.29497300
H	1.92118900	-2.94742500	-0.65129000
C	-1.46101900	-3.88205200	1.67120900
H	-1.34889400	-4.97331500	1.62903100
H	-0.64244000	-3.48713500	2.27512200
H	-2.40584500	-3.67448200	2.17894300
C	0.32211500	3.43495400	-0.90124900
C	0.69071800	4.76244500	-0.68775900
C	0.46989900	5.36218300	0.55650700
C	-0.11218400	4.62908600	1.59349800
C	-0.48914700	3.30239600	1.38472700

C	-0.28224600	2.69383900	0.13398400
H	1.17054300	5.32153700	-1.48505300
H	0.76448100	6.39419600	0.72055900
H	-0.27486700	5.09069700	2.56254600
H	-0.94049400	2.72277000	2.18420500
C	0.22520800	-0.86516100	2.75132400
C	1.12748800	-1.21271800	3.75257500
C	2.45933900	-0.79908000	3.66505100
C	2.85848200	-0.00127100	2.59506200
C	1.94991200	0.37828300	1.60143000
C	0.60986100	-0.08111500	1.64596200
H	-0.80426900	-1.20254900	2.80197700
H	0.79506900	-1.81329300	4.59407800
H	3.17508300	-1.07951600	4.43117500
H	3.87833600	0.35954900	2.51515800
H	0.54902700	2.94689700	-1.84268600
N	2.44046700	1.23947900	0.57163700
H	1.89181300	2.07442100	0.38655400
S	2.93186500	0.59191700	-0.91540200
O	2.82306200	1.70886300	-1.86201000
O	2.22530000	-0.67393600	-1.16134400
C	4.98706300	-1.05252700	-0.12454100
C	6.32885100	-1.33441900	0.12490600
C	7.33000400	-0.38856400	-0.13912100
C	6.95477000	0.85675800	-0.66828200
C	5.61992400	1.16161800	-0.91786700
C	4.64742700	0.19865000	-0.64165500

H	4.21551500	-1.79008900	0.06593700
H	6.60421100	-2.30736300	0.52210700
H	7.72071400	1.59411900	-0.89198000
H	5.32964200	2.11936000	-1.33583000
C	-0.64744900	1.28400900	-0.04897200
C	-0.37435100	0.14196800	0.58490000
C	8.77915800	-0.68957500	0.15291800
H	9.08329300	-0.23797700	1.10497200
H	8.96165500	-1.76497700	0.22455800
H	9.43459800	-0.28189500	-0.62243500
C	-2.56020200	3.20009700	-2.56105700
H	-1.81079400	3.91218500	-2.20227600
H	-2.03686900	2.41527700	-3.10742500
H	-3.24321000	3.72613700	-3.23072500

Zero-point correction= 0.711867 (Hartree/Particle)

Thermal correction to Energy= 0.757817

Thermal correction to Enthalpy= 0.758762

Thermal correction to Gibbs Free Energy= 0.630326

Sum of electronic and zero-point Energies= -2428.474033

Sum of electronic and thermal Energies= -2428.428082

Sum of electronic and thermal Enthalpies= -2428.427138

Sum of electronic and thermal Free Energies= -2428.555574

E(RB3LYP) = -2429.185900 A.U.

B-5d

1 1

Number of imaginary frequencies: 0

C	-0.87354100	3.47464900	-1.27891300

C	-2.78332300	2.15503100	-0.52727100
C	-3.57750900	3.34156700	-0.45844500
C	-2.98856700	4.57117500	-0.83901100
C	-1.67807400	4.63188000	-1.25838600
C	-3.28448000	0.85523400	-0.24062200
C	-4.91822800	3.22426200	-0.02038200
H	-3.58967600	5.47537100	-0.80431900
H	-1.22740900	5.56816200	-1.56523500
C	-5.40702400	1.98327900	0.32671300
C	-4.59916600	0.82721600	0.21462800
H	-5.53598400	4.11436400	0.03931700
H	-6.42794300	1.88518600	0.68344600
H	-5.03405900	-0.12574400	0.50079400
N	-1.45442600	2.32595300	-0.90275200
O	-0.64745400	1.17833800	-0.84165800
Rh	-2.05875500	-0.72776800	-0.62627800
C	-2.96465500	-2.66015000	-0.42988600
C	-3.46653600	-2.17495900	-1.71784400
C	-2.35565000	-1.99503300	-2.55683300
C	-1.15698300	-2.47194800	-1.84976100
C	-1.53787400	-2.94874900	-0.58239500
C	-3.82315500	-3.13428900	0.69953600
H	-4.71790200	-2.51614000	0.81029100
H	-4.15453100	-4.16325000	0.50947600
H	-3.27937800	-3.12392800	1.64520400
C	-4.90703300	-1.93819900	-2.04325100
H	-5.41506100	-2.89364400	-2.22035600

H	-5.43003700	-1.43880800	-1.22421500
H	-5.02468400	-1.32340200	-2.93755400
C	-2.34494700	-1.47815400	-3.96239700
H	-1.51489200	-0.78350700	-4.12210700
H	-2.21796700	-2.30272400	-4.67440600
H	-3.27279700	-0.95954300	-4.21109200
C	0.21291600	-2.48747000	-2.45433000
H	0.99260300	-2.63342100	-1.70646500
H	0.29000000	-3.29727200	-3.19059900
H	0.41846700	-1.55249700	-2.98588300
C	-0.66381700	-3.60043800	0.44496100
H	-0.73136900	-4.69145200	0.35607500
H	0.38372400	-3.31461100	0.32513100
H	-0.96945700	-3.32756700	1.45680400
C	0.22763500	-1.05029400	2.99893300
C	0.22943500	-1.67139100	4.24727200
C	-0.97405600	-1.97556300	4.88755000
C	-2.18825700	-1.65839400	4.27095600
C	-2.19610100	-1.05661700	3.01429300
C	-0.98853200	-0.74032500	2.36553900
H	1.17723100	-1.91778600	4.71599800
H	-0.96749800	-2.45827000	5.86008300
H	-3.12728100	-1.88650700	4.76673800
H	-3.13313700	-0.81537900	2.52257800
C	0.59233600	2.84461200	1.91642300
C	1.66158900	3.62493600	2.35214400
C	2.96217800	3.28758600	1.96453000

C	3.20014700	2.18104000	1.15019100
C	2.13123900	1.38857700	0.72246400
C	0.81119300	1.72130000	1.10647700
H	-0.42530400	3.08531700	2.20884100
H	1.48583100	4.48588200	2.98867000
H	3.80018100	3.89328700	2.29545200
H	4.20946900	1.92990300	0.84341500
H	1.17092300	-0.82302100	2.51735300
N	2.35029400	0.26905300	-0.11964200
H	1.48405400	-0.16773800	-0.43059700
S	3.33953300	-1.03394900	0.42940000
O	2.74192100	-2.19593600	-0.24506700
O	3.46632400	-0.97919900	1.88781600
C	5.97542000	-0.27632100	0.54560700
C	7.21777000	-0.00396400	-0.02548700
C	7.42811500	-0.14042300	-1.40479400
C	6.35578300	-0.55869800	-2.21098300
C	5.10798400	-0.83493100	-1.66291600
C	4.93116100	-0.68395100	-0.28524100
H	5.81280100	-0.18526300	1.61391500
H	8.03814400	0.31244500	0.61223400
H	6.50590300	-0.67303600	-3.28083700
H	4.28617700	-1.17007200	-2.28652200
C	-0.29186400	0.89541900	0.61179000
C	-1.03528800	-0.12345000	1.03854600
C	8.78454000	0.12032000	-2.01009800
H	9.37461100	0.80600800	-1.39633700

H	9.35121200	-0.81463500	-2.09635300
H	8.70019800	0.54316700	-3.01536200
C	0.56860600	3.50312900	-1.68255600
H	1.19880600	3.67945500	-0.80491700
H	0.88082800	2.55906600	-2.12861500
H	0.72892900	4.31869100	-2.39038400

Zero-point correction= 0.711725 (Hartree/Particle)

Thermal correction to Energy= 0.757778

Thermal correction to Enthalpy= 0.758722

Thermal correction to Gibbs Free Energy= 0.630303

Sum of electronic and zero-point Energies= -2428.473039

Sum of electronic and thermal Energies= -2428.426986

Sum of electronic and thermal Enthalpies= -2428.426041

Sum of electronic and thermal Free Energies= -2428.554461

E(RB3LYP) = -2429.184764 A.U.

B-5e

1 1

Number of imaginary frequencies: 0

C	2.48367800	-0.81633900	1.85080700
C	3.48804600	-0.62892500	2.78399100
C	3.22960700	0.30576400	3.79548200
C	2.01484700	1.00005700	3.82472600
C	1.02266900	0.78371800	2.86075600
C	1.25369400	-0.14061100	1.84176700
H	4.42752100	-1.16748900	2.72757700
H	3.97701100	0.48556800	4.56100100
H	1.83453900	1.71811900	4.61897000

H	0.08886700	1.32185400	2.89975500
C	1.23102000	-3.95504600	-0.73300200
C	0.98725200	-4.92207000	-1.70674700
C	0.38556100	-4.56070400	-2.91425600
C	0.03047900	-3.22848700	-3.13485800
C	0.27606400	-2.25955400	-2.16381200
C	0.87689100	-2.60920300	-0.94626700
H	1.67149600	-4.26589000	0.21279200
H	1.26193100	-5.95566700	-1.52048000
H	0.19738000	-5.31181500	-3.67496600
H	-0.43461100	-2.93951100	-4.07299500
H	-0.01385600	-1.23050800	-2.32481500
N	2.51557400	-1.65852200	0.67862300
S	3.89770600	-0.91787600	-0.61202200
O	5.12152500	-1.12258500	0.15509300
O	3.59070700	-1.61205500	-1.85242600
C	2.36353900	1.14048600	-1.50800900
C	1.93774700	2.46315900	-1.47559000
C	2.50096500	3.38896900	-0.58232000
C	3.53120700	2.96778300	0.27587200
C	3.98757900	1.65713100	0.25937000
C	3.39621400	0.76135200	-0.64129700
H	1.92371000	0.42030800	-2.18773400
H	1.15676600	2.78782800	-2.15317700
H	3.98256000	3.67869500	0.96103200
H	4.78244300	1.32838600	0.91746000
C	1.15062600	-1.60627800	0.09649400

C	0.41133500	-0.64658700	0.73497300
C	1.99017100	4.80364000	-0.52442500
H	2.77454800	5.50276600	-0.22327800
H	1.58757500	5.12296500	-1.48908200
H	1.17637300	4.87454400	0.20684900
C	-1.27497900	1.97372200	-3.08884100
C	-1.41659400	2.32579300	-0.71127900
C	-1.45385000	3.73676600	-0.90328700
C	-1.37588200	4.24179500	-2.22502900
C	-1.28659700	3.36986700	-3.28747900
C	-1.49279600	1.68980000	0.55711900
C	-1.57966300	4.55246200	0.24958100
H	-1.39884200	5.31450000	-2.39058100
H	-1.23541100	3.73394200	-4.30734800
C	-1.68071400	3.96026400	1.49016000
C	-1.64402000	2.55132500	1.63634500
H	-1.61302300	5.63126200	0.13400200
H	-1.79741000	4.58026000	2.37468200
H	-1.75265400	2.14549800	2.63760100
N	-1.33837800	1.50688600	-1.82642900
O	-1.34364400	0.19066400	-1.63583600
Rh	-1.58851300	-0.33758900	0.44358800
C	-3.65294200	-0.52501200	1.45402300
C	-3.71079900	-1.27152500	0.25521600
C	-2.74939000	-2.36902700	0.33913600
C	-2.08806300	-2.27036600	1.58112200
C	-2.56452300	-1.06809200	2.25368200

C	-4.54463400	0.60556100	1.86360600
H	-5.07919000	1.02836700	1.01074300
H	-5.28913000	0.25492200	2.58807200
H	-3.98060000	1.41468200	2.33322600
C	-4.60151400	-1.04585600	-0.92756800
H	-5.31573800	-1.86962700	-1.03943400
H	-5.16746200	-0.11673300	-0.83950300
H	-4.00658300	-0.99532600	-1.84554700
C	-2.61102700	-3.44626000	-0.69231800
H	-3.44409600	-4.15627600	-0.61681800
H	-2.62200600	-3.02915100	-1.70196500
H	-1.67910600	-4.00194500	-0.58003900
C	-1.09066100	-3.22975900	2.15254200
H	-0.32325600	-2.70708100	2.72887800
H	-1.59252600	-3.93349500	2.82745800
H	-0.59738700	-3.80602800	1.36837800
C	-2.25011700	-0.69169900	3.67052700
H	-2.84202000	-1.29114200	4.37367300
H	-1.19387600	-0.85029200	3.90058000
H	-2.48268200	0.35854100	3.86345200
C	-1.20880500	0.96574700	-4.19049100
H	-0.29053400	0.37235700	-4.12206100
H	-2.04194600	0.26035600	-4.11142700
H	-1.23874000	1.46040700	-5.16233100
H	2.89096200	-2.59994400	0.82574400

Zero-point correction= 0.713218 (Hartree/Particle)

Thermal correction to Energy= 0.758506

Thermal correction to Enthalpy= 0.759450

Thermal correction to Gibbs Free Energy= 0.637388

Sum of electronic and zero-point Energies= -2428.495150

Sum of electronic and thermal Energies= -2428.449863

Sum of electronic and thermal Enthalpies= -2428.448918

Sum of electronic and thermal Free Energies= -2428.570980

E(RB3LYP) = -2429.208368 A.U.

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Number of imaginary frequencies: 0

C	-1.02927700	-3.40812400	0.38325000
C	-0.60717500	-1.49540700	1.80963400
C	-1.24349500	-2.15263500	2.90405500
C	-1.80497600	-3.43336100	2.67829100
C	-1.70798300	-4.03651600	1.44734900
C	-0.05903400	-0.18867900	1.90770100
C	-1.29482000	-1.49540800	4.15342700
H	-2.30710600	-3.94034000	3.49659300
H	-2.13015100	-5.01694100	1.26298000
C	-0.72755600	-0.24145900	4.27546800
C	-0.13285300	0.39942200	3.17620200
H	-1.77899000	-1.98482700	4.99159400
H	-0.75785900	0.27517300	5.22944500
H	0.25407700	1.40268200	3.30265800
N	-0.56155600	-2.16813500	0.60806000
O	0.25112900	-1.61217100	-0.42432400
Rh	2.29455900	-0.34219100	-0.00545100

C	3.91005200	0.97194200	-0.63402600
C	4.35992600	0.46196200	0.66476500
C	4.46566600	-0.92971800	0.54319600
C	4.18375800	-1.29981900	-0.85362900
C	3.92361200	-0.12649000	-1.59157100
C	3.83807900	2.42378100	-0.99530900
H	3.23002600	2.99394100	-0.28989700
H	4.84841700	2.85214100	-0.98763400
H	3.42907000	2.56822900	-1.99684100
C	4.71245500	1.29632700	1.85894300
H	5.79836900	1.44465400	1.91132200
H	4.25709000	2.28718800	1.80621300
H	4.39905300	0.82551000	2.79443300
C	4.87464500	-1.89924400	1.60970200
H	5.92740900	-2.18429800	1.48917800
H	4.75714200	-1.47086500	2.60750700
H	4.28527500	-2.81989600	1.56426000
C	4.25328700	-2.70240000	-1.37424500
H	3.75678600	-2.80000300	-2.34171300
H	5.29706400	-3.01705800	-1.49762500
H	3.78594000	-3.40704100	-0.67936500
C	3.68962800	0.00404900	-3.06588700
H	4.56341200	0.44785000	-3.55813000
H	3.50669600	-0.96797500	-3.52847100
H	2.82635000	0.63940300	-3.28269100
C	-0.90994400	2.62196500	0.33242400
C	-1.10272800	3.99721100	0.45940300

C	-0.12782300	4.79281600	1.06671100
C	1.04146000	4.20125700	1.54933500
C	1.23629700	2.82521300	1.41054800
C	0.26854500	2.02143300	0.79502200
H	-2.01849500	4.44416300	0.08387300
H	-0.27885500	5.86339100	1.16532000
H	1.80191300	4.80862300	2.03140000
H	2.13768500	2.35635600	1.78863300
C	0.44868500	1.58690000	-2.33506600
C	-0.02947100	2.28517600	-3.43769300
C	-1.15811100	1.82030500	-4.11689000
C	-1.78465800	0.65396200	-3.69194800
C	-1.31965500	-0.03376400	-2.56238700
C	-0.19360300	0.43303200	-1.84766900
H	1.31284700	1.95514700	-1.79937200
H	0.48246100	3.18318800	-3.76841300
H	-1.53319600	2.34697800	-4.98848200
H	-2.64081800	0.25009100	-4.22023500
H	-1.67182700	2.01202800	-0.13594000
N	-1.98561200	-1.22397800	-2.17915700
H	-1.44441100	-1.82169000	-1.58005600
S	-3.62243100	-1.29148900	-1.73127700
O	-3.71695500	-2.61165100	-1.08892100
O	-4.41839600	-0.91816400	-2.89528400
C	-4.24095900	1.25225900	-0.85954600
C	-4.35405900	2.23420700	0.12323100
C	-4.06143300	1.95761700	1.46774400

C	-3.69042600	0.65018500	1.81747000
C	-3.59012000	-0.34856000	0.85322200
C	-3.84833500	-0.03425500	-0.48229600
H	-4.46729800	1.46643100	-1.89775600
H	-4.66874400	3.23483400	-0.15947100
H	-3.48039900	0.41106700	2.85598600
H	-3.34578700	-1.36789300	1.12697400
C	0.43447200	0.52913600	0.71842100
C	0.34042200	-0.13718800	-0.57807300
C	-4.09866700	3.05148900	2.50314800
H	-4.28968400	2.65530300	3.50408800
H	-3.13249200	3.57094000	2.52724000
H	-4.86674300	3.79586500	2.27571300
C	-0.83361600	-4.09379900	-0.93395500
H	-1.72938500	-3.94400200	-1.54876000
H	0.04029800	-3.72713400	-1.47104600
H	-0.72870100	-5.16703400	-0.76271900

Zero-point correction= 0.713136 (Hartree/Particle)

Thermal correction to Energy= 0.758566

Thermal correction to Enthalpy= 0.759510

Thermal correction to Gibbs Free Energy= 0.636194

Sum of electronic and zero-point Energies= -2428.481196

Sum of electronic and thermal Energies= -2428.435766

Sum of electronic and thermal Enthalpies= -2428.434822

Sum of electronic and thermal Free Energies= -2428.558138

E(RB3LYP) = -2429.194332 A.U.

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Number of imaginary frequencies: 0

Rh	-1.51517100	-1.14302300	0.75384100
C	0.30395700	-2.35640600	0.05416500
C	-0.69670300	-3.24353900	0.58656700
C	-0.20638500	-1.78322400	-1.19036100
C	-1.85151600	-3.13413900	-0.25804900
C	-1.52230800	-2.23977900	-1.36617500
C	1.70080200	-2.23998200	0.57258200
H	2.27468700	-3.12548300	0.27217500
H	2.21158600	-1.36551100	0.17637600
H	1.71479600	-2.18031900	1.66270900
C	-0.57862600	-4.08294700	1.82079100
H	-1.03749400	-5.06348900	1.66830800
H	0.46726700	-4.23651400	2.09289800
H	-1.08320800	-3.58452500	2.65828200
C	-3.11735300	-3.92119700	-0.13875800
H	-3.09210000	-4.77383600	-0.82906800
H	-3.25338800	-4.30836200	0.87236600
H	-3.99052400	-3.31754300	-0.39986900
C	-2.42028000	-1.93450000	-2.52222400
H	-2.33427800	-2.72200200	-3.28119800
H	-3.46768100	-1.88723700	-2.21591600
H	-2.15989200	-0.98297400	-2.98971600
C	0.54312300	-0.93271300	-2.17023300
H	1.58658900	-0.81237700	-1.88499800
H	0.52425800	-1.39834300	-3.16100200

H	0.09077600	0.05880300	-2.27516800
O	-1.98732400	-1.32023600	2.47707800
C	-3.28056600	0.73740100	-0.83590500
C	-4.56719300	-0.57133400	0.65106300
C	-2.08802800	1.49045200	-1.10831000
C	-4.39160200	0.86876700	-1.73021500
C	-5.71203000	-0.40447300	-0.16979000
C	-2.02785900	2.21227300	-2.29554700
C	-4.26031400	1.59209200	-2.94138900
C	-5.61337900	0.25696600	-1.36566800
H	-6.65330800	-0.83086600	0.15735900
C	-3.07941700	2.23100100	-3.23278800
H	-1.15090300	2.81538600	-2.49503600
H	-5.10919800	1.64184000	-3.61664400
H	-6.46974600	0.34226900	-2.02861200
H	-2.96453700	2.79172400	-4.15434100
N	-3.38117700	-0.06816800	0.27845800
C	-0.56827100	0.69140500	0.72530600
C	-1.00945500	1.66003300	-0.09887700
C	0.49094600	0.79575900	1.73572600
C	1.83857900	1.07215300	1.36147400
C	0.18206700	0.69126400	3.10570500
C	2.80473400	1.29652500	2.35294900
H	3.81081900	1.57373500	2.07018100
C	1.14208600	0.90873700	4.08082100
C	2.45308600	1.21908400	3.69536900
H	-0.83271000	0.42156400	3.38121400

H	0.87948100	0.83504400	5.13065400
H	3.21395300	1.39522200	4.44960800
C	-0.48423000	3.05972300	0.10509800
C	0.48426900	3.63265800	-0.73285700
C	-0.97086100	3.79704300	1.19371200
C	0.95930800	4.92033300	-0.47908500
H	0.90299700	3.07684900	-1.56612900
C	-0.49945300	5.08601000	1.43921500
H	-1.71217900	3.35071400	1.84985000
C	0.46850800	5.64950500	0.60467100
H	1.72314600	5.34244300	-1.12446600
H	-0.88324500	5.64656900	2.28615700
H	0.84242900	6.64937700	0.80180300
N	2.13189700	1.08353200	-0.00144600
H	1.33827500	1.04189400	-0.62576800
S	3.54469400	1.49310900	-0.84240100
O	4.32387500	2.43358400	-0.04474200
O	3.03434100	1.80802900	-2.18031500
C	4.31476200	-0.83434500	-2.08904700
C	4.91782700	-2.09037600	-2.12078400
C	5.61759600	-2.58854800	-1.01189300
C	5.70877000	-1.78670100	0.13721800
C	5.11872200	-0.52667000	0.18767900
C	4.41212600	-0.06644100	-0.92662600
H	3.78888800	-0.44138600	-2.95220700
H	4.85348800	-2.68890400	-3.02518400
H	6.25949900	-2.15058700	1.00004600

H	5.21419700	0.08964800	1.07364000
C	6.29695700	-3.93401200	-1.06529000
H	7.34381700	-3.82179200	-1.37168200
H	6.29624700	-4.42347600	-0.08710600
H	5.81556000	-4.60087400	-1.78577600
C	-4.72140800	-1.32174700	1.94519700
H	-4.18043200	-2.27122700	1.93054900
H	-4.30114800	-0.74852000	2.77105600
H	-5.77732000	-1.52590600	2.13232600

Zero-point correction= 0.711843 (Hartree/Particle)

Thermal correction to Energy= 0.757919

Thermal correction to Enthalpy= 0.758863

Thermal correction to Gibbs Free Energy= 0.632756

Sum of electronic and zero-point Energies= -2428.466300

Sum of electronic and thermal Energies= -2428.420224

Sum of electronic and thermal Enthalpies= -2428.419280

Sum of electronic and thermal Free Energies= -2428.545387

E(RB3LYP) = -2429.178143 A.U.

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Number of imaginary frequencies: 0

C	-1.30296100	-0.08845700	-2.51297200
C	-1.43877300	1.49258200	-0.76729400
C	-2.15977800	2.41734900	-1.59703800
C	-2.37456500	2.03636700	-2.94726300
C	-1.90842400	0.82913000	-3.41299100
C	-0.94523200	1.90937900	0.51981500

C	-2.55561300	3.65925000	-1.06277900
H	-2.88781400	2.72445000	-3.61399100
H	-2.02907000	0.54693600	-4.45331400
C	-2.17810000	4.01120600	0.22565800
C	-1.34080000	3.17148400	0.97697500
H	-3.11868800	4.35036300	-1.68362200
H	-2.47632500	4.97157300	0.63382200
H	-0.95256000	3.51521800	1.93023000
N	-1.08719600	0.23724400	-1.23552000
O	-1.26691200	-0.75510900	1.56136600
Rh	-2.70430300	-0.35190200	0.24627100
C	-4.04512100	-2.06007900	0.04522000
C	-4.20826500	-1.47240900	1.35115800
C	-4.65801000	-0.11316200	1.16206000
C	-4.84887000	0.11023500	-0.26105800
C	-4.45894600	-1.07620300	-0.94672700
C	-3.60105500	-3.45930700	-0.23045800
H	-2.96921700	-3.83611400	0.57593800
H	-4.47359000	-4.11917800	-0.31914700
H	-3.03879500	-3.52438200	-1.16467700
C	-3.89123300	-2.14556200	2.64985500
H	-4.29956600	-3.15993500	2.66266400
H	-2.80544500	-2.20707500	2.78761500
H	-4.31198900	-1.59758500	3.49441400
C	-4.95863600	0.87845100	2.23912100
H	-6.02134700	0.82860300	2.50777300
H	-4.37039400	0.68151200	3.13691200

H	-4.74496300	1.89698900	1.90699500
C	-5.38146300	1.36850600	-0.86625900
H	-5.18749600	1.41074200	-1.93903700
H	-6.46555100	1.42854800	-0.71435900
H	-4.93003900	2.25283600	-0.40780900
C	-4.54246300	-1.32022900	-2.41934400
H	-5.53784900	-1.70244800	-2.67468600
H	-4.37561000	-0.40463400	-2.98894900
H	-3.80993900	-2.06150900	-2.74324100
C	1.82326400	2.81978900	0.48027400
C	3.01613100	3.51902500	0.65574400
C	3.81045400	3.27823300	1.77901000
C	3.39581900	2.33705500	2.72605200
C	2.19749800	1.64797400	2.55982400
C	1.38849300	1.86809100	1.42738600
H	3.33122600	4.24019700	-0.09226500
H	4.73942600	3.82268400	1.91927100
H	4.00151200	2.14971200	3.60748200
H	1.87951900	0.93909800	3.31443400
C	1.06494900	-1.73734400	3.16711800
C	2.05313500	-2.66928300	3.47304600
C	2.98555600	-3.01650200	2.49238600
C	2.93479900	-2.45068700	1.22035500
C	1.95023200	-1.50042200	0.91564200
C	1.01902200	-1.12404100	1.91075600
H	0.32339200	-1.45562600	3.90929300
H	2.09362100	-3.12299800	4.45777100

H	3.75717800	-3.74825500	2.71138600
H	3.64109800	-2.76432700	0.46228100
H	1.23277300	2.99582200	-0.41330100
N	1.85172600	-0.88488900	-0.34411700
H	0.99967400	-0.37324800	-0.56139500
S	2.72785600	-1.22127400	-1.73269600
O	2.11431000	-0.31474500	-2.71776900
O	2.77524800	-2.66133000	-2.00394500
C	5.45810600	-1.46908300	-1.71089800
C	6.74691800	-1.04325800	-1.39653100
C	6.96528100	0.14146500	-0.67795300
C	5.85266600	0.89531600	-0.27362500
C	4.55763000	0.49255000	-0.58278400
C	4.37420500	-0.69106200	-1.29994500
H	5.28704700	-2.39486500	-2.24908800
H	7.59648800	-1.64488000	-1.70711300
H	5.99700300	1.80667200	0.29950200
H	3.70628600	1.07393700	-0.25141300
C	0.11479100	1.14395200	1.21315400
C	-0.07644700	-0.17789600	1.55856100
C	8.36586200	0.60558300	-0.36424900
H	8.75012600	1.24155400	-1.17108000
H	8.39714000	1.19298400	0.55781100
H	9.05440500	-0.23733500	-0.25789100
C	-0.87395900	-1.45055900	-2.96161700
H	0.12315800	-1.36847000	-3.41082600
H	-0.79172100	-2.12970900	-2.11046600

H	-1.55460300	-1.86347100	-3.71104800

Zero-point correction= 0.711859 (Hartree/Particle)

Thermal correction to Energy= 0.758137

Thermal correction to Enthalpy= 0.759082

Thermal correction to Gibbs Free Energy= 0.629943

Sum of electronic and zero-point Energies= -2428.566401

Sum of electronic and thermal Energies= -2428.520123

Sum of electronic and thermal Enthalpies= -2428.519179

Sum of electronic and thermal Free Energies= -2428.648317

E(RB3LYP) = -2429.278260 A.U.

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0 1

Number of imaginary frequencies: 0

C	0.37760600	-3.90949900	1.06960100
C	1.30015000	-1.84422800	1.59022600
C	2.27431600	-2.42224600	2.44708900
C	2.19868900	-3.81644100	2.64461400
C	1.24275100	-4.55910500	1.97751400
C	1.25962700	-0.38366700	1.43765100
C	3.32904900	-1.61024800	2.99549200
H	2.91060400	-4.29945600	3.30926700
H	1.16900400	-5.63220700	2.12196100
C	3.38763900	-0.27721200	2.71984400
C	2.35020500	0.36561600	1.96581300
H	4.08628100	-2.08946100	3.61059500
H	4.19664000	0.34083700	3.09417100
H	2.27338000	1.43874600	2.04783900

N	0.42338100	-2.58963800	0.89450600
O	-1.65138100	-0.80262000	1.41028500
Rh	2.29899200	0.33266300	-0.36542700
C	3.85470000	0.59504300	-1.93938500
C	4.35150700	-0.38318600	-1.03578100
C	3.44680200	-1.50902300	-1.09224500
C	2.42342400	-1.23698000	-2.06608700
C	2.65281800	0.07760200	-2.57845900
C	4.48822300	1.90727900	-2.27445900
H	3.72533400	2.65760500	-2.49219800
H	5.09551400	2.27358900	-1.44696300
H	5.12293600	1.79563600	-3.16275900
C	5.56597700	-0.25175700	-0.16955500
H	5.49332800	-0.90783400	0.70152300
H	6.47777900	-0.51639900	-0.71940800
H	5.64915100	0.77401700	0.19711200
C	3.67685100	-2.83342600	-0.43912400
H	4.35005000	-3.43420000	-1.06426600
H	4.14544800	-2.72378800	0.53977400
H	2.74837400	-3.39141900	-0.31483200
C	1.37450700	-2.22514200	-2.48083300
H	0.70571600	-1.81569700	-3.23760700
H	1.84793900	-3.12567700	-2.89031000
H	0.76185500	-2.52192500	-1.62503700
C	1.94634100	0.77176300	-3.70313200
H	2.62154400	0.89938700	-4.55799600
H	1.08101900	0.20302300	-4.04296400

H	1.60738000	1.76808200	-3.40185200
C	-0.35927800	1.98535600	2.44336300
C	-0.83622400	3.23032700	2.85626400
C	-1.16923700	4.20258400	1.91057500
C	-1.03411900	3.90995000	0.55081800
C	-0.55612400	2.66672100	0.14184900
C	-0.18934200	1.69239600	1.08068000
H	-0.95056000	3.43686000	3.91668000
H	-1.53430700	5.17510900	2.22879800
H	-1.29179600	4.65559800	-0.19588800
H	-0.43030300	2.46407100	-0.91315900
C	-1.03699800	-0.00179600	-2.06422300
C	-1.60824800	-0.07398100	-3.32945800
C	-2.74071200	-0.86903800	-3.52654100
C	-3.30439000	-1.56766500	-2.46424200
C	-2.76774600	-1.45048000	-1.17410400
C	-1.60019000	-0.66595600	-0.96382600
H	-0.13713800	0.57710600	-1.90305700
H	-1.17499200	0.47844100	-4.15704700
H	-3.18552100	-0.95068700	-4.51420600
H	-4.17980300	-2.18960800	-2.60577400
H	-0.12156800	1.22640800	3.18104500
N	-3.39629600	-2.12239900	-0.09985400
H	-2.87725300	-1.95061400	0.76959800
S	-5.03365500	-1.73657600	0.24659300
O	-5.23677700	-2.24700600	1.60208800
O	-5.86198100	-2.17957700	-0.87765800

C	-5.62839600	0.75420700	-0.78278700
C	-5.52669800	2.14481500	-0.80843200
C	-4.82235400	2.83767200	0.18482900
C	-4.22003200	2.10517700	1.22020200
C	-4.32603300	0.71939900	1.27299300
C	-5.03047900	0.05535400	0.26485600
H	-6.15639800	0.21023500	-1.55764900
H	-5.99230200	2.69851600	-1.61957100
H	-3.64256800	2.62379100	1.97959300
H	-3.84075300	0.16064400	2.06427300
C	0.25713000	0.31126100	0.65837200
C	-1.03294600	-0.47320100	0.39368200
C	-4.72636100	4.34326300	0.16110700
H	-5.51154800	4.79233700	0.78191700
H	-3.76386400	4.67955900	0.55533100
H	-4.84343700	4.73864000	-0.85227900
C	-0.62407700	-4.66576200	0.23534800
H	-1.60742000	-4.18890700	0.28808300
H	-0.32167000	-4.65724400	-0.81876700
H	-0.71461400	-5.70691900	0.55480300
O	4.13134700	2.64537200	0.87365000
C	3.11667100	3.10874500	0.34323400
O	2.18260300	2.42958000	-0.26219200
C	2.82572700	4.60638900	0.34541500
H	3.59294600	5.14012000	0.90790300
H	2.79691600	4.97833400	-0.68394800
H	1.83805500	4.78371000	0.78148300

Zero-point correction= 0.765558 (Hartree/Particle)

Thermal correction to Energy= 0.816004

Thermal correction to Enthalpy= 0.816948

Thermal correction to Gibbs Free Energy= 0.682769

Sum of electronic and zero-point Energies= -2657.214303

Sum of electronic and thermal Energies= -2657.163857

Sum of electronic and thermal Enthalpies= -2657.162913

Sum of electronic and thermal Free Energies= -2657.297092

E(RB3LYP) = -2657.979861 A.U.

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Number of imaginary frequencies: 0

C	5.37671500	-0.43793300	0.25902900
C	3.30821700	-0.43328200	-0.77263800
C	3.66955400	-1.49699200	-1.64975900
C	4.95307600	-2.05759900	-1.47433900
C	5.79876800	-1.54852400	-0.50911600
C	1.99314400	0.17890500	-0.91547700
C	2.76470300	-1.94327900	-2.67181200
H	5.26378900	-2.88629900	-2.10616300
H	6.78687300	-1.97162200	-0.35379600
C	1.54967000	-1.34582000	-2.83183200
C	1.13443700	-0.26984200	-1.98236500
H	3.08378300	-2.74863600	-3.32866800
H	0.88368800	-1.65190100	-3.63346300
H	0.31431400	0.35631500	-2.31353200
N	4.16916200	0.09802400	0.11579000

O	2.34130600	1.16695500	2.09256200
Rh	0.22914700	-0.68980500	0.08547400
C	1.25673300	-2.14194300	1.63656200
C	0.11016800	-1.58466000	2.26598700
C	-1.04669400	-1.95931500	1.48065300
C	-0.61699900	-2.80049400	0.40190900
C	0.81106400	-2.88110700	0.47778100
C	2.65705600	-2.02038400	2.14522700
H	3.38127100	-2.44696700	1.44885600
H	2.91728300	-0.96916900	2.30355400
H	2.75540800	-2.54427300	3.10400900
C	0.11401600	-0.84098600	3.56246500
H	-0.78640700	-0.23714800	3.68691200
H	0.16824200	-1.54860500	4.40051600
H	0.97933600	-0.17565400	3.62503600
C	-2.46309600	-1.66026300	1.85689700
H	-2.56239700	-0.64475600	2.24316700
H	-3.14101700	-1.76692500	1.01043500
H	-2.78393800	-2.35228000	2.64618400
C	-1.46734400	-3.60434200	-0.53407700
H	-1.12384600	-3.51137800	-1.56883400
H	-1.42615500	-4.66922800	-0.26807600
H	-2.50946700	-3.29022700	-0.49731000
C	1.63403300	-3.82858400	-0.33407900
H	1.51618100	-4.84141000	0.07329900
H	1.31406100	-3.84833800	-1.37706400
H	2.69422300	-3.57901900	-0.31131000

C	0.18346400	3.51881800	-0.66854500
C	0.03048500	4.63724300	-1.48419300
C	0.80147700	4.79656300	-2.63404000
C	1.74657600	3.82029100	-2.95442500
C	1.89415300	2.69887600	-2.14684300
C	1.10161100	2.49866300	-0.98944200
H	-0.71593000	5.37887900	-1.21735700
H	0.67367500	5.66950400	-3.26760600
H	2.37710800	3.93276200	-3.83186400
H	2.65578400	1.97189900	-2.40336700
C	-1.18082700	1.58530800	1.36017200
C	-2.32428200	1.99971100	2.06950400
C	-2.22206900	2.70695500	3.26481300
C	-0.97154800	3.00699100	3.80947100
C	0.17040500	2.58377300	3.13699300
C	0.09246900	1.89031400	1.92316600
H	1.15878800	2.77137700	3.54350200
H	-3.30078900	1.76198300	1.67118900
H	-3.13002500	3.01200100	3.77809000
H	-0.89007200	3.55060500	4.74549200
H	-0.44676600	3.44690000	0.20119200
N	-1.26450800	0.83914200	0.16492100
S	-2.30113900	1.27349900	-1.04175700
O	-1.64486800	0.99798100	-2.33207800
O	-2.87084500	2.60500800	-0.77600700
C	-4.82258700	0.42771200	-0.24414500
C	-5.85800200	-0.50117600	-0.15866000

C	-5.77631700	-1.73932500	-0.81200800
C	-4.62763200	-2.01836000	-1.56627000
C	-3.57990800	-1.10205100	-1.65249200
C	-3.67647600	0.11327800	-0.97547400
H	-4.90603900	1.40026800	0.22831100
H	-6.74888000	-0.25759200	0.41471800
H	-4.55306800	-2.96612500	-2.09406500
H	-2.69175300	-1.31523200	-2.23629700
C	1.44039000	1.30253300	-0.16186800
C	1.40737500	1.42179600	1.33369200
C	-6.91647800	-2.72664300	-0.74403100
H	-6.56265800	-3.75646700	-0.85143000
H	-7.45790600	-2.64912500	0.20362200
H	-7.63965900	-2.54433800	-1.54860900
C	6.29141600	0.20860000	1.26790100
H	5.69694900	0.76427400	1.99543000
H	6.90804400	-0.53373600	1.78510000
H	6.97173500	0.91464100	0.77546400

Zero-point correction= 0.700158 (Hartree/Particle)

Thermal correction to Energy= 0.745136

Thermal correction to Enthalpy= 0.746080

Thermal correction to Gibbs Free Energy= 0.624124

Sum of electronic and zero-point Energies= -2428.139111

Sum of electronic and thermal Energies= -2428.094134

Sum of electronic and thermal Enthalpies= -2428.093190

Sum of electronic and thermal Free Energies= -2428.215145

E(RB3LYP) = -2428.839270 A.U.

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Number of imaginary frequencies: 0

C	4.03129700	-0.08334200	1.58109900
C	2.65916400	1.54820300	0.66166400
C	3.75307600	2.44915400	0.48122500
C	5.03132600	2.01020200	0.91461200
C	5.17449600	0.75975800	1.46062500
C	1.33919200	1.93525600	0.26822000
C	3.52617600	3.71184500	-0.11856300
H	5.88567400	2.67356200	0.80377800
H	6.14198300	0.40204700	1.80061000
C	2.25304000	4.06447600	-0.50406200
C	1.16501500	3.18492000	-0.29631400
H	4.36334300	4.39012300	-0.26252800
H	2.06742500	5.03151600	-0.96116600
H	0.17363700	3.50899200	-0.58382600
N	2.83341600	0.30968500	1.19669100
O	0.44329300	1.20257200	3.03740100
C	-1.69649100	1.98205600	-0.92474100
C	-2.70502200	2.98770300	-1.10761400
C	-3.25705200	3.65783700	-0.04878100
C	-2.80259900	3.38559200	1.27780900
C	-1.80623300	2.47253500	1.50902700
C	-1.22931000	1.70819700	0.43132000
H	-3.00581300	3.22747800	-2.12462200
H	-4.01681300	4.41728800	-0.21221700

H	-3.22558200	3.93714000	2.11307700
H	-1.43284400	2.33336000	2.51528000
C	0.16774900	-1.40518600	0.69873500
C	0.20088400	-2.77344100	0.41889300
C	0.38365900	-3.65884800	1.48681700
C	0.49906800	-3.21490200	2.81108500
C	0.43740900	-1.84834800	3.08197000
C	0.28621200	-0.96585200	2.01792400
H	0.53060800	-1.45009600	4.08731700
H	0.07277000	-3.14056100	-0.58823700
H	0.41787400	-4.72390600	1.27530400
H	0.62628500	-3.93175900	3.61587000
H	-1.05277400	1.79591300	-1.77212900
N	0.01126200	-0.29703700	-0.21262500
S	0.71507400	-0.50848100	-1.83779400
O	0.57947000	0.77739900	-2.51805200
O	0.06141900	-1.71603600	-2.34928300
C	2.92822700	-2.12709000	-1.39966800
C	4.30108100	-2.34467500	-1.30328900
C	5.21642000	-1.30721700	-1.52254900
C	4.72394900	-0.04333700	-1.87913200
C	3.35856700	0.19747000	-1.97337000
C	2.46816200	-0.84672400	-1.70875200
H	2.23254800	-2.94019800	-1.24655100
H	4.66507800	-3.33753500	-1.05390600
H	5.41981900	0.76883000	-2.06757500
H	2.97888200	1.17699800	-2.23691000

C	0.14468400	1.03430100	0.59892300
C	0.31792400	0.49593400	2.05728900
C	6.69792500	-1.52212100	-1.34455300
H	7.03134400	-1.08010700	-0.39697700
H	6.95652000	-2.58421900	-1.32688300
H	7.27198500	-1.04207300	-2.14334400
C	4.16445200	-1.47023600	2.15422200
H	3.19039000	-1.96027200	2.18420100
H	4.84385100	-2.07364200	1.54197200
H	4.57847900	-1.43548200	3.16847700
Rh	-2.31513600	-0.01397600	-0.29972200
C	-3.61389900	-1.72344600	0.77837700
C	-4.29158700	-0.50053000	0.86297500
C	-4.52489000	-0.01713300	-0.50422700
C	-4.06632100	-1.01128500	-1.42561400
C	-3.39459400	-1.99476900	-0.64399500
C	-3.19209800	-2.61333900	1.90777800
H	-2.18823600	-3.01238700	1.75130500
H	-3.18180200	-2.07315500	2.85798000
H	-3.86990600	-3.47106700	2.02041000
C	-4.73235300	0.23571000	2.08953300
H	-4.38296900	1.27453500	2.06446100
H	-5.82711600	0.25736400	2.16843700
H	-4.33842900	-0.22563300	2.99856600
C	-5.41167700	1.14439900	-0.82982500
H	-5.24946800	1.97555600	-0.14094100
H	-5.23365000	1.51633200	-1.84163700

H	-6.46609100	0.84499200	-0.75831100
C	-4.23942100	-1.02657500	-2.91504900
H	-3.37759300	-1.48753000	-3.40621900
H	-5.13435500	-1.59097400	-3.21549800
H	-4.34074200	-0.01335000	-3.31392500
C	-2.78027500	-3.24554800	-1.20314900
H	-3.56086200	-3.91312500	-1.59048300
H	-2.09398100	-3.01444100	-2.02195900
H	-2.22771500	-3.79553700	-0.43924100

Zero-point correction= 0.699930 (Hartree/Particle)

Thermal correction to Energy= 0.744975

Thermal correction to Enthalpy= 0.745919

Thermal correction to Gibbs Free Energy= 0.624798

Sum of electronic and zero-point Energies= -2428.145149

Sum of electronic and thermal Energies= -2428.100104

Sum of electronic and thermal Enthalpies= -2428.099160

Sum of electronic and thermal Free Energies= -2428.220281

E(RB3LYP) = -2428.845079 A.U.

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Number of imaginary frequencies: 0

C	0.93537000	-3.08863800	-0.42056300
C	1.07560100	-4.47693600	-0.54055500
C	0.52914500	-5.15811300	-1.62398700
C	-0.19004300	-4.46963800	-2.60730300
C	-0.32836300	-3.09184700	-2.51305700
C	0.25115000	-2.38337000	-1.44228500

H	1.61616200	-5.00295300	0.23617700
H	0.64474900	-6.23564900	-1.68992900
H	-0.63633200	-5.00569900	-3.43888700
H	-0.87057500	-2.53765500	-3.27299800
C	1.04533600	2.59993400	-1.10322600
C	1.39152700	3.85686900	-1.59246100
C	1.43180400	4.10152800	-2.96780300
C	1.14272700	3.06895800	-3.86468300
C	0.79512800	1.80669500	-3.38729300
C	0.72535300	1.56487900	-2.00012600
H	1.00531600	2.40677800	-0.04134900
H	1.63448300	4.65018100	-0.89181500
H	1.69889000	5.08628100	-3.33962200
H	1.19042300	3.24467900	-4.93527100
H	0.57708300	0.99830700	-4.07768700
N	1.44542300	-2.43892700	0.72038100
H	0.90166000	-1.67067300	1.12135700
S	3.10472900	-2.33777500	1.03222300
O	3.72643400	-3.45868500	0.31997000
O	3.25185300	-2.15713400	2.47227000
C	3.48021000	0.39016200	0.91098000
C	3.85463900	1.56696800	0.26400000
C	4.34181600	1.55228000	-1.04954200
C	4.44440200	0.32078000	-1.71395500
C	4.08166400	-0.86746400	-1.08556600
C	3.60589000	-0.81912400	0.22672200
H	3.08639700	0.40407900	1.92019200

H	3.75578900	2.51206400	0.79030100
H	4.82250400	0.29374800	-2.73294400
H	4.17989800	-1.82470100	-1.58601500
C	0.32502300	0.25929900	-1.55592600
C	0.18765900	-0.96088100	-1.44805100
C	4.73834300	2.82650800	-1.75388600
H	4.65233000	3.69419300	-1.09453400
H	5.77250900	2.77404100	-2.11231200
H	4.09628100	3.00517900	-2.62290400
Rh	-1.74381000	0.11141700	-0.27210700
C	-3.92291400	0.12287800	0.03943600
C	-3.41749200	1.46399600	0.13581400
C	-2.83447300	1.83115600	-1.13984000
C	-2.98485400	0.70747100	-2.01603000
C	-3.62471400	-0.36866600	-1.29280000
O	-2.80837800	-2.97402900	0.63949200
C	-1.86302700	-2.51767900	1.27856800
O	-1.19513100	-1.42674400	0.98519500
C	-1.32978400	-3.17801400	2.53876000
C	-4.05154000	-1.68107400	-1.86784200
H	-3.88245300	-2.47125200	-1.13650000
H	-5.11417000	-1.64325000	-2.13922600
H	-3.48191600	-1.91907300	-2.76880200
C	-4.66098600	-0.59166200	1.12474400
H	-4.19255400	-0.40074000	2.09371200
H	-5.69351200	-0.22236900	1.16604400
H	-4.66025700	-1.66670800	0.95839000

C	-3.46187700	2.34051500	1.34365500
H	-2.57483600	2.97368500	1.39569500
H	-4.35029300	2.98313000	1.30081900
H	-3.48767600	1.74942500	2.25891800
C	-2.26743300	3.17666500	-1.46621000
H	-1.63412100	3.14869900	-2.35353900
H	-3.07825100	3.89396400	-1.64225700
H	-1.65804200	3.54935700	-0.64043400
C	-2.56950000	0.64441000	-3.44997400
H	-3.44541900	0.79691700	-4.09188400
H	-1.83252700	1.41092900	-3.68850000
H	-2.14263100	-0.33093600	-3.69402600
H	-0.26905800	-3.41352300	2.41948600
H	-1.40569000	-2.46603900	3.36588900
H	-1.89886100	-4.08283200	2.75472200
S	-0.24909900	0.80480600	2.52925200
O	-0.46361800	1.23094300	1.07368300
O	-1.49957300	0.60083600	3.27273300
C	0.43738500	2.43067900	3.12692400
O	0.85133600	-0.15169900	2.70911100
F	-0.45514300	3.41690700	2.93220600
F	1.55589400	2.73691700	2.43620500
F	0.73877200	2.37057500	4.42367900

Zero-point correction= 0.633101 (Hartree/Particle)

Thermal correction to Energy= 0.683652

Thermal correction to Enthalpy= 0.684596

Thermal correction to Gibbs Free Energy= 0.545882

Sum of electronic and zero-point Energies= -3102.854698

Sum of electronic and thermal Energies= -3102.804147

Sum of electronic and thermal Enthalpies= -3102.803203

Sum of electronic and thermal Free Energies= -3102.941918

E(RB3LYP) = -3103.487799 A.U.

B-12

0 1

Number of imaginary frequencies: 0

C	0.24996400	-2.41190600	0.63993000
C	1.23973000	-3.38783000	0.73216700
C	1.16207900	-4.38016900	1.70281200
C	0.08978000	-4.39636900	2.59971900
C	-0.90730200	-3.43304200	2.50907900
C	-0.85653100	-2.42980800	1.52022100
H	2.06716800	-3.35610800	0.03789600
H	1.94326100	-5.13071000	1.76845600
H	0.03356100	-5.15909900	3.37008300
H	-1.74475300	-3.43685800	3.19856400
C	-3.84835200	1.40479800	0.54260500
C	-4.95598900	2.24314700	0.45108600
C	-6.15375900	1.90926800	1.09027200
C	-6.24122200	0.72522100	1.82909800
C	-5.14063300	-0.12353800	1.92516900
C	-3.93207200	0.20794800	1.27945100
H	-2.92896000	1.66580900	0.03669700
H	-4.87575400	3.16093600	-0.12380600
H	-7.01430900	2.56774900	1.01533200

H	-7.16876800	0.46163200	2.32906700
H	-5.20410400	-1.04705200	2.49208900
N	0.37538900	-1.36380000	-0.33273700
H	-0.34037000	-0.64608700	-0.15628100
S	0.08111000	-1.87967500	-2.04537800
O	0.46385900	-3.29143600	-2.11167200
O	0.74192900	-0.88106700	-2.88307800
C	-2.18517100	-0.39869400	-2.36609600
C	-3.55786700	-0.20930400	-2.27856600
C	-4.42063200	-1.26910000	-1.95588800
C	-3.87769100	-2.54654400	-1.75821600
C	-2.50416400	-2.76683400	-1.84216600
C	-1.67830200	-1.68334500	-2.14339800
H	-1.52338000	0.43669100	-2.55598600
H	-3.95831800	0.78909300	-2.42145000
H	-4.53596300	-3.37622400	-1.51676600
H	-2.07574000	-3.74829000	-1.67166300
C	-2.81881300	-0.67631500	1.35649300
C	-1.89798900	-1.46754600	1.42817700
C	-5.89252500	-1.00653200	-1.76807800
H	-6.05616700	-0.46884700	-0.82676000
H	-6.29084400	-0.38110100	-2.57330200
H	-6.47037700	-1.93406400	-1.73375700
Rh	2.00834300	0.20388600	-0.04961100
C	3.66587600	1.58355200	-0.36518800
C	4.02384500	0.66630900	0.67665400
C	3.99068100	-0.66542800	0.12807900

C	3.69837500	-0.55157900	-1.29702800
C	3.47220800	0.81794600	-1.59679400
O	0.93595200	0.41584700	1.69358800
C	1.22628500	-0.18809200	2.81355300
O	2.15136400	-0.98212800	2.99626600
C	0.24505400	0.17907200	3.91897400
C	3.09411000	1.40827800	-2.91700000
H	2.39407700	2.23489100	-2.77794800
H	3.98775700	1.79059100	-3.42618700
H	2.61334600	0.66505100	-3.55292800
C	3.63917000	3.07313000	-0.26368200
H	3.51639400	3.39916000	0.76960700
H	4.58911500	3.47420100	-0.64027100
H	2.82471600	3.49465700	-0.85371800
C	4.38025300	1.02096200	2.08355900
H	4.10065800	0.21757500	2.76404400
H	5.46093100	1.20078200	2.15001000
H	3.86592100	1.93049800	2.40045600
C	4.37644600	-1.90586400	0.86995000
H	4.29386300	-2.79183100	0.23800900
H	5.41765700	-1.82898400	1.20538000
H	3.73418400	-2.02030100	1.74692400
C	3.68319300	-1.69564100	-2.26032300
H	4.71578200	-1.98973400	-2.48555400
H	3.16936400	-2.56835500	-1.85174000
H	3.17966400	-1.42915200	-3.18759400
H	-0.73102000	-0.25464100	3.68153300

H	0.59660800	-0.20215400	4.87855500
H	0.11312700	1.26350600	3.95559500
S	-0.23654700	2.68174300	-0.98500600
O	0.18705800	1.23295000	-0.85358200
O	0.77001700	3.53784100	-1.63413000
C	-0.27919700	3.27205600	0.78449000
O	-1.62691400	2.77903600	-1.45649400
F	0.95773300	3.25754000	1.31025400
F	-1.07680100	2.49790200	1.52689700
F	-0.74022400	4.52875900	0.82322300

Zero-point correction= 0.634682 (Hartree/Particle)

Thermal correction to Energy= 0.684683

Thermal correction to Enthalpy= 0.685627

Thermal correction to Gibbs Free Energy= 0.550934

Sum of electronic and zero-point Energies= -3102.869860

Sum of electronic and thermal Energies= -3102.819858

Sum of electronic and thermal Enthalpies= -3102.818914

Sum of electronic and thermal Free Energies= -3102.953608

E(RB3LYP) = -3103.504542 A.U.

B-13a

0 1

Number of imaginary frequencies: 0

C	-1.98269100	-1.78302700	0.64833600
C	-3.25797800	-2.38748200	0.66072500
C	-3.58962400	-3.30514800	1.65420800
C	-2.68105600	-3.66838500	2.65537900
C	-1.41626400	-3.09162100	2.65685500

C	-1.06800900	-2.15420800	1.67150400
H	-3.96665600	-2.15851700	-0.12255700
H	-4.57670600	-3.75908800	1.63441900
H	-2.95500400	-4.39209400	3.41594900
H	-0.68569700	-3.34865800	3.41793000
C	2.81953500	0.83510900	2.32536100
C	4.05043100	1.34460800	2.72602200
C	5.02462200	0.49417700	3.25672400
C	4.76550200	-0.87489100	3.38513400
C	3.54620300	-1.39880800	2.96542100
C	2.56379900	-0.54456100	2.42263100
H	2.04914800	1.47532900	1.92315800
H	4.24012300	2.40781000	2.62054500
H	5.98253800	0.89539300	3.57441900
H	5.51856200	-1.53437900	3.80617000
H	3.34193800	-2.46181100	3.05215000
N	-1.50841100	-0.85477000	-0.27176900
S	-2.54238000	-0.04523900	-1.29479400
O	-3.40528100	-0.98707600	-2.04300700
O	-1.70672200	0.88450800	-2.06093200
C	-2.99416700	1.87412600	0.61380700
C	-3.80069600	2.60614200	1.47789100
C	-5.18322600	2.37107500	1.56213800
C	-5.74674500	1.38337200	0.74574700
C	-4.95610300	0.63740300	-0.12983300
C	-3.58724300	0.88848300	-0.18094200
H	-1.93176700	2.07388200	0.54300600

H	-3.35001300	3.38166100	2.09163300
H	-6.81635700	1.19585700	0.79108000
H	-5.38784900	-0.11978100	-0.77479900
C	1.31789800	-1.06601900	1.97677100
C	0.21685700	-1.52908800	1.66957200
C	-6.03188600	3.16516800	2.52569300
H	-5.84025500	2.85740100	3.56090300
H	-5.80773100	4.23516200	2.46167200
H	-7.09939500	3.02920100	2.33106900
Rh	0.60281200	-0.78598200	-0.55830400
C	2.22131500	-0.80957700	-2.19227100
C	2.53589800	-1.75636300	-1.18427900
C	1.43069100	-2.71046300	-1.10501400
C	0.45530600	-2.34013700	-2.08775200
C	0.90599500	-1.11673400	-2.72189100
C	0.26222100	-0.40856700	-3.86686000
H	0.31008800	0.67018800	-3.71613900
H	0.78925100	-0.67123000	-4.79403900
H	-0.78773700	-0.67964400	-3.96515300
C	3.11951200	0.27177500	-2.69000800
H	3.88431100	0.53065300	-1.95785100
H	3.62045200	-0.08652800	-3.59915900
H	2.55194200	1.16919100	-2.93201700
C	3.82438700	-1.82018700	-0.42763900
H	3.75038500	-2.47233500	0.44200500
H	4.61944900	-2.20756300	-1.07634000
H	4.12498500	-0.83143500	-0.07320600

C	1.38727700	-3.92702900	-0.23588100
H	0.35953100	-4.19112000	0.02031700
H	1.84460900	-4.77749300	-0.75578700
H	1.92887800	-3.76230600	0.69723700
C	-0.79556800	-3.09453800	-2.40510600
H	-0.57334400	-3.85614800	-3.16303500
H	-1.18873800	-3.59750100	-1.51934300
H	-1.58236200	-2.44058400	-2.78097400
S	0.67591200	2.56331500	-0.76398100
O	0.59009600	1.28587000	0.07202300
O	0.88649900	2.34213800	-2.20036900
C	2.32741400	3.23643800	-0.20492700
O	-0.29490800	3.56735800	-0.32747900
F	3.28904900	2.29581300	-0.33118900
F	2.29144800	3.61482600	1.08677600
F	2.67174000	4.29171800	-0.94600600

Zero-point correction= 0.569784 (Hartree/Particle)

Thermal correction to Energy= 0.614322

Thermal correction to Enthalpy= 0.615266

Thermal correction to Gibbs Free Energy= 0.490893

Sum of electronic and zero-point Energies= -2873.801906

Sum of electronic and thermal Energies= -2873.757369

Sum of electronic and thermal Enthalpies= -2873.756424

Sum of electronic and thermal Free Energies= -2873.880798

E(RB3LYP) = -2874.371691 A.U.

B-13c

0 1

Number of imaginary frequencies: 0

Rh	0.61620900	-1.24164600	-0.37620500
C	0.11719200	-2.26470800	-2.25082100
C	1.48426400	-1.84863000	-2.32742100
C	2.24722900	-2.64722700	-1.36072200
C	1.34913300	-3.45654600	-0.65198600
C	-0.00407800	-3.18258400	-1.14504000
C	-0.98263000	-1.87066800	-3.18841300
H	-0.83725700	-0.85829700	-3.57133600
H	-1.00003900	-2.55866200	-4.04246700
H	-1.95575900	-1.91332000	-2.69643400
C	2.08061200	-0.98958800	-3.39876300
H	2.43855800	-1.62197200	-4.22183500
H	1.34353800	-0.29417100	-3.80561700
H	2.91939200	-0.41111500	-3.01253500
C	3.73493900	-2.63462800	-1.18279100
H	4.15255200	-3.59438100	-1.51086900
H	4.20037100	-1.83003400	-1.74913200
H	4.00695700	-2.48350300	-0.13486100
C	1.71158400	-4.46882100	0.38786300
H	1.85742000	-5.44865100	-0.08632700
H	2.64581400	-4.19950000	0.88705700
H	0.92739100	-4.55839500	1.13938300
C	-1.22020800	-3.96968600	-0.77631500
H	-1.16182700	-4.96614700	-1.23455700
H	-1.27741200	-4.07082100	0.30725900
H	-2.13420400	-3.48580800	-1.12404500

C	-1.59559900	2.10741600	-1.88984700
C	-1.64253300	3.27534700	-2.63274200
C	-0.41625800	3.76916100	-3.09408000
C	0.77402100	3.09303000	-2.80125000
C	0.78781600	1.91451100	-2.04663400
C	-0.42201100	1.40842600	-1.56465600
H	-2.57684100	3.78792500	-2.83003500
H	-0.39438000	4.68058200	-3.68270800
H	1.71648000	3.48983300	-3.16637200
H	1.71912100	1.41033700	-1.84106600
C	-4.30626300	-1.08221700	-0.88282600
C	-5.18538000	-2.05478900	-0.41087100
C	-4.87012900	-2.78816700	0.73700900
C	-3.67277000	-2.53787400	1.41001300
C	-2.80205700	-1.55394400	0.94929200
C	-3.10042000	-0.81874200	-0.20584600
H	-4.55981700	-0.54806700	-1.79669400
H	-6.11139200	-2.24699900	-0.94480200
H	-5.55212300	-3.55313600	1.09656200
H	-3.38872400	-3.11489600	2.28389900
H	-1.87025900	-1.35926900	1.45611200
N	-2.69713700	1.42577800	-1.25807700
S	-3.44784800	2.61123000	0.25875600
O	-3.46637900	3.92924000	-0.37004600
O	-4.66350100	1.88882300	0.61580200
C	-2.28156000	1.40345700	2.37612400
C	-1.16986600	1.09764500	3.14319400

C	0.06522200	1.73108200	2.92568000
C	0.15055000	2.74185600	1.95261700
C	-0.94842700	3.08767100	1.18087400
C	-2.15540600	2.40571700	1.40410300
H	-3.21693500	0.87041400	2.49628900
H	-1.24439600	0.31963800	3.89467600
H	1.10077600	3.22740200	1.76916400
H	-0.87605600	3.84446900	0.40846100
C	-2.13887800	0.16665300	-0.70931600
C	-0.77603300	0.18539500	-0.80469100
C	1.29125300	1.27441100	3.65625100
H	1.98877500	2.09327600	3.83704400
H	1.04162500	0.79802700	4.60680700
H	1.78901700	0.53280500	3.02130100
H	-3.53602300	1.31632900	-1.83259600
O	-0.56515900	-3.28405000	2.21180500
C	0.11026800	-2.28708200	2.50186800
O	0.33658700	-1.25472000	1.75034500
C	0.73647800	-2.18294400	3.89380700
H	1.76218700	-1.81322200	3.82468500
H	0.17086800	-1.47220800	4.50529600
H	0.71140000	-3.15772200	4.38335700
S	3.37062800	0.56807900	0.21441800
O	1.86931300	0.51583500	0.37536100
O	4.11390600	-0.25507100	1.17670200
C	3.70489700	2.34136200	0.68929700
O	3.80755000	0.53329800	-1.19744200

F	3.47576600	2.55640400	1.99774600
F	2.90403000	3.16987000	-0.00997100
F	4.97564900	2.65609700	0.42710500

Zero-point correction= 0.636777 (Hartree/Particle)

Thermal correction to Energy= 0.685300

Thermal correction to Enthalpy= 0.686244

Thermal correction to Gibbs Free Energy= 0.557038

Sum of electronic and zero-point Energies= -3102.846720

Sum of electronic and thermal Energies= -3102.798197

Sum of electronic and thermal Enthalpies= -3102.797253

Sum of electronic and thermal Free Energies= -3102.926459

E(RB3LYP) = -3103.483497 A.U.

B-14

1 1

Number of imaginary frequencies: 0

C	-1.42979500	0.41373200	1.59182800
C	-2.65118800	0.38608200	2.28727000
C	-2.88570500	1.32374400	3.28924000
C	-1.93591400	2.29989300	3.62451700
C	-0.71555000	2.33073100	2.95990200
C	-0.45747700	1.38021300	1.96167000
H	-3.38858200	-0.37446700	2.07123800
H	-3.82588400	1.28545300	3.83076900
H	-2.14373200	3.01539400	4.41266800
H	0.04304800	3.06433500	3.21198400
C	2.80899500	2.37834600	-1.60973000
C	3.88570800	2.99735600	-2.23551500

C	4.97824400	3.43656300	-1.47988900
C	4.98792600	3.26970900	-0.09114400
C	3.91147700	2.66012200	0.54744700
C	2.81480400	2.20002100	-0.21143500
H	1.95613700	2.03072100	-2.18393700
H	3.87572700	3.14020700	-3.31131900
H	5.81827400	3.91641300	-1.97213600
H	5.83173500	3.62167100	0.49358700
H	3.90441200	2.53641000	1.62539600
N	-1.03562100	-0.40140300	0.52503400
S	-2.18233100	-1.36562600	-0.28677900
O	-2.77690700	-2.33964100	0.64092700
O	-1.48248600	-1.83955800	-1.48917300
C	-3.07214500	0.89461100	-1.57983000
C	-4.05948400	1.78530700	-1.98627100
C	-5.40375100	1.59577600	-1.62328100
C	-5.73494600	0.48610100	-0.83336400
C	-4.75947900	-0.41426900	-0.40834900
C	-3.43471700	-0.19591200	-0.78476300
H	-2.03655500	1.04399200	-1.86673600
H	-3.78783100	2.64162800	-2.59714100
H	-6.76953500	0.32381900	-0.54519900
H	-5.01360200	-1.27274300	0.20383100
C	1.69755100	1.59223400	0.43784100
C	0.74657400	1.31983100	1.20380300
C	-6.46795200	2.55166500	-2.10041700
H	-6.08919700	3.57615200	-2.15894200

H	-6.81119200	2.27289600	-3.10403900
H	-7.34032600	2.54442000	-1.44175000
Rh	0.95635400	-0.56724500	0.10130600
C	1.75212400	-2.27174800	-1.29452000
C	2.84773800	-1.40546100	-0.89313900
C	2.94710700	-1.43996900	0.53070000
C	1.86831500	-2.27633500	1.02727400
C	1.16585100	-2.82404000	-0.12040700
C	0.13294100	-3.90100000	-0.04594800
H	-0.40831600	-4.00492000	-0.98352600
H	0.63951800	-4.84700300	0.18409600
H	-0.60243700	-3.71205100	0.73825400
C	1.34220600	-2.56197500	-2.69801700
H	1.67259200	-1.77866800	-3.38279200
H	1.79695300	-3.50566500	-3.02616300
H	0.25845200	-2.65700800	-2.76832600
C	3.80509100	-0.74895100	-1.83498800
H	4.38996800	0.03029600	-1.34738400
H	4.49956600	-1.50264400	-2.22604000
H	3.29039000	-0.30089900	-2.68723300
C	4.00732000	-0.80994400	1.37408300
H	3.61617700	-0.51204100	2.34932500
H	4.81348100	-1.53369900	1.54443900
H	4.44003900	0.06786400	0.89346300
C	1.62207100	-2.65316800	2.45030700
H	2.19716000	-3.55500400	2.69784700
H	1.92966000	-1.86060600	3.13521900

H	0.56611400	-2.87035300	2.62173700

Zero-point correction= 0.540182 (Hartree/Particle)

Thermal correction to Energy= 0.576278

Thermal correction to Enthalpy= 0.577222

Thermal correction to Gibbs Free Energy= 0.471017

Sum of electronic and zero-point Energies= -1912.177155

Sum of electronic and thermal Energies= -1912.141060

Sum of electronic and thermal Enthalpies= -1912.140115

Sum of electronic and thermal Free Energies= -1912.246320

E(RB3LYP) = -1912.717337 A.U.

B-15

1 1

Number of imaginary frequencies: 0

Rh	1.95849800	-0.07064500	-0.29696800
C	3.41680900	-1.57715400	0.28259500
C	3.32642000	-1.51922600	-1.14635800
C	3.77690200	-0.19159900	-1.56252700
C	4.19953000	0.53205500	-0.40098200
C	3.93704500	-0.28843900	0.73557400
C	3.13043300	-2.76612600	1.14448600
H	2.28490900	-3.34138700	0.76038600
H	4.00592900	-3.42552000	1.18219600
H	2.89185200	-2.46806800	2.16713800
C	2.98932000	-2.64271100	-2.07480000
H	3.90936700	-3.04027100	-2.52064200
H	2.49414400	-3.45918800	-1.54833200
H	2.33988500	-2.31249000	-2.88850400

C	3.86704000	0.26579500	-2.98205900
H	4.82882400	-0.04228500	-3.41160200
H	3.07575500	-0.17535100	-3.59210900
H	3.79946300	1.35236900	-3.06236200
C	4.76608900	1.91826500	-0.36040800
H	5.83827800	1.88585100	-0.13669400
H	4.64015000	2.43128000	-1.31516000
H	4.27985800	2.52574200	0.40800700
C	4.17865700	0.09223000	2.15979800
H	5.18458100	-0.22275700	2.46499900
H	4.11071800	1.17302400	2.30021700
H	3.46388200	-0.38905800	2.83095200
C	-1.67211000	-1.61785200	1.03272000
C	-2.57780000	-2.55276000	1.53014300
C	-2.42343700	-3.87545200	1.10925800
C	-1.39705000	-4.25740700	0.22931400
C	-0.49048400	-3.31753700	-0.25183700
C	-0.62558900	-1.98082500	0.14621800
H	-3.35343500	-2.26992300	2.22962200
H	-3.11154700	-4.62724300	1.48267000
H	-1.31157000	-5.29634700	-0.07260700
H	0.29693300	-3.60230900	-0.94158300
C	0.34798200	2.35741100	1.70714700
C	1.12825700	3.49753100	1.63867400
C	1.71467900	3.90942700	0.42259800
C	1.49343800	3.18083500	-0.73310300
C	0.70264900	2.01085200	-0.69342500

C	0.13192400	1.58093700	0.54274100
H	-0.09766700	2.04281300	2.64178900
H	1.29491100	4.08255200	2.53793200
H	2.31306800	4.81454900	0.39243700
H	1.90036800	3.51277600	-1.68307200
H	0.36045000	1.56187500	-1.62055300
N	-1.56677100	-0.21977100	1.30266600
S	-2.99240000	0.75060500	1.68557500
O	-3.70288000	-0.00737500	2.70652800
O	-2.47402400	2.09358000	1.91771000
C	-3.58257500	1.65992500	-0.82845400
C	-4.26344300	1.60552300	-2.04071500
C	-5.23996600	0.62547500	-2.28321600
C	-5.52899000	-0.30193500	-1.27049100
C	-4.86097600	-0.26913500	-0.04943100
C	-3.89119600	0.71508200	0.15456800
H	-2.84753600	2.43306100	-0.63167400
H	-4.04579000	2.34362600	-2.80732900
H	-6.29408100	-1.05451400	-1.43706100
H	-5.09711500	-0.97535900	0.73777300
C	-0.50327100	0.25874700	0.54325100
C	0.13066600	-0.78695300	-0.14092000
C	-5.95232600	0.56035300	-3.61044400
H	-6.96991600	0.17602500	-3.50017400
H	-6.00570200	1.54297300	-4.08670200
H	-5.42213600	-0.11034600	-4.29765300

Zero-point correction= 0.541629 (Hartree/Particle)

Thermal correction to Energy= 0.577390

Thermal correction to Enthalpy= 0.578334

Thermal correction to Gibbs Free Energy= 0.470129

Sum of electronic and zero-point Energies= -1912.190395

Sum of electronic and thermal Energies= -1912.154633

Sum of electronic and thermal Enthalpies= -1912.153689

Sum of electronic and thermal Free Energies= -1912.261895

E(RB3LYP) = -1912.732024 A.U.

B-TSa1

1 1

Number of imaginary frequencies: 1

Rh	-0.82112900	0.05961900	0.05079200
C	-2.27823500	-0.74064500	1.45642700
C	-2.81608500	-0.90353100	0.12541400
C	-1.91539900	-1.73071200	-0.62003600
C	-0.83509200	-2.14443900	0.27227800
C	-1.07605200	-1.54926600	1.54777400
O	-0.05061100	2.52037000	-1.77807900
O	-1.68921200	1.91755300	-0.36811100
C	-1.12111800	2.75217100	-1.16177300
C	-1.79523900	4.09500500	-1.32248300
H	-1.40858700	4.76655500	-0.54847600
H	-1.55605400	4.51993800	-2.29787200
H	-2.87398500	4.00411100	-1.18890300
C	-2.91660700	0.03288800	2.56532100
H	-2.17193700	0.40136200	3.27396500
H	-3.46658000	0.89107800	2.17393900

H	-3.62167400	-0.60214800	3.11570400
C	-4.05653700	-0.23483400	-0.37267300
H	-4.91843900	-0.55679700	0.22108500
H	-3.96017900	0.85131700	-0.27753500
H	-4.25321600	-0.47259300	-1.41871900
C	-2.09789800	-2.19135400	-2.03169600
H	-2.69992800	-3.10780100	-2.04950900
H	-2.61088900	-1.43999100	-2.63532600
H	-1.13976700	-2.41330900	-2.50407400
C	0.26747300	-3.09401800	-0.07910200
H	-0.07309100	-4.12891200	0.04084500
H	0.59172700	-2.96206600	-1.11275100
H	1.13840900	-2.95060500	0.56344000
C	-0.22389600	-1.66468300	2.76964600
H	-0.69736800	-2.33682500	3.49438900
H	0.76595700	-2.06039500	2.53662300
H	-0.10181800	-0.68807400	3.24445800
C	2.92419200	0.89238600	1.65842800
C	2.08046600	0.14169900	-0.45868400
C	3.33702100	-0.42289600	-0.78969700
C	4.40620500	-0.28215600	0.13118400
C	4.19742700	0.38892100	1.31383300
C	0.96536100	0.12476000	-1.34214300
C	3.44210700	-1.09902100	-2.03548700
H	5.38007600	-0.69821500	-0.10635700
H	5.00074700	0.52437400	2.02873800
C	2.36135300	-1.16771500	-2.89135700

C	1.14156200	-0.53897100	-2.55360000
H	4.39289800	-1.54812700	-2.30615000
H	2.45923900	-1.67531700	-3.84576500
H	0.33190700	-0.52902100	-3.27765600
N	1.91212200	0.72829900	0.78523600
O	0.68770100	1.13238000	1.14036800
H	0.33843300	1.20356200	-1.46282000
C	2.60881900	1.57312200	2.94867400
H	2.20129100	2.57167100	2.76210400
H	1.83464600	1.02015600	3.49046900
H	3.50215700	1.65241300	3.56896000

Zero-point correction= 0.439873 (Hartree/Particle)

Thermal correction to Energy= 0.468782

Thermal correction to Enthalpy= 0.469726

Thermal correction to Gibbs Free Energy= 0.380493

Sum of electronic and zero-point Energies= -1244.008261

Sum of electronic and thermal Energies= -1243.979351

Sum of electronic and thermal Enthalpies= -1243.978407

Sum of electronic and thermal Free Energies= -1244.067640

E(RB3LYP) = -1244.448134 A.U.

B-TSb1

1 1

Number of imaginary frequencies: 1

Rh	1.03317100	-0.10498800	-0.06815700
C	3.14330300	0.11617300	-0.62953900
C	3.02912800	0.15237900	0.79458600
C	2.44580100	-1.10638300	1.23328600

C	2.25733500	-1.93316700	0.06246000
C	2.64511400	-1.17546200	-1.09212300
O	0.06909900	1.21568200	1.31828500
O	0.42721100	2.84238900	-0.17701300
C	0.08984700	2.44297900	0.98682800
C	-0.30299200	3.47626900	2.01007000
H	-0.58693900	3.00500400	2.95036400
H	0.53901000	4.15644500	2.16986800
H	-1.13073600	4.07438300	1.61950800
H	0.37660800	1.79516500	-0.93438100
C	3.68352000	1.20641800	-1.49903300
H	3.28212800	1.14419300	-2.51222800
H	3.43913100	2.19186600	-1.09720300
H	4.77496900	1.12523900	-1.56502500
C	3.40939000	1.28282300	1.69654900
H	4.38116700	1.08244900	2.16210100
H	3.48277200	2.22386800	1.14893300
H	2.67243100	1.40670100	2.49341400
C	2.17749100	-1.48761300	2.65363300
H	3.09139400	-1.86943100	3.12434200
H	1.83475400	-0.62504900	3.22916400
H	1.41019300	-2.26075600	2.72084100
C	1.65672600	-3.30306200	0.02211600
H	2.31583200	-3.98655400	-0.52223900
H	1.49939300	-3.70324400	1.02408300
H	0.68985400	-3.28057200	-0.49227800
C	2.63844400	-1.67321000	-2.50315200

H	3.59844500	-2.14544500	-2.74337800
H	1.85169500	-2.41587900	-2.65364700
H	2.48370000	-0.86097800	-3.21720000
C	-1.57992700	0.70852200	-1.45256800
C	-3.05847400	-0.62602700	-0.10252400
C	-4.15877100	0.20582900	-0.46135600
C	-3.92385600	1.30784500	-1.31903600
C	-2.65708200	1.55131600	-1.79678300
C	-3.22667700	-1.72158000	0.76807600
C	-5.43548000	-0.10422100	0.07452500
H	-4.75040200	1.95668900	-1.59173900
H	-2.45405200	2.39094600	-2.45110100
C	-5.59622300	-1.17897600	0.92020800
C	-4.48570300	-1.98505900	1.26805300
H	-6.27956000	0.52262300	-0.19625100
H	-6.57541400	-1.41092400	1.32576300
H	-4.62670400	-2.82548200	1.94018700
N	-1.81157200	-0.32974400	-0.62538900
O	-0.78952900	-1.13914300	-0.28100600
H	-2.36798300	-2.32680900	1.02330000
C	-0.17446900	0.92870200	-1.87217500
H	0.23081600	0.05135800	-2.38299000
H	-0.10711200	1.75848800	-2.58214600

Zero-point correction= 0.439675 (Hartree/Particle)

Thermal correction to Energy= 0.468434

Thermal correction to Enthalpy= 0.469378

Thermal correction to Gibbs Free Energy= 0.378497

Sum of electronic and zero-point Energies= -1243.995386

Sum of electronic and thermal Energies= -1243.966627

Sum of electronic and thermal Enthalpies= -1243.965683

Sum of electronic and thermal Free Energies= -1244.056564

E(RB3LYP) = -1244.435061 A.U.

B-TSc1

1 1

Number of imaginary frequencies: 1

Rh	-0.82260200	-0.03073300	-0.00716300
C	-2.34573300	0.38601100	1.52787500
C	-2.96363400	0.50150000	0.24958800
C	-2.83694400	-0.78022000	-0.43302900
C	-2.19194600	-1.69670800	0.46334400
C	-1.82466300	-0.96921200	1.65641200
O	1.57096700	2.09866000	-1.65612400
O	-0.38022400	0.99399500	-1.94492700
C	0.39589100	2.09314900	-1.97718200
C	-0.34609300	3.31808500	-2.47066000
H	-1.13613800	3.57375000	-1.75615200
H	0.34225300	4.15692900	-2.57335400
H	-0.82838900	3.10626500	-3.42881100
C	-2.17348600	1.45140100	2.56323100
H	-1.11754900	1.55143100	2.83297100
H	-2.52641600	2.42102100	2.21024700
H	-2.73197600	1.19130900	3.46906100
C	-3.57836100	1.71525500	-0.36753500
H	-4.65794600	1.56997900	-0.48867100

H	-3.41989800	2.60683900	0.24040200
H	-3.15220000	1.89309700	-1.35970900
C	-3.38145600	-1.07153700	-1.79563600
H	-4.46935000	-1.19994100	-1.75091900
H	-3.16422300	-0.24953300	-2.48196400
H	-2.95281500	-1.98374300	-2.21443400
C	-1.93601000	-3.14886900	0.21697400
H	-2.75819100	-3.73911500	0.63916500
H	-1.87892100	-3.37410900	-0.84926600
H	-1.00882400	-3.47893700	0.68877100
C	-1.17061700	-1.52689300	2.88049700
H	-1.93015100	-1.85982900	3.59821900
H	-0.53642800	-2.38283800	2.64129500
H	-0.55385000	-0.77076900	3.37122700
C	3.00031900	1.21111200	1.22318600
C	2.09875700	-0.55662800	-0.10937000
C	3.35847500	-1.19984900	-0.16251400
C	4.45958300	-0.58431100	0.48273500
C	4.27638900	0.61835200	1.12625700
C	0.97279900	-1.01730900	-0.84863700
C	3.43901900	-2.41913200	-0.88907900
H	5.43827700	-1.05171100	0.44498000
H	5.10588500	1.13318900	1.59662600
C	2.33624800	-2.92996900	-1.54443300
C	1.11690700	-2.21757600	-1.54108200
H	4.39317200	-2.93601200	-0.93128200
H	2.41781600	-3.85794900	-2.10082000

H	0.28782600	-2.58212700	-2.14086800
N	1.95490200	0.57288400	0.66474100
O	0.72987800	1.06372400	0.88090900
H	0.40112000	-0.11482300	-1.53647800
C	2.71506300	2.49609000	1.92220500
H	2.23820400	3.18618700	1.21832200
H	2.00885500	2.34042900	2.74407500
H	3.63460400	2.93629200	2.30877400

Zero-point correction= 0.439479 (Hartree/Particle)

Thermal correction to Energy= 0.468294

Thermal correction to Enthalpy= 0.469238

Thermal correction to Gibbs Free Energy= 0.380318

Sum of electronic and zero-point Energies= -1243.984652

Sum of electronic and thermal Energies= -1243.955836

Sum of electronic and thermal Enthalpies= -1243.954892

Sum of electronic and thermal Free Energies= -1244.043812

E(RB3LYP) = -1244.424130 A.U.

B-TSd1

1 1

Number of imaginary frequencies: 1

Rh	1.17265900	-0.02863300	-0.16357600
C	3.06591500	-1.00581000	-0.76168000
C	3.36043700	0.18075600	-0.02371900
C	2.79018600	0.03356700	1.31105900
C	2.14533900	-1.24286900	1.38056200
C	2.26611700	-1.87835800	0.08495900
O	-1.48220300	2.55818600	-0.36928900

O	0.71498300	2.10827100	-0.60906100
C	-0.33175400	2.73450700	-0.02175500
C	0.08757400	3.67238800	1.08734200
H	-0.77095000	4.24515400	1.43732500
H	0.49830300	3.08583600	1.91630300
H	0.87489100	4.34554900	0.73751900
H	0.31020200	1.19286200	-1.45625700
C	3.48918900	-1.30969300	-2.16298800
H	2.76703000	-1.95182800	-2.67165100
H	3.61649900	-0.40025500	-2.75264400
H	4.44909300	-1.83973400	-2.14821900
C	4.11994100	1.38259200	-0.48796700
H	5.06389800	1.46830800	0.06182400
H	4.35068600	1.32844100	-1.55258800
H	3.53765400	2.29176500	-0.31408300
C	2.90343900	1.05450300	2.39561800
H	3.87894500	0.96887900	2.88947200
H	2.82552000	2.06474600	1.98691000
H	2.12815200	0.92908200	3.15330500
C	1.38729500	-1.81556500	2.53517000
H	1.84727500	-2.75638400	2.85553400
H	1.37203800	-1.13468900	3.38672800
H	0.35291700	-2.02251500	2.24297200
C	1.78751800	-3.25472300	-0.25167000
H	2.55442500	-3.99455600	0.00818100
H	0.88065300	-3.50097600	0.30462400
H	1.57461900	-3.35936100	-1.31780900

C	-1.56549300	-0.08985800	-1.62387800
C	-3.04026000	-0.41816200	0.24125200
C	-4.16848500	-0.35948200	-0.62459200
C	-3.95461600	-0.16124200	-2.01055400
C	-2.67568800	-0.03095200	-2.49152000
C	-3.19957300	-0.59480900	1.63019300
C	-5.45999700	-0.49278100	-0.05371500
H	-4.80681300	-0.10690700	-2.68049000
H	-2.48376700	0.13238800	-3.54538300
C	-5.61087500	-0.66967500	1.30356200
C	-4.47471000	-0.71770400	2.14453200
H	-6.32441600	-0.44909700	-0.70900500
H	-6.60214400	-0.76866700	1.73329100
H	-4.60693400	-0.85027600	3.21358100
N	-1.77511700	-0.28495900	-0.31335000
O	-0.74772600	-0.32125300	0.56403400
H	-2.32555900	-0.62104700	2.26528100
C	-0.15383400	0.07683100	-2.08007300
H	0.31614900	-0.90382400	-2.23935100
H	-0.10865500	0.56791800	-3.05731900

Zero-point correction= 0.438887 (Hartree/Particle)

Thermal correction to Energy= 0.467775

Thermal correction to Enthalpy= 0.468719

Thermal correction to Gibbs Free Energy= 0.378806

Sum of electronic and zero-point Energies= -1243.970978

Sum of electronic and thermal Energies= -1243.942090

Sum of electronic and thermal Enthalpies= -1243.941146

Sum of electronic and thermal Free Energies= -1244.031060

E(RB3LYP) = -1244.409865 A.U.

B-TSa2

1 1

Number of imaginary frequencies: 1

C	-3.77288100	2.36513600	-0.85615100
C	-3.62617900	0.48670500	0.66246600
C	-4.75785400	0.96029400	1.38744600
C	-5.38983900	2.14817000	0.94202500
C	-4.91567500	2.81812700	-0.16203600
C	-2.94252400	-0.71766300	0.96861800
C	-5.18955900	0.20547800	2.50546000
H	-6.26055400	2.51835900	1.47530700
H	-5.40112400	3.71680000	-0.52406400
C	-4.51407700	-0.94709800	2.84641900
C	-3.40940300	-1.40006000	2.08417000
H	-6.04755200	0.54685300	3.07556300
H	-4.83564600	-1.52471700	3.70811600
H	-2.91876800	-2.31941900	2.39017600
N	-3.17824800	1.24650300	-0.41097800
O	-2.01942500	0.84182400	-1.01061100
Rh	-1.50678600	-1.23089900	-0.37397900
C	-2.36423500	-3.22681700	-0.98142100
C	-2.02932900	-2.51846000	-2.16469000
C	-0.58001400	-2.32011500	-2.20548000
C	-0.03688700	-2.88545200	-1.03366800
C	-1.14131800	-3.36951000	-0.21241400

C	-3.70599900	-3.75339300	-0.57814400
H	-4.51329200	-3.27365500	-1.13497500
H	-3.76128400	-4.83216400	-0.76593500
H	-3.89480500	-3.59052300	0.48591800
C	-2.96287800	-2.05995000	-3.24079700
H	-2.81517300	-2.64944500	-4.15316900
H	-4.00789600	-2.15543100	-2.94070100
H	-2.77386400	-1.01213600	-3.49525600
C	0.16413500	-1.68363600	-3.33996500
H	1.10072100	-1.23940000	-3.00251700
H	0.38618100	-2.42461600	-4.11803500
H	-0.43197800	-0.89314400	-3.80399000
C	1.40427300	-3.01970200	-0.65943000
H	1.57426800	-2.71665700	0.37691300
H	1.70516800	-4.07082100	-0.75177700
H	2.04123100	-2.40904900	-1.29547100
C	-0.98495200	-4.19926600	1.02413300
H	-0.83433500	-5.25212700	0.75358600
H	-0.12219300	-3.88089400	1.61180200
H	-1.87390400	-4.15182400	1.65785600
C	0.15401300	3.40254400	-0.87755500
C	0.12519600	4.79336000	-0.91158000
C	-0.62022700	5.50460100	0.03676000
C	-1.32813500	4.82809400	1.03587700
C	-1.29499700	3.43722600	1.08897300
C	-0.55411100	2.71153600	0.13061700
H	0.68378200	5.32335500	-1.67619900

H	-0.64244300	6.58967800	0.00156800
H	-1.89768700	5.38549500	1.77276300
H	-1.83324200	2.89647700	1.86113900
C	0.52328200	-1.29954700	2.50799300
C	1.49959900	-1.79420800	3.36818500
C	2.80298600	-1.29544000	3.30361000
C	3.10157400	-0.26968700	2.41011300
C	2.11889300	0.25323400	1.56184200
C	0.81104500	-0.28886700	1.57257500
H	-0.48448700	-1.69628800	2.53717600
H	1.24554300	-2.57324500	4.08060200
H	3.57492100	-1.68484100	3.95956300
H	4.09533100	0.16237000	2.36699000
H	0.73250800	2.84660600	-1.60623800
N	2.50316300	1.33596800	0.71468400
H	1.84727800	2.10680500	0.63764100
S	3.12218000	1.01109800	-0.83825200
O	3.08682000	2.31389100	-1.51385600
O	2.44077200	-0.14860800	-1.43239100
C	5.14784400	-0.81275400	-0.47416200
C	6.45708500	-1.16660000	-0.15221400
C	7.41781700	-0.19172800	0.15088000
C	7.03602000	1.16045600	0.12543100
C	5.73472900	1.53522100	-0.19158000
C	4.80161600	0.53821900	-0.48854900
H	4.40507400	-1.56530700	-0.71242800
H	6.73731100	-2.21602500	-0.13808600

H	7.77105400	1.92683900	0.35472300
H	5.44236200	2.57942700	-0.21723100
C	-0.55342700	1.28151100	0.17753300
C	-0.24091300	0.11098800	0.62796800
C	8.84109900	-0.57777900	0.46695500
H	9.27176800	0.07505800	1.23187300
H	8.91081200	-1.61095200	0.81736300
H	9.47008200	-0.48947300	-0.42703600
C	-3.21431300	3.06949200	-2.05159800
H	-2.38686700	3.72313600	-1.76032500
H	-2.82554600	2.35479300	-2.77881000
H	-3.99088200	3.68286800	-2.51204400

Zero-point correction= 0.710304 (Hartree/Particle)

Thermal correction to Energy= 0.756130

Thermal correction to Enthalpy= 0.757074

Thermal correction to Gibbs Free Energy= 0.629461

Sum of electronic and zero-point Energies= -2428.466058

Sum of electronic and thermal Energies= -2428.420232

Sum of electronic and thermal Enthalpies= -2428.419288

Sum of electronic and thermal Free Energies= -2428.546901

E(RB3LYP) = -2429.176362 A.U.

B-TSb2

1 1

Number of imaginary frequencies: 1

C	-1.03377100	3.59483000	-0.83612700
C	-2.86060500	2.13952800	-0.19067500
C	-3.68203900	3.26942100	0.09385500

C	-3.14098100	4.56153000	-0.11738600
C	-1.85488700	4.71397100	-0.58438700
C	-3.30042500	0.79555200	-0.06164900
C	-4.99447800	3.03020700	0.56995900
H	-3.75586700	5.43348900	0.08548800
H	-1.43746300	5.69740700	-0.76599600
C	-5.42652900	1.73262200	0.74375200
C	-4.58771400	0.63463600	0.43213700
H	-5.63805400	3.87453100	0.79480300
H	-6.42696000	1.54437100	1.12214200
H	-4.97402400	-0.36801400	0.59134200
N	-1.56025900	2.37873000	-0.61689100
O	-0.75631400	1.28500100	-0.77767400
Rh	-1.96470400	-0.59284700	-0.69973200
C	-2.81808400	-2.56838700	-0.94025700
C	-3.30200500	-1.80055700	-2.07727300
C	-2.17164800	-1.40060900	-2.82785400
C	-0.98093200	-2.01732800	-2.23728600
C	-1.38002900	-2.77248500	-1.11679200
C	-3.67985100	-3.31148400	0.03237800
H	-4.60656700	-2.77021800	0.24014100
H	-3.95481200	-4.29116100	-0.37844100
H	-3.16271400	-3.47606900	0.97902500
C	-4.73884000	-1.51583500	-2.38121300
H	-5.20401800	-2.39211700	-2.84802100
H	-5.30473300	-1.28657700	-1.47559300
H	-4.84864800	-0.67163200	-3.06452800

C	-2.15012300	-0.55798800	-4.06530100
H	-1.33077800	0.16650300	-4.03092000
H	-1.99665300	-1.18182300	-4.95420800
H	-3.08384800	-0.00810000	-4.19758900
C	0.39891500	-1.87405500	-2.80411200
H	1.16480300	-2.22871500	-2.11407700
H	0.48706700	-2.44693200	-3.73536400
H	0.61543700	-0.82876500	-3.04901500
C	-0.51801500	-3.61992300	-0.23301300
H	-0.59320900	-4.67092700	-0.53771800
H	0.53211600	-3.32564400	-0.28153800
H	-0.83609200	-3.55379500	0.80969200
C	0.11012500	-1.69337400	2.90059800
C	0.03156500	-2.57493100	3.97847200
C	-1.21087700	-2.98849600	4.46469800
C	-2.38347400	-2.51938000	3.86530800
C	-2.31341800	-1.65453800	2.77464600
C	-1.06612400	-1.23139200	2.28594100
H	0.94651400	-2.93677000	4.43746200
H	-1.26634500	-3.67351800	5.30517800
H	-3.35205300	-2.83374500	4.24275600
H	-3.21642000	-1.29338200	2.29420800
C	0.61130600	2.70465200	2.14994200
C	1.67961900	3.52148400	2.50009200
C	2.95802900	3.23476000	2.00345600
C	3.17606000	2.14942000	1.15511400
C	2.11157600	1.31621700	0.80279700

C	0.81633300	1.58398200	1.32070100
H	-0.38868400	2.89923900	2.52364900
H	1.52576800	4.37324700	3.15398500
H	3.79442400	3.87363300	2.27010100
H	4.16452900	1.95099400	0.75640900
H	1.08067900	-1.37936500	2.53168400
N	2.29864600	0.24140600	-0.09138100
H	1.42428700	-0.17042400	-0.41532000
S	3.30415500	-1.08410600	0.37760300
O	2.76169500	-2.19409400	-0.41677000
O	3.36880200	-1.15307300	1.83975800
C	5.91757600	-0.29915700	0.66713500
C	7.17028100	0.05878700	0.17078600
C	7.42434000	0.08565100	-1.20779000
C	6.38550100	-0.25550700	-2.09103200
C	5.12827600	-0.61521200	-1.61885300
C	4.90819800	-0.62737500	-0.23877600
H	5.71996200	-0.33116900	1.73286800
H	7.96424200	0.31467900	0.86638400
H	6.56966800	-0.24210800	-3.16153300
H	4.33186100	-0.88780700	-2.30297900
C	-0.25232700	0.70867000	0.97914200
C	-1.01206700	-0.33299700	1.12206600
C	8.79158900	0.43927500	-1.73629400
H	9.35732700	1.04154200	-1.02070600
H	9.37206900	-0.47005800	-1.93319000
H	8.72614400	0.99281500	-2.67750100

C	0.37166900	3.70886300	-1.34081400
H	1.08670600	3.64149100	-0.51552700
H	0.60091300	2.90284500	-2.03988100
H	0.50615900	4.67398300	-1.83254100

Zero-point correction= 0.710266 (Hartree/Particle)

Thermal correction to Energy= 0.756145

Thermal correction to Enthalpy= 0.757089

Thermal correction to Gibbs Free Energy= 0.629362

Sum of electronic and zero-point Energies= -2428.468324

Sum of electronic and thermal Energies= -2428.422445

Sum of electronic and thermal Enthalpies= -2428.421501

Sum of electronic and thermal Free Energies= -2428.549228

E(RB3LYP) = -2429.178590 A.U.

B-TSc2

1 1

Number of imaginary frequencies: 1

C	-0.97513700	2.51212100	1.59580300
C	-1.16653400	3.69761000	2.29697900
C	-0.08322600	4.57114300	2.43575900
C	1.15377300	4.25449700	1.86965500
C	1.33192500	3.06064500	1.16788300
C	0.26679400	2.17130000	1.02395700
H	-2.14165000	3.94449900	2.70059400
H	-0.21236700	5.50100700	2.97969500
H	1.98724300	4.94140800	1.97929100
H	2.28934500	2.80682600	0.73707400
C	-1.43289000	-1.70883500	-1.05557800

C	-2.11383700	-2.89810400	-1.29127600
C	-2.92920900	-3.45149100	-0.29980100
C	-3.04750000	-2.81353900	0.93883600
C	-2.34755300	-1.63687000	1.19009500
C	-1.53611300	-1.06371600	0.19307500
H	-0.79467400	-1.27762300	-1.81324200
H	-2.01311000	-3.39157200	-2.25316700
H	-3.46628800	-4.37598400	-0.48862100
H	-3.67923300	-3.23799400	1.71260200
H	-2.42675800	-1.15634500	2.15931700
N	-2.00907000	1.54232600	1.33769100
S	-3.23344100	2.21637000	0.18522200
O	-3.89956100	3.29791600	0.90933400
O	-2.48651300	2.44634600	-1.04787200
C	-4.27904200	0.06274000	-1.14284600
C	-5.14974500	-1.01371500	-1.25876800
C	-6.07186700	-1.31726800	-0.24420100
C	-6.12454600	-0.49295300	0.88960400
C	-5.27167400	0.59964400	1.02303700
C	-4.34612900	0.85206900	0.00743600
H	-3.56018200	0.29427600	-1.91930600
H	-5.10782900	-1.63784100	-2.14606600
H	-6.84913700	-0.70177600	1.67092000
H	-5.33985800	1.25744500	1.88354400
C	-0.78493600	0.13177000	0.43727000
C	0.28817100	0.85876200	0.38112800
C	-6.96836300	-2.52132500	-0.37545000

H	-6.38314000	-3.44299200	-0.27050300
H	-7.75120200	-2.53233700	0.38639500
H	-7.44667100	-2.55379400	-1.35926300
H	-2.51748800	1.26389200	2.17937700
C	3.32221900	1.05785000	-2.14110300
C	3.20907300	-0.32233600	-2.51591600
C	1.86042800	-0.53227100	-3.02664300
C	1.13686600	0.67235400	-2.90187500
C	2.02678100	1.65827600	-2.29729500
C	4.58228600	1.75714200	-1.73823100
H	5.22853900	1.11115800	-1.14039800
H	5.14153100	2.05873900	-2.63185400
H	4.37547800	2.66178200	-1.16159700
C	4.30966600	-1.33832700	-2.55443100
H	4.78277200	-1.36980300	-3.54386300
H	5.08495500	-1.11060200	-1.81938900
H	3.92399100	-2.33794000	-2.33712700
C	1.36542200	-1.85780200	-3.51972000
H	2.02219600	-2.24507200	-4.30539200
H	1.35682800	-2.58704200	-2.70129600
H	0.35587600	-1.78821400	-3.92996500
C	-0.26728600	0.97469000	-3.33256700
H	-0.86031600	1.39136700	-2.51323300
H	-0.26351200	1.71537100	-4.14088400
H	-0.77743500	0.08474400	-3.70800100
C	1.67231100	3.10693200	-2.15699400
H	1.68786800	3.58686600	-3.14347900

H	0.66966800	3.23227900	-1.74157000
H	2.37374900	3.64297700	-1.51627800
C	1.62561500	-3.41619800	1.61035600
C	2.79274100	-1.31357700	1.60830600
C	3.43851500	-1.64100800	2.83279600
C	3.13339700	-2.88497200	3.43977800
C	2.24078300	-3.74208000	2.83688900
C	2.98546100	-0.09230000	0.91055900
C	4.34754200	-0.69285800	3.36572600
H	3.60680500	-3.15158200	4.37962200
H	1.99237100	-4.69702400	3.28581900
C	4.57461100	0.48530800	2.68870300
C	3.90057400	0.78071600	1.47652600
H	4.85616900	-0.91343500	4.29881900
H	5.27841500	1.20924900	3.08939800
H	4.12219800	1.72554100	0.99277900
N	1.92828000	-2.23419800	1.04512000
O	1.38120800	-1.92946600	-0.13557700
Rh	1.85707600	0.02600100	-0.77515600
C	0.66135300	-4.29598900	0.88454100
H	-0.30453200	-3.79485900	0.77315900
H	1.02199100	-4.50626500	-0.12741300
H	0.52419300	-5.23478100	1.42319900

Zero-point correction= 0.710933 (Hartree/Particle)

Thermal correction to Energy= 0.756220

Thermal correction to Enthalpy= 0.757164

Thermal correction to Gibbs Free Energy= 0.632846

Sum of electronic and zero-point Energies= -2428.472130

Sum of electronic and thermal Energies= -2428.426843

Sum of electronic and thermal Enthalpies= -2428.425899

Sum of electronic and thermal Free Energies= -2428.550218

E(RB3LYP) = -2429.183063 A.U.

B-TSd2

1 1

Number of imaginary frequencies: 1

C	-1.76678300	2.56934900	1.47287500
C	-2.32851400	3.63186100	2.14833600
C	-1.40148200	4.58763200	2.59515300
C	-0.02542000	4.44324900	2.35513400
C	0.50743700	3.35062700	1.65712500
C	-0.41088000	2.40938600	1.20342300
H	-3.39426700	3.73784900	2.30968300
H	-1.75707800	5.45926500	3.13425200
H	0.64975000	5.20997600	2.72247400
H	1.56888400	3.25270300	1.48296700
C	-0.80599400	-1.70195700	-1.64115900
C	-1.47534500	-2.90294900	-1.86325500
C	-2.06567200	-3.59351400	-0.79668500
C	-1.99169700	-3.06189200	0.49147600
C	-1.33973000	-1.84603600	0.71177300
C	-0.73594900	-1.14942700	-0.35049400
H	-0.32531800	-1.18330300	-2.46093500
H	-1.52549000	-3.31140500	-2.86828200
H	-2.56842800	-4.54016000	-0.97044700

H	-2.43866000	-3.59178100	1.32745800
H	-1.25167100	-1.45097500	1.72057500
N	-2.24073000	1.34788700	0.82480800
S	-3.36083100	1.61903000	-0.64806800
O	-3.93315200	2.93825700	-0.40553400
O	-2.52656400	1.32054000	-1.80383100
C	-5.72902200	0.67788300	0.33901800
C	-6.66651600	-0.32477100	0.55907400
C	-6.46334200	-1.62972800	0.07650900
C	-5.28790700	-1.91078700	-0.63633400
C	-4.33304300	-0.92688900	-0.87428900
C	-4.57046700	0.35698300	-0.37933000
H	-5.89272500	1.68955100	0.69403600
H	-7.57479600	-0.09256800	1.10727700
H	-5.11115600	-2.91406100	-1.01103900
H	-3.42928200	-1.14832200	-1.42850600
C	0.01293000	0.08795500	-0.07380300
C	-0.51810700	1.13041000	0.51721100
C	-7.50661800	-2.69485600	0.29495200
H	-8.27595200	-2.63738900	-0.48448300
H	-7.07352000	-3.69764200	0.25549300
H	-8.01004500	-2.57179800	1.25792900
C	3.50949700	1.73786500	-1.29198900
C	3.86819300	0.48238600	-1.87193200
C	2.80745300	0.10369400	-2.79880900
C	1.79499000	1.08645900	-2.75349900
C	2.19626900	2.08550800	-1.77390300

C	4.37203500	2.56779800	-0.39252300
H	4.93407300	1.94820700	0.30975800
H	5.09229800	3.14253800	-0.98661500
H	3.78110200	3.28301000	0.18464200
C	5.15328500	-0.26644900	-1.68843700
H	5.86311100	-0.03615200	-2.49257300
H	5.62926300	-0.01196800	-0.73866400
H	4.97862500	-1.34582300	-1.69773900
C	2.81683600	-1.16824800	-3.58895600
H	3.67723300	-1.19539000	-4.26641500
H	2.89188100	-2.02936000	-2.91591500
H	1.91013300	-1.28191500	-4.18600500
C	0.54983500	1.18531300	-3.58352900
H	-0.33449400	1.36858600	-2.96783600
H	0.63538100	2.01690800	-4.29363500
H	0.37717800	0.27779100	-4.16620300
C	1.47295600	3.38487300	-1.59307400
H	1.60755700	4.00883500	-2.48555600
H	0.39967000	3.22760200	-1.46169900
H	1.84201000	3.95074300	-0.73754800
C	2.01986000	-3.66560400	1.07205900
C	2.48890900	-1.40636000	1.75027500
C	2.74103200	-1.83076600	3.08391700
C	2.59844800	-3.20819400	3.38726100
C	2.23516000	-4.09419500	2.39823000
C	2.54826800	-0.05346700	1.32142200
C	3.11443600	-0.83778900	4.02503200

H	2.77440700	-3.55353900	4.40136800
H	2.11418300	-5.15035300	2.61071200
C	3.22507200	0.47457900	3.62017700
C	2.94242800	0.86045400	2.28474900
H	3.31584100	-1.12992000	5.05084200
H	3.52635900	1.23447100	4.33581700
H	3.04688400	1.90755600	2.02576500
N	2.17118600	-2.35809500	0.79717300
O	2.01915900	-1.94775700	-0.46347700
Rh	2.02213400	0.16127100	-0.63063500
C	1.64221600	-4.56139500	-0.06127100
H	0.70058800	-4.22641400	-0.50709800
H	2.39871000	-4.51919400	-0.85172500
H	1.53909100	-5.59078200	0.28528200
H	-2.67314400	0.64215700	1.42767400

Zero-point correction= 0.710045 (Hartree/Particle)

Thermal correction to Energy= 0.755702

Thermal correction to Enthalpy= 0.756646

Thermal correction to Gibbs Free Energy= 0.630792

Sum of electronic and zero-point Energies= -2428.443438

Sum of electronic and thermal Energies= -2428.397782

Sum of electronic and thermal Enthalpies= -2428.396837

Sum of electronic and thermal Free Energies= -2428.522691

E(RB3LYP) = -2429.153483 A.U.

B-TSe2

1 1

Number of imaginary frequencies: 1

C	-0.40576100	2.84952100	-2.24908400
C	-2.26317600	1.80916600	-1.13608800
C	-3.12742700	2.86545000	-1.53097200
C	-2.56711000	3.95853500	-2.24023300
C	-1.22848000	3.95465900	-2.55642200
C	-2.69971500	0.72071900	-0.32669700
C	-4.50370300	2.75218000	-1.20531600
H	-3.20315700	4.78786900	-2.53316000
H	-0.77835400	4.78129800	-3.09374300
C	-4.96374400	1.64412100	-0.52209600
C	-4.06694500	0.65862600	-0.06394500
H	-5.18148000	3.54491200	-1.50558100
H	-6.01981600	1.55044600	-0.28964400
H	-4.43857800	-0.13147700	0.57990000
N	-0.95592700	1.81679500	-1.58186900
O	-0.22521800	0.71314700	-1.39242300
Rh	-1.35642000	-0.95371900	-0.55314400
C	-0.50171700	-2.53234500	-1.88183700
C	-0.57620200	-3.06996300	-0.56007100
C	-1.96378900	-3.01406000	-0.16175000
C	-2.75185100	-2.57596100	-1.31275100
C	-1.85694000	-2.25229700	-2.35591100
C	0.72121400	-2.34508300	-2.72087900
H	1.62285800	-2.68128200	-2.21166100
H	0.61291400	-2.90494400	-3.65679700
H	0.86573800	-1.29048300	-2.97412100
C	0.56105600	-3.59087700	0.26278200

H	0.64533900	-4.67659600	0.13239600
H	1.51064800	-3.13846500	-0.02735000
H	0.40886200	-3.39253400	1.32591500
C	-2.51152200	-3.50475500	1.14309300
H	-2.72090000	-4.58014600	1.09401100
H	-1.79534200	-3.34050700	1.95184800
H	-3.44272300	-2.99559600	1.40368800
C	-4.24517200	-2.50235300	-1.36535900
H	-4.65018600	-3.44491600	-1.75229400
H	-4.67711200	-2.34360600	-0.37502800
H	-4.58646500	-1.69608700	-2.01790100
C	-2.18642700	-1.75042400	-3.72747900
H	-2.19337100	-2.57392200	-4.45180600
H	-3.16818100	-1.27232600	-3.75608400
H	-1.44112300	-1.02415600	-4.06251700
C	-2.76466000	2.46085700	2.37537200
C	-3.51990500	3.02914800	3.39704500
C	-4.06190400	2.22199300	4.40294300
C	-3.84336600	0.84315700	4.38647000
C	-3.07824500	0.26962500	3.37064700
C	-2.52630200	1.07658000	2.36234000
H	-3.68884900	4.10146400	3.41108100
H	-4.65477800	2.66801800	5.19543100
H	-4.26699100	0.21420000	5.16338600
H	-2.91502100	-0.80335000	3.34329500
C	0.35100700	-1.20761700	3.26031200
C	1.41906900	-1.70163700	4.00040400

C	2.71264200	-1.60039200	3.48227400
C	2.93644700	-1.00438900	2.24489300
C	1.86464300	-0.52293600	1.48046100
C	0.54947300	-0.62757400	1.99267000
H	-0.65895200	-1.26779500	3.64995700
H	1.24639700	-2.15397500	4.97137900
H	3.55812600	-1.97735300	4.04907500
H	3.94864000	-0.91415700	1.87199900
H	-2.35183400	3.07996800	1.58495200
N	2.07846600	0.10857800	0.23600200
H	1.25587000	0.45103800	-0.27236000
S	3.24025900	-0.42088100	-0.87687700
O	2.81751000	0.19704100	-2.13992300
O	3.41557700	-1.87720200	-0.78354500
C	5.90149400	-0.43961300	-0.20944100
C	7.09209700	0.16688100	0.18886900
C	7.14689800	1.53617700	0.48232600
C	5.96856100	2.29393800	0.37336100
C	4.77146900	1.70908600	-0.02445500
C	4.74962900	0.34133200	-0.30936700
H	5.85564600	-1.50052400	-0.42871500
H	7.99210200	-0.43516300	0.27441500
H	5.99268400	3.35434900	0.60839800
H	3.86186100	2.29656800	-0.09012600
C	-1.69630300	0.46860800	1.32156300
C	-0.60249500	-0.21200200	1.21701100
C	8.44407800	2.19176200	0.88490900

H	8.92787500	2.65135000	0.01455900
H	8.28065100	2.98358000	1.62178900
H	9.14671200	1.46881200	1.30745400
C	1.02191300	2.71809500	-2.65812900
H	1.66882800	2.61093700	-1.78226100
H	1.17817700	1.80203800	-3.23436900
H	1.33433500	3.58687200	-3.23847400

Zero-point correction= 0.709983 (Hartree/Particle)

Thermal correction to Energy= 0.755779

Thermal correction to Enthalpy= 0.756724

Thermal correction to Gibbs Free Energy= 0.629483

Sum of electronic and zero-point Energies= -2428.473555

Sum of electronic and thermal Energies= -2428.427758

Sum of electronic and thermal Enthalpies= -2428.426814

Sum of electronic and thermal Free Energies= -2428.554054

E(RB3LYP) = -2429.183537 A.U.

B-TSa3

1 1

Number of imaginary frequencies: 1

C	2.99961800	0.06415900	3.89083400
C	3.71464800	1.19661200	3.58785900
C	3.38921600	1.98131000	2.45253300
C	2.31981200	1.55028000	1.59862100
C	1.94643400	-0.35733900	3.05968100
H	4.87680000	3.50472400	2.79858100
H	3.22386500	-0.52981400	4.76884300
H	4.52797100	1.52011900	4.22995500

C	4.05663300	3.18950800	2.16283100
C	1.89310300	2.33137800	0.47281200
C	2.55892800	3.55791200	0.29381900
C	3.62321700	3.96636400	1.10291600
H	2.22788000	4.20638200	-0.50765900
H	4.10939000	4.91400900	0.89340000
Rh	1.25623100	-1.24155500	-0.56965400
O	0.60666700	-0.10919900	1.25651900
N	1.66928600	0.38557800	1.96856900
C	0.78136100	1.91698900	-0.34499200
C	0.36204800	0.60930700	-0.28838900
C	-0.73631700	-0.10145900	-0.95991900
C	-1.54491900	-1.12756000	-0.37171000
C	-0.87863500	0.11804300	-2.36617800
C	-2.36994800	-1.92048800	-1.20401600
C	-1.71943000	-0.64803800	-3.14418300
H	-0.29144900	0.90652300	-2.81867900
C	-2.45122700	-1.70155800	-2.56534200
H	-2.98498300	-2.68407400	-0.73647000
H	-1.80174800	-0.44414100	-4.20673600
H	-3.10490300	-2.31688400	-3.17519900
C	0.04464100	2.88112400	-1.21247700
C	-1.27233600	3.24919100	-0.89190300
C	0.62809200	3.39668600	-2.38208100
C	-1.98515400	4.11142600	-1.72572800
H	-1.72112100	2.85603500	0.01408200
C	-0.08468500	4.26681000	-3.20933500

H	1.64008800	3.10086000	-2.64686300
C	-1.39536000	4.62323200	-2.88450700
H	-3.00091000	4.39397400	-1.46375300
H	0.38021800	4.65941500	-4.10899000
H	-1.95175400	5.29737300	-3.52864100
C	2.12084200	-2.02330600	-2.42213200
C	3.03295600	-1.03500500	-1.91439400
C	2.15933000	-3.20677000	-1.54262200
C	3.43844900	-1.49938500	-0.62390100
C	2.94386500	-2.88190500	-0.43880800
C	1.42459100	-4.47996100	-1.82549300
H	0.38811500	-4.28093500	-2.11732100
H	1.89490000	-5.02451900	-2.65352800
H	1.41003400	-5.14140400	-0.95673700
C	3.28475300	-3.73924200	0.74108100
H	2.60133300	-4.58527700	0.83931400
H	4.30190800	-4.13910300	0.64649500
H	3.25114500	-3.16761400	1.67328800
C	4.41113300	-0.82371900	0.29164500
H	4.15650500	-0.98854400	1.34200200
H	5.41952900	-1.22758800	0.13579600
H	4.45011000	0.25239100	0.11350900
C	3.40230400	0.27464200	-2.54088300
H	3.38551700	1.08319200	-1.80332200
H	4.40696400	0.23425100	-2.97775300
H	2.70358600	0.54288000	-3.33645800
C	1.44139300	-2.01022100	-3.75536400

H	1.33888100	-0.99708600	-4.14733100
H	2.02054100	-2.59891000	-4.47736500
H	0.44106800	-2.44609200	-3.69400500
N	-1.65502100	-1.29830200	1.03142700
H	-1.99199700	-2.21598500	1.30802200
S	-2.46305800	-0.11668200	1.98674400
O	-1.89415400	1.17916500	1.62305700
O	-2.37296700	-0.66461500	3.34204100
C	-5.08850500	-0.93494600	2.12151900
C	-6.39070900	-1.00724900	1.63250100
C	-6.76794200	-0.32526300	0.46528800
C	-5.80283100	0.44045900	-0.20775700
C	-4.49694800	0.53315500	0.26537400
C	-4.15423600	-0.16024000	1.43071600
H	-4.79904400	-1.45118900	3.03069200
H	-7.12839200	-1.59795900	2.16817200
H	-6.08095100	0.97655200	-1.11076100
H	-3.75907000	1.13958900	-0.24931900
C	-8.18967100	-0.38431700	-0.03438600
H	-8.78931400	0.41199500	0.42280300
H	-8.24110200	-0.25036900	-1.11844600
H	-8.66518200	-1.33603700	0.21839200
C	1.10951500	-1.56865300	3.31692600
H	0.06791500	-1.28764400	3.50838200
H	1.09788600	-2.22379600	2.43884200
H	1.50390800	-2.11390400	4.17561700

Zero-point correction= 0.710732 (Hartree/Particle)

Thermal correction to Energy= 0.756122

Thermal correction to Enthalpy= 0.757066

Thermal correction to Gibbs Free Energy= 0.630485

Sum of electronic and zero-point Energies= -2428.447565

Sum of electronic and thermal Energies= -2428.402175

Sum of electronic and thermal Enthalpies= -2428.401231

Sum of electronic and thermal Free Energies= -2428.527813

E(RB3LYP) = -2429.158297 A.U.

B-TSb3

1 1

Number of imaginary frequencies: 1

Rh	-0.08320900	-1.00136300	0.71312800
C	-1.39956000	-0.88487000	2.47725500
C	-2.06635200	-1.97542600	1.73322200
C	-0.12318200	-1.36959000	2.94191400
C	-1.15452700	-3.01326600	1.60433800
C	0.10391400	-2.59408900	2.26574000
C	-2.09474900	0.36840100	2.90112400
H	-2.70748400	0.16431200	3.78945100
H	-1.38795500	1.16196900	3.14653700
H	-2.75888600	0.73211300	2.11308700
C	-3.47139600	-1.89337800	1.23358100
H	-3.74351600	-2.76524800	0.63559600
H	-4.17292400	-1.82947000	2.07361400
H	-3.61775600	-1.00225400	0.61884000
C	-1.34584600	-4.35503800	0.97219800
H	-1.37663200	-5.13097800	1.74642100

H	-2.27566800	-4.41150800	0.40477800
H	-0.51941900	-4.60653600	0.30091100
C	1.32097900	-3.45722400	2.38740800
H	1.17577100	-4.20870100	3.17360200
H	1.52655000	-3.99125900	1.45595800
H	2.20204000	-2.86583100	2.64434800
C	0.77023500	-0.75863500	3.97654200
H	0.44000500	0.24339600	4.24583600
H	0.74724900	-1.37398000	4.88315900
H	1.80764800	-0.70202600	3.63691600
O	-0.33862000	-0.40659700	-1.12774800
C	2.19427800	-1.88759900	-1.19550400
C	0.08416800	-2.85726400	-1.81910300
C	2.97190900	-0.83092900	-0.61381300
C	2.87237100	-2.96150800	-1.87327300
C	0.73741000	-3.91501400	-2.47954800
C	4.36149000	-0.92771400	-0.73026700
C	4.28632200	-3.00925400	-1.92073200
C	2.10863700	-3.97444700	-2.49307800
H	0.13546600	-4.65874800	-2.98852400
C	5.02246600	-2.00036600	-1.34960600
H	4.95751100	-0.12159100	-0.31943600
H	4.76371600	-3.84713400	-2.41928000
H	2.62217100	-4.78364200	-3.00383400
H	6.10664700	-2.01518200	-1.38320900
N	0.80882500	-1.93831900	-1.14893300
C	1.26845700	0.50016900	0.67995300

C	2.44141900	0.39399900	0.03246700
C	0.69764400	1.74917300	1.19788400
C	0.99474800	2.21853200	2.48958500
C	-0.17218800	2.52786600	0.37334600
C	0.39545500	3.36025700	3.00358200
H	1.72571400	1.67614000	3.07566900
C	-0.78395600	3.68071900	0.90703000
C	-0.51230300	4.07575300	2.20887000
H	0.64672900	3.70862800	4.00017900
H	-1.41407000	4.29159600	0.27505800
H	-0.98031100	4.97546000	2.59605300
C	3.28562100	1.63263800	-0.09336500
C	4.05788700	2.10272200	0.97648900
C	3.26882500	2.35159300	-1.29693300
C	4.80274800	3.27621200	0.84686800
H	4.07171400	1.54652400	1.90966800
C	4.00730000	3.52834600	-1.42216500
H	2.66155500	1.99794300	-2.12520800
C	4.77646300	3.99160300	-0.35189100
H	5.39868800	3.63259200	1.68176900
H	3.97729900	4.08549400	-2.35355900
H	5.35085700	4.90750500	-0.45129600
N	-0.30146300	2.14097100	-0.95820800
H	0.09326600	1.22171500	-1.21972400
S	-1.49931100	2.59872000	-2.08157100
O	-1.02222500	2.02585500	-3.33650200
O	-1.75062400	4.02766200	-1.91040300

C	-3.76717100	2.20346300	-0.54699300
C	-4.91384300	1.49900000	-0.18253100
C	-5.28820900	0.32416200	-0.85338500
C	-4.46931500	-0.14308600	-1.89331000
C	-3.31110900	0.53800100	-2.26029800
C	-2.97164100	1.71002400	-1.58339600
H	-3.50813300	3.13136800	-0.05074500
H	-5.54129800	1.88010800	0.61852100
H	-4.75022800	-1.04623100	-2.42863500
H	-2.68293400	0.19185600	-3.07270800
C	-6.55777100	-0.40241600	-0.48427900
H	-7.40639900	-0.00958600	-1.05668700
H	-6.48726100	-1.47225200	-0.70135100
H	-6.79757200	-0.28051100	0.57597400
C	-1.40575500	-2.73414000	-1.94412900
H	-1.87617700	-2.33717900	-1.04903000
H	-1.62286800	-2.02302300	-2.74679000
H	-1.84070800	-3.70221700	-2.20115300

Zero-point correction= 0.710436 (Hartree/Particle)

Thermal correction to Energy= 0.755774

Thermal correction to Enthalpy= 0.756718

Thermal correction to Gibbs Free Energy= 0.632123

Sum of electronic and zero-point Energies= -2428.429254

Sum of electronic and thermal Energies= -2428.383916

Sum of electronic and thermal Enthalpies= -2428.382971

Sum of electronic and thermal Free Energies= -2428.507567

E(RB3LYP) = -2429.139690 A.U.

B-TSa4

1 1

Number of imaginary frequencies: 1

C	0.05931600	2.34037300	-2.29200500
C	-0.11860400	-0.05639700	-2.45920200
C	-0.35843500	0.01241100	-3.84692200
C	-0.31749300	1.29417300	-4.45666700
C	-0.08516600	2.42117400	-3.68972600
C	-0.06380600	-1.24806800	-1.71753700
C	-0.58727900	-1.20665400	-4.53344000
H	-0.48889900	1.38552400	-5.52464700
H	-0.06320800	3.40610000	-4.14231400
C	-0.57016900	-2.39205300	-3.82255600
C	-0.30701100	-2.42029700	-2.43596400
H	-0.74876600	-1.19463200	-5.60634200
H	-0.74386300	-3.33067700	-4.33893300
H	-0.28584200	-3.37349000	-1.92247100
N	0.12026100	1.10468900	-1.73517300
O	-0.61952600	1.07490500	-0.36733100
Rh	1.86494000	0.38535400	0.00433700
C	3.50818900	1.89766300	0.47149300
C	3.26175600	1.15785200	1.65639500
C	3.48421200	-0.23239800	1.33035700
C	4.05414800	-0.30807100	-0.02690300
C	4.02320800	0.99163900	-0.55890400
C	3.38899600	3.38100000	0.30429400
H	2.65080200	3.81007500	0.98637000

H	4.35051300	3.86660300	0.51309500
H	3.11119100	3.64934700	-0.71853900
C	2.80172900	1.67928700	2.98287800
H	2.41648400	2.69795200	2.90145800
H	2.00587500	1.05634600	3.40145900
H	3.62901100	1.69321200	3.70256500
C	3.47962200	-1.35746900	2.31653900
H	4.50689000	-1.55871500	2.64613900
H	2.89088300	-1.10848100	3.20065900
H	3.08155700	-2.27855700	1.88648000
C	4.65283100	-1.52808600	-0.65562900
H	5.74362200	-1.51690700	-0.53589500
H	4.28814900	-2.44248200	-0.18499200
H	4.43856600	-1.58414600	-1.72594700
C	4.46501900	1.42211200	-1.92378300
H	4.59694100	0.56709300	-2.59000000
H	3.73736600	2.09922400	-2.38397200
H	5.41929700	1.96050100	-1.87350000
C	-0.84757800	-3.03100900	1.03614400
C	-0.84579800	-4.32829000	1.54895600
C	0.28262900	-5.14064300	1.40690400
C	1.40575200	-4.65093900	0.73715400
C	1.40234600	-3.35050000	0.22798000
C	0.28707300	-2.51895100	0.38790400
H	-1.72807800	-4.70641900	2.05694000
H	0.28266900	-6.14981600	1.80694900
H	2.28114100	-5.28039100	0.60700600

H	2.25836200	-2.97055200	-0.31833500
C	-0.03980900	-0.67428300	2.84463200
C	-0.47384400	-0.65176200	4.16363000
C	-1.42409000	0.28815900	4.57447200
C	-1.88131400	1.23284100	3.66433200
C	-1.44258800	1.22533700	2.33300100
C	-0.55221600	0.21553700	1.87575700
H	0.69196500	-1.40954800	2.54569900
H	-0.06822700	-1.36954200	4.86971900
H	-1.77414600	0.30830400	5.60132100
H	-2.57752600	2.01102500	3.95630700
H	-1.72525100	-2.40334400	1.14203200
N	-1.90181700	2.28863700	1.50936800
H	-1.27644600	2.51285700	0.74931500
S	-3.49070300	2.29819000	0.87549800
O	-3.41092700	3.31283700	-0.18340400
O	-4.40559300	2.38588700	2.00887300
C	-4.06537300	-0.39567300	0.90800200
C	-4.10367700	-1.66383000	0.33344500
C	-3.77568800	-1.86121500	-1.01758200
C	-3.45300300	-0.74298100	-1.79879200
C	-3.41282000	0.53418300	-1.24332300
C	-3.70315700	0.69424600	0.11206500
H	-4.31713700	-0.24469000	1.95172800
H	-4.38631000	-2.51730900	0.94398700
H	-3.21948100	-0.87629800	-2.85127200
H	-3.16305500	1.40142600	-1.84462100

C	0.24398300	-1.17051800	-0.26570600
C	-0.13604800	0.04028900	0.45423900
C	-3.74258500	-3.25420900	-1.59321600
H	-2.90843700	-3.82095600	-1.16129300
H	-4.66096100	-3.80344800	-1.36306100
H	-3.61472600	-3.24117300	-2.67839400
C	0.04042700	3.54454500	-1.40556700
H	0.63896100	3.39646800	-0.50606800
H	0.41238800	4.41773500	-1.94545300
H	-0.99617400	3.75632100	-1.10366500

Zero-point correction= 0.711297 (Hartree/Particle)

Thermal correction to Energy= 0.756304

Thermal correction to Enthalpy= 0.757249

Thermal correction to Gibbs Free Energy= 0.635022

Sum of electronic and zero-point Energies= -2428.457794

Sum of electronic and thermal Energies= -2428.412786

Sum of electronic and thermal Enthalpies= -2428.411842

Sum of electronic and thermal Free Energies= -2428.534068

E(RB3LYP) = -2429.169090 A.U.

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0 1

Number of imaginary frequencies: 1

C	-3.71326800	3.17582600	-0.63899400
C	-3.63841200	1.17640200	0.55324200
C	-5.06454900	1.17143700	0.70858400
C	-5.78692300	2.27331700	0.18309600
C	-5.12391800	3.27366700	-0.47753100

C	-2.86111900	0.08918800	1.08889900
C	-5.71957300	0.07612300	1.31960400
H	-6.86762600	2.29979600	0.29988000
H	-5.65544700	4.12412500	-0.89360800
C	-4.97213600	-0.99110300	1.76111900
C	-3.56625600	-0.96954100	1.65733900
H	-6.80171900	0.08983200	1.41787100
H	-5.45438500	-1.84914000	2.22057400
H	-3.01099300	-1.80704100	2.06060300
N	-3.01297500	2.16986900	-0.14399800
O	-1.15053200	2.23913200	2.06119100
Rh	-0.54951400	-1.03140800	-0.59689400
C	-1.19461500	-0.30299700	-2.51880800
C	-0.15622700	-1.24951700	-2.97228000
C	-0.52676900	-2.52185400	-2.55888800
C	-1.79383600	-2.39983200	-1.81652000
C	-2.29158300	-1.07937400	-1.98519200
C	-1.27435200	1.13701300	-2.91110200
H	-0.28641600	1.59834300	-2.94699400
H	-1.73464800	1.23295600	-3.90379100
H	-1.87410100	1.68466400	-2.18508500
C	1.06628200	-0.86555600	-3.74321100
H	0.87571300	-0.95153200	-4.82071800
H	1.34326400	0.17096400	-3.54147400
H	1.91674500	-1.49352900	-3.47535600
C	0.15237500	-3.81792300	-2.85217300
H	-0.41336600	-4.35974100	-3.62215400

H	1.16684600	-3.66086900	-3.22244600
H	0.21607300	-4.44214400	-1.96069100
C	-2.54186800	-3.54998700	-1.21913700
H	-3.26456400	-3.20051400	-0.47793200
H	-3.08564300	-4.10295600	-1.99645900
H	-1.85539900	-4.24682800	-0.73146900
C	-3.72372600	-0.66903400	-1.88012800
H	-4.25259400	-1.06918500	-2.75556600
H	-4.21144500	-1.06726700	-0.98958100
H	-3.84009600	0.41251000	-1.88870800
C	-0.92129500	-0.31703400	3.58322300
C	-0.50851800	-1.12260400	4.63983900
C	-0.02157500	-2.41310800	4.40537300
C	0.04175400	-2.89400600	3.10093200
C	-0.39145200	-2.08790400	2.04541100
C	-0.85680300	-0.78720300	2.26138000
H	-0.55911900	-0.73814400	5.65499500
H	0.31114700	-3.03227100	5.23380700
H	0.43881100	-3.88084900	2.88669300
H	-0.31503000	-2.51236400	1.04208300
C	1.19157900	1.27343900	-0.49275000
C	2.02872000	1.85241500	-1.45428600
C	1.87996900	3.19658100	-1.79460200
C	0.92884900	3.97981700	-1.13420300
C	0.11271900	3.40576800	-0.16087800
C	0.20199900	2.04400900	0.14580700
H	-0.62749600	3.99205700	0.37089500

H	2.81207500	1.24601600	-1.89642100
H	2.52622000	3.63664300	-2.54855400
H	0.82654800	5.03396000	-1.37509000
H	-1.28018500	0.68807700	3.76610500
N	1.39498600	-0.08704900	-0.08427800
S	2.32309200	-0.10409200	1.42073400
O	2.65386600	-1.49886200	1.70614500
O	1.66134200	0.74753900	2.41352200
C	3.99979200	2.07876700	1.33441700
C	5.15016500	2.75900500	0.93989800
C	6.12271400	2.13570700	0.14658300
C	5.91479400	0.80515000	-0.24812500
C	4.77437700	0.10536900	0.13835000
C	3.82435300	0.75562600	0.92919500
H	3.23971400	2.55822000	1.94070300
H	5.29151500	3.79133700	1.24896900
H	6.65698100	0.31050300	-0.86956800
H	4.59656200	-0.90833400	-0.19990800
C	-1.34569600	0.05856300	1.07799100
C	-0.77237800	1.50397100	1.16423300
C	7.38015900	2.86883100	-0.25353100
H	7.73752900	2.54537400	-1.23599500
H	7.22165000	3.95079400	-0.28588500
H	8.18684200	2.67762600	0.46502900
C	-2.98005600	4.25803000	-1.39361600
H	-2.80577200	5.12252500	-0.74076800
H	-2.00871000	3.90631900	-1.74083800

H	-3.56628100	4.61013000	-2.24858500
H	2.04714900	-0.89187700	-0.79521600
O	1.37830500	-3.27949800	-0.28850900
C	2.48200200	-2.95902500	-0.74619100
O	2.76040300	-1.80472000	-1.29108600
C	3.65535200	-3.91958200	-0.67297000
H	3.30839300	-4.94667300	-0.54887500
H	4.29321100	-3.82926300	-1.55602400
H	4.24925900	-3.64290600	0.20547200

Zero-point correction= 0.758941 (Hartree/Particle)

Thermal correction to Energy= 0.809319

Thermal correction to Enthalpy= 0.810263

Thermal correction to Gibbs Free Energy= 0.675943

Sum of electronic and zero-point Energies= -2657.190749

Sum of electronic and thermal Energies= -2657.140371

Sum of electronic and thermal Enthalpies= -2657.139427

Sum of electronic and thermal Free Energies= -2657.273747

E(RB3LYP) = -2657.949690 A.U.

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0 1

Number of imaginary frequencies: 1

C	4.80974500	0.84942100	-0.59606800
C	2.93084700	0.40925300	0.68576800
C	3.40720100	1.20131900	1.77219500
C	4.66346900	1.80822100	1.60404600
C	5.37627100	1.62927800	0.42654000
C	1.64915400	-0.30263400	0.83857500

C	2.61374700	1.36309900	2.96874500
H	5.07043000	2.41628100	2.40887600
H	6.35091700	2.08709700	0.28899800
C	1.37500800	0.81319700	3.05722700
C	0.82299000	0.00169600	1.99631400
H	3.02346700	1.95857000	3.78060000
H	0.77902200	0.95268500	3.95578800
H	0.06100000	-0.71397300	2.27841800
N	3.61725600	0.26484700	-0.45584800
O	2.82152700	-2.29066100	-1.63003900
Rh	0.04286700	0.99995700	0.20658300
C	0.87557200	2.92767900	-0.80607100
C	-0.18265600	2.47430800	-1.62094800
C	-1.39065500	2.47311200	-0.80924400
C	-1.08045500	2.99845200	0.48006800
C	0.34366100	3.19803800	0.51734600
C	2.29299400	3.12799300	-1.24013000
H	2.98144900	3.10031800	-0.39400400
H	2.60524500	2.35217400	-1.94353300
H	2.40839300	4.10151700	-1.73445600
C	-0.08434700	2.12791300	-3.07464000
H	-0.88392300	1.45388500	-3.38267400
H	-0.14798600	3.02831700	-3.70057800
H	0.86330400	1.63141000	-3.30124600
C	-2.76044700	2.18381900	-1.34274300
H	-2.73897200	1.36607400	-2.06468700
H	-3.46052500	1.91530900	-0.55237200

H	-3.15493600	3.06716000	-1.86230200
C	-2.03598500	3.39288900	1.56473100
H	-1.68140100	3.07514900	2.55018800
H	-2.15755400	4.48462000	1.59754300
H	-3.02136600	2.95517200	1.40514900
C	1.07436300	3.90190300	1.61821700
H	0.96571200	4.98871400	1.50382100
H	0.68389300	3.62376600	2.59912200
H	2.14003900	3.66928200	1.61158300
C	0.72542200	-3.96075500	0.21593900
C	0.65768500	-5.17760300	0.88008900
C	1.14199200	-5.29035200	2.18679300
C	1.69106900	-4.17602000	2.82577200
C	1.73905300	-2.94860300	2.17377800
C	1.25517300	-2.82167100	0.85714000
H	0.22131500	-6.03776100	0.38237500
H	1.09179300	-6.24394100	2.70455000
H	2.07923300	-4.26288500	3.83616400
H	2.16831400	-2.08871500	2.67390200
C	-0.57866100	-1.15466600	-1.80819800
C	-1.63941300	-1.04640400	-2.72311600
C	-1.39837000	-1.16858900	-4.08952000
C	-0.10598400	-1.39302000	-4.58422400
C	0.94511900	-1.53482800	-3.68685500
C	0.71037000	-1.42618900	-2.31099700
H	1.95542300	-1.76079600	-4.01365900
H	-2.64417700	-0.87104300	-2.36450500

H	-2.23241700	-1.08245400	-4.78074000
H	0.06470300	-1.47605100	-5.65278600
H	0.31904500	-3.87480900	-0.78553900
N	-0.69527600	-1.00922100	-0.40290000
S	-1.93859400	-1.86832200	0.36452800
O	-1.49828500	-2.07574300	1.75055700
O	-2.31103100	-3.01914500	-0.47509600
C	-4.44554200	-0.97848700	-0.40447600
C	-5.59020500	-0.19636100	-0.25727100
C	-5.70034100	0.73369200	0.78570900
C	-4.62797700	0.86380400	1.68163700
C	-3.46852300	0.10497800	1.53719300
C	-3.38523900	-0.81031100	0.48600200
H	-4.37900000	-1.73409800	-1.17988900
H	-6.41689400	-0.32249200	-0.95133200
H	-4.70364000	1.57024300	2.50408400
H	-2.63977600	0.20650000	2.22784000
C	1.38961500	-1.55599000	0.12783300
C	1.76510000	-1.75570000	-1.33778700
C	-6.95680900	1.54960600	0.96932000
H	-6.73039100	2.55335000	1.34196300
H	-7.51119400	1.65022200	0.03195800
H	-7.62572400	1.07536500	1.69797800
C	5.49007300	0.65603500	-1.92667400
H	5.32655600	-0.36494200	-2.28097400
H	5.05946800	1.33445500	-2.67446300
H	6.56363600	0.85728000	-1.87008700

Zero-point correction= 0.698397 (Hartree/Particle)

Thermal correction to Energy= 0.743285

Thermal correction to Enthalpy= 0.744230

Thermal correction to Gibbs Free Energy= 0.622793

Sum of electronic and zero-point Energies= -2428.125755

Sum of electronic and thermal Energies= -2428.080866

Sum of electronic and thermal Enthalpies= -2428.079922

Sum of electronic and thermal Free Energies= -2428.201358

E(RB3LYP) = -2428.824152 A.U.

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0 1

Number of imaginary frequencies: 1

C	-0.24615200	-0.50724700	1.72633200
C	0.63811700	-0.98900100	2.69596900
C	0.60372700	-0.52540300	4.00570700
C	-0.33502700	0.44259100	4.37269400
C	-1.23988300	0.91301500	3.43197300
C	-1.22610200	0.44370800	2.10135600
H	1.35358600	-1.73948600	2.39671000
H	1.31384600	-0.90823000	4.73233800
H	-0.35765700	0.83031200	5.38639500
H	-1.97421100	1.66424400	3.70064800
C	-4.23186700	1.48276200	-1.67061900
C	-5.32262900	1.84929600	-2.45407900
C	-6.44173700	2.45508900	-1.87415800
C	-6.46137300	2.69849800	-0.49812200
C	-5.37473000	2.33578800	0.29564200

C	-4.24582800	1.71845900	-0.28029800
H	-3.36149400	1.00250500	-2.10072200
H	-5.30189600	1.66148700	-3.52429400
H	-7.29039100	2.73825000	-2.49002400
H	-7.32558400	3.17266800	-0.04157400
H	-5.38665100	2.52119200	1.36504500
N	-0.13033600	-0.97444100	0.36524400
H	-0.74101100	-0.25641000	-0.61739300
S	-0.72040300	-2.57134600	0.14609700
O	-0.29505800	-3.43900800	1.25472600
O	-0.37025000	-2.92695500	-1.24008100
C	-3.20867100	-2.03808000	-0.89651100
C	-4.56013500	-1.73793600	-0.77881100
C	-5.19530900	-1.72957900	0.47255100
C	-4.45114900	-2.08019300	1.60630900
C	-3.09705400	-2.39553900	1.51004800
C	-2.48683300	-2.35591100	0.25607700
H	-2.70584500	-2.00980300	-1.85520500
H	-5.12762700	-1.46815500	-1.66448100
H	-4.93269900	-2.09145700	2.58013300
H	-2.51565200	-2.65717000	2.38676300
C	-3.15339100	1.31020800	0.53352400
C	-2.22640800	0.91857100	1.21349600
C	-6.63639700	-1.29969000	0.58261000
H	-6.71238300	-0.21367700	0.44966900
H	-7.25339500	-1.76586500	-0.19259600
H	-7.06217500	-1.55191400	1.55767900

Rh	1.88388800	-0.54762300	-0.54487800
C	3.01226700	-2.45490900	-0.23873000
C	3.00034300	-2.05269400	-1.61616500
C	3.72438600	-0.79028800	-1.71879000
C	4.14244300	-0.41971300	-0.40983400
C	3.63876000	-1.40506100	0.52598100
O	-1.18374500	0.22442900	-1.57461600
C	-0.30402700	0.40772100	-2.48397800
O	0.91280800	0.11323900	-2.37550400
C	-0.79815700	1.02345500	-3.77020500
C	3.96418500	-1.40022200	1.98654600
H	3.51558700	-2.24976800	2.50358000
H	5.05101400	-1.46074200	2.12260600
H	3.61383200	-0.47290500	2.44680800
C	2.55326200	-3.77572200	0.28226200
H	1.75359100	-4.19134300	-0.32916500
H	3.40728700	-4.46552800	0.25997800
H	2.18008600	-3.71481700	1.30333600
C	2.44995200	-2.82447000	-2.77150400
H	2.09109000	-2.14206300	-3.54484300
H	3.23088300	-3.46064500	-3.20678200
H	1.61048900	-3.44461100	-2.45859100
C	3.97147600	-0.04720100	-2.99138900
H	4.33458900	0.96269000	-2.79536000
H	4.71203300	-0.57448500	-3.60417600
H	3.04301600	0.03485500	-3.56190800
C	5.03269500	0.71335300	-0.02728900

H	6.01881000	0.29841100	0.21994900
H	5.15496200	1.43425900	-0.83343000
H	4.64601000	1.22940300	0.85195100
H	-1.24615700	1.99557300	-3.54463700
H	0.01723700	1.14357300	-4.48292700
H	-1.58084200	0.38944700	-4.19740100
S	1.74461400	2.32742200	1.15109500
O	0.70975500	3.07015600	1.86608600
O	2.84161300	1.72543700	1.93157200
C	2.56480900	3.58425100	0.04142300
O	1.17500300	1.38963800	0.09342200
F	3.38807600	4.37039000	0.74453300
F	1.64714200	4.34175300	-0.56487700
F	3.29093700	2.96165800	-0.91469000

Zero-point correction= 0.629896 (Hartree/Particle)

Thermal correction to Energy= 0.679313

Thermal correction to Enthalpy= 0.680257

Thermal correction to Gibbs Free Energy= 0.544770

Sum of electronic and zero-point Energies= -3102.862496

Sum of electronic and thermal Energies= -3102.813079

Sum of electronic and thermal Enthalpies= -3102.812135

Sum of electronic and thermal Free Energies= -3102.947622

E(RB3LYP) = -3103.492392 A.U.

B-TSb7

0 1

Number of imaginary frequencies: 1

C	-2.95876600	1.42345200	-0.29819100

C	-4.30911500	1.70034700	-0.07816300
C	-4.84474300	2.92288100	-0.49192400
C	-4.05290700	3.87600500	-1.13352700
C	-2.70174800	3.61402300	-1.34627400
C	-2.14678600	2.39888700	-0.91904400
H	-4.94595800	0.98670500	0.42288800
H	-5.89527000	3.12519900	-0.30688700
H	-4.48023300	4.82027800	-1.45493900
H	-2.05952200	4.34545000	-1.82588900
C	2.61083800	1.21764700	-2.11664100
C	3.93716600	1.42797800	-2.48608800
C	4.41589200	2.72961200	-2.65611700
C	3.57796200	3.83167900	-2.44290300
C	2.26007300	3.63655900	-2.04597800
C	1.76716000	2.32027400	-1.88337100
H	2.26475400	0.21080600	-1.92355200
H	4.59874900	0.57239200	-2.58254800
H	5.45220100	2.88767300	-2.94004900
H	3.95701900	4.84098700	-2.57365900
H	1.60307300	4.48192900	-1.86398800
N	-2.27100100	0.20477200	0.02147600
S	-3.03263200	-0.99112700	0.98676300
O	-3.59609800	-0.33737500	2.17917700
O	-2.01678500	-2.03802600	1.10987200
C	-5.68025200	-1.58315200	0.55639300
C	-6.73904200	-2.12431800	-0.17113300
C	-6.52934600	-2.70720600	-1.42764300

C	-5.22223900	-2.74641400	-1.93901300
C	-4.14758200	-2.22076700	-1.22850000
C	-4.39499000	-1.62937700	0.01457300
H	-5.83922700	-1.13582800	1.53151500
H	-7.74149100	-2.09567000	0.24671600
H	-5.04187400	-3.20184400	-2.90892800
H	-3.14403900	-2.25605800	-1.63786800
C	0.42902600	2.15234100	-1.44057400
C	-0.74266300	2.13896800	-1.04863000
C	-7.67896900	-3.26574800	-2.22921000
H	-8.56540500	-3.42255300	-1.60889700
H	-7.95625900	-2.57949300	-3.03849900
H	-7.41226700	-4.22057400	-2.69293000
Rh	-0.09799500	0.67109200	0.65334900
C	1.30697000	-0.02979600	2.26088300
C	1.76422800	1.20938800	1.68437500
C	0.75363900	2.22426400	1.95682100
C	-0.34054100	1.60009400	2.62767600
C	0.01119800	0.19539700	2.82936900
C	-0.75098100	-0.79553600	3.64520800
H	-0.71291900	-1.78790500	3.19606400
H	-0.29549600	-0.84361800	4.64280700
H	-1.79802900	-0.51691700	3.75059900
C	2.05291700	-1.31416200	2.18055500
H	2.24320800	-1.57272400	1.13141800
H	3.03598000	-1.20641200	2.64830500
H	1.51184700	-2.12843300	2.66302300

C	3.12057400	1.40132500	1.09341900
H	3.19164900	2.32097700	0.51266300
H	3.85722000	1.44659700	1.90534500
H	3.38872100	0.55395500	0.45673800
C	0.86654300	3.66702600	1.58655100
H	-0.11481200	4.11551500	1.41965400
H	1.36061500	4.21487200	2.39816100
H	1.46470900	3.79510400	0.68260800
C	-1.59368100	2.25919900	3.11298800
H	-1.48499200	2.55322400	4.16408200
H	-1.81675200	3.15635200	2.53135700
H	-2.44468000	1.58061600	3.02975900
H	-1.84435100	-0.35640000	-0.94835800
O	0.52248500	-0.86944300	-0.60337400
C	-0.10810300	-1.39458100	-1.57238900
O	-1.29035800	-1.06256700	-1.91269200
C	0.61112200	-2.48023900	-2.32941300
H	0.41843100	-2.37290800	-3.39960700
H	1.67869900	-2.45465100	-2.10396700
H	0.19978900	-3.44469500	-2.01102200
S	4.74334400	-1.98184600	-0.96272800
O	3.38679600	-1.37928900	-0.76740700
O	4.73187600	-3.36361600	-1.46622100
C	5.32071100	-2.14312600	0.80212200
O	5.73026100	-1.05438300	-1.55826400
F	4.53483900	-2.99624500	1.49221200
F	5.25827200	-0.94514200	1.43974300

F	6.58194600	-2.58270800	0.87985600

Zero-point correction= 0.630378 (Hartree/Particle)

Thermal correction to Energy= 0.679684

Thermal correction to Enthalpy= 0.680628

Thermal correction to Gibbs Free Energy= 0.545956

Sum of electronic and zero-point Energies= -3102.842776

Sum of electronic and thermal Energies= -3102.793470

Sum of electronic and thermal Enthalpies= -3102.792526

Sum of electronic and thermal Free Energies= -3102.927197

E(RB3LYP) = -3103.473154 A.U.

B-TSc7

0 1

Number of imaginary frequencies: 1

C	0.95241000	2.83878900	-0.66890300
C	1.05738700	4.17638600	-1.02805600
C	-0.07359700	4.98493600	-0.87608500
C	-1.26672400	4.44327800	-0.39321000
C	-1.35064500	3.09742100	-0.02982500
C	-0.22506200	2.28068200	-0.14432700
H	1.98931500	4.57261800	-1.41450800
H	-0.02422500	6.03129900	-1.15986300
H	-2.15117300	5.06825600	-0.31916600
H	-2.29248100	2.66307400	0.26934200
C	2.43403600	-1.74828100	0.11300200
C	3.04212300	-2.87387300	-0.43572500
C	2.90389700	-3.14900300	-1.79723800
C	2.12706300	-2.31630400	-2.61124300

C	1.49756500	-1.20176600	-2.06603000
C	1.67160900	-0.89956800	-0.69962600
H	2.52013700	-1.53250300	1.16995800
H	3.61281100	-3.54174500	0.20159400
H	3.38048800	-4.02802500	-2.22254300
H	1.98725500	-2.55611500	-3.66094500
H	0.82306900	-0.58606200	-2.65368200
N	2.00933200	1.85797900	-0.79451700
S	3.46272300	2.32068000	0.14704700
O	4.10251800	3.39389700	-0.61756300
O	2.98961700	2.51667800	1.51348100
C	4.80082700	0.20307600	1.23287000
C	5.61851700	-0.92296300	1.16060000
C	6.07303600	-1.40902500	-0.07155700
C	5.72285500	-0.71688700	-1.24258900
C	4.93374500	0.42481900	-1.19185800
C	4.46305300	0.85926900	0.05043600
H	4.42273300	0.56900000	2.18078900
H	5.89017500	-1.44253300	2.07485900
H	6.07385900	-1.08021400	-2.20379600
H	4.69508900	0.96808000	-2.10043900
C	1.01403200	0.27327400	-0.18660200
C	-0.11890200	0.84277700	0.12151100
C	6.88416000	-2.67613500	-0.15671700
H	6.24423600	-3.50756200	-0.47678000
H	7.69200700	-2.58718400	-0.88936500
H	7.32175700	-2.94419600	0.80827000

H	2.29220800	1.69855300	-1.76442300
C	-2.68076100	0.70747800	2.63237000
C	-3.23892200	-0.63976300	2.51876100
C	-2.21086400	-1.56874100	2.79450600
C	-0.97324600	-0.82268100	2.99320300
C	-1.30520500	0.59155800	2.98010200
C	-3.51036100	1.94566900	2.49824600
H	-4.06794700	1.92818300	1.55643600
H	-4.23835100	1.99884700	3.31689100
H	-2.90269600	2.85121600	2.52806700
C	-4.65952600	-0.90912700	2.12923700
H	-5.35254100	-0.48877600	2.86760000
H	-4.87314100	-0.44604100	1.15953800
H	-4.85782100	-1.97887600	2.04508300
C	-2.34375200	-3.05652800	2.87235400
H	-2.45494500	-3.35848500	3.92194500
H	-3.22285800	-3.40679600	2.32695800
H	-1.46378500	-3.54224300	2.45128500
C	0.34328000	-1.41742900	3.38553100
H	1.14946700	-0.69079500	3.25413100
H	0.33329900	-1.72251400	4.44011400
H	0.54778700	-2.28502900	2.75584000
C	-0.35248400	1.71033800	3.27537200
H	-0.24289500	1.83440200	4.35930700
H	0.63703200	1.51736200	2.85414500
H	-0.70360100	2.65462400	2.85593500
Rh	-1.60407100	-0.31018300	0.97781400

O	-1.28415000	-1.81559000	-0.40420400
C	-0.67959600	-2.94021600	-0.19150700
O	-0.03544800	-3.26297700	0.81543500
C	-0.83763000	-3.92123200	-1.35084300
H	0.10819200	-4.44164300	-1.51504300
H	-1.59071800	-4.66750400	-1.07410600
H	-1.16387000	-3.41252800	-2.25797600
S	-2.82225300	0.67969500	-2.01306200
O	-3.01680900	0.45050400	-0.51416600
O	-3.52623600	1.88991700	-2.45332800
C	-3.81346100	-0.73041500	-2.72217900
O	-1.44664100	0.47040700	-2.49069000
F	-5.04913800	-0.72808400	-2.19547700
F	-3.24822900	-1.91555400	-2.46646100
F	-3.91412800	-0.58561600	-4.05193000

Zero-point correction= 0.633034 (Hartree/Particle)

Thermal correction to Energy= 0.682393

Thermal correction to Enthalpy= 0.683337

Thermal correction to Gibbs Free Energy= 0.547096

Sum of electronic and zero-point Energies= -3102.810324

Sum of electronic and thermal Energies= -3102.760965

Sum of electronic and thermal Enthalpies= -3102.760021

Sum of electronic and thermal Free Energies= -3102.896262

E(RB3LYP) = -3103.443358 A.U.

B-TSa8

1 1

Number of imaginary frequencies: 1

C	2.54930600	3.14208100	-0.71724800
C	2.08594200	2.04516400	0.01994300
C	1.27535400	1.10514600	-0.61760600
C	0.88463700	1.30720800	-1.97736600
C	1.34250600	2.43130600	-2.68253300
C	2.19354300	3.33837500	-2.05728700
H	3.18894400	3.86635600	-0.22169600
H	2.34363600	1.95399100	1.06580000
H	1.02784800	2.56601000	-3.71221500
H	2.56786700	4.20182100	-2.59701400
C	-0.06059600	0.32915700	-2.42267700
C	-0.21831600	-0.63829000	-1.49757000
C	-1.12965800	-1.75874700	-1.34923100
C	-2.00286400	-2.04786100	-2.44344200
C	-1.35325600	-2.40617500	-0.10144500
C	-3.05366200	-2.92186600	-2.27320200
H	-1.82634700	-1.54703400	-3.38762700
C	-2.45070200	-3.28655300	0.04059800
H	-0.59923800	-2.38322600	0.67449700
C	-3.29641000	-3.53798400	-1.02167800
H	-3.70659600	-3.13913100	-3.11324500
H	-2.59260200	-3.79095300	0.99108500
H	-4.12437300	-4.23173500	-0.91408400
N	0.69719500	-0.07799000	-0.06891500
S	1.57156900	-0.76002500	1.30164000
O	1.06298000	-2.11927200	1.49639600
O	1.44786000	0.21242200	2.39937400

C	3.25640400	-0.84483800	0.74155900
C	3.54707000	-1.60551000	-0.39472600
C	4.25232200	-0.18391800	1.45986000
C	4.86797700	-1.68655900	-0.81958500
H	2.75803200	-2.11783900	-0.93546700
C	5.57043400	-0.28834100	1.02010500
H	3.99677800	0.39302600	2.34161900
C	5.89872600	-1.03450600	-0.12072600
H	5.10768100	-2.26739000	-1.70548400
H	6.35597900	0.21929100	1.57202700
C	7.32967400	-1.16319500	-0.57706500
H	7.94845300	-0.34451900	-0.20108000
H	7.76418500	-2.10104800	-0.21071600
H	7.40105200	-1.17681600	-1.66848000
Rh	-1.53652900	0.05776300	0.12685700
C	-1.84087200	1.94424700	1.20202800
C	-2.48438700	2.04740800	-0.07647900
C	-3.48950000	0.99824700	-0.14277600
C	-3.50694100	0.31076500	1.12678600
C	-2.46343100	0.85974900	1.94776100
C	-4.44722100	-0.79125100	1.49070800
H	-5.42605600	-0.36803200	1.74552900
H	-4.58740300	-1.48524100	0.65812400
H	-4.08953600	-1.35954100	2.35028800
C	-2.08020500	0.45462900	3.33490700
H	-2.48446800	1.16976500	4.06179000
H	-2.46474600	-0.53528300	3.58542600

H	-0.99243700	0.43582500	3.44471800
C	-4.40443900	0.72664600	-1.29279100
H	-4.66448900	-0.33263700	-1.34656800
H	-5.33306500	1.29953300	-1.18094900
H	-3.94308100	1.00936100	-2.24087300
C	-2.16575800	3.05052600	-1.13530600
H	-2.52480300	2.72832900	-2.11342800
H	-2.63735300	4.01064000	-0.89331800
H	-1.08763900	3.21453400	-1.21377800
C	-0.75513100	2.82340500	1.72613500
H	-0.02744100	2.24569600	2.30019700
H	-0.22813100	3.33570200	0.92088600
H	-1.19231100	3.58154200	2.38754100

Zero-point correction= 0.538834 (Hartree/Particle)

Thermal correction to Energy= 0.574032

Thermal correction to Enthalpy= 0.574976

Thermal correction to Gibbs Free Energy= 0.471862

Sum of electronic and zero-point Energies= -1912.113885

Sum of electronic and thermal Energies= -1912.078688

Sum of electronic and thermal Enthalpies= -1912.077744

Sum of electronic and thermal Free Energies= -1912.180858

E(RB3LYP) = -1912.652720 A.U.

C-Re3

0 1

Number of imaginary frequencies: 0

C	-1.84459400	-1.35049600	0.01366200
C	-3.06218700	-1.36046700	0.69813000

C	-4.22454000	-1.49181100	-0.06033700
C	-4.17983800	-1.63168200	-1.45823600
C	-2.96415700	-1.64146400	-2.13218100
C	-1.78291300	-1.48921800	-1.39292800
H	-3.09853600	-1.27044900	1.77444500
H	-5.18430000	-1.50070800	0.44719400
H	-5.10583800	-1.74368900	-2.01428500
H	-2.92300600	-1.76443800	-3.21030300
C	2.52840000	-2.08861300	0.38688200
C	3.92019100	-2.10706200	0.38102000
C	4.63300000	-1.36748200	-0.56638000
C	3.94400700	-0.60501300	-1.51131000
C	2.55039800	-0.58098200	-1.50617500
C	1.82661100	-1.32327800	-0.55803200
H	1.97491700	-2.65459700	1.12612600
H	4.45081600	-2.70120700	1.11882900
H	5.71891500	-1.38317800	-0.56516200
H	4.49061400	-0.02171800	-2.24660500
H	2.00863300	0.02996300	-2.22157600
N	-0.51045000	-1.27442800	0.50506700
S	-0.15353400	-0.15472300	1.80105800
O	-1.31152800	-0.18806300	2.69096200
O	1.18309300	-0.47024100	2.29057700
C	1.12459400	1.92560200	0.53592100
C	1.14236200	3.11418100	-0.18992200
C	-0.04518400	3.78682800	-0.51041500
C	-1.26507900	3.23930200	-0.08535100

C	-1.30753300	2.05439400	0.64334300
C	-0.10558000	1.41175100	0.94712400
H	2.03953200	1.39730100	0.77708200
H	2.09460700	3.52416200	-0.51466800
H	-2.19349600	3.74822300	-0.32892300
H	-2.24952600	1.63072200	0.97251700
C	0.35937500	-1.33032000	-0.63231300
C	-0.39473400	-1.47126200	-1.76102800
C	-0.01290700	5.08949200	-1.27120300
H	0.00658400	5.94109400	-0.58021500
H	0.87524000	5.16235400	-1.90513100
H	-0.89692900	5.20485500	-1.90509200
H	0.01080400	-1.63010400	-2.75057100

Zero-point correction= 0.329299 (Hartree/Particle)

Thermal correction to Energy= 0.349959

Thermal correction to Enthalpy= 0.350903

Thermal correction to Gibbs Free Energy= 0.277367

Sum of electronic and zero-point Energies= -1413.548615

Sum of electronic and thermal Energies= -1413.527955

Sum of electronic and thermal Enthalpies= -1413.527011

Sum of electronic and thermal Free Energies= -1413.600547

E(RB3LYP) = -1413.877914 A.U.

C-1

1 1

Number of imaginary frequencies: 0

Rh	2.03031500	-0.37166500	-0.12206100
C	1.63994500	-2.16989900	-1.66227500

C	2.32440700	-1.14988100	-2.34119700
C	3.55295000	-0.86911700	-1.59811100
C	3.65444900	-1.83136100	-0.52565100
C	2.42162400	-2.54876900	-0.48053400
C	1.67178900	2.47205700	-1.33908700
C	2.23300900	2.40707700	0.91902300
C	2.07911500	3.81770000	1.04502300
C	1.73959200	4.54667300	-0.12235600
C	1.55646300	3.87789800	-1.31156600
H	1.47249900	1.92132800	-2.24869000
C	2.63279500	1.59973400	2.01264100
C	2.26657600	4.40062500	2.32471100
H	1.62604400	5.62554800	-0.06562400
H	1.29199300	4.40167600	-2.22247500
C	2.59460200	3.60449000	3.40153100
C	2.78636200	2.20929800	3.24571500
H	2.14323000	5.47310700	2.44136900
H	2.72777800	4.05041300	4.38227800
H	3.08190300	1.61252100	4.10414200
N	1.97978600	1.75711700	-0.26677900
C	2.90559900	0.15387800	1.71334400
H	3.98311100	0.00844400	1.59603300
H	2.55980400	-0.51339500	2.50731100
C	0.38272800	-2.84746100	-2.09871100
H	-0.27880900	-2.19126600	-2.66551000
H	0.63954500	-3.69928300	-2.74137600
H	-0.17798200	-3.24483800	-1.25242800

C	1.94321700	-0.52239200	-3.64686700
H	2.44342700	-1.03627300	-4.47702800
H	0.86797700	-0.58162500	-3.82786800
H	2.24521400	0.52708900	-3.70006700
C	4.62239900	0.08030200	-2.04123600
H	5.24292000	-0.37941700	-2.82018900
H	4.19176000	0.99492600	-2.45652300
H	5.27494800	0.36301300	-1.21283100
C	4.85234000	-2.08786000	0.33306600
H	5.42971800	-2.91841200	-0.09020300
H	5.51453400	-1.22121800	0.38576800
H	4.56867400	-2.36694500	1.35039200
C	2.11539100	-3.69423800	0.43407700
H	2.52153900	-4.62782600	0.02488600
H	2.55447200	-3.54086300	1.42182800
H	1.04260300	-3.82697300	0.57072200
C	-1.16424800	-2.22140700	1.08609900
C	-1.52083100	-3.53898900	1.40125200
C	-0.98222000	-4.08830100	2.56385400
C	-0.10332500	-3.36336100	3.38655900
C	0.26912600	-2.06649700	3.05294100
C	-0.25699100	-1.49106700	1.88909700
H	-2.19468700	-4.10764300	0.77872000
H	-1.25468700	-5.10300600	2.83586600
H	0.28701700	-3.82231600	4.28934800
H	0.94363000	-1.50032800	3.68689100
C	-1.60436000	2.22044300	0.12845700

C	-1.93685200	3.40759800	-0.52160600
C	-1.90028800	3.47642900	-1.91584600
C	-1.50729000	2.35760200	-2.65499500
C	-1.16672800	1.17135800	-2.00744900
C	-1.23243400	1.08287400	-0.60847900
H	-1.66244500	2.15882500	1.21020900
H	-2.23543700	4.27338800	0.06111400
H	-2.17115000	4.39720100	-2.42363400
H	-1.46216400	2.40753800	-3.73875300
H	-0.85729400	0.31012900	-2.58120700
N	-1.53631000	-1.38075700	-0.00098300
S	-2.94533400	-1.67156300	-1.03124600
O	-2.57816000	-1.25069400	-2.37870000
O	-3.32304400	-3.05040000	-0.75191500
C	-4.70567900	-0.86559300	0.89603600
C	-5.62274500	0.02138200	1.44769800
C	-5.98880800	1.20093100	0.77603800
C	-5.40675600	1.47504000	-0.46969900
C	-4.48222000	0.60472500	-1.04215700
C	-4.14267200	-0.55588300	-0.34661500
H	-4.43420000	-1.78078400	1.41172300
H	-6.06877600	-0.20508400	2.41180300
H	-5.67787300	2.38293900	-1.00024100
H	-4.02357700	0.82155500	-1.99929600
C	-0.90104500	-0.14205500	0.14610800
C	-0.06531400	-0.20182500	1.26294700
C	-7.01179100	2.13290000	1.37421100

H	-8.02587500	1.78237000	1.14768700
H	-6.92128200	2.18097700	2.46326800
H	-6.91762400	3.14590600	0.97434500
H	0.32471300	0.68239700	1.74421500

Zero-point correction= 0.709544 (Hartree/Particle)

Thermal correction to Energy= 0.753654

Thermal correction to Enthalpy= 0.754598

Thermal correction to Gibbs Free Energy= 0.631917

Sum of electronic and zero-point Energies= -2353.365026

Sum of electronic and thermal Energies= -2353.320916

Sum of electronic and thermal Enthalpies= -2353.319972

Sum of electronic and thermal Free Energies= -2353.442652

E(RB3LYP) = -2354.074570 A.U.

C-2a

1 1

Number of imaginary frequencies: 0

Rh	-0.67791400	-1.43594800	0.35409900
C	1.28543200	-2.49780300	0.52724900
C	0.57679000	-2.71602200	1.73311400
C	-0.66801700	-3.35674100	1.37931500
C	-0.60291800	-3.74415300	-0.03824000
C	0.57088700	-3.19588300	-0.56177600
C	-3.70136900	-1.75735500	0.37073800
C	-3.03650300	-0.18847800	-1.22485000
C	-4.37958500	-0.10307300	-1.71914200
C	-5.37511200	-0.90572600	-1.11329200
C	-5.04102100	-1.71919500	-0.05568100

H	-3.41806200	-2.38428900	1.20516800
C	-2.03428300	0.66728600	-1.76567700
C	-4.68124200	0.79529100	-2.77569800
H	-6.39626000	-0.85383400	-1.47971300
H	-5.77933800	-2.32737900	0.45444200
C	-3.69659900	1.59532600	-3.30340300
C	-2.38315600	1.53272800	-2.78710700
H	-5.70044300	0.84285700	-3.14712300
H	-3.92300100	2.29010300	-4.10528900
H	-1.62730200	2.20586900	-3.18052200
N	-2.72577700	-1.05303800	-0.19728500
C	2.64771800	-1.89428900	0.42075500
H	2.75522300	-1.04100000	1.09304700
H	3.40835900	-2.63683700	0.69295500
H	2.86160300	-1.55855500	-0.59163900
C	1.06575300	-2.45164200	3.11510300
H	1.56259000	-3.35552900	3.49145300
H	1.78287900	-1.63205900	3.14540900
H	0.25161200	-2.21048600	3.79976100
C	-1.66046200	-3.87604300	2.37290800
H	-1.23348800	-4.74098300	2.89593500
H	-1.90450600	-3.12509600	3.12903800
H	-2.58244300	-4.21448700	1.89608700
C	-1.65367900	-4.53798300	-0.74978900
H	-1.50811900	-4.52208000	-1.83140900
H	-1.63428600	-5.58416700	-0.42302900
H	-2.65630200	-4.15050200	-0.54258000

C	1.06432300	-3.25237800	-1.97310200
H	1.87274500	-3.98860700	-2.06074300
H	0.27435700	-3.53363800	-2.67192000
H	1.47683700	-2.28856000	-2.28438300
C	-0.63552500	0.72773700	-1.21649600
H	-0.15848000	-0.28878700	-1.19023700
H	-0.02471700	1.25268400	-1.94696200
C	1.36954200	1.29276000	1.76504200
C	2.50630100	1.57885100	2.51776500
C	2.46370600	1.32076200	3.89619300
C	1.31687800	0.81306300	4.51066000
C	0.19251900	0.50553600	3.73871600
C	0.23196300	0.70962900	2.36112300
H	3.37151400	2.05535200	2.07995800
H	3.33512200	1.56028700	4.49762100
H	1.29762100	0.66255200	5.58513000
H	-0.70812300	0.11027500	4.20036400
C	-2.52126600	2.82707800	0.34133600
C	-3.20120500	4.02520000	0.54987400
C	-2.49223100	5.19915500	0.80769300
C	-1.10124100	5.15047100	0.87205000
C	-0.42110500	3.95019700	0.65795200
C	-1.11651900	2.77113500	0.36135900
H	-3.10434800	1.92998500	0.17662700
H	-4.28678800	4.03599100	0.51955400
H	-3.01855600	6.13432900	0.97209400
H	-0.53203500	6.04776900	1.09430000

H	0.65622300	3.95646300	0.74918900
N	1.09057100	1.51955900	0.38723000
S	2.14867500	2.36752800	-0.65623200
O	1.32574500	2.84802700	-1.76933300
O	2.95447400	3.28659000	0.14716700
C	4.44986800	0.84380700	-0.63986400
C	5.29981100	-0.13339900	-1.15482600
C	4.97306300	-0.84107100	-2.32109400
C	3.76422000	-0.53900600	-2.96906500
C	2.89981900	0.43158300	-2.46676300
C	3.24515400	1.10679700	-1.29340800
H	4.72449400	1.40712700	0.24401600
H	6.23836400	-0.34137200	-0.64901300
H	3.50649900	-1.05835400	-3.88807500
H	1.98695600	0.68520500	-2.99351700
C	-0.40320800	1.41805800	0.17273800
C	-0.79163300	0.45991300	1.33803500
C	5.91876400	-1.86846000	-2.89043000
H	6.64784900	-1.39084200	-3.55571300
H	6.48188400	-2.37591900	-2.10216200
H	5.38802500	-2.62364900	-3.47686200
H	-1.81992100	0.58281200	1.67160900

Zero-point correction= 0.711655 (Hartree/Particle)

Thermal correction to Energy= 0.754555

Thermal correction to Enthalpy= 0.755499

Thermal correction to Gibbs Free Energy= 0.638477

Sum of electronic and zero-point Energies= -2353.336004

Sum of electronic and thermal Energies= -2353.293104

Sum of electronic and thermal Enthalpies= -2353.292160

Sum of electronic and thermal Free Energies= -2353.409182

E(RB3LYP) = -2354.047659 A.U.

C-2b

1 1

Number of imaginary frequencies: 0

Rh	-1.45958900	-0.31640600	0.75879500
C	-2.09092000	-2.26912300	1.64031600
C	-0.84721700	-1.90880600	2.22460000
C	-1.04971500	-0.62375000	2.85924100
C	-2.49632400	-0.33729600	2.86782400
C	-3.12199600	-1.31855900	2.10206600
C	-1.41196400	2.69558500	1.23375100
C	-2.18180700	2.25514200	-0.92042500
C	-2.38207900	3.65511500	-1.14852200
C	-2.08526100	4.56061000	-0.10201600
C	-1.58807100	4.08300000	1.08617400
H	-0.98062900	2.30339100	2.14412900
C	-2.42323300	1.33345400	-1.97931200
C	-2.83545100	4.10361100	-2.41540800
H	-2.23334700	5.62474300	-0.26126400
H	-1.31687400	4.74355500	1.90156700
C	-3.06449900	3.20138200	-3.42631000
C	-2.85596900	1.82289000	-3.19912300
H	-2.98786400	5.16749200	-2.57041000
H	-3.40578000	3.53850200	-4.39945200

H	-3.03840800	1.12358300	-4.01049600
N	-1.71603600	1.80646800	0.29685600
C	-2.40883800	-3.51616700	0.88057800
H	-1.51313000	-3.99396100	0.48936400
H	-2.92747800	-4.22441100	1.53886800
H	-3.06875800	-3.31031900	0.03458500
C	0.42664000	-2.68943900	2.25028600
H	0.27725000	-3.69763400	1.86367000
H	1.19149700	-2.20854300	1.63185100
H	0.79411800	-2.76662000	3.27876000
C	-0.04068900	0.07122400	3.71828100
H	-0.21852700	-0.18615900	4.77029400
H	0.97610600	-0.23304200	3.46576400
H	-0.10076900	1.15950600	3.63900200
C	-3.13976400	0.80415600	3.58833200
H	-4.10056600	1.07616900	3.14660100
H	-3.31705400	0.53203200	4.63599300
H	-2.50621000	1.69353100	3.59365800
C	-4.57600400	-1.44099000	1.77206900
H	-5.03847300	-2.23084500	2.37629800
H	-5.11723800	-0.51250900	1.96320100
H	-4.72307700	-1.71348700	0.72290500
C	1.49288800	1.29684800	0.69246800
C	2.08400500	2.53347200	0.92035100
C	2.07659200	3.50539100	-0.08568100
C	1.49029500	3.21166500	-1.31677000
C	0.90038500	1.96500300	-1.54266600

C	0.87660600	0.99407000	-0.53507100
H	2.56360300	2.73469200	1.87350700
H	2.53397200	4.47515200	0.08519900
H	1.49300200	3.95169300	-2.11154200
H	0.45818600	1.75701300	-2.50950800
C	-1.44123700	-3.07407800	-2.63280300
C	-1.16649500	-4.43940000	-2.48627300
C	-0.11802300	-4.86975800	-1.66701100
C	0.67230500	-3.94798800	-0.97243000
C	0.38295100	-2.59516000	-1.12736100
C	-0.65257200	-2.15265000	-1.95151500
H	-2.24737000	-2.75103900	-3.28576200
H	-1.76804800	-5.16882800	-3.01945600
H	0.09116600	-5.93046500	-1.57148400
H	1.50516300	-4.26641700	-0.35946300
H	1.50759400	0.53933000	1.46556500
N	1.08915100	-1.48487600	-0.53315500
H	-0.27234600	-0.23605200	-2.84373200
S	2.66272800	-1.35918800	-1.44828500
O	2.41149000	-0.63218000	-2.69961100
O	3.18103400	-2.72862000	-1.45814800
C	4.05214300	-0.87214300	0.87064500
C	4.92070200	-0.12840200	1.66236200
C	5.49554600	1.06261600	1.18677600
C	5.17432600	1.49352200	-0.10768800
C	4.29197200	0.77424300	-0.91007000
C	3.73166100	-0.39539300	-0.40230600

H	3.63058900	-1.80501100	1.22926000
H	5.17208400	-0.48171300	2.65868700
H	5.61189800	2.41115100	-0.48997300
H	4.01634800	1.11999700	-1.89924500
C	-0.71528000	-0.63794100	-1.92217000
C	0.17875600	-0.32518300	-0.68533100
C	6.46729200	1.83985300	2.03938600
H	6.24400000	1.73244700	3.10482300
H	7.49045500	1.47748000	1.88313600
H	6.45756800	2.90475400	1.79067500
C	-2.18534400	-0.14431900	-1.81790500
H	-2.66203100	-0.51634800	-0.87689700
H	-2.76261000	-0.67011400	-2.58377200

Zero-point correction= 0.710341 (Hartree/Particle)

Thermal correction to Energy= 0.753711

Thermal correction to Enthalpy= 0.754656

Thermal correction to Gibbs Free Energy= 0.635894

Sum of electronic and zero-point Energies= -2353.335403

Sum of electronic and thermal Energies= -2353.292033

Sum of electronic and thermal Enthalpies= -2353.291088

Sum of electronic and thermal Free Energies= -2353.409850

E(RB3LYP) = -2354.045744 A.U.

C-2c

1 1

Number of imaginary frequencies: 0

Rh	-2.23759700	-0.85824800	-0.13062800
C	-4.11736300	-1.86950900	0.89416800

C	-3.87923700	-0.59541900	1.44373700
C	-3.92068000	0.37350600	0.35186000
C	-4.34175400	-0.33962800	-0.85198900
C	-4.40185800	-1.71035700	-0.53439900
C	-0.39073800	2.34790900	1.95809000
C	-0.64990300	2.30496800	-0.40838000
C	-0.81727800	3.73732600	-0.36289100
C	-0.85677800	4.40423600	0.87930500
C	-0.75956000	3.68692800	2.05093300
H	-0.13966200	1.78603800	2.84528800
C	-1.01351500	1.59933000	-1.59632300
C	-1.06627000	4.46878500	-1.55010600
H	-1.01247500	5.47883400	0.89511300
H	-0.86572400	4.14184000	3.02772800
C	-1.24765600	3.79495300	-2.73214000
C	-1.26923700	2.38981300	-2.72126400
H	-1.15331200	5.54875500	-1.49054100
H	-1.43921800	4.33126400	-3.65562300
H	-1.52723600	1.87114000	-3.63925600
N	-0.22398600	1.70852500	0.78918100
C	-4.16483300	-3.17738700	1.62516400
H	-3.60807100	-3.13770800	2.56484100
H	-5.19900500	-3.45172400	1.86698500
H	-3.75105700	-3.98855900	1.01922600
C	-3.61347400	-0.25823600	2.87895400
H	-4.53723800	0.04538600	3.38564400
H	-3.20201500	-1.10997700	3.42670800

H	-2.90568100	0.57171400	2.96582400
C	-3.90378700	1.86303400	0.50951700
H	-4.90596000	2.23510000	0.75838900
H	-3.22795100	2.17317700	1.31044400
H	-3.58345900	2.35587800	-0.41050700
C	-4.66778500	0.30893200	-2.16162900
H	-4.54593100	-0.38354900	-2.99779500
H	-5.70656700	0.66006600	-2.16734900
H	-4.02699300	1.17515000	-2.34813900
C	-4.75943300	-2.83809300	-1.45336100
H	-5.79320200	-3.16313900	-1.28162200
H	-4.67123700	-2.54740300	-2.50197600
H	-4.11349900	-3.70535400	-1.28990700
C	-1.29580000	0.13449700	-1.72182700
H	-1.98657600	0.01360700	-2.56181000
H	-0.40245400	-0.42229300	-1.99344400
C	0.96100600	-1.47216200	-0.51135700
C	1.52625600	-2.33447500	-1.43467300
C	1.05950200	-3.66195300	-1.45987300
C	0.05717800	-4.10390800	-0.59821500
C	-0.51740200	-3.22152700	0.32850000
C	-0.06090000	-1.89602800	0.37479600
H	2.29045900	-2.00721300	-2.12737700
H	1.49697500	-4.35295600	-2.17335300
H	-0.27461900	-5.13617600	-0.63653000
H	-1.27692700	-3.55956800	1.02605700
C	1.74184200	-0.70033300	2.87112500

C	2.77365600	-0.72911500	3.81356100
C	3.60746700	0.37565600	3.97994100
C	3.40412900	1.51191000	3.19316600
C	2.38372500	1.54119400	2.24499500
C	1.53441600	0.43282300	2.07195500
H	1.12138000	-1.57923600	2.75063600
H	2.91846800	-1.61976100	4.41716000
H	4.40691100	0.35348900	4.71393800
H	4.04924700	2.37755800	3.30636900
H	2.26951300	2.41538300	1.61855700
N	1.20306000	-0.09319500	-0.29884200
S	2.29780800	0.81150300	-1.24912700
O	1.89733000	0.63035800	-2.64417700
O	2.29408800	2.14924200	-0.65057300
C	4.30822600	-0.48514300	0.18730600
C	5.56495800	-1.07702500	0.27617700
C	6.40232100	-1.18640300	-0.84404000
C	5.93862900	-0.69616200	-2.07397500
C	4.68237200	-0.10734900	-2.18909800
C	3.87784000	-0.00209700	-1.04969300
H	3.67528800	-0.42700200	1.06104300
H	5.89757600	-1.46532300	1.23456200
H	6.56653300	-0.78232900	-2.95612200
H	4.32092100	0.25268800	-3.14564000
C	0.49452900	0.35393700	0.92594800
C	-0.56999000	-0.73087800	1.10780800
C	7.77542000	-1.79796200	-0.72655900

H	8.52347700	-1.02221700	-0.52279100
H	7.82460200	-2.52318100	0.09022800
H	8.07130100	-2.30034500	-1.65168300
H	-0.88394300	-0.84058500	2.14534100

Zero-point correction= 0.710319 (Hartree/Particle)

Thermal correction to Energy= 0.753546

Thermal correction to Enthalpy= 0.754490

Thermal correction to Gibbs Free Energy= 0.635003

Sum of electronic and zero-point Energies= -2353.282385

Sum of electronic and thermal Energies= -2353.239159

Sum of electronic and thermal Enthalpies= -2353.238215

Sum of electronic and thermal Free Energies= -2353.357701

E(RB3LYP) = -2353.992704 A.U.

C-2d

1 1

Number of imaginary frequencies: 0

Rh	1.31251400	-1.18762300	0.18513100
C	1.11696400	-2.92895700	-1.50005300
C	1.48142500	-1.72013800	-2.10772500
C	2.70387100	-1.24958800	-1.45780400
C	3.15371300	-2.29429700	-0.54313300
C	2.13316300	-3.25959600	-0.49372200
C	1.19403500	2.88253200	-1.02090800
C	2.86732200	1.94556000	0.39030200
C	3.84109100	2.77631600	-0.26167900
C	3.44228700	3.59623900	-1.34196600
C	2.13536100	3.58730800	-1.77392500

H	0.13791000	2.95795800	-1.23666800
C	3.28614200	0.90632900	1.28363500
C	5.20308300	2.70798700	0.12427100
H	4.18868800	4.20611900	-1.84240000
H	1.80250400	4.16165500	-2.62962800
C	5.58861600	1.79919900	1.07994600
C	4.64270100	0.90406000	1.61683300
H	5.92108200	3.35914800	-0.36340600
H	6.62567900	1.73341300	1.39271100
H	4.98802000	0.14052700	2.30687300
N	1.53294700	2.14883300	0.04534100
C	-0.01045900	-3.84890000	-1.84757200
H	-0.67470500	-3.41630400	-2.59245800
H	0.39132600	-4.79311100	-2.23496800
H	-0.61553800	-4.09448400	-0.96909400
C	0.83817100	-1.01203500	-3.25795600
H	1.51433600	-1.01541900	-4.12179300
H	-0.10311300	-1.47512200	-3.54570200
H	0.62144000	0.03199200	-3.01336500
C	3.55457600	-0.14363800	-1.99838500
H	4.08149500	-0.48961000	-2.89727900
H	2.94972600	0.71909600	-2.28805000
H	4.30654600	0.18256200	-1.27898800
C	4.47701900	-2.34788600	0.15274200
H	4.41198600	-2.86945800	1.11125200
H	5.20553300	-2.88474000	-0.46668800
H	4.87671100	-1.34923100	0.33558200

C	2.10423200	-4.50167400	0.34202000
H	2.41291300	-5.37006000	-0.25348700
H	2.77575600	-4.42818700	1.19985100
H	1.09638200	-4.70326200	0.71432500
C	2.43297100	-0.23852300	1.73094300
H	3.08684600	-1.01371900	2.13931100
H	1.74111100	0.02169700	2.53177400
C	-1.70043600	2.06401100	0.03038800
C	-2.82112100	2.81206700	-0.34487900
C	-2.98021800	4.07891000	0.22570700
C	-2.05349100	4.60857900	1.13104300
C	-0.91175500	3.87408500	1.45997500
C	-0.74807300	2.61216900	0.89924200
H	-3.54869600	2.43787200	-1.05132400
H	-3.85418500	4.66313900	-0.04566200
H	-2.21463700	5.59095000	1.56185700
H	-0.15918800	4.28088800	2.12993000
C	-0.72089200	-0.10679700	3.03576800
C	-1.07199600	-0.97195200	4.06621100
C	-1.36404200	-2.31624100	3.79997000
C	-1.34101800	-2.77024800	2.48584400
C	-1.00930700	-1.90049400	1.43803000
C	-0.65917400	-0.55092800	1.69573700
H	-0.52293900	0.93177300	3.27747100
H	-1.12611100	-0.59723700	5.08408100
H	-1.62872700	-2.98797500	4.61053500
H	-1.60501600	-3.79852000	2.25717000

H	-1.10132400	-2.24090600	0.41498900
N	-1.28397800	0.76791500	-0.35790600
S	-2.15053700	-0.09758900	-1.51727200
O	-2.16659800	0.70148500	-2.74585100
O	-1.59286300	-1.45157100	-1.53225500
C	-4.07528300	-0.44039800	0.45693300
C	-5.39487900	-0.52903300	0.89058000
C	-6.46768300	-0.35468900	0.00239600
C	-6.18320800	-0.07480600	-1.34204600
C	-4.86991400	0.02437600	-1.79663100
C	-3.82535500	-0.16327800	-0.88860600
H	-3.25947900	-0.56313000	1.15897200
H	-5.59621300	-0.73147100	1.93877200
H	-7.00017600	0.07303700	-2.04254700
H	-4.65179100	0.25761300	-2.83298400
C	-0.15281500	0.30002900	0.54257700
C	0.41081500	1.66589800	0.97341900
C	-7.89225500	-0.48646700	0.47935300
H	-8.22790000	-1.52767100	0.40113100
H	-7.99457100	-0.18827100	1.52651500
H	-8.57470100	0.12225300	-0.12001900
H	0.87626400	1.64355200	1.95040700

Zero-point correction= 0.711604 (Hartree/Particle)

Thermal correction to Energy= 0.754584

Thermal correction to Enthalpy= 0.755528

Thermal correction to Gibbs Free Energy= 0.636398

Sum of electronic and zero-point Energies= -2353.289075

Sum of electronic and thermal Energies= -2353.246095

Sum of electronic and thermal Enthalpies= -2353.245151

Sum of electronic and thermal Free Energies= -2353.364281

E(RB3LYP) = -2354.000679 A.U.

C-11

0 1

Number of imaginary frequencies: 0

Rh	-1.62709600	-0.32914200	-0.69557700
C	-1.14320100	-2.10967100	-1.97195600
C	-2.19108600	-2.43933400	-1.04461500
C	-3.29930400	-1.56732400	-1.32366500
C	-2.91900800	-0.66319500	-2.39123100
C	-1.57467100	-1.00770700	-2.79762100
C	0.15046600	-2.83728300	-2.11175200
H	0.46044700	-3.29539800	-1.17262300
H	0.01969800	-3.64190800	-2.84694900
H	0.95372800	-2.19112000	-2.46417800
C	-2.16714600	-3.50584400	0.00460100
H	-2.67878000	-4.40883700	-0.35012300
H	-1.14646500	-3.77416900	0.28040900
H	-2.66871400	-3.15999100	0.91087000
C	-4.62508400	-1.59702400	-0.64063000
H	-5.26626800	-2.33419200	-1.14073600
H	-4.52755400	-1.87828800	0.40859000
H	-5.11387100	-0.62360500	-0.68171100
C	-3.80627400	0.37473400	-2.99477800
H	-4.49835500	-0.09754500	-3.70413800

H	-4.39083000	0.86970200	-2.21502200
H	-3.21493000	1.13561600	-3.50100000
C	-0.84532200	-0.43460900	-3.97108200
H	-1.33475800	-0.75482500	-4.89930200
H	-0.86501000	0.65496100	-3.91538600
H	0.18975600	-0.78079000	-4.00658800
C	1.30279000	-2.16234400	1.11378500
C	1.52708900	-3.50404400	1.44575700
C	0.73602400	-4.05081400	2.45673500
C	-0.26357000	-3.30396600	3.10723500
C	-0.50130100	-1.98067000	2.75627300
C	0.29216700	-1.40515900	1.75491500
H	2.28567700	-4.09005100	0.94798300
H	0.89886000	-5.08604500	2.74160500
H	-0.86206400	-3.77257400	3.88251000
H	-1.28786300	-1.39123700	3.21344500
C	1.71533000	1.30910000	-1.88757800
C	2.13055000	2.49760900	-2.48316600
C	2.58452400	3.55856000	-1.69545000
C	2.60342800	3.43300300	-0.30456900
C	2.17452900	2.24918000	0.29341600
C	1.74226800	1.17083000	-0.49427000
H	1.35165600	0.49450800	-2.49603800
H	2.07987500	2.60059900	-3.56228600
H	2.90629000	4.48430600	-2.16340900
H	2.94524400	4.25661900	0.31511800
H	2.18801200	2.14390100	1.37338000

N	1.89288900	-1.31672000	0.13606100
S	3.35599100	-1.64334700	-0.73270000
O	3.70011400	-3.02431600	-0.40460400
O	3.13635900	-1.23371400	-2.11844900
C	4.95088000	0.59642200	-0.65992200
C	5.83646400	1.46551500	-0.02671500
C	6.29231400	1.21638100	1.27458900
C	5.84164700	0.06325200	1.93900700
C	4.96158000	-0.82136900	1.32547900
C	4.52403700	-0.53808100	0.02850400
H	4.57248600	0.80371000	-1.65375100
H	6.16480000	2.35921000	-0.54915100
H	6.18536400	-0.14095200	2.94917900
H	4.61653100	-1.71307100	1.83849600
C	1.27554300	-0.04505500	0.20107800
C	0.28613700	-0.09301400	1.16227500
C	7.26681800	2.15280700	1.94490600
H	8.29669100	1.80110100	1.80762100
H	7.20609700	3.16167000	1.52758300
H	7.08542000	2.21500200	3.02201300
H	-0.28697000	0.76311200	1.47975300
O	-1.43980800	2.34367100	-2.69971700
C	-1.33045100	2.56237800	-1.49301700
O	-1.27637200	1.66396700	-0.54655900
C	-1.21473200	3.97145600	-0.93325200
H	-1.34312500	4.70640700	-1.72874100
H	-1.96523300	4.11058300	-0.15142300

H	-0.22959600	4.09144200	-0.47295200
S	-3.72108100	0.79388500	1.59523100
O	-2.56506900	-0.15572200	1.27834300
O	-4.19584300	1.55324100	0.42901900
C	-2.84928000	2.01228200	2.70205300
O	-4.71451300	0.14863400	2.46007900
F	-1.87943100	2.66729400	2.04325400
F	-2.27948500	1.35205000	3.72600500
F	-3.71437200	2.90664500	3.18941600

Zero-point correction= 0.635606 (Hartree/Particle)

Thermal correction to Energy= 0.685109

Thermal correction to Enthalpy= 0.686053

Thermal correction to Gibbs Free Energy= 0.548003

Sum of electronic and zero-point Energies= -3102.894723

Sum of electronic and thermal Energies= -3102.845220

Sum of electronic and thermal Enthalpies= -3102.844276

Sum of electronic and thermal Free Energies= -3102.982326

E(RB3LYP) = -3103.530329 A.U.

C-12

1 1

Number of imaginary frequencies: 0

Rh	-2.15319900	-0.33497800	-0.15880700
C	-2.26347700	1.01899100	1.64090900
C	-3.09516700	1.53705500	0.57561000
C	-4.10599500	0.54972300	0.28803500
C	-3.87210300	-0.59767800	1.12918700
C	-2.72516400	-0.29879300	1.96598000

C	-1.19827700	1.77551000	2.35950400
H	-0.69202900	2.48767100	1.70850900
H	-1.66430500	2.34885300	3.17076400
H	-0.45010000	1.11738100	2.79976300
C	-3.02041900	2.91301600	-0.00086300
H	-3.70723400	3.57634300	0.53876700
H	-2.01533500	3.32693400	0.07714900
H	-3.29884400	2.92287600	-1.05577100
C	-5.18150200	0.65446400	-0.74281600
H	-6.15173400	0.79657800	-0.25276100
H	-5.01143600	1.49626800	-1.41487400
H	-5.23213700	-0.25738900	-1.34371100
C	-4.68828200	-1.84886700	1.18107500
H	-5.41550900	-1.79241200	1.99979200
H	-5.23925300	-2.00085600	0.25097400
H	-4.05363800	-2.72165400	1.35021200
C	-2.16544800	-1.21434900	3.00574200
H	-2.83489800	-1.24198700	3.87379500
H	-2.07749000	-2.23364200	2.62000600
H	-1.18346000	-0.88399600	3.34745100
C	0.59534400	2.20044900	-0.58676400
C	0.81091200	3.57464600	-0.42658100
C	0.21630800	4.42634600	-1.35797200
C	-0.58028200	3.93947000	-2.40920200
C	-0.81557800	2.57568100	-2.54394700
C	-0.22651600	1.70126600	-1.62325200
H	1.42097200	3.96333600	0.37530400

H	0.38257000	5.49493600	-1.26601400
H	-1.01607800	4.63651100	-3.11771500
H	-1.43704500	2.18599900	-3.34436600
C	0.95534100	-2.17297200	0.97865900
C	1.49379100	-3.45031900	1.10937900
C	2.21865700	-4.02067500	0.05909300
C	2.39204200	-3.31294300	-1.13160200
C	1.84812300	-2.03620800	-1.26834600
C	1.14084600	-1.45006600	-0.20642700
H	0.38963700	-1.73388700	1.78740500
H	1.34224700	-4.00455300	2.03037000
H	2.63957100	-5.01570400	0.16684700
H	2.95158800	-3.75043700	-1.95252300
H	1.99366300	-1.47731200	-2.18769200
N	1.07037300	1.07659800	0.14476600
S	2.22502500	1.13574500	1.48138000
O	2.31985400	2.55279500	1.80920700
O	1.75034600	0.16153500	2.45938300
C	4.15966600	-0.73446000	0.94239500
C	5.33199300	-1.15395700	0.31914800
C	6.06725200	-0.29052700	-0.50568300
C	5.60002800	1.02165700	-0.69724800
C	4.43475700	1.46675400	-0.08462900
C	3.72571600	0.57465400	0.72768000
H	3.58784400	-1.40619000	1.57086500
H	5.67840700	-2.17103900	0.47562000
H	6.16216700	1.70225000	-1.33000200

H	4.08479800	2.48411000	-0.22328300
C	0.59311100	-0.09445500	-0.43830300
C	-0.26458800	0.26031000	-1.49214300
C	7.35103400	-0.74408300	-1.15226600
H	8.21286000	-0.41992100	-0.55666000
H	7.39891000	-1.83290100	-1.23466800
H	7.46836300	-0.31570300	-2.15188200
H	-0.53421800	-0.42141700	-2.28629900
O	-1.69892900	-2.44058200	-0.50105800
C	-2.23386100	-2.40670000	-1.65729000
O	-2.73599300	-1.29798500	-2.04798500
C	-2.22584300	-3.61848200	-2.54051200
H	-2.55686300	-4.49173600	-1.97299400
H	-2.86082600	-3.46599400	-3.41351200
H	-1.19693100	-3.80830300	-2.86368300

Zero-point correction= 0.606539 (Hartree/Particle)

Thermal correction to Energy= 0.647311

Thermal correction to Enthalpy= 0.648255

Thermal correction to Gibbs Free Energy= 0.530901

Sum of electronic and zero-point Energies= -2141.284096

Sum of electronic and thermal Energies= -2141.243324

Sum of electronic and thermal Enthalpies= -2141.242380

Sum of electronic and thermal Free Energies= -2141.359734

E(RB3LYP) = -2141.890635 A.U.

C-13

1 1

Number of imaginary frequencies: 0

Rh	1.95849800	-0.07064500	-0.29696800
C	3.41680900	-1.57715400	0.28259500
C	3.32642000	-1.51922600	-1.14635800
C	3.77690200	-0.19159900	-1.56252700
C	4.19953000	0.53205500	-0.40098200
C	3.93704500	-0.28843900	0.73557400
C	3.13043300	-2.76612600	1.14448600
H	2.28490900	-3.34138700	0.76038600
H	4.00592900	-3.42552000	1.18219600
H	2.89185200	-2.46806800	2.16713800
C	2.98932000	-2.64271100	-2.07480000
H	3.90936700	-3.04027100	-2.52064200
H	2.49414400	-3.45918800	-1.54833200
H	2.33988500	-2.31249000	-2.88850400
C	3.86704000	0.26579500	-2.98205900
H	4.82882400	-0.04228500	-3.41160200
H	3.07575500	-0.17535100	-3.59210900
H	3.79946300	1.35236900	-3.06236200
C	4.76608900	1.91826500	-0.36040800
H	5.83827800	1.88585100	-0.13669400
H	4.64015000	2.43128000	-1.31516000
H	4.27985800	2.52574200	0.40800700
C	4.17865700	0.09223000	2.15979800
H	5.18458100	-0.22275700	2.46499900
H	4.11071800	1.17302400	2.30021700
H	3.46388200	-0.38905800	2.83095200
C	-1.67211000	-1.61785200	1.03272000

C	-2.57780000	-2.55276000	1.53014300
C	-2.42343700	-3.87545200	1.10925800
C	-1.39705000	-4.25740700	0.22931400
C	-0.49048400	-3.31753700	-0.25183700
C	-0.62558900	-1.98082500	0.14621800
H	-3.35343500	-2.26992300	2.22962200
H	-3.11154700	-4.62724300	1.48267000
H	-1.31157000	-5.29634700	-0.07260700
H	0.29693300	-3.60230900	-0.94158300
C	0.34798200	2.35741100	1.70714700
C	1.12825700	3.49753100	1.63867400
C	1.71467900	3.90942700	0.42259800
C	1.49343800	3.18083500	-0.73310300
C	0.70264900	2.01085200	-0.69342500
C	0.13192400	1.58093700	0.54274100
H	-0.09766700	2.04281300	2.64178900
H	1.29491100	4.08255200	2.53793200
H	2.31306800	4.81454900	0.39243700
H	1.90036800	3.51277600	-1.68307200
H	0.36045000	1.56187500	-1.62055300
N	-1.56677100	-0.21977100	1.30266600
S	-2.99240000	0.75060500	1.68557500
O	-3.70288000	-0.00737500	2.70652800
O	-2.47402400	2.09358000	1.91771000
C	-3.58257500	1.65992500	-0.82845400
C	-4.26344300	1.60552300	-2.04071500
C	-5.23996600	0.62547500	-2.28321600

C	-5.52899000	-0.30193500	-1.27049100
C	-4.86097600	-0.26913500	-0.04943100
C	-3.89119600	0.71508200	0.15456800
H	-2.84753600	2.43306100	-0.63167400
H	-4.04579000	2.34362600	-2.80732900
H	-6.29408100	-1.05451400	-1.43706100
H	-5.09711500	-0.97535900	0.73777300
C	-0.50327100	0.25874700	0.54325100
C	0.13066600	-0.78695300	-0.14092000
C	-5.95232600	0.56035300	-3.61044400
H	-6.96991600	0.17602500	-3.50017400
H	-6.00570200	1.54297300	-4.08670200
H	-5.42213600	-0.11034600	-4.29765300

Zero-point correction= 0.541629 (Hartree/Particle)

Thermal correction to Energy= 0.577390

Thermal correction to Enthalpy= 0.578334

Thermal correction to Gibbs Free Energy= 0.470129

Sum of electronic and zero-point Energies= -1912.190395

Sum of electronic and thermal Energies= -1912.154633

Sum of electronic and thermal Enthalpies= -1912.153689

Sum of electronic and thermal Free Energies= -1912.261895

E(RB3LYP) = -1912.732024 A.U.

C-TSa2

1 1

Number of imaginary frequencies: 1

Rh	1.36254800	0.34139100	0.72872700
C	1.53631200	2.26802100	1.90297600

C	0.47574800	1.50098600	2.49293000
C	1.04197300	0.26491800	2.92951700
C	2.50082000	0.34104600	2.74902700
C	2.79531400	1.57645000	2.15291500
C	1.35921100	-2.75053700	0.97854700
C	2.59632400	-1.99380300	-0.84136000
C	2.92103300	-3.33323300	-1.21724800
C	2.44323500	-4.38765600	-0.40087000
C	1.66845900	-4.09579800	0.69680400
H	0.69659200	-2.50547500	1.79605600
C	3.05409100	-0.89983300	-1.62630900
C	3.67806100	-3.55445600	-2.39672200
H	2.68258500	-5.41463000	-0.66120600
H	1.26905400	-4.87486900	1.33586600
C	4.07653300	-2.48956200	-3.17264000
C	3.75751500	-1.16673600	-2.78938900
H	3.92102900	-4.57359000	-2.68183900
H	4.64201500	-2.65834400	-4.08326400
H	4.08888200	-0.33974100	-3.41122100
N	1.80259300	-1.73419800	0.24991800
C	1.44693800	3.67393400	1.39617100
H	0.41549500	4.01946100	1.35749500
H	2.01029900	4.34272000	2.05755700
H	1.86381300	3.77167100	0.38978100
C	-0.94678200	1.93539500	2.64371600
H	-0.99711500	2.88387700	3.18878800
H	-1.41491100	2.07342100	1.66331400

H	-1.52866100	1.19589400	3.19842800
C	0.33583200	-0.78291500	3.73743200
H	0.15277700	-0.41070000	4.75260100
H	-0.63054300	-1.05308600	3.30580000
H	0.93489300	-1.69062200	3.83279700
C	3.46546700	-0.71644200	3.18724300
H	4.45161000	-0.57382500	2.74077600
H	3.58449200	-0.69938100	4.27707600
H	3.11398300	-1.71486600	2.91126600
C	4.14000700	2.12378100	1.78998800
H	4.49309800	2.81248100	2.56667100
H	4.89033900	1.33661400	1.68254100
H	4.09912000	2.69191900	0.85543700
C	-1.54535700	-1.44558400	0.52587200
C	-2.04569200	-2.73920100	0.63103000
C	-1.88694000	-3.63645000	-0.42937400
C	-1.24199100	-3.21726700	-1.59455400
C	-0.74887600	-1.91525000	-1.70162500
C	-0.88122400	-1.01709700	-0.63603000
H	-2.56835400	-3.04297300	1.53286500
H	-2.27251600	-4.64845300	-0.35270900
H	-1.13009200	-3.90122400	-2.43043900
H	-0.27515900	-1.59837000	-2.62388700
C	1.32650300	3.22642100	-2.39822200
C	0.91933300	4.56112200	-2.32415700
C	-0.21764400	4.91828600	-1.58937000
C	-0.98052300	3.95357600	-0.92758200

C	-0.57735400	2.62405900	-1.02641800
C	0.57249600	2.25583400	-1.73860400
H	2.20932000	2.95988500	-2.97172800
H	1.49008600	5.32659400	-2.83995500
H	-0.51795000	5.95983800	-1.53725000
H	-1.87433700	4.22146900	-0.38065700
H	-1.67089700	-0.74359900	1.34185100
N	-1.24237300	1.47157600	-0.47816900
H	0.96879400	0.18896000	-2.45987100
S	-2.79137000	1.29329900	-1.45315100
O	-2.43600000	0.66151500	-2.72773300
O	-3.39923900	2.62274600	-1.40237100
C	-4.21375700	0.57692600	0.78351000
C	-5.06322800	-0.26543600	1.49276200
C	-5.55314200	-1.45191300	0.92026600
C	-5.16471700	-1.77831800	-0.38664800
C	-4.29864500	-0.96058400	-1.10778500
C	-3.82497900	0.20267000	-0.50456900
H	-3.85562100	1.50329500	1.21894300
H	-5.36605200	0.00594200	2.50027200
H	-5.53638600	-2.69098000	-0.84320000
H	-3.97065900	-1.22502000	-2.10613700
C	0.77158600	0.79694600	-1.58272300
C	-0.30000400	0.35474700	-0.66767800
C	-6.50707700	-2.33536900	1.68456900
H	-6.32307500	-2.28992200	2.76182500
H	-7.54267300	-2.01570500	1.51745300

H	-6.43268300	-3.37856900	1.36519500
C	2.74156900	0.48569200	-1.19549400
H	3.33631800	0.79986200	-0.33653400
H	2.94215800	1.21469800	-1.97387600

Zero-point correction= 0.708797 (Hartree/Particle)

Thermal correction to Energy= 0.751908

Thermal correction to Enthalpy= 0.752852

Thermal correction to Gibbs Free Energy= 0.634823

Sum of electronic and zero-point Energies= -2353.303730

Sum of electronic and thermal Energies= -2353.260619

Sum of electronic and thermal Enthalpies= -2353.259675

Sum of electronic and thermal Free Energies= -2353.377704

E(RB3LYP) = -2354.012527 A.U.

C-TSb2

1 1

Number of imaginary frequencies: 1

Rh	-0.65565400	-1.25699500	0.29755600
C	1.22502300	-2.49980800	0.07678300
C	0.51183500	-3.03363200	1.19918000
C	-0.77054000	-3.44658500	0.73728700
C	-0.78880200	-3.32706300	-0.72684300
C	0.44244900	-2.78277200	-1.12593400
C	-3.69034400	-1.46886400	0.76784000
C	-3.09011900	-0.08412300	-1.01347900
C	-4.45825300	0.05872000	-1.40051100
C	-5.43662100	-0.65101600	-0.66122100
C	-5.05682000	-1.40026100	0.42983600

H	-3.36385300	-2.02725300	1.63654700
C	-2.07036900	0.67631600	-1.65007400
C	-4.78378800	0.94567200	-2.45798300
H	-6.48191600	-0.56911100	-0.94507700
H	-5.78235300	-1.92641900	1.03994200
C	-3.79467700	1.69711200	-3.05308000
C	-2.45155200	1.57897900	-2.63226200
H	-5.82127400	1.04562800	-2.76214100
H	-4.04456100	2.39957600	-3.84162700
H	-1.69469000	2.21219900	-3.08570500
N	-2.74023100	-0.86565500	0.06214100
C	2.64599900	-2.02965900	0.11158900
H	2.83301000	-1.39665200	0.98157000
H	3.32795300	-2.88760100	0.16708400
H	2.90370500	-1.46049600	-0.77968100
C	1.06501600	-3.26415100	2.56537500
H	1.48991200	-4.27549300	2.60875800
H	1.85632800	-2.55804400	2.81254900
H	0.29581100	-3.19807100	3.33766600
C	-1.78457400	-4.18999700	1.55214300
H	-1.47976600	-5.23919400	1.65387000
H	-1.87544200	-3.77854400	2.56124200
H	-2.76997700	-4.18538000	1.08274300
C	-1.92283700	-3.76515500	-1.60164800
H	-1.85966800	-3.32192600	-2.59759200
H	-1.92110000	-4.85538000	-1.71922500
H	-2.88770500	-3.48396900	-1.17032800

C	0.88447000	-2.51496300	-2.53043800
H	1.43371000	-3.37845800	-2.92451700
H	0.03724700	-2.33129200	-3.19632900
H	1.55606700	-1.65655200	-2.58273300
C	-0.65597300	0.57103400	-1.21501900
H	-0.10247000	-0.25781800	-1.66388000
H	-0.11398200	1.46803400	-1.48772700
C	1.71740300	0.99521200	1.97316200
C	2.97340700	1.15060200	2.55446700
C	3.20888400	0.50720800	3.77580200
C	2.21197100	-0.23963900	4.41130300
C	0.95508100	-0.38069600	3.81849500
C	0.71754300	0.21324900	2.57971700
H	3.71464400	1.81551600	2.13579200
H	4.17417500	0.63381600	4.25554300
H	2.40875100	-0.69208900	5.37784200
H	0.16570400	-0.93640100	4.31453500
C	-2.58666600	2.29786700	0.93163900
C	-3.48517200	3.35901800	0.97341400
C	-3.02581000	4.67275600	0.86633100
C	-1.65649600	4.90502500	0.74992300
C	-0.75558900	3.84159000	0.69738000
C	-1.20697000	2.51286200	0.75180200
H	-2.96634600	1.29590300	1.06215700
H	-4.54387000	3.15630200	1.10381800
H	-3.72336400	5.50381300	0.90094200
H	-1.27531700	5.92049100	0.70943600

H	0.29724500	4.07330400	0.65490500
N	1.15614500	1.61365100	0.81640400
S	2.13123400	2.49087300	-0.31597500
O	1.20971300	3.01719700	-1.32348200
O	2.97342000	3.36871500	0.48978000
C	4.43232800	0.97750100	-0.59171900
C	5.26893900	0.11108600	-1.29036800
C	4.89505400	-0.41703700	-2.53533900
C	3.64993200	-0.04905500	-3.06847200
C	2.79148500	0.80393300	-2.37836900
C	3.18444900	1.29909100	-1.13194600
H	4.75628600	1.41320800	0.34366200
H	6.23712100	-0.14469600	-0.86987300
H	3.35389500	-0.42565800	-4.04356000
H	1.84457200	1.10448100	-2.81054800
C	-0.26042500	1.34560700	0.76494900
C	-0.50216900	0.28166600	1.76909500
C	5.82952300	-1.31758200	-3.30199200
H	6.53067800	-0.72139200	-3.89805700
H	6.42405100	-1.94275200	-2.62999100
H	5.28620200	-1.96963900	-3.99114900
H	-1.44855700	0.32526200	2.29960800

Zero-point correction= 0.709431 (Hartree/Particle)

Thermal correction to Energy= 0.752444

Thermal correction to Enthalpy= 0.753388

Thermal correction to Gibbs Free Energy= 0.635652

Sum of electronic and zero-point Energies= -2353.301437

Sum of electronic and thermal Energies= -2353.258424

Sum of electronic and thermal Enthalpies= -2353.257480

Sum of electronic and thermal Free Energies= -2353.375216

E(RB3LYP) = -2354.010868 A.U.

C-TSc2

1 1

Number of imaginary frequencies: 1

Rh	-2.13285600	-0.94145600	0.07461900
C	-3.90986200	-1.83473900	1.35538600
C	-3.71691400	-0.47695000	1.67489900
C	-3.86187300	0.30522700	0.44916000
C	-4.24424300	-0.60982500	-0.61134900
C	-4.20768400	-1.92295600	-0.07328200
C	-0.51989400	2.72561500	1.44944400
C	-0.91481600	2.30025500	-0.82385900
C	-1.21443100	3.69809000	-1.01284000
C	-1.19580600	4.56553300	0.10515800
C	-0.94081400	4.06299800	1.35849100
H	-0.19370900	2.32904000	2.40274600
C	-1.26581600	1.36531500	-1.85352700
C	-1.62828800	4.17842200	-2.27997700
H	-1.43457600	5.61539200	-0.03888400
H	-0.98993200	4.67353200	2.25239400
C	-1.84445700	3.28753600	-3.30213200
C	-1.70591400	1.90649700	-3.06065600
H	-1.80911400	5.24139400	-2.40618100
H	-2.17188900	3.63217200	-4.27774900

H	-1.97475400	1.21483600	-3.85348100
N	-0.41986000	1.91559500	0.40689700
C	-3.89179200	-2.99598400	2.30320500
H	-3.23402900	-2.81324300	3.15728100
H	-4.89604500	-3.18980500	2.69935400
H	-3.56034800	-3.91355300	1.80989300
C	-3.41639600	0.10516800	3.02135700
H	-4.33444400	0.46893500	3.49824400
H	-2.96642300	-0.63161300	3.69133800
H	-2.73157100	0.95360500	2.93727900
C	-3.95441900	1.79705300	0.38032000
H	-4.97098000	2.12155000	0.63719100
H	-3.26727300	2.27768400	1.07942800
H	-3.73015100	2.16514400	-0.62181100
C	-4.66064200	-0.21090500	-1.99285800
H	-4.48612400	-1.01238700	-2.71438900
H	-5.73037600	0.02904200	-2.01274600
H	-4.11516200	0.67213200	-2.33361000
C	-4.51320700	-3.19513800	-0.80134900
H	-5.54550500	-3.50997900	-0.60304600
H	-4.40120700	-3.07693500	-1.88071100
H	-3.85412000	-4.00621800	-0.48145500
C	-1.31542500	-0.12069200	-1.70030500
H	-1.95556700	-0.52151600	-2.49216400
H	-0.33775000	-0.55757200	-1.86734200
C	0.96655500	-1.61131500	-0.43174000
C	1.38383700	-2.55191300	-1.35405300

C	0.82204700	-3.84006000	-1.26956100
C	-0.13524200	-4.15899900	-0.30948200
C	-0.56731000	-3.19475500	0.61551100
C	-0.00390600	-1.90695500	0.55979700
H	2.10275600	-2.31490000	-2.12539600
H	1.14875700	-4.59745300	-1.97463600
H	-0.53878500	-5.16510100	-0.26115900
H	-1.26432700	-3.45326700	1.40447400
C	1.97278900	0.00849000	2.92897800
C	2.94530300	0.35225200	3.86994400
C	3.58018300	1.59138200	3.80256500
C	3.23953800	2.48098300	2.78041500
C	2.28124300	2.13551400	1.82941000
C	1.62578400	0.89361200	1.89340400
H	1.50851400	-0.96929400	2.98616200
H	3.20071200	-0.35330300	4.65439400
H	4.33138900	1.86341400	4.53751900
H	3.72742000	3.44833500	2.71310900
H	2.05403900	2.82603100	1.03144700
N	1.32740400	-0.24541800	-0.27660100
S	2.39064300	0.55805300	-1.40035500
O	1.95977800	0.11309700	-2.72253100
O	2.34215200	1.96611900	-1.02298600
C	4.60272600	0.04860400	0.17851500
C	5.84689200	-0.52792800	0.40842100
C	6.48862500	-1.29951800	-0.57444100
C	5.84511200	-1.48333200	-1.80633800

C	4.59590300	-0.92078900	-2.05878500
C	3.98369500	-0.16341900	-1.05707200
H	4.13016600	0.64958800	0.94415400
H	6.33125900	-0.37370700	1.36839300
H	6.32742100	-2.07304700	-2.58037400
H	4.10420000	-1.05679200	-3.01537500
C	0.67786100	0.32216200	0.84918700
C	-0.33602100	-0.67233000	1.26070000
C	7.85307800	-1.88714000	-0.31864400
H	8.63418600	-1.15172000	-0.54627400
H	7.97428600	-2.17700500	0.72896900
H	8.03721500	-2.76519500	-0.94311300
H	-0.63417500	-0.65690300	2.30390800

Zero-point correction= 0.708650 (Hartree/Particle)

Thermal correction to Energy= 0.751736

Thermal correction to Enthalpy= 0.752681

Thermal correction to Gibbs Free Energy= 0.633510

Sum of electronic and zero-point Energies= -2353.270502

Sum of electronic and thermal Energies= -2353.227416

Sum of electronic and thermal Enthalpies= -2353.226472

Sum of electronic and thermal Free Energies= -2353.345643

E(RB3LYP) = -2353.979153 A.U.

C-TSd2

1 1

Number of imaginary frequencies: 1

Rh	1.48232200	-0.82925600	-0.14853400
C	1.50948500	-2.80669800	-1.04394600

C	1.30087200	-1.97821900	-2.22736000
C	2.38518700	-1.09383200	-2.30109800
C	3.36511900	-1.44180000	-1.26061000
C	2.86208200	-2.54044300	-0.54079100
C	1.94472100	2.55120300	-0.72370700
C	2.98412000	1.44061600	1.09375000
C	4.16408600	2.22794600	0.88889400
C	4.19361600	3.14439900	-0.18758600
C	3.11262900	3.25237600	-1.03782500
H	1.03477800	2.70208300	-1.29040800
C	3.01227200	0.30870400	1.96792200
C	5.30860900	1.99741200	1.69585800
H	5.09033500	3.73457800	-0.35370200
H	3.12093300	3.90886400	-1.89968700
C	5.30000800	0.96710700	2.60613100
C	4.17603800	0.11866700	2.70716500
H	6.18868800	2.61522500	1.54921800
H	6.17350700	0.77152600	3.21985900
H	4.22450700	-0.74187400	3.36768400
N	1.85763100	1.71950800	0.31742400
C	0.65686900	-3.97435400	-0.66627300
H	-0.40076300	-3.73117000	-0.77333600
H	0.88253600	-4.82214500	-1.32657500
H	0.84554200	-4.29643100	0.36024700
C	0.21858400	-2.12445700	-3.25135300
H	0.63973200	-2.58806500	-4.15221400
H	-0.59560100	-2.74885500	-2.89151000

H	-0.21461100	-1.16450300	-3.53963200
C	2.57718900	-0.01361000	-3.31820200
H	3.25038800	-0.35374400	-4.11514500
H	1.62906700	0.27131300	-3.77902600
H	3.03026000	0.87826600	-2.87481500
C	4.69790600	-0.78013200	-1.08449200
H	5.06266700	-0.87904000	-0.05954700
H	5.44455800	-1.22498800	-1.75352200
H	4.64597500	0.28672100	-1.31795900
C	3.56641100	-3.31369300	0.52921100
H	4.14037800	-4.13533900	0.08464800
H	4.26405200	-2.68423600	1.08788300
H	2.86089100	-3.75112900	1.23904700
C	1.93467200	-0.72729700	1.92231700
H	2.31732100	-1.67905100	2.29464900
H	1.06575600	-0.47505500	2.52906200
C	-1.41325200	1.88593300	-0.67562000
C	-2.19168900	2.69298400	-1.51974700
C	-2.21435700	4.06384400	-1.27094600
C	-1.47114600	4.65002200	-0.23077600
C	-0.64826100	3.85502400	0.56044000
C	-0.61579800	2.47680600	0.32496000
H	-2.74402000	2.26468700	-2.34385500
H	-2.82681500	4.69733300	-1.90558900
H	-1.52778800	5.71974500	-0.06091900
H	-0.02945200	4.29137400	1.33966100
C	-2.02373900	0.26248700	2.39324300

C	-2.78810500	-0.29663900	3.41897700
C	-2.71930300	-1.66597700	3.67713200
C	-1.87926500	-2.46961500	2.90135100
C	-1.10904700	-1.90451200	1.88517300
C	-1.16454300	-0.53149700	1.61497600
H	-2.11575900	1.32524100	2.19109100
H	-3.44250400	0.33861300	4.00828000
H	-3.31362800	-2.10394200	4.47337000
H	-1.82235100	-3.53801200	3.08805200
H	-0.45500000	-2.52155800	1.28538000
N	-1.24509300	0.50214600	-0.65479900
S	-2.32760900	-0.56493900	-1.43420300
O	-2.37599400	-0.10852800	-2.82683900
O	-1.86496800	-1.90274300	-1.06785800
C	-4.29255500	-1.00939100	0.43784400
C	-5.55685700	-0.81443300	0.98445400
C	-6.48506400	0.05070800	0.38615700
C	-6.11659600	0.71520900	-0.79317800
C	-4.85693400	0.53528000	-1.35798100
C	-3.94645100	-0.31583500	-0.72452900
H	-3.59163500	-1.69282200	0.89915600
H	-5.82615000	-1.34699800	1.89195200
H	-6.82926100	1.37336300	-1.28201600
H	-4.59614700	1.01714600	-2.29187900
C	-0.34268300	0.08862000	0.48235500
C	0.23107600	1.43467400	0.91896700
C	-7.86349600	0.22683300	0.97177500

H	-8.55384800	-0.51834000	0.55827700
H	-7.85743400	0.09822200	2.05777300
H	-8.27424800	1.21429300	0.74382000
H	0.46785200	1.51630600	1.97452300

Zero-point correction= 0.709641 (Hartree/Particle)

Thermal correction to Energy= 0.752293

Thermal correction to Enthalpy= 0.753237

Thermal correction to Gibbs Free Energy= 0.636353

Sum of electronic and zero-point Energies= -2353.276712

Sum of electronic and thermal Energies= -2353.234060

Sum of electronic and thermal Enthalpies= -2353.233116

Sum of electronic and thermal Free Energies= -2353.350001

E(RB3LYP) = -2353.986353 A.U.

C-TSa11

1 1

Number of imaginary frequencies: 1

Rh	2.10928700	-0.39318400	0.26769600
C	2.65540600	0.31489400	-1.73276500
C	3.61005200	0.74490900	-0.72623000
C	4.32005200	-0.43998600	-0.22133600
C	3.74086700	-1.56906800	-0.82156600
C	2.68704000	-1.10801800	-1.74224300
C	1.82136500	1.21359600	-2.59128600
H	1.52502000	2.11344000	-2.04864300
H	2.38817600	1.51941600	-3.47789700
H	0.91125200	0.71237100	-2.92463200
C	3.97049900	2.15576400	-0.41010200

H	4.73194200	2.49942600	-1.12282400
H	3.10754000	2.81906800	-0.48744400
H	4.38934500	2.24467400	0.59439600
C	5.40457200	-0.39206000	0.80591400
H	5.68793300	-1.39053600	1.14045400
H	6.29401000	0.09764600	0.39373600
H	5.08356900	0.17903700	1.68219600
C	4.08426000	-3.00755500	-0.60526700
H	3.18235400	-3.62443500	-0.56568400
H	4.69661300	-3.37700200	-1.43699100
H	4.64283000	-3.15738000	0.31973200
C	1.88684200	-2.02999300	-2.60013400
H	1.35952400	-2.77675700	-1.99911600
H	1.14544800	-1.49582300	-3.19078800
H	2.55804100	-2.56504400	-3.28253400
C	-0.82734100	2.62590400	-0.25199200
C	-1.10091300	3.99174800	-0.36139500
C	-0.27630800	4.86307100	0.34901000
C	0.78569800	4.39324600	1.14132400
C	1.05812000	3.03073300	1.22795900
C	0.25197000	2.13610200	0.51374900
H	-1.92124400	4.36011000	-0.96072800
H	-0.46364600	5.93013000	0.28604900
H	1.39975400	5.10315900	1.68671800
H	1.88321800	2.65847500	1.82816600
C	-1.44239900	-1.26726000	-2.28004600
C	-1.66310300	-2.57961900	-2.69614900

C	-1.52870800	-3.63935000	-1.79555100
C	-1.17248900	-3.38119100	-0.46781800
C	-0.95146200	-2.07304700	-0.04339200
C	-1.08668800	-0.99941600	-0.94704300
H	-1.54801700	-0.45046900	-2.98267500
H	-1.93735600	-2.77353500	-3.72851600
H	-1.70767400	-4.65874300	-2.12331900
H	-1.08634000	-4.19819100	0.24215500
H	-0.72726700	-1.87216600	0.99942600
N	-1.46093200	1.50175100	-0.85568500
S	-3.21768300	1.50655800	-1.26314200
O	-3.66901300	2.84293600	-0.90011500
O	-3.34102200	1.00076100	-2.62501600
C	-4.36969100	-0.88598300	-0.57102300
C	-4.79230900	-1.83333900	0.35860400
C	-4.66882900	-1.60402600	1.73633800
C	-4.11471300	-0.38783300	2.17284100
C	-3.69616500	0.57783500	1.26500000
C	-3.82441100	0.30809700	-0.10098000
H	-4.43956300	-1.06972200	-1.63652500
H	-5.21662800	-2.76901200	0.00683800
H	-4.01244900	-0.19730800	3.23705500
H	-3.27157000	1.51646300	1.60665300
C	-0.77251500	0.35611800	-0.48354000
C	0.28461400	0.68122600	0.38686300
C	-5.14619200	-2.62708800	2.73544100
H	-6.16955100	-2.39854500	3.05646700

H	-5.15373100	-3.63386500	2.30942700
H	-4.51914000	-2.63461900	3.63165900
H	0.09731600	0.12466100	1.57947800
C	1.22911100	-0.61452400	3.13938500
O	0.05129000	-0.28843900	2.79408600
O	2.22292600	-0.66731700	2.33797700
C	1.49012500	-0.93493500	4.58898100
H	0.56633500	-1.23054500	5.08652700
H	2.24942400	-1.71376300	4.67443600
H	1.87450500	-0.03176400	5.07572100

Zero-point correction= 0.600468 (Hartree/Particle)

Thermal correction to Energy= 0.641280

Thermal correction to Enthalpy= 0.642224

Thermal correction to Gibbs Free Energy= 0.523229

Sum of electronic and zero-point Energies= -2141.249406

Sum of electronic and thermal Energies= -2141.208594

Sum of electronic and thermal Enthalpies= -2141.207650

Sum of electronic and thermal Free Energies= -2141.326645

E(RB3LYP) = -2141.849874 A.U.

C-TSb11

1 1

Number of imaginary frequencies: 1

Rh	2.49632400	-0.20413400	0.08909800
C	3.66697700	1.20458200	-1.14475500
C	4.41487200	-0.00463700	-0.86422200
C	3.73991200	-1.11937300	-1.51990400
C	2.54495200	-0.62292100	-2.10259500

C	2.47609700	0.81743800	-1.83974600
C	4.08596700	2.59810000	-0.80674900
H	4.71065200	2.62376200	0.08777900
H	4.66992700	3.01082600	-1.63842900
H	3.22520400	3.24602400	-0.63807100
C	5.73734300	-0.09222700	-0.17438800
H	6.54897800	0.01245500	-0.90535800
H	5.85298400	0.69565000	0.57237100
H	5.85593100	-1.05835400	0.32090000
C	4.22500800	-2.53351400	-1.48034500
H	3.55610400	-3.20514900	-2.01958500
H	5.22041800	-2.60593000	-1.93099400
H	4.29262500	-2.88168600	-0.44459000
C	1.51301100	-1.39915100	-2.85667100
H	0.50283100	-1.08170400	-2.59007100
H	1.63969200	-1.23969000	-3.93447000
H	1.58924100	-2.46946000	-2.65958700
C	1.39361700	1.72874100	-2.32419400
H	0.41659800	1.24044800	-2.30457500
H	1.32828400	2.62858300	-1.71057600
H	1.59473600	2.03159300	-3.35877600
C	-0.33054900	1.77421400	0.65736000
C	-0.01869700	3.12165500	0.85638300
C	1.18054000	3.42549700	1.51391500
C	2.09993300	2.42608600	1.86461000
C	1.80222300	1.06401200	1.70253000
C	0.52610000	0.75320600	1.16060400

H	-0.67065500	3.90675500	0.50028100
H	1.42362300	4.46888600	1.69186000
H	3.07557600	2.71864900	2.24479500
H	2.40892000	0.06767800	2.65417300
C	-2.30633400	-1.26993700	-1.98574600
C	-3.10352000	-2.26838100	-2.54354000
C	-3.65649000	-3.26303300	-1.73349900
C	-3.40074700	-3.26442600	-0.35999200
C	-2.59736700	-2.27457900	0.20241700
C	-2.05299200	-1.26160300	-0.60373600
H	-1.90253800	-0.48445200	-2.61317500
H	-3.29461600	-2.26697500	-3.61230100
H	-4.28235300	-4.03483500	-2.17092300
H	-3.83056900	-4.03360400	0.27413400
H	-2.41177700	-2.26047700	1.27182500
N	-1.36101100	1.13082700	-0.04759200
S	-2.80231100	1.94480900	-0.69681400
O	-2.73003600	3.28770600	-0.13366000
O	-2.77905400	1.71833000	-2.13823100
C	-4.97469800	0.27368700	-0.74426800
C	-5.98782400	-0.45585000	-0.12906100
C	-6.15459900	-0.43606800	1.26333900
C	-5.28030900	0.34564600	2.03809300
C	-4.26427600	1.08752500	1.44671000
C	-4.12012100	1.03066000	0.05730700
H	-4.82980800	0.24310000	-1.81701400
H	-6.65436700	-1.05662300	-0.74039700

H	-5.40227600	0.37425200	3.11692400
H	-3.59592400	1.69552900	2.04778200
C	-1.17534500	-0.25516100	0.01702700
C	-0.04391300	-0.51675000	0.77285300
C	-7.26871800	-1.21358400	1.91621900
H	-8.16362100	-0.58742900	2.01513300
H	-7.54686900	-2.09026900	1.32511800
H	-6.99177100	-1.54651200	2.92037100
H	0.27592800	-1.51038300	1.05285300
C	2.90590900	-1.83461500	2.65112800
O	2.75625700	-0.76401100	3.34208500
O	2.73256800	-1.90113600	1.40020800
C	3.31345000	-3.07156100	3.40582200
H	2.57664400	-3.27586100	4.18753000
H	3.39780900	-3.92396000	2.73276900
H	4.26955600	-2.88672200	3.90439800

Zero-point correction= 0.600729 (Hartree/Particle)

Thermal correction to Energy= 0.641393

Thermal correction to Enthalpy= 0.642337

Thermal correction to Gibbs Free Energy= 0.524592

Sum of electronic and zero-point Energies= -2141.236650

Sum of electronic and thermal Energies= -2141.195985

Sum of electronic and thermal Enthalpies= -2141.195041

Sum of electronic and thermal Free Energies= -2141.312787

E(RB3LYP) = -2141.837378 A.U.