Metal-Dependent Pathway Selection in Co(III)- *and* Rh(III)-Catalyzed C–H Activation–Alkyne Coupling: A DFT Study

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Figures S1 and S2 compare the energy profiles obtained at the M06 and M06-L levels and support the reliability of the computational protocol.

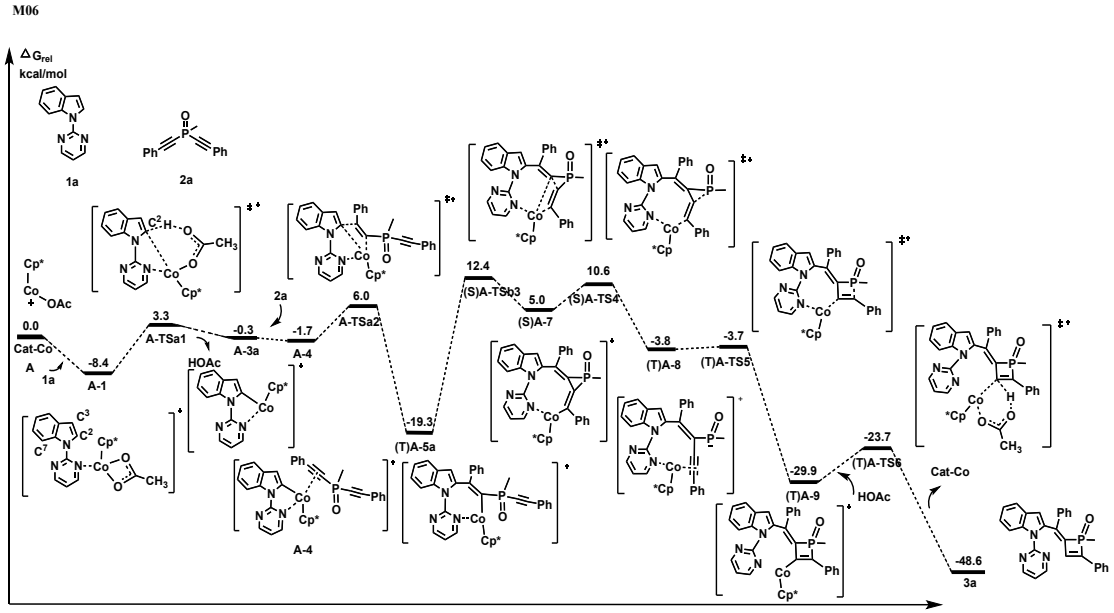

Figure S1. Energy trend graph for optimizing the overall reaction in M06 mode. Species labeled with "S" and "T" correspond to singlet and triplet states, respectively. The relative free energies are reported in kcal/mol.

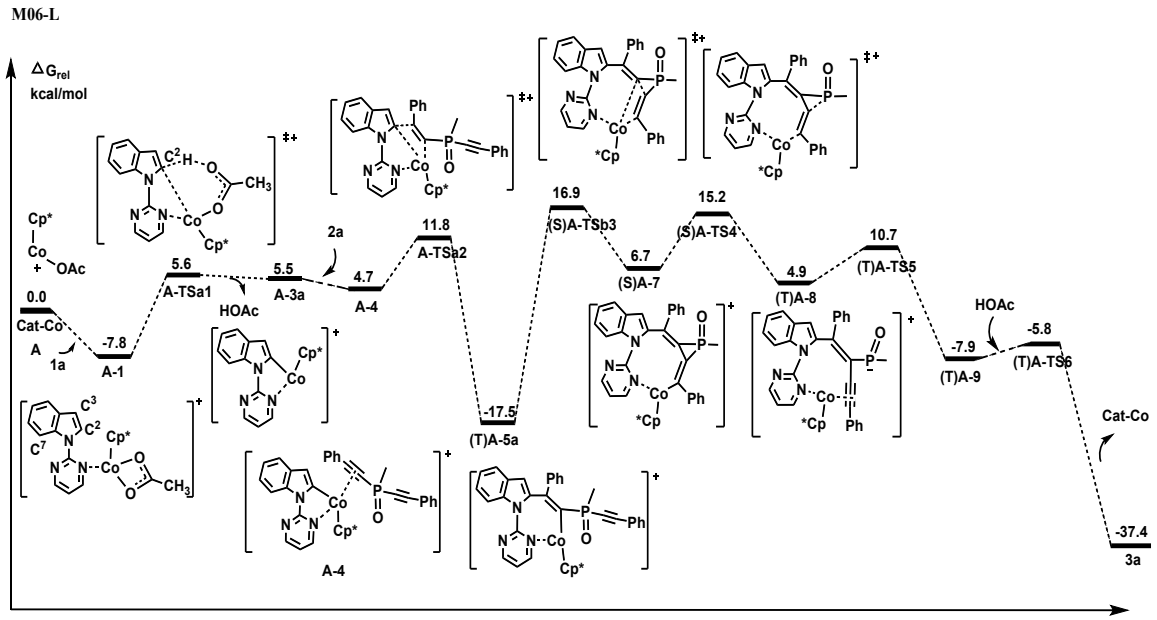

Figure S2. Energy trend graph for optimizing the overall reaction in M06L mode. Species labeled with "S" and "T" correspond to singlet and triplet states, respectively. The relative free energies are reported in kcal/mol.

Figure S3 describes the alternative C–H activation pathway through a σ-bond metathesis mechanism

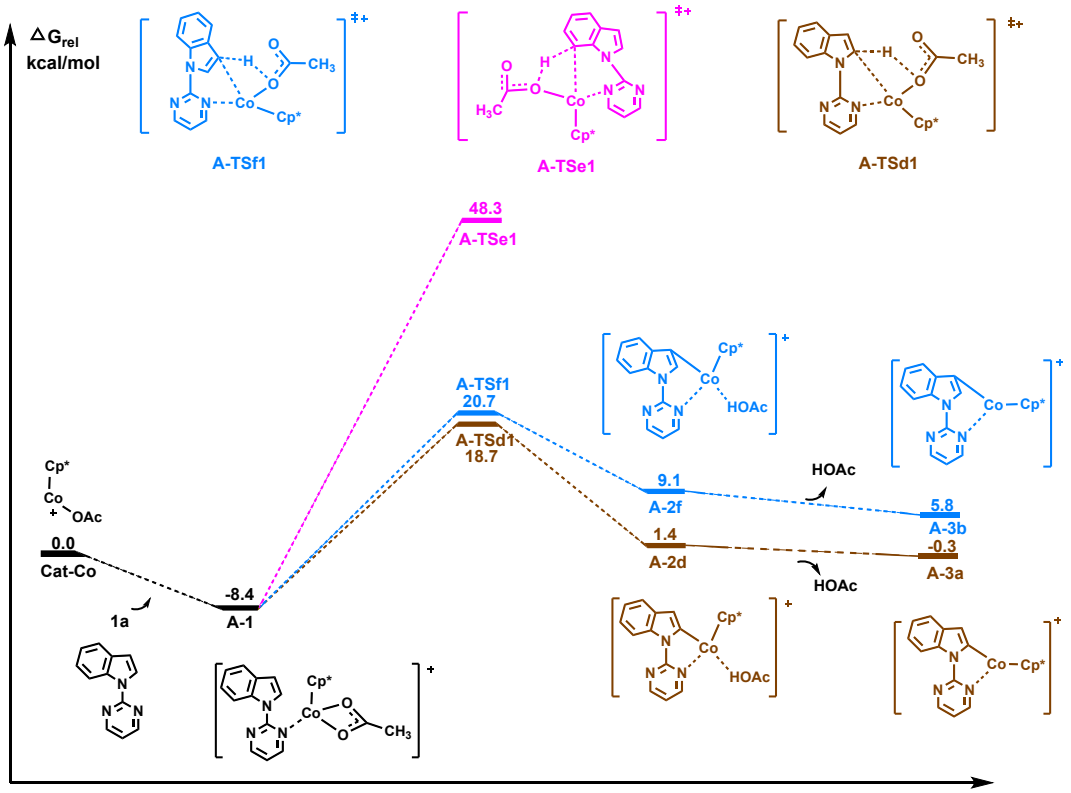

Figure S3. Free energy profile for the A-series C-H activation (σ bond metathesis mechanism). The relative free energies are reported in kcal/mol.

Figure S4 presents the O-bound coordination mode of the phosphine oxide substrate and explains why this pathway is not productive for the subsequent alkyne migratory insertion.

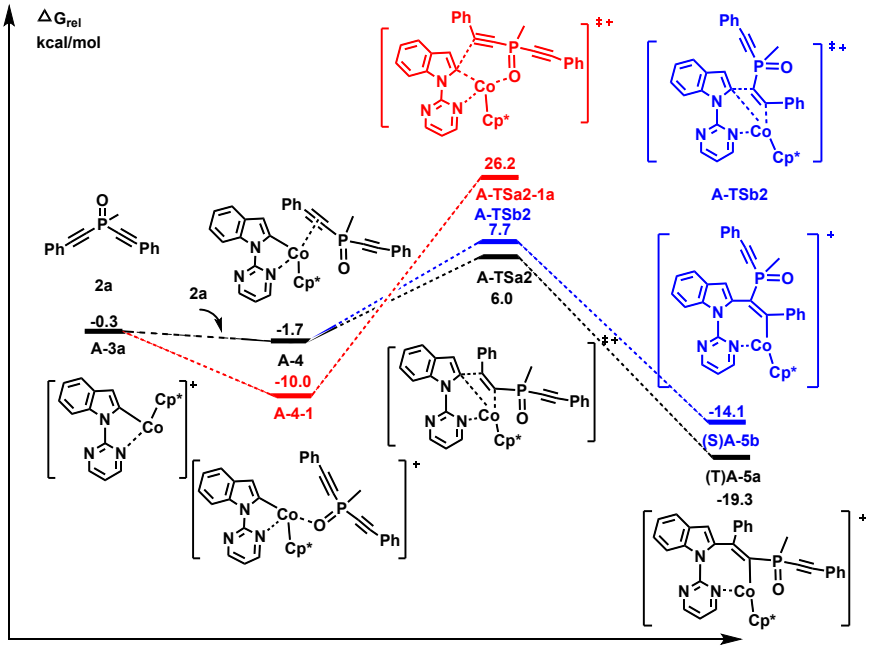

Figure S4. Calculated free energy profile for the alkyne migration insertion. The relative free energies are reported in kcal/mol.

Figures S5 and S6 discuss alternative reaction sequences and regioisomeric migratory insertion pathways.

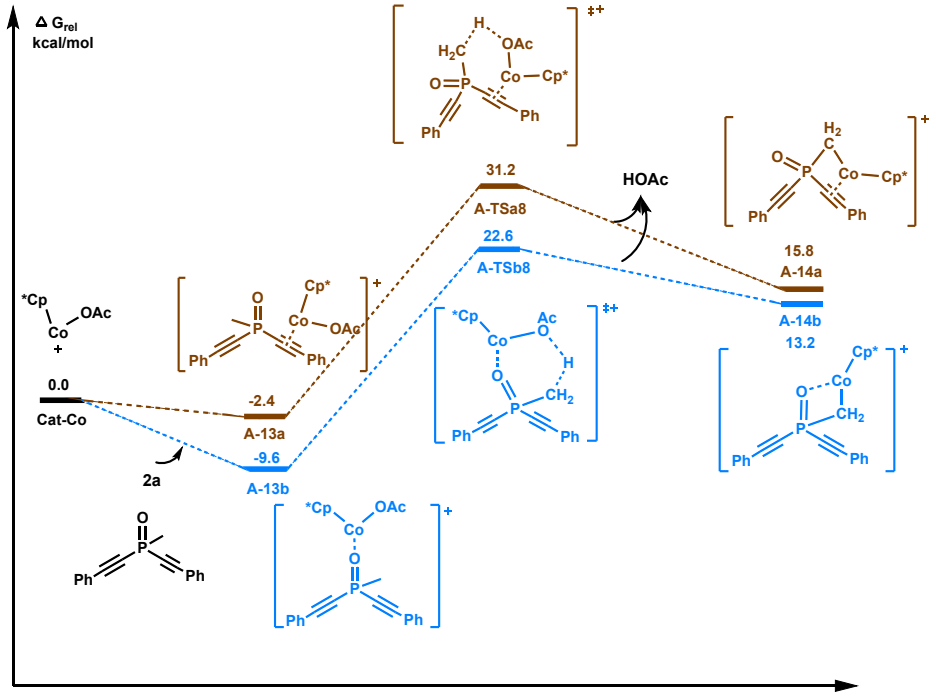

Figure S5. The computational energy distribution map of substrate **2a** participating in the CMD process.The relative free energies are reported in kcal/mol.

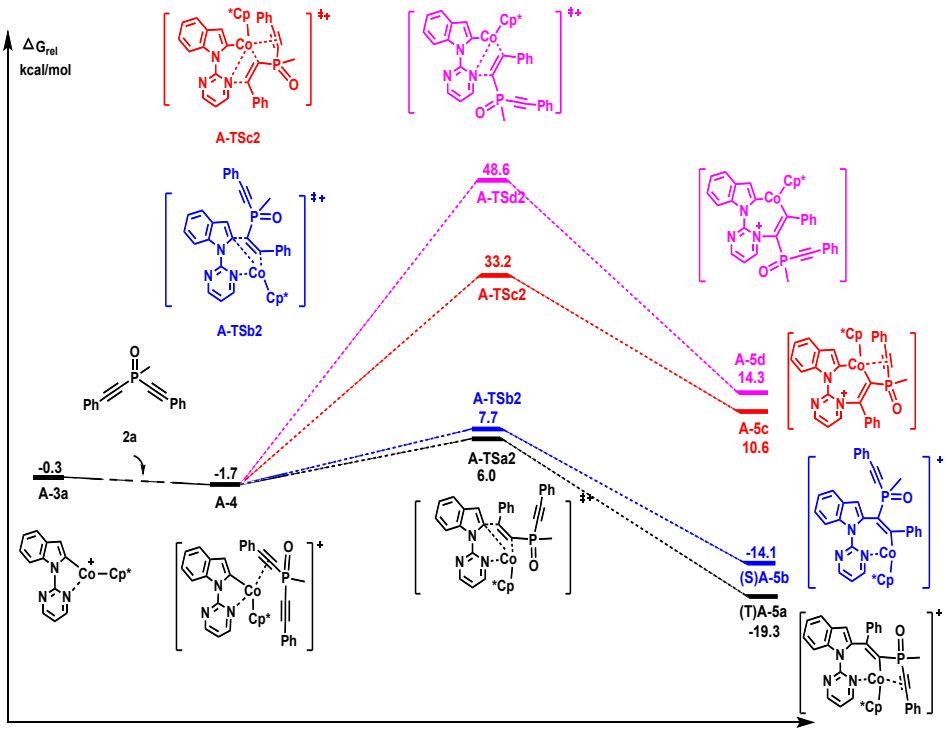

Figure S6. Free energy profile for the A-series alkyne migration insertion. The relative free energies are reported in kcal/mol.

Figure S7 provides the complete post-insertion pathway, including β-C(alkynyl) elimination, second alkyne migratory insertion, anti-elimination, cyclization, and catalyst regeneration.

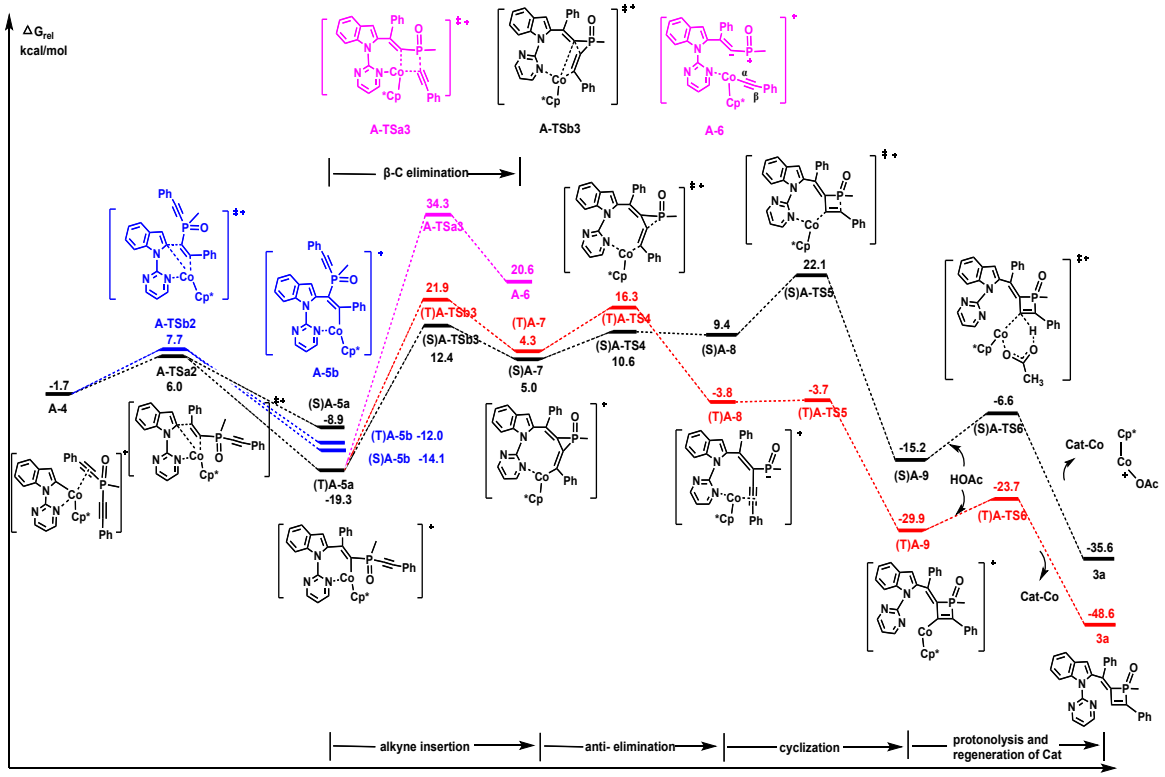

Figure S7. Calculated the free energy profile of *β*-C (alkynyl) elimination process from the post-insertion alkenyl-cobalt intermediate **A-5a**. Species labeled with "S" and "T" correspond to singlet and triplet states, respectively. Free energies are given in kcal/mol.

Figures S8 and S9 compare the Co- and Rh-catalyzed pathways for the 2-pyridone substrates.

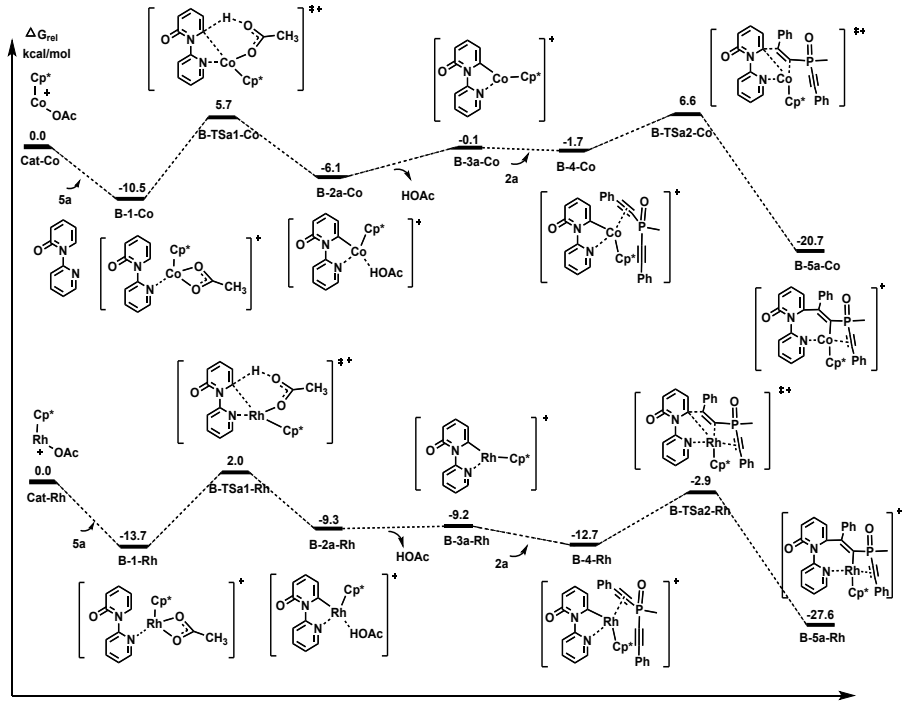

Figure S8. Calculated the free energy distribution of the cobalt/rhodium-catalyzed catalytic cycles were compared

for the 2-pyridone substrates. The relative free energies are reported in kcal/mol.

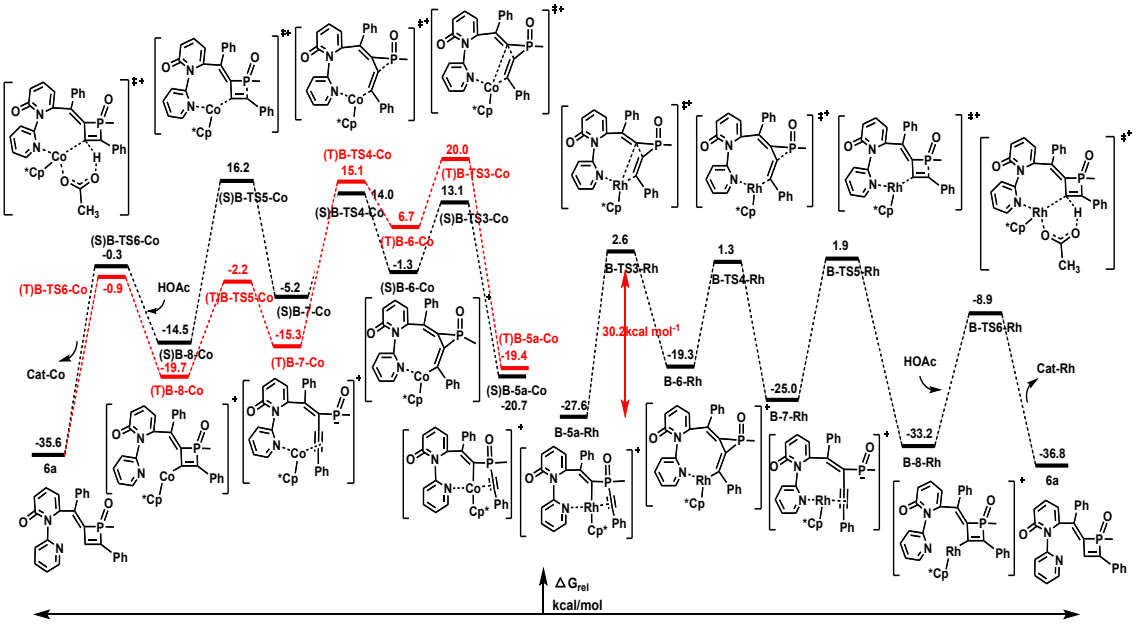

Figure S9. Calculated the free energy distribution of the Co and Rh-catalyzed catalytic cycles was compared for the 2-pyridone substrates. Species labeled with "S" and "T" correspond to singlet and triplet states, respectively. The relative free energies are reported in kcal/mol.

Figure S10 provides additional charge/structural analysis of key transition states, and Figure S11 evaluates representative intermolecular exchange pathways relevant to the crossover experiment.

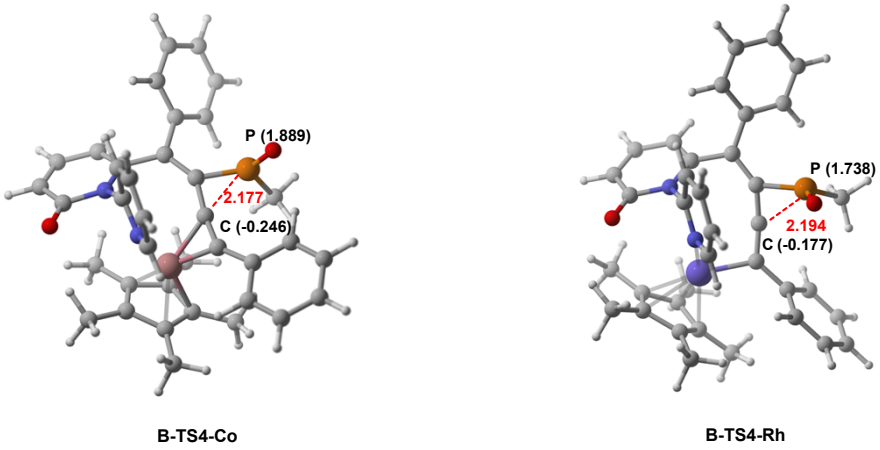

Figure S10. Calculated NPA charges on transition states **B-TS4-Co** and **B-TS4-Rh** (black numerals indicate NPA charges (in a.u.), and Red numerals represent bond lengths (in Å))

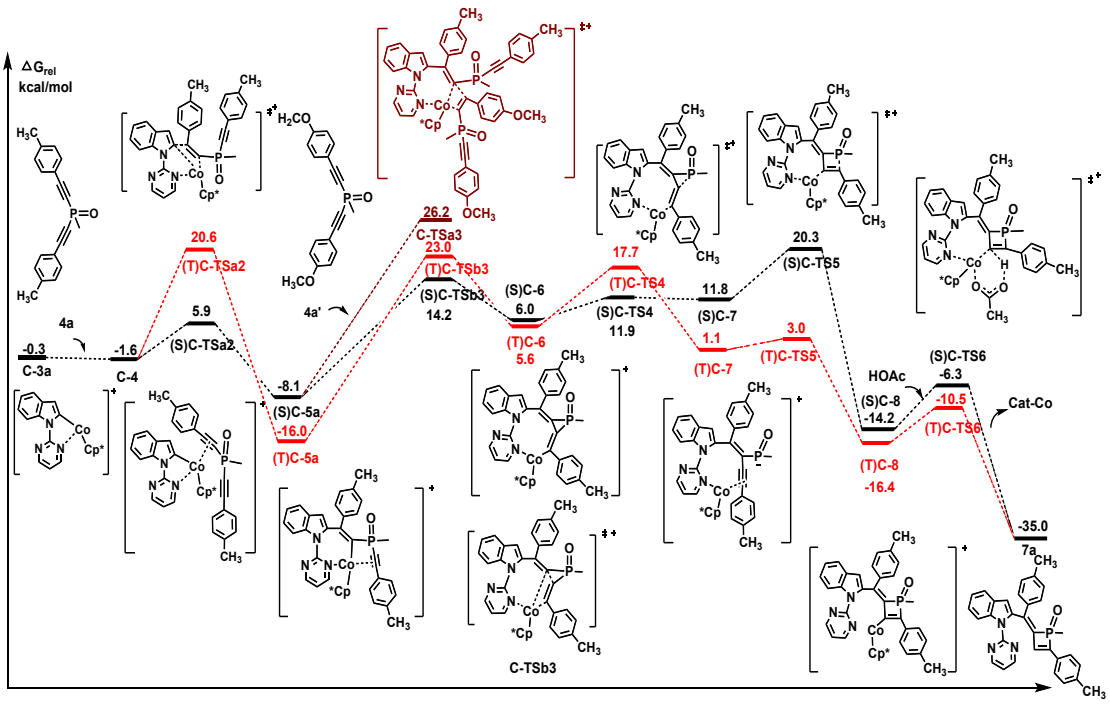

Figure S11. Calculated the free energy profile of representative intermolecular exchange pathways involving alkyne dissociation and recombination between distinct phosphine oxide substrates. Species labeled with "S" and "T" correspond to singlet and triplet states, respectively. Free energies are given in kcal/mol.

The Cartesian coordinates of the stationary points

Cat-Co

1 1

Number of imaginary frequencies: 0

C	1.06787400	-1.17619800	0.68946500
C	1.63878700	-0.73015900	-0.52828200
C	1.63883200	0.72991200	-0.52850200
C	1.06795500	1.17636600	0.68911100
C	0.65691600	0.00021600	1.43352000
O	-1.83807900	1.08358100	-0.43936100
C	-2.52189900	0.00002000	-0.53620200
O	-1.83806900	-1.08357200	-0.43943400
C	-3.98569000	-0.00006000	-0.72452400
C	-0.05156600	0.00044600	2.73258700
H	-0.67567800	-0.88712300	2.85748500
H	0.67716300	0.00064300	3.55291400
H	-0.67574900	0.88801700	2.85712800
C	0.79087300	-2.57492800	1.09369000
H	0.87337900	-3.26887400	0.25634500
H	1.50484500	-2.89243800	1.86152400
H	-0.21052100	-2.68040500	1.51844000
C	2.11114300	-1.57235400	-1.65328200
H	1.84661800	-1.14689500	-2.62488300
H	3.20490700	-1.64494900	-1.63095900
H	1.71372400	-2.58712100	-1.60612200
C	2.11120500	1.57172600	-1.65377900

H	1.71379200	2.58651100	-1.60697200
H	3.20497000	1.64432600	-1.63145800
H	1.84670300	1.14593200	-2.62523900
C	0.79105400	2.57523800	1.09291700
H	1.50499000	2.89289200	1.86072500
H	0.87370500	3.26894300	0.25538800
H	-0.21036700	2.68093100	1.51755200
H	-4.30602400	-0.89766800	-1.25305800
H	-4.46591300	-0.00407500	0.25910600
H	-4.30712700	0.90073800	-1.24685100
Co	-0.24433800	-0.00003000	-0.30300100

Zero-point correction= 0.274414 (Hartree/Particle)

Thermal correction to Energy= 0.293319

Thermal correction to Enthalpy= 0.294263

Thermal correction to Gibbs Free Energy= 0.226618

Sum of electronic and zero-point Energies= -763.984521

Sum of electronic and thermal Energies= -763.965616

Sum of electronic and thermal Enthalpies= -763.964672

Sum of electronic and thermal Free Energies= -764.032317

E(RM06L) = -764.258935 A.U.

Cat-Rh

1 1

Number of imaginary frequencies: 0

Rh	-0.35218600	-0.00014200	-0.19468600
C	1.33795200	-1.18254100	0.56694600
C	1.65461500	-0.73414300	-0.74457300
C	1.65421100	0.73480900	-0.74444300

C	1.33735400	1.18281200	0.56718000
C	1.08818100	0.00000400	1.38216500
O	-2.15128900	1.09293600	-0.18069000
C	-2.82562300	-0.00020600	-0.22796600
O	-2.15129900	-1.09337400	-0.18124000
C	-4.31278400	-0.00026100	-0.30478000
C	0.75088800	-0.00021700	2.83255500
H	0.18303500	-0.88850700	3.11462100
H	1.68328500	0.00000600	3.41329600
H	0.18252200	0.88770000	3.11476800
C	1.24438100	-2.59514000	1.04446900
H	1.09095400	-3.29055800	0.21835800
H	2.17394300	-2.87297900	1.55552200
H	0.42177800	-2.72277200	1.75151400
C	1.96089400	-1.58439900	-1.93211600
H	1.56584700	-1.14691300	-2.85191400
H	3.04879300	-1.66877900	-2.04846400
H	1.55366800	-2.59074600	-1.82591000
C	1.95997300	1.58543300	-1.93185500
H	1.55228500	2.59156900	-1.82541700
H	3.04781900	1.67034300	-2.04830600
H	1.56503000	1.14793200	-2.85169200
C	1.24300200	2.59527800	1.04494500
H	2.17238500	2.87352200	1.55610100
H	1.08924900	3.29075800	0.21894800
H	0.42028500	2.72234400	1.75196000
H	-4.66401900	-0.89965900	-0.81319300

H	-4.71135100	-0.00502500	0.71659400
H	-4.66469100	0.90307000	-0.80561600

Zero-point correction= 0.273780 (Hartree/Particle)

Thermal correction to Energy= 0.293059

Thermal correction to Enthalpy= 0.294004

Thermal correction to Gibbs Free Energy= 0.224356

Sum of electronic and zero-point Energies= -727.697709

Sum of electronic and thermal Energies= -727.678429

Sum of electronic and thermal Enthalpies= -727.677485

Sum of electronic and thermal Free Energies= -727.747133

E(RB3LYP) = -727.971488 A.U.

1a

0 1

Number of imaginary frequencies: 0

C	2.15549000	0.85004200	0.00003500
C	1.09784600	-0.09450600	0.00005400
C	1.34470700	-1.46705600	-0.00005500
C	2.67334600	-1.87893800	-0.00021900
C	3.73043800	-0.95992800	-0.00027200
C	3.48075500	0.40464500	-0.00012800
C	1.56675100	2.15687200	0.00027500
C	0.21878400	2.00093800	0.00027200
H	0.53167400	-2.17909300	-0.00002800
H	2.89112000	-2.94315600	-0.00031500
H	4.75476200	-1.32153700	-0.00038900
H	4.29760500	1.12136300	-0.00013100
H	2.09059900	3.10217600	0.00035500

H	-0.58619000	2.71722400	0.00035400
C	-1.40777700	0.17051200	0.00007900
N	-1.58703200	-1.15656900	0.00050800
C	-2.85617000	-1.56376300	0.00040900
C	-3.93512800	-0.68880400	-0.00016200
C	-3.61424700	0.66531500	-0.00054600
N	-2.36281400	1.11511100	-0.00039000
H	-3.00687300	-2.64276900	0.00076400
H	-4.96055500	-1.03798200	-0.00028700
H	-4.39286000	1.42759100	-0.00090400
N	-0.09987800	0.63920100	0.00018700

Zero-point correction= 0.187208 (Hartree/Particle)

Thermal correction to Energy= 0.197689

Thermal correction to Enthalpy= 0.198633

Thermal correction to Gibbs Free Energy= 0.150279

Sum of electronic and zero-point Energies= -626.712256

Sum of electronic and thermal Energies= -626.701775

Sum of electronic and thermal Enthalpies= -626.700831

Sum of electronic and thermal Free Energies= -626.749185

E(RM06L) = -626.899464 A.U.

2a

0 1

Number of imaginary frequencies: 0

C	2.36297500	0.39245100	-0.03106800
C	3.48952100	-0.46784900	0.02790900
C	4.79036000	0.05258100	-0.08643400
C	3.31718200	-1.85253400	0.19936600

C	5.88794100	-0.79549200	-0.02943800
H	4.92207700	1.12141700	-0.22268100
C	4.42201500	-2.69115300	0.25468100
H	2.31193300	-2.25308300	0.28595200
C	5.70829300	-2.16692900	0.14118700
H	6.88903200	-0.38448000	-0.11997900
H	4.27905300	-3.75955900	0.38670600
H	6.56986400	-2.82666900	0.18474200
C	1.38746500	1.12448900	-0.07342400
P	0.03282600	2.23187500	-0.24020300
C	-2.34976800	0.45937000	-0.04869100
C	-3.50159400	-0.36774300	-0.01547300
C	-4.35892000	-0.36020500	1.09848800
C	-3.79768100	-1.20787800	-1.10332800
C	-5.48218100	-1.17567900	1.11952500
H	-4.13070800	0.28973300	1.93761000
C	-4.92332400	-2.01932600	-1.07127800
H	-3.13619100	-1.20984300	-1.96390000
C	-5.76743400	-2.00654300	0.03762900
H	-6.13894000	-1.16284500	1.98430600
H	-5.14424100	-2.66450500	-1.91637500
H	-6.64743300	-2.64263100	0.05844200
C	-1.34961900	1.15785100	-0.08109100
C	0.03669100	3.15955400	1.31407500
H	-0.84138600	3.80806400	1.34242900
H	0.02286700	2.49174800	2.17810400
H	0.93284400	3.78211100	1.35283100

O	0.04841400	3.06532900	-1.47511900

Zero-point correction= 0.245085 (Hartree/Particle)

Thermal correction to Energy= 0.263097

Thermal correction to Enthalpy= 0.264041

Thermal correction to Gibbs Free Energy= 0.193906

Sum of electronic and zero-point Energies= -1071.792494

Sum of electronic and thermal Energies= -1071.774481

Sum of electronic and thermal Enthalpies= -1071.773537

Sum of electronic and thermal Free Energies= -1071.843672

E(RM06L) = -1072.037578 A.U.

3a

0 1

Number of imaginary frequencies: 0

C	-1.23084000	1.09462400	-0.46355600
C	-1.87771100	2.36366200	-0.12277000
C	-1.42068200	3.57309900	-0.67026900
C	-2.95610700	2.40490700	0.77582600
C	-2.00438600	4.78232900	-0.31793700
H	-0.62389900	3.54664500	-1.40962400
C	-3.54033200	3.61532900	1.12575600
H	-3.31004100	1.47622400	1.21476500
C	-3.06684500	4.80850900	0.58338500
H	-1.64018700	5.70630800	-0.75831000
H	-4.36552200	3.62930200	1.83221500
H	-3.52759600	5.75356000	0.85623200
C	0.10279800	1.02497600	-0.74822200
P	1.59878000	1.96505800	-0.27097500

C	2.21153400	0.31505000	-0.72771700
C	3.48545800	-0.35197300	-0.66572300
C	4.61917400	0.33690800	-0.19818600
C	3.62616100	-1.70463800	-1.03135800
C	5.85097800	-0.29878800	-0.11416300
H	4.51535200	1.37252300	0.11900900
C	4.85904200	-2.33421200	-0.94770300
H	2.75387800	-2.25662600	-1.37424700
C	5.97738200	-1.63425300	-0.49186900
H	6.71593400	0.24751100	0.25102900
H	4.95207900	-3.37754200	-1.23621900
H	6.94106100	-2.13083700	-0.42589000
C	0.95311600	-0.08945000	-1.09337400
C	2.09251500	3.08856400	-1.61446400
H	3.17739600	3.21997400	-1.59278200
H	1.80212200	2.69439800	-2.59108000
H	1.63231500	4.06691200	-1.46071400
O	1.78680900	2.54615400	1.09444800
C	-3.54285200	-1.76300900	-0.86666900
C	-2.45608500	-2.34452900	-0.16525400
C	-2.43179500	-3.69392000	0.18000300
C	-3.51528900	-4.46971700	-0.21242300
C	-4.59445300	-3.91996800	-0.92346000
C	-4.61863500	-2.57455000	-1.25344200
C	-3.25223600	-0.37574300	-1.01813600
C	-2.03398400	-0.12492900	-0.43640400
H	-1.58680200	-4.11855600	0.70923200

H	-3.52113800	-5.52843800	0.03008500
H	-5.42034600	-4.56140800	-1.21698800
H	-5.45754700	-2.14898400	-1.79726800
H	-3.83521300	0.35894000	-1.55714300
C	-0.47852900	-1.40111400	1.02254600
N	0.29752100	-2.48678800	0.94343300
C	1.36852400	-2.47466500	1.74380300
C	1.68640900	-1.39581400	2.55818900
C	0.76828400	-0.34948700	2.58188500
N	-0.34363700	-0.35584300	1.84422100
H	2.00526700	-3.35737500	1.70121200
H	2.59166800	-1.37600600	3.15358300
H	0.91732300	0.52566600	3.21043000
N	-1.54193800	-1.32727400	0.10483500
H	0.64043300	-1.04116500	-1.52567400

Zero-point correction= 0.436966 (Hartree/Particle)

Thermal correction to Energy= 0.464864

Thermal correction to Enthalpy= 0.465809

Thermal correction to Gibbs Free Energy= 0.377141

Sum of electronic and zero-point Energies= -1698.597232

Sum of electronic and thermal Energies= -1698.569333

Sum of electronic and thermal Enthalpies= -1698.568389

Sum of electronic and thermal Free Energies= -1698.657056

E(RM06L) = -1699.034197 A.U.

4a

0 1

Number of imaginary frequencies: 0

C	2.36640400	0.73161900	-0.04363200
C	3.49581300	-0.12395200	0.00357500
C	4.79697600	0.39768200	-0.09449300
C	3.33543200	-1.51240100	0.15218900
C	5.89512100	-0.44765700	-0.04610400
H	4.93086900	1.46903700	-0.20788000
C	4.44381700	-2.34391600	0.19854200
H	2.33389000	-1.92368700	0.23270800
C	5.74212100	-1.83109800	0.09786500
H	6.89602900	-0.02852800	-0.12083700
H	4.30343400	-3.41601400	0.31710700
C	1.38695600	1.45940900	-0.07657200
P	0.02532300	2.55904900	-0.22863000
C	-2.34727700	0.77226600	-0.05170700
C	-3.49482900	-0.05917900	-0.02256000
C	-4.35034300	-0.07153200	1.09241800
C	-3.79567600	-0.89419600	-1.11238200
C	-5.46666300	-0.89355600	1.10900800
H	-4.12436200	0.56693700	1.94105600
C	-4.91581300	-1.71063400	-1.07990500
H	-3.13889000	-0.89256400	-1.97669900
C	-5.77309900	-1.72537400	0.02595000
H	-6.11722300	-0.89451000	1.98073700
H	-5.13347600	-2.35369700	-1.92966800
C	-1.35053400	1.47632400	-0.08009300
C	0.02420200	3.46859400	1.33706400
H	-0.85769600	4.11152800	1.37361200

H	0.01468700	2.79032700	2.19297200
H	0.91674100	4.09585800	1.38314500
O	0.03489200	3.41006400	-1.45204800
C	6.93180300	-2.73981900	0.11679400
H	6.75330400	-3.62818700	0.72851200
H	7.17684600	-3.09225300	-0.89190900
H	7.82128300	-2.23467600	0.50221700
C	-6.99774400	-2.58648500	0.04029200
H	-7.24801000	-2.91797600	1.05163400
H	-7.86946200	-2.04160600	-0.34043400
H	-6.87694400	-3.47280500	-0.58792300

Zero-point correction= 0.299654 (Hartree/Particle)

Thermal correction to Energy= 0.320687

Thermal correction to Enthalpy= 0.321631

Thermal correction to Gibbs Free Energy= 0.242051

Sum of electronic and zero-point Energies= -1150.368068

Sum of electronic and thermal Energies= -1150.347035

Sum of electronic and thermal Enthalpies= -1150.346090

Sum of electronic and thermal Free Energies= -1150.425671

E(RM06L) = -1150.667722 A.U.

4a'

0 1

Number of imaginary frequencies: 0

C	2.36751200	1.00058100	0.04071300
C	3.52056700	0.18532500	0.14402700
C	4.21861200	-0.21392700	-1.00604700
C	3.99597700	-0.24435100	1.39928500

C	5.35028200	-1.01358600	-0.91758600
H	3.86322900	0.11215800	-1.97853100
C	5.12081900	-1.03922600	1.49476100
H	3.46601200	0.05653600	2.29765600
C	5.80688800	-1.43043300	0.33712000
H	5.86825700	-1.30557400	-1.82411500
H	5.49459800	-1.37518400	2.45633500
C	1.36986300	1.69874400	-0.05186200
P	-0.00443600	2.76713800	-0.27661300
C	-2.36317300	0.95684800	-0.17383500
C	-3.49958900	0.11270000	-0.17118100
C	-4.48305500	0.22667800	0.82286400
C	-3.66936100	-0.86516900	-1.17238800
C	-5.59849100	-0.60046400	0.82851000
H	-4.36618600	0.97663400	1.59921100
C	-4.77549100	-1.69116500	-1.17276100
H	-2.91719300	-0.96231000	-1.94878700
C	-5.74885600	-1.56577900	-0.17243900
H	-6.34168800	-0.48776500	1.60980000
H	-4.91514900	-2.44630100	-1.93922100
C	-1.37407500	1.67318700	-0.17742800
C	-0.09095100	3.68947600	1.28020900
H	-0.98901000	4.31066200	1.27516600
H	-0.12073600	3.01733200	2.14057600
H	0.78401600	4.33801100	1.35756400
O	0.05052400	3.60531600	-1.50814600
C	7.61668200	-2.62165200	-0.61089200

H	8.44549000	-3.22815500	-0.24764800
H	6.99341200	-3.22478800	-1.28299900
H	8.01227600	-1.76364500	-1.16877800
C	-7.79988100	-2.32063600	0.73113800
H	-7.39831500	-2.51352800	1.73396700
H	-8.27591000	-1.33202100	0.72379800
H	-8.54291800	-3.07961500	0.48911800
O	-6.79644700	-2.42281200	-0.26031800
O	6.89850800	-2.21030700	0.53632000

Zero-point correction= 0.310439 (Hartree/Particle)

Thermal correction to Energy= 0.333482

Thermal correction to Enthalpy= 0.334426

Thermal correction to Gibbs Free Energy= 0.252686

Sum of electronic and zero-point Energies= -1300.754399

Sum of electronic and thermal Energies= -1300.731355

Sum of electronic and thermal Enthalpies= -1300.730411

Sum of electronic and thermal Free Energies= -1300.812151

E(RM06L) = -1301.064837 A.U.

5a

0 1

Number of imaginary frequencies: 0

C	1.21505100	-1.36870300	0.26622000
C	2.56468800	-1.53362700	0.27452100
C	3.39589800	-0.39960400	0.04818300
C	2.83933800	0.82415200	-0.16959400
C	1.40623400	1.04356000	-0.18199700
C	-0.81335900	-0.08743700	0.02993500

C	-2.74054100	-1.24807400	-0.41008400
C	-3.54510000	-0.17664500	-0.03055800
C	-2.91341000	0.98618700	0.41144500
C	-1.52370200	1.04519300	0.45160100
H	0.51840800	-2.18295100	0.40814000
H	2.98203700	-2.51656000	0.45364000
H	4.47646400	-0.51410200	0.04922500
H	3.43458300	1.71054500	-0.35362600
H	-3.18109700	-2.18085900	-0.75541400
H	-4.62603900	-0.25426400	-0.07710500
H	-3.49572200	1.84545900	0.72984700
H	-1.00190400	1.93106900	0.77844500
N	0.62464200	-0.13764500	0.06290700
N	-1.40403000	-1.20847500	-0.38725900
O	0.87980000	2.13431300	-0.38759100

Zero-point correction= 0.162534 (Hartree/Particle)

Thermal correction to Energy= 0.172117

Thermal correction to Enthalpy= 0.173061

Thermal correction to Gibbs Free Energy= 0.126760

Sum of electronic and zero-point Energies= -570.474145

Sum of electronic and thermal Energies= -570.464562

Sum of electronic and thermal Enthalpies= -570.463618

Sum of electronic and thermal Free Energies= -570.509919

E(RB3LYP) = -570.636679 A.U.

6a

0 1

Number of imaginary frequencies: 0

C	1.52973900	-0.40943100	-0.64567900
C	2.59010500	-1.32743600	-0.18791600
C	2.48892700	-2.71785200	-0.37542700
C	3.73350700	-0.83179600	0.46881600
C	3.46759600	-3.58094600	0.10759400
H	1.65094400	-3.11976500	-0.93138600
C	4.71342800	-1.69593200	0.95089800
H	3.85292900	0.23858000	0.60111000
C	4.58326500	-3.07528300	0.77842100
H	3.36468400	-4.65032900	-0.05041700
H	5.58122600	-1.29002700	1.46228100
H	5.34844000	-3.74862700	1.15241300
C	0.22879300	-0.76727700	-0.77759500
P	-0.91728800	-2.09139600	-0.16915900
C	-2.00043700	-0.70970800	-0.70333700
C	-3.41049500	-0.40216300	-0.59091100
C	-4.33625600	-1.40474200	-0.24614300
C	-3.87822000	0.91349000	-0.79115600
C	-5.69124800	-1.10751500	-0.12738100
H	-3.98557300	-2.41634300	-0.06278400
C	-5.23293800	1.20499400	-0.67165100
H	-3.16683200	1.70298900	-1.01342500
C	-6.14449100	0.19599700	-0.34337600
H	-6.39415500	-1.89117700	0.13876900
H	-5.58031800	2.22233600	-0.82554500
H	-7.20095100	0.42772000	-0.24694500
C	-0.93558900	0.01477400	-1.16232600

C	-1.07909200	-3.40317300	-1.44060700
H	-2.06874400	-3.85825000	-1.34307900
H	-0.96786900	-2.98943300	-2.44547200
H	-0.32844100	-4.17781700	-1.26822800
O	-0.87956000	-2.61678500	1.23101200
H	-0.93110800	0.98135100	-1.65587000
C	1.92470800	1.00220800	-0.94119100
C	0.49706400	1.77206100	0.92314000
C	0.04629200	0.82199400	3.06561500
C	-1.27049100	1.25605100	2.92015800
C	-1.61704700	1.94284000	1.75731400
N	-0.75721600	2.18737400	0.76084200
H	0.35787300	0.27329600	3.94822500
H	-2.01607200	1.05897200	3.68272000
H	-2.63614700	2.28705300	1.60094200
N	1.39532000	2.03421700	-0.17915600
C	2.80454700	1.28621400	-1.95263100
H	3.21528200	0.46837300	-2.53083900
C	1.74373000	3.41697900	-0.37038400
C	2.63570900	3.65570900	-1.48781300
H	2.88925800	4.69383300	-1.66670700
C	3.14857500	2.63625900	-2.23271700
H	3.83091200	2.85032300	-3.05106300
O	1.31423800	4.27188800	0.39244500
C	0.96115400	1.10220700	2.05370100
H	1.99481700	0.78478200	2.11870700

Zero-point correction= 0.412492 (Hartree/Particle)

Thermal correction to Energy= 0.439598

Thermal correction to Enthalpy= 0.440542

Thermal correction to Gibbs Free Energy= 0.352430

Sum of electronic and zero-point Energies= -1642.486702

Sum of electronic and thermal Energies= -1642.459596

Sum of electronic and thermal Enthalpies= -1642.458652

Sum of electronic and thermal Free Energies= -1642.546764

E(RB3LYP) = -1642.899194 A.U.

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Number of imaginary frequencies: 0

H	1.70162000	-0.81898900	0.00042000
C	0.09213200	0.12640300	-0.00029600
O	0.76202500	-1.05257400	0.00000000
O	0.65508800	1.19679100	0.00006300
C	-1.38740500	-0.09831600	-0.00001000
H	-1.67975500	-0.67717300	0.87889100
H	-1.90755100	0.85720300	-0.00312000
H	-1.67958300	-0.68329900	-0.87486300

Zero-point correction= 0.062248 (Hartree/Particle)

Thermal correction to Energy= 0.066832

Thermal correction to Enthalpy= 0.067776

Thermal correction to Gibbs Free Energy= 0.034868

Sum of electronic and zero-point Energies= -229.004490

Sum of electronic and thermal Energies= -228.999906

Sum of electronic and thermal Enthalpies= -228.998962

Sum of electronic and thermal Free Energies= -229.031870

E(RM06L) = -229.066738 A.U.

A-1

1 1

Number of imaginary frequencies: 0

C	-0.42020500	-0.83158900	-1.65436200
C	-1.20041800	-1.85556200	-1.04948300
C	-2.57256700	-1.41117100	-1.00268700
C	-2.63881600	-0.12706500	-1.65243500
C	-1.31335400	0.25619700	-2.00781700
O	-1.62938700	-0.93884400	1.82799500
O	-2.85817100	0.70617700	1.14305000
C	-2.57158200	-0.11808600	2.07814400
C	-3.71421100	-2.16674300	-0.42555600
H	-4.14903700	-2.84445400	-1.16855400
H	-3.39891200	-2.77560900	0.42569800
H	-4.51120500	-1.49794000	-0.09056100
C	-0.70272400	-3.12207100	-0.46084400
H	-1.08630300	-3.26102800	0.55480200
H	-1.04847600	-3.97399000	-1.05677100
H	0.38710400	-3.15184500	-0.41917900
C	1.02367700	-0.89512300	-1.99273900
H	1.58695600	-1.54002500	-1.31405500
H	1.13802400	-1.30033300	-3.00503900
H	1.49708100	0.09003900	-1.99323800
C	-0.89819600	1.51845900	-2.67250500
H	0.09689600	1.83778600	-2.34957900
H	-0.85277300	1.38206400	-3.75870600

H	-1.59515400	2.33696100	-2.47708700
C	-3.86276500	0.69895500	-1.78196900
H	-3.63302300	1.74458600	-1.99614200
H	-4.48242200	0.32225300	-2.60312300
H	-4.46635100	0.66278600	-0.87173000
C	4.18082400	0.74805400	-0.34393400
C	3.24175600	-0.02210700	0.33815900
C	3.50605300	-1.36019400	0.71309500
C	4.74712200	-1.93160400	0.41620200
C	5.69034300	-1.16641400	-0.25365700
C	5.40517400	0.15180300	-0.63043400
H	3.98218500	1.77469700	-0.61874200
H	4.96208700	-2.95584100	0.70584800
H	6.66097500	-1.59112700	-0.48908400
H	6.15957000	0.73283700	-1.15149400
C	1.38767200	-0.89391300	1.34800100
H	0.40593100	-0.86465000	1.79126200
C	2.33014300	-1.87077800	1.35812500
H	2.21325100	-2.84492300	1.81293800
N	1.90879100	0.25109200	0.72765000
C	1.21675700	1.42308800	0.53558000
N	-0.14822300	1.39580000	0.53583800
C	-0.76034000	2.60124300	0.52655100
C	-0.07001700	3.79328000	0.43540200
C	1.31126100	3.68878700	0.28528000
N	1.94643000	2.52650900	0.35069000
H	-1.84491400	2.57069700	0.56921300

H	-0.58721000	4.74419300	0.43284400
H	1.93337700	4.56491100	0.11244700
Co	-1.43706300	-0.10325500	0.00299700
C	-3.32213800	-0.14424800	3.35795600
H	-3.75893500	0.83027600	3.57457100
H	-4.13882100	-0.86818800	3.27457700
H	-2.67842600	-0.46790800	4.17592200

Zero-point correction= 0.465277 (Hartree/Particle)

Thermal correction to Energy= 0.495196

Thermal correction to Enthalpy= 0.496140

Thermal correction to Gibbs Free Energy= 0.404774

Sum of electronic and zero-point Energies= -1390.756594

Sum of electronic and thermal Energies= -1390.726674

Sum of electronic and thermal Enthalpies= -1390.725730

Sum of electronic and thermal Free Energies= -1390.817097

E(RM06L) = -1391.221871 A.U.

A-3a

1 1

Number of imaginary frequencies: 0

C	-2.95519000	-1.44152600	-0.00007400
C	-2.98639900	-0.02086800	-0.00001100
C	-4.17320300	0.69674400	-0.00009800
C	-5.35337800	-0.04692300	-0.00024300
C	-5.35163400	-1.45116000	-0.00030400
C	-4.16168700	-2.15951300	-0.00023100
C	-1.59003200	-1.83999700	0.00007500
C	-0.76869400	-0.71820600	0.00015500

H	-4.18036000	1.77902100	-0.00005900
H	-6.30244500	0.48017300	-0.00030900
H	-6.29717100	-1.98315400	-0.00041000
H	-4.15613900	-3.24517300	-0.00027200
H	-1.24428200	-2.86537300	0.00009700
C	-1.10346900	1.63736800	-0.00009100
N	-1.86119300	2.72892300	-0.00008800
C	-1.21225300	3.89255400	-0.00017800
C	0.18020900	3.98841900	-0.00018900
C	0.88552500	2.79960800	-0.00026600
N	0.26469600	1.60678000	-0.00027500
H	-1.83492900	4.78442100	-0.00013700
H	0.68938700	4.94341600	-0.00017000
H	1.97163900	2.77093400	-0.00033800
N	-1.65093600	0.39161700	0.00009100
C	1.95635800	-1.98690700	-0.00027400
C	2.31819300	-1.21521900	-1.15332000
C	2.95892500	0.00241700	-0.70814500
C	2.95797300	0.00212300	0.70970000
C	2.31669700	-1.21575600	1.15358300
C	2.08633600	-1.59247500	2.56955400
H	1.22824400	-2.25866200	2.68033300
H	2.96306700	-2.11749500	2.96877800
H	1.92238400	-0.71710700	3.20274700
C	1.39093600	-3.36022100	-0.00100000
H	0.78045300	-3.55095400	-0.88690900
H	2.19951800	-4.09943800	-0.00144500

H	0.78058700	-3.55192300	0.88478700
C	2.08942700	-1.59112500	-2.56975700
H	1.92426400	-0.71549100	-3.20228900
H	2.96741500	-2.11409700	-2.96891000
H	1.23266900	-2.25882200	-2.68169100
C	3.47569600	1.05922700	-1.61867000
H	3.82462600	1.94029600	-1.07530800
H	4.32534000	0.68406300	-2.19902200
H	2.71971800	1.38538500	-2.34068400
C	3.47338700	1.05866000	1.62129800
H	4.32205100	0.68326400	2.20292900
H	3.82323200	1.93982500	1.07868400
H	2.71627900	1.38472200	2.34217100
Co	1.02793100	-0.19897800	-0.00036100

Zero-point correction= 0.400896 (Hartree/Particle)

Thermal correction to Energy= 0.425428

Thermal correction to Enthalpy= 0.426372

Thermal correction to Gibbs Free Energy= 0.347648

Sum of electronic and zero-point Energies= -1161.701802

Sum of electronic and thermal Energies= -1161.677269

Sum of electronic and thermal Enthalpies= -1161.676325

Sum of electronic and thermal Free Energies= -1161.755049

E(RM06L) = -1162.102697 A.U.

A-3b

1 1

Number of imaginary frequencies: 0

C	1.93976400	-1.64362800	0.01245100

C	2.62332800	-0.64542300	-0.72902300
C	3.96593200	-0.38408800	-0.53908300
C	4.65502800	-1.21459500	0.34966300
C	4.00487200	-2.22221000	1.07486600
C	2.63835100	-2.42799300	0.93761600
C	0.56290300	-1.54778400	-0.35981200
C	0.45399600	-0.67772700	-1.46138400
H	4.46001900	0.42131700	-1.07259500
H	5.72296200	-1.07149700	0.48327600
H	4.57931700	-2.84345400	1.75378200
H	2.12599500	-3.20161200	1.50078200
H	-0.13346900	-0.72901900	-2.36976000
C	1.46429300	1.29151000	-0.68102700
N	2.22725000	2.34599800	-0.88642900
C	2.12458600	3.35159300	-0.00725200
C	1.28310700	3.29303400	1.09576000
C	0.50172400	2.15493200	1.22579100
N	0.55648800	1.15076800	0.33554900
H	2.74830900	4.22096700	-0.20084800
H	1.23075000	4.09301900	1.82402200
H	-0.18486600	2.01961600	2.05703700
N	1.67866600	0.13376800	-1.49869300
C	-2.49690100	-1.16251000	0.81260000
C	-2.44288300	0.20393200	1.19996600
C	-2.43198200	1.00561300	-0.00561800
C	-2.50044400	0.13258700	-1.12699000
C	-2.48415800	-1.21638000	-0.63690200

C	-2.55467000	-2.44954100	-1.46415800
H	-2.11335600	-3.30610300	-0.95017100
H	-3.59533300	-2.70330100	-1.69439100
H	-2.03494300	-2.33401200	-2.41947400
C	-2.55275000	-2.32758000	1.73176400
H	-2.04708800	-2.12393500	2.67844500
H	-3.59619600	-2.56970000	1.96747500
H	-2.10233100	-3.21908100	1.29171500
C	-2.47245300	0.70341200	2.60313600
H	-2.27581400	1.77652500	2.66485600
H	-3.46129300	0.54270700	3.04666400
H	-1.75096200	0.18693500	3.24362800
C	-2.41822600	2.48996400	-0.08403600
H	-1.77626600	2.85090000	-0.89407400
H	-3.42623800	2.87105000	-0.28179800
H	-2.08122300	2.95550000	0.84507700
C	-2.55208300	0.55615200	-2.55028600
H	-3.57411100	0.83966800	-2.82594700
H	-1.91723800	1.42556900	-2.74464300
H	-2.25292500	-0.24425100	-3.23134500
Co	-0.80179800	-0.32782100	0.04766800

Zero-point correction= 0.398248 (Hartree/Particle)

Thermal correction to Energy= 0.422994

Thermal correction to Enthalpy= 0.423939

Thermal correction to Gibbs Free Energy= 0.345048

Sum of electronic and zero-point Energies= -1161.604661

Sum of electronic and thermal Energies= -1161.579915

Sum of electronic and thermal Enthalpies= -1161.578971

Sum of electronic and thermal Free Energies= -1161.657861

E(RM06L) = -1162.002909 A.U.

A-4

1 1

Number of imaginary frequencies: 0

C	-4.40950400	-0.34042500	-0.97681900
C	-5.68571900	0.22056600	-0.72973900
C	-5.83874600	1.61627600	-0.64177300
C	-6.80779700	-0.61259300	-0.57195900
C	-7.09205700	2.16141500	-0.40191100
H	-4.96987900	2.25603100	-0.76868600
C	-8.05531700	-0.05414500	-0.33232500
H	-6.68564500	-1.68869300	-0.64365600
C	-8.20020900	1.32965000	-0.24716700
H	-7.20741600	3.23894000	-0.33863100
H	-8.91923300	-0.70044000	-0.21392300
H	-9.17906300	1.76112100	-0.06200700
C	-3.30901800	-0.82382600	-1.19933900
P	-1.72393100	-1.49979000	-1.43899600
C	-0.55099300	0.80667700	-0.17181100
C	-0.55820900	2.20205900	0.03122800
C	0.38281200	3.03277400	-0.60992300
C	-1.56564700	2.78026300	0.83153800
C	0.32844000	4.40646900	-0.42829000
H	1.14676100	2.58726500	-1.23872400
C	-1.61265800	4.15601100	0.99867800

H	-2.31103000	2.13792800	1.29366500
C	-0.66154400	4.96773200	0.37826300
H	1.06053100	5.04099900	-0.91790300
H	-2.39093100	4.59908600	1.61178900
H	-0.69864700	6.04388400	0.51768700
C	-0.71396000	-0.40740300	-0.42920800
C	-1.24169500	-1.06935100	-3.12532300
H	-1.39116600	-0.00484700	-3.31732800
H	-0.18752000	-1.31784000	-3.27621800
H	-1.84351900	-1.65079000	-3.82692300
O	-1.57921400	-2.94971200	-1.09300400
C	3.65347100	2.20397100	0.14457100
C	3.89293000	1.26530000	-0.88559400
C	4.85326800	1.45883500	-1.87226000
C	5.58521500	2.64241500	-1.81396700
C	5.36085500	3.59224100	-0.80980100
C	4.39961800	3.38566600	0.17289100
C	2.59645800	1.68413100	0.97372400
C	2.18573600	0.48120500	0.47471100
H	5.02042700	0.72185500	-2.64733600
H	6.34504100	2.82942800	-2.56621300
H	5.95036900	4.50402100	-0.79909100
H	4.23147300	4.12508700	0.95119300
H	2.16986700	2.19349500	1.82889400
C	2.76717400	-0.93131200	-1.35818400
N	3.49940400	-1.23988900	-2.42861900
C	3.21020600	-2.39399700	-3.02630700

C	2.19554200	-3.24341600	-2.59045000
C	1.47242600	-2.83601500	-1.47972600
N	1.75228000	-1.68632000	-0.84577200
H	3.81595100	-2.64196700	-3.89579800
H	1.96260100	-4.17209000	-3.09554600
H	0.62113300	-3.39541700	-1.10441000
N	2.98319100	0.21720800	-0.66733500
C	1.55694500	-0.94405300	2.77073400
C	0.16333400	-0.63936900	2.70128000
C	-0.51641200	-1.78717000	2.13562300
C	0.45643900	-2.75020200	1.78430900
C	1.75573400	-2.20084100	2.11491400
C	3.06755800	-2.87112300	1.91943900
H	3.86775500	-2.14369800	1.75680100
H	3.33802800	-3.46278300	2.80157000
H	3.05258400	-3.55297700	1.06519300
C	2.59813600	-0.16791500	3.48788200
H	2.75314400	-0.62449800	4.47290200
H	3.55649500	-0.16729600	2.96613600
H	2.30229500	0.86914500	3.65197800
C	-0.49056300	0.56741800	3.27069200
H	-1.50528400	0.69033600	2.88640700
H	-0.56500700	0.49097400	4.36168800
H	0.06587000	1.48273400	3.04503200
C	-1.98870800	-1.92802700	2.00132000
H	-2.25587700	-2.69328200	1.26974100
H	-2.42381200	-2.20822000	2.96769600

H	-2.46235900	-0.98896800	1.69728400
C	0.19513200	-4.12524200	1.28435300
H	-0.05907000	-4.77652100	2.12881500
H	-0.63759800	-4.15195700	0.57738600
H	1.07683000	-4.56230400	0.80910100
Co	0.88638600	-0.91178100	0.78988300

Zero-point correction= 0.649192 (Hartree/Particle)

Thermal correction to Energy= 0.692201

Thermal correction to Enthalpy= 0.693145

Thermal correction to Gibbs Free Energy= 0.572431

Sum of electronic and zero-point Energies= -2233.539577

Sum of electronic and thermal Energies= -2233.496568

Sum of electronic and thermal Enthalpies= -2233.495624

Sum of electronic and thermal Free Energies= -2233.616338

E(RM06L) = -2234.188769 A.U.

（S）A-5a

1 1

Number of imaginary frequencies: 0

C	-4.34772100	-0.17468100	-0.46113400
C	-5.59196300	-0.06729700	0.20621000
C	-6.25268600	1.17168000	0.28270600
C	-6.17264900	-1.19960100	0.80514000
C	-7.46878600	1.26989500	0.94378300
H	-5.80181000	2.04371800	-0.18257700
C	-7.38945700	-1.08859200	1.46323800
H	-5.66142200	-2.15585100	0.73920700
C	-8.03890000	0.14287200	1.53388600

H	-7.97610000	2.22805100	0.99773900
H	-7.83562300	-1.96619800	1.92052600
H	-8.99172100	0.22406000	2.04785400
C	-3.26937700	-0.26992000	-1.02929200
P	-1.69658700	-0.43731600	-1.77375000
C	0.11000600	1.20550600	-0.21231600
C	-0.36235100	2.59192600	-0.36062100
C	0.54704500	3.65516200	-0.46876300
C	-1.73704200	2.87496400	-0.38988100
C	0.09442400	4.95756100	-0.63988500
H	1.61648500	3.45656900	-0.43349400
C	-2.18591900	4.17949100	-0.55577600
H	-2.45018100	2.06338300	-0.25656300
C	-1.27283900	5.22418100	-0.68671400
H	0.81029300	5.76827900	-0.73609500
H	-3.25274000	4.38415300	-0.56691400
H	-1.62463300	6.24355700	-0.81170600
C	-0.48423100	0.04231300	-0.55021900
C	-1.66381000	0.79858700	-3.09546700
H	-1.92449300	1.79875100	-2.74521900
H	-0.65824400	0.82263100	-3.52451200
H	-2.36698000	0.49118100	-3.87205500
O	-1.38201900	-1.82325600	-2.27297600
C	3.19516600	1.65173600	1.79462000
C	3.72886600	1.24518600	0.54130900
C	5.10244000	1.19454500	0.29945300
C	5.93372900	1.59574300	1.33433700

C	5.42798500	2.02400500	2.57894600
C	4.06932200	2.05520800	2.82119900
C	1.79249200	1.49723800	1.72519200
C	1.44070200	0.99071900	0.47978800
H	5.49360300	0.89100700	-0.66431800
H	7.00769700	1.59042700	1.17603800
H	6.12225200	2.33358500	3.35313500
H	3.67683100	2.37774200	3.78089500
H	1.07007100	1.79287300	2.47642800
C	2.73718800	0.10390900	-1.42232800
N	3.65838400	0.36920600	-2.33456100
C	3.60865700	-0.37844200	-3.44293900
C	2.61826500	-1.33150300	-3.66334400
C	1.71761100	-1.56156000	-2.63353900
N	1.81479600	-0.88039000	-1.47870400
H	4.38049400	-0.18326400	-4.18357100
H	2.55630700	-1.88642300	-4.59120500
H	0.89412900	-2.26870800	-2.69601200
N	2.66430600	0.87312900	-0.26621500
C	1.63879100	-2.01121600	1.94478000
C	0.20957400	-1.75598700	2.04860000
C	-0.44918800	-2.53179600	1.04749800
C	0.56125300	-3.16661000	0.25184200
C	1.85431000	-2.85519200	0.83804100
C	3.17474100	-3.30711000	0.32240100
H	3.96495700	-2.58399100	0.54893600
H	3.47068000	-4.26241800	0.76977600

H	3.15763200	-3.45550900	-0.76168200
C	2.69886100	-1.47873700	2.84121200
H	3.04747700	-2.26881400	3.51588400
H	3.57505000	-1.12335400	2.28784800
H	2.34358000	-0.65220500	3.45961500
C	-0.47387100	-0.92540500	3.07722000
H	-1.26344500	-0.31071000	2.63278400
H	-0.94459800	-1.55397600	3.84161000
H	0.22214400	-0.25718800	3.58946600
C	-1.91568700	-2.69052400	0.88020700
H	-2.18605300	-2.85610800	-0.16556300
H	-2.25695200	-3.55724400	1.45952200
H	-2.46411600	-1.81759400	1.24300300
C	0.30862500	-4.11048100	-0.86585900
H	0.01726700	-5.08957500	-0.46625000
H	-0.50113500	-3.75387200	-1.50840300
H	1.20207900	-4.27308400	-1.47485200
Co	0.81897500	-1.14919800	0.20911000

Zero-point correction= 0.651106 (Hartree/Particle)

Thermal correction to Energy= 0.692598

Thermal correction to Enthalpy= 0.693542

Thermal correction to Gibbs Free Energy= 0.579140

Sum of electronic and zero-point Energies= -2233.550353

Sum of electronic and thermal Energies= -2233.508861

Sum of electronic and thermal Enthalpies= -2233.507917

Sum of electronic and thermal Free Energies= -2233.622319

E(RM06L) = -2234.201459 A.U.

（T）A-5a

1 3

Number of imaginary frequencies: 0

C	4.17829000	-0.03028000	0.36295200
C	5.45394900	-0.03153700	-0.25029400
C	6.16467200	1.17224300	-0.40637000
C	6.01678200	-1.23418200	-0.71495400
C	7.41165700	1.16682400	-1.01457000
H	5.72719100	2.09823400	-0.04488100
C	7.26483500	-1.22597700	-1.32135800
H	5.46936500	-2.16375300	-0.58774000
C	7.96317100	-0.02897300	-1.47227800
H	7.95711100	2.09787600	-1.13155800
H	7.69669500	-2.15662500	-1.67564000
H	8.93987600	-0.02816200	-1.94612300
C	3.07087000	-0.02877700	0.88260200
P	1.46576200	-0.01319600	1.55529800
C	-0.40789200	1.59090800	0.07361400
C	0.19726100	2.92492600	0.26464200
C	-0.57220400	4.02317200	0.67774000
C	1.57628200	3.10282500	0.06894900
C	0.02751800	5.25411600	0.91702000
H	-1.64209200	3.90049500	0.82488900
C	2.17178200	4.33595600	0.30572100
H	2.17162400	2.26697400	-0.29478400
C	1.39999600	5.41402700	0.73555100
H	-0.57832200	6.09220900	1.24804800

H	3.23766200	4.46211700	0.13876300
H	1.86421900	6.37858000	0.91688000
C	0.24874600	0.43966100	0.36776700
C	1.53987700	1.11376600	2.96302700
H	1.91290100	2.09547600	2.66263600
H	0.53447000	1.22573400	3.37744200
H	2.19750900	0.69627600	3.72844700
O	0.96694900	-1.41907900	1.93610500
C	-3.59105700	1.84072700	-1.79857600
C	-3.87104100	0.77962900	-0.91186500
C	-5.08645300	0.10071400	-0.92697600
C	-6.02432100	0.49575900	-1.87284800
C	-5.75876100	1.53757800	-2.77574300
C	-4.55045600	2.21512300	-2.74918500
C	-2.27764000	2.30447700	-1.49439100
C	-1.74832400	1.53047100	-0.49847300
H	-5.30288900	-0.69694900	-0.22358600
H	-6.98210400	-0.01322700	-1.91203000
H	-6.51552100	1.81538700	-3.50233100
H	-4.34752600	3.02153600	-3.44723400
H	-1.73836200	3.10447000	-1.98466300
C	-2.84838700	-0.02252000	1.15800800
N	-3.91773100	0.28883900	1.88031900
C	-4.00315200	-0.25657300	3.09540600
C	-3.01283500	-1.08242000	3.62218900
C	-1.94212900	-1.37413500	2.79493100
N	-1.88095500	-0.87854500	1.54731900

H	-4.89186100	-0.00328800	3.66943000
H	-3.07821700	-1.49174500	4.62275500
H	-1.10845700	-2.00821700	3.08407900
N	-2.72711100	0.54242900	-0.12789000
C	-1.51670100	-2.77049500	-0.99469600
C	-0.77619700	-1.88511800	-1.82613700
C	0.62487600	-2.03849400	-1.49328500
C	0.74343000	-3.07033100	-0.51337000
C	-0.57497700	-3.46846000	-0.15061800
C	-0.92424500	-4.46489400	0.89728600
H	-1.94050100	-4.31917100	1.27488100
H	-0.87471800	-5.48726100	0.50550800
H	-0.23434600	-4.41350000	1.74519400
C	-2.99521800	-2.94436500	-0.97671700
H	-3.29471900	-3.84895600	-1.51740900
H	-3.38383900	-3.04460600	0.04338800
H	-3.50678900	-2.09962800	-1.44740300
C	-1.30837000	-0.96162200	-2.86306500
H	-0.75383700	-0.01855600	-2.88397900
H	-1.22112500	-1.40750500	-3.86105700
H	-2.36440300	-0.72442900	-2.70352900
C	1.73953300	-1.33605400	-2.18351500
H	2.67810200	-1.42413600	-1.63226600
H	1.89798500	-1.76024700	-3.18195700
H	1.52873900	-0.27003100	-2.31392900
C	2.00913600	-3.56008300	0.08921800
H	2.43660200	-4.37194000	-0.51145700

H	2.75620000	-2.76409000	0.15463800
H	1.85415300	-3.93842400	1.10117800
Co	-0.48948400	-1.33648500	0.19943800

Zero-point correction= 0.648826 (Hartree/Particle)

Thermal correction to Energy= 0.691705

Thermal correction to Enthalpy= 0.692649

Thermal correction to Gibbs Free Energy= 0.570862

Sum of electronic and zero-point Energies= -2233.567611

Sum of electronic and thermal Energies= -2233.524733

Sum of electronic and thermal Enthalpies= -2233.523788

Sum of electronic and thermal Free Energies= -2233.645576

E(RM06L) = -2234.216438 A.U.

(S)A-5b

1 1

Number of imaginary frequencies: 0

C	-3.05790400	2.22890900	0.25525700
C	-4.36501600	1.88633400	-0.16899000
C	-5.24318400	1.23738000	0.71726700
C	-4.77901000	2.14310000	-1.48849900
C	-6.50816800	0.85978900	0.28805700
H	-4.91678000	1.03566400	1.73317900
C	-6.04725800	1.76248700	-1.90534800
H	-4.09867900	2.64607800	-2.16994800
C	-6.91300900	1.12089300	-1.02013600
H	-7.18296200	0.36192500	0.97789700
H	-6.36510900	1.97120900	-2.92237800
H	-7.90570600	0.82894400	-1.34943200

C	-1.93060500	2.52242400	0.63087700
P	-0.25624000	2.43397600	1.13379200
C	1.73312600	1.01276500	-0.30094000
C	2.87853200	1.89367700	-0.29016800
C	2.99451500	2.92359100	-1.23951600
C	3.92580900	1.70236700	0.62721800
C	4.11870300	3.74086100	-1.26049800
H	2.19198000	3.06826700	-1.95988700
C	5.03928200	2.53335500	0.61352200
H	3.83884500	0.91245600	1.37033000
C	5.14288700	3.55069700	-0.33475900
H	4.19482700	4.53194300	-2.00055700
H	5.82978300	2.38834900	1.34389400
H	6.01805700	4.19244300	-0.35090000
C	0.43034600	1.21731800	-0.05163900
C	0.47513700	4.04814300	0.80320700
H	1.54437800	4.02105600	1.02272700
H	0.32478700	4.35422300	-0.23423000
H	0.00294200	4.77785700	1.46424200
O	-0.05436400	1.90937100	2.52671000
C	-2.47227600	-0.91782700	-0.79418400
C	-2.17658300	-1.26652300	0.55461700
C	-3.01445200	-2.08730500	1.30970900
C	-4.17554700	-2.53025900	0.69243500
C	-4.50125800	-2.18097200	-0.63414300
C	-3.66313500	-1.38052500	-1.38424600
C	-1.40940900	-0.11896200	-1.26946000

C	-0.44724000	0.00932700	-0.26671000
H	-2.77903600	-2.33377000	2.33796200
H	-4.86168800	-3.15597400	1.25525200
H	-5.43079200	-2.54098400	-1.06338200
H	-3.91451000	-1.10252000	-2.40368800
H	-1.35945400	0.39564200	-2.22117100
C	-0.10030400	-0.99495400	1.91226000
N	-0.59209900	-1.28252800	3.10666200
C	0.30476800	-1.45515800	4.07709800
C	1.67615300	-1.33172600	3.86420800
C	2.08752200	-1.12092700	2.55916400
N	1.20710400	-0.99174200	1.55585400
H	-0.09333600	-1.69663400	5.05971800
H	2.39263800	-1.43166600	4.66958800
H	3.13813700	-1.08053900	2.28236000
N	-0.95852700	-0.69159800	0.86955800
C	1.10817000	-2.60402000	-1.61717200
C	1.65092900	-1.49485900	-2.38320400
C	2.95566400	-1.19825000	-1.87637000
C	3.17317300	-2.02545300	-0.72913000
C	2.03342900	-2.92212900	-0.60363400
C	1.85937900	-3.95997600	0.44708100
H	0.80388900	-4.12063100	0.68772900
H	2.26668200	-4.92244700	0.11791000
H	2.37719300	-3.69596600	1.37408600
C	-0.19963600	-3.27612600	-1.84504100
H	-0.86065300	-2.68347200	-2.48052400

H	-0.05338000	-4.24428600	-2.33681800
H	-0.73490200	-3.47081000	-0.90914800
C	1.03499500	-0.85082700	-3.57526800
H	1.15620400	0.23716700	-3.55048000
H	1.50617900	-1.20716200	-4.49838900
H	-0.03311100	-1.06733600	-3.64913000
C	3.92286000	-0.23141100	-2.45417400
H	4.58044000	0.20194900	-1.69557400
H	4.55790200	-0.74084100	-3.18821300
H	3.42313100	0.59266700	-2.96923300
C	4.42274600	-2.06532400	0.07691200
H	5.20514100	-2.62462600	-0.44972400
H	4.81908200	-1.06069300	0.25974500
H	4.27771600	-2.56193100	1.04002600
Co	1.51994600	-0.89179600	-0.45010700

Zero-point correction= 0.649309 (Hartree/Particle)

Thermal correction to Energy= 0.691833

Thermal correction to Enthalpy= 0.692777

Thermal correction to Gibbs Free Energy= 0.574431

Sum of electronic and zero-point Energies= -2233.552645

Sum of electronic and thermal Energies= -2233.510120

Sum of electronic and thermal Enthalpies= -2233.509176

Sum of electronic and thermal Free Energies= -2233.627522

E(RM06L) = -2234.201953 A.U.

A-5c

1 1

Number of imaginary frequencies: 0

C	-2.79010900	-0.91338000	-1.02759400
C	-4.07614900	-0.44061000	-1.32895700
C	-4.22266200	0.73050000	-2.10625700
C	-5.22639300	-1.12510500	-0.87932700
C	-5.48949100	1.20305700	-2.41001600
H	-3.33245400	1.23707100	-2.46831500
C	-6.48621000	-0.64011000	-1.18920200
H	-5.10916500	-2.03392300	-0.29507800
C	-6.61834400	0.52241300	-1.95138000
H	-5.60213200	2.09902500	-3.01174500
H	-7.36967500	-1.16720300	-0.84412200
H	-7.60830400	0.89587000	-2.19507100
C	-1.62771900	-1.25120800	-0.73874900
P	-0.14167200	-2.07477700	-1.36340300
C	0.88934500	-1.19724400	-0.19517500
C	3.12185700	-1.29367800	-1.40468100
C	4.03378900	-0.41225900	-2.00808700
C	3.11859300	-2.63581600	-1.80537800
C	4.89389500	-0.86004900	-3.00238500
H	4.04723200	0.63723900	-1.71931100
C	3.97777600	-3.08118300	-2.80109200
H	2.44778300	-3.33368400	-1.31002500
C	4.86667800	-2.19425200	-3.40361000
H	5.58132600	-0.16368400	-3.47249700
H	3.96151600	-4.12453800	-3.09976200
H	5.54053100	-2.54243500	-4.17997700
C	2.16265100	-0.82021400	-0.39389700

C	-0.37542400	-3.77159000	-0.76631800
H	-0.48801700	-3.79925800	0.31859000
H	-1.26777200	-4.19083900	-1.23605800
H	0.48338900	-4.37890200	-1.06124000
O	0.08299400	-1.95633100	-2.83319400
C	-0.56628300	3.22477800	-0.69952400
C	0.80250000	3.17072600	-0.37442000
C	1.66558600	4.22728600	-0.63597900
C	1.11915100	5.37406500	-1.20916600
C	-0.24179600	5.45560000	-1.51939700
C	-1.09168200	4.38388600	-1.27513200
C	-1.14045600	1.95797500	-0.34927800
C	-0.18492100	1.11638300	0.14093400
H	2.71909200	4.18440300	-0.39164200
H	1.76821700	6.21965500	-1.41252300
H	-0.63472800	6.36512800	-1.96309500
H	-2.14543100	4.43740000	-1.53480600
H	-2.18993200	1.69902700	-0.41822600
C	2.25071500	1.48166900	0.63778000
N	2.98176100	2.42503500	1.24318700
C	4.14728800	2.11123500	1.77966600
C	4.65742700	0.80574500	1.77506200
C	3.92212700	-0.12533700	1.09434000
N	2.73784300	0.19226600	0.49815100
H	4.69574700	2.92869300	2.24351800
H	5.59280500	0.54064400	2.24990800
H	4.23320200	-1.15543100	0.95807900

N	1.04991600	1.85185300	0.11827200
C	-0.92397300	0.37074500	2.76223400
C	-2.04441300	-0.39604000	2.37113000
C	-1.63009500	-1.78586200	2.29074200
C	-0.25358800	-1.86277500	2.60284800
C	0.21060000	-0.51842400	2.85055000
C	1.53754800	-0.17632800	3.42701100
H	1.84641900	0.84768600	3.19687800
H	1.50029900	-0.25024300	4.52126000
H	2.31788700	-0.86526100	3.09266700
C	-0.90254400	1.82963200	3.04871700
H	-1.67933700	2.36241400	2.49557600
H	-1.07130900	2.00734000	4.11706600
H	0.05720300	2.28709600	2.78905500
C	-3.42865900	0.10970300	2.16413900
H	-4.03266500	-0.59165000	1.58258900
H	-3.94128700	0.26317000	3.12096600
H	-3.43663100	1.07004400	1.63785700
C	-2.55481200	-2.91302300	1.99343800
H	-2.04087300	-3.87637500	1.96628900
H	-3.32969100	-2.97877000	2.76499100
H	-3.06452900	-2.77915600	1.03299600
C	0.60252600	-3.07755000	2.70737900
H	0.96044200	-3.21214700	3.73412100
H	0.06416900	-3.98845000	2.43610300
H	1.48648800	-3.01052600	2.06159500
Co	-0.50041800	-0.57968000	0.93951500

Zero-point correction= 0.649462 (Hartree/Particle)

Thermal correction to Energy= 0.691534

Thermal correction to Enthalpy= 0.692478

Thermal correction to Gibbs Free Energy= 0.575691

Sum of electronic and zero-point Energies= -2233.509458

Sum of electronic and thermal Energies= -2233.467386

Sum of electronic and thermal Enthalpies= -2233.466442

Sum of electronic and thermal Free Energies= -2233.583230

E(RM06L) = -2234.158920 A.U.

A-5d

1 1

Number of imaginary frequencies: 0

C	-3.09431000	1.73296200	-0.76850900
C	-4.23384900	0.96312600	-1.10605400
C	-5.45937000	1.17836700	-0.45019300
C	-4.14113000	-0.03021300	-2.09667500
C	-6.56684900	0.41253900	-0.78586900
H	-5.52708100	1.94962500	0.31080000
C	-5.25631200	-0.78825900	-2.42304400
H	-3.18965300	-0.19916000	-2.59296600
C	-6.46847800	-0.56962100	-1.77080000
H	-7.51249800	0.58498800	-0.28133000
H	-5.17796100	-1.55788800	-3.18510600
H	-7.33897300	-1.16426000	-2.03136300
C	-2.11249400	2.41162700	-0.49996900
P	-0.65145400	3.22551500	-0.00043000
C	1.26019300	1.06540900	-0.17910800

C	1.94894300	1.15901600	-1.44347800
C	1.71085800	0.15714300	-2.42325000
C	3.00658300	2.08318100	-1.65848800
C	2.52429000	0.09194400	-3.56546600
H	0.82357200	-0.46114500	-2.35043300
C	3.76382100	2.02118100	-2.80832000
H	3.19170900	2.85009500	-0.91007500
C	3.53705000	1.01331000	-3.76353000
H	2.31908000	-0.66432800	-4.31769300
H	4.54470200	2.75700300	-2.97759300
H	4.14277800	0.97625600	-4.66347500
C	0.37235900	1.79773900	0.49390600
C	0.08002900	3.88898600	-1.50539500
H	1.05817500	4.32124900	-1.28621900
H	0.17781800	3.12903900	-2.28356100
H	-0.57495500	4.68342200	-1.86871700
O	-0.81410900	4.17960700	1.14366600
C	-1.70974200	-2.40945200	-0.52485600
C	-2.00633100	-1.58943800	0.58125100
C	-3.26517800	-1.57319400	1.17194600
C	-4.22512100	-2.43984100	0.65690000
C	-3.94030100	-3.28547400	-0.42091400
C	-2.69056400	-3.27076900	-1.02617900
C	-0.35717500	-2.12979800	-0.91132300
C	0.18477200	-1.16575000	-0.10723800
H	-3.49827800	-0.92721900	2.00901500
H	-5.21503100	-2.45179700	1.10232300

H	-4.71271300	-3.95073000	-0.79563300
H	-2.47566300	-3.91046700	-1.87753900
H	0.19414400	-2.64226300	-1.69193300
C	-0.77219700	0.07145700	1.87686700
N	-1.40731800	-0.25044900	3.00293300
C	-1.34505200	0.56877700	4.04314300
C	-0.60585100	1.75352500	4.03623700
C	0.00318500	2.08900900	2.85275700
N	-0.08975700	1.27107600	1.76596800
H	-1.89700200	0.25617700	4.92721100
H	-0.53405300	2.40244900	4.89884600
H	0.54932100	3.00864100	2.68610500
N	-0.84720000	-0.79733500	0.82564100
C	2.54913900	-2.38374300	0.90255100
C	3.42620300	-2.17940100	-0.18237700
C	4.10892000	-0.91544000	0.02855700
C	3.64102400	-0.33794000	1.23531400
C	2.62499900	-1.21046800	1.76273700
C	1.95819000	-1.08622700	3.08527400
H	0.99321800	-1.59971500	3.10880200
H	2.57850300	-1.54496100	3.86512300
H	1.80721800	-0.04250900	3.37783200
C	1.71122400	-3.58191200	1.16551400
H	1.46754800	-4.12034400	0.24723600
H	2.24792100	-4.27444200	1.82428900
H	0.76710300	-3.32663700	1.65382800
C	3.66009800	-3.09090200	-1.33528400

H	3.80693400	-2.53495400	-2.26631100
H	4.55951800	-3.69829700	-1.18035100
H	2.82532800	-3.78033300	-1.48311100
C	5.17269800	-0.38592600	-0.86241100
H	5.40700600	0.65963000	-0.65332000
H	6.09404900	-0.96433400	-0.72723900
H	4.89958100	-0.46452100	-1.91905600
C	4.08529600	0.94982900	1.83386800
H	4.92259600	0.79784200	2.52405800
H	4.42088100	1.65631100	1.06923000
H	3.28215300	1.43078200	2.39986100
Co	2.02926600	-0.61029600	-0.05980600

Zero-point correction= 0.649776 (Hartree/Particle)

Thermal correction to Energy= 0.691888

Thermal correction to Enthalpy= 0.692832

Thermal correction to Gibbs Free Energy= 0.575672

Sum of electronic and zero-point Energies= -2233.506832

Sum of electronic and thermal Energies= -2233.464720

Sum of electronic and thermal Enthalpies= -2233.463776

Sum of electronic and thermal Free Energies= -2233.580936

E(RM06L) = -2234.156608 A.U.

A-6

1 1

Number of imaginary frequencies: 0

C	-0.47358200	-1.73088700	-0.38834200
C	-1.56009700	-1.60558500	-1.38963800
C	-1.52165700	-0.58885500	-2.35390500

C	-2.66960400	-2.45814200	-1.35390100
C	-2.57654400	-0.40967700	-3.24033700
H	-0.66923200	0.08743600	-2.36906700
C	-3.71424400	-2.29302800	-2.25567200
H	-2.69760800	-3.25778800	-0.61733200
C	-3.67704600	-1.26326100	-3.19401800
H	-2.54107600	0.39717200	-3.96792600
H	-4.56372400	-2.96890100	-2.22348700
H	-4.49991800	-1.13014100	-3.88993700
C	-0.72204700	-2.08130500	0.87768100
P	-1.44954300	-2.58421600	2.22498100
C	-2.37420800	1.13891900	0.40381600
C	-1.14484600	1.29416400	0.46667500
C	-1.87021700	-1.22938300	3.34575100
H	-1.26853300	-1.28477300	4.25570000
H	-1.72585800	-0.27191200	2.83674300
H	-2.91843700	-1.32924900	3.63809900
O	-1.64510000	-3.96195800	2.76343900
C	2.78395800	-1.92327900	-2.06557200
C	3.16778200	-1.64529400	-0.73070600
C	4.50250400	-1.60773400	-0.33240700
C	5.45943400	-1.87104500	-1.30569200
C	5.10188400	-2.15589600	-2.63468300
C	3.77341800	-2.18573300	-3.02461300
C	1.36547100	-1.83921500	-2.12434500
C	0.88794700	-1.51071700	-0.87399300
H	4.78166400	-1.42454300	0.69930800

H	6.50807700	-1.87298900	-1.02540500
H	5.88142000	-2.36239700	-3.36082100
H	3.49731600	-2.40619400	-4.05133500
H	0.73492500	-2.09315700	-2.96560700
C	1.95843100	-0.92867500	1.30309000
N	2.70099100	-1.58214100	2.18879700
C	2.57633200	-1.22443400	3.46567700
C	1.67713800	-0.24344800	3.87954100
C	1.01600500	0.44853800	2.87938900
N	1.19822800	0.16136700	1.57777500
H	3.20578200	-1.75513400	4.17641200
H	1.52831400	0.00042800	4.92442900
H	0.34126700	1.27528300	3.08788300
N	2.00224800	-1.35875500	-0.01597100
C	2.54044900	2.39010500	0.08712800
C	2.01456200	2.16620700	-1.20997300
C	0.73203200	2.83773100	-1.30470000
C	0.49855300	3.51710800	-0.07397800
C	1.59316000	3.19780600	0.81403400
C	1.75072500	3.68911700	2.20560700
H	2.35582700	3.01246200	2.81509400
H	2.26003600	4.66050500	2.20867700
H	0.78647800	3.83308100	2.70030800
C	3.81521000	1.85713700	0.63640500
H	4.15731200	0.97333300	0.09041700
H	4.60922100	2.60886900	0.57210100
H	3.72057800	1.58509700	1.69300800

C	2.64659600	1.39873700	-2.30887500
H	1.93056000	0.74529600	-2.81660500
H	3.03843400	2.09243900	-3.06252700
H	3.47895700	0.78106600	-1.96515200
C	-0.16150400	2.86777300	-2.49314200
H	-1.20825900	2.72129500	-2.20787600
H	-0.08804300	3.83380800	-3.00550800
H	0.10147800	2.09409100	-3.21825900
C	-0.65533200	4.39787800	0.23464400
H	-0.41197000	5.43157400	-0.03750100
H	-1.54397300	4.10249300	-0.32614500
H	-0.91050700	4.38617100	1.29607900
Co	0.64615300	1.52671000	0.23923500
C	-3.75071800	0.87527900	0.25040200
C	-4.29984000	-0.34432100	0.69902700
C	-4.59486800	1.80599500	-0.39240300
C	-5.64536400	-0.61927200	0.51507700
H	-3.63541400	-1.07371700	1.15544300
C	-5.94022000	1.52522200	-0.56892100
H	-4.17295900	2.74339700	-0.74522300
C	-6.46823300	0.31466000	-0.11537600
H	-6.05635000	-1.56482200	0.85573800
H	-6.58378000	2.24714100	-1.06191500
H	-7.52301100	0.09857300	-0.25610800

Zero-point correction= 0.648045 (Hartree/Particle)

Thermal correction to Energy= 0.691405

Thermal correction to Enthalpy= 0.692349

Thermal correction to Gibbs Free Energy= 0.572301

Sum of electronic and zero-point Energies= -2233.488267

Sum of electronic and thermal Energies= -2233.444907

Sum of electronic and thermal Enthalpies= -2233.443963

Sum of electronic and thermal Free Energies= -2233.564012

E(RM06L) = -2234.136313 A.U.

A-7

1 1

Number of imaginary frequencies: 0

C	-1.60220300	1.50082700	0.15133000
C	-2.44290600	2.71949400	0.03601400
C	-2.16707300	3.68095600	-0.94691800
C	-3.50812200	2.94913600	0.91933700
C	-2.92394800	4.84294600	-1.03894300
H	-1.37631900	3.48843300	-1.66857700
C	-4.25514100	4.11816200	0.83508800
H	-3.72957400	2.21345100	1.68775100
C	-3.96564200	5.06837700	-0.14191400
H	-2.70810500	5.56850200	-1.81759400
H	-5.06298600	4.29068500	1.53955000
H	-4.55339000	5.97865900	-0.20754300
C	-0.24108300	1.73175000	0.16151500
P	0.88254000	3.05878400	0.24598200
C	2.13054400	0.35231300	0.22558100
C	3.49767600	0.55168400	0.63666600
C	3.95156800	1.77066400	1.18672700
C	4.40525700	-0.52280000	0.56030700

C	5.27041400	1.90580200	1.59376800
H	3.26115100	2.59960400	1.32416300
C	5.72086400	-0.38504700	0.97751200
H	4.04411000	-1.47071200	0.16947100
C	6.16100700	0.83607500	1.48642400
H	5.60557300	2.85010000	2.01177200
H	6.40406100	-1.22645400	0.90967300
H	7.18993900	0.95016400	1.81346000
C	1.11398300	1.25602400	0.18440800
C	1.33167200	3.80952400	-1.33458200
H	2.41546500	3.94675800	-1.36415100
H	1.01797800	3.18754500	-2.17428600
H	0.86345900	4.79377500	-1.40757400
O	1.22234600	3.87924700	1.44904900
C	-4.06255700	-1.21125800	-0.05616700
C	-3.00076200	-1.87817600	0.59648400
C	-3.10193000	-3.20426000	1.01236000
C	-4.28914000	-3.86782400	0.73370200
C	-5.34705800	-3.23255400	0.05748500
C	-5.24735700	-1.91225300	-0.34065600
C	-3.63283400	0.11687600	-0.27644700
C	-2.33595800	0.26437600	0.19393500
H	-2.29493400	-3.69985900	1.54381600
H	-4.40299200	-4.90066700	1.04736700
H	-6.25556600	-3.79007200	-0.14549900
H	-6.06696000	-1.41913600	-0.85411100
H	-4.19109800	0.90660200	-0.75883500

C	-0.91688200	-1.25930700	1.64528900
N	-1.33835700	-1.47341100	2.88749500
C	-0.42309300	-1.81752000	3.79327200
C	0.92308500	-1.95252700	3.46899300
C	1.27430500	-1.68745000	2.15895900
N	0.35883000	-1.34946400	1.22401800
H	-0.78579900	-1.97898600	4.80593300
H	1.66984400	-2.23176800	4.20206600
H	2.30389700	-1.73373400	1.81539100
N	-1.91642100	-0.99925400	0.68684000
C	-0.10953300	-1.57863600	-2.24677600
C	0.96516600	-0.70055300	-2.63160400
C	2.21940100	-1.28110100	-2.24351100
C	1.92024900	-2.47971500	-1.52093800
C	0.47746000	-2.65451700	-1.54207300
C	-0.22510300	-3.81110600	-0.92986500
H	-1.29653700	-3.63039900	-0.81990800
H	-0.10328700	-4.70196800	-1.55682800
H	0.18337800	-4.06310400	0.05467800
C	-1.54111100	-1.39206700	-2.59977000
H	-1.84312500	-0.34198600	-2.54539900
H	-1.72810800	-1.72794600	-3.62662900
H	-2.20550600	-1.96219400	-1.94528800
C	0.78732200	0.59013900	-3.34630900
H	1.68327000	1.21302300	-3.28762400
H	0.57478000	0.41771700	-4.40792800
H	-0.06006900	1.15607800	-2.94132500

C	3.55532100	-0.73126700	-2.60214400
H	4.36934900	-1.27070000	-2.11523500
H	3.71263000	-0.80088400	-3.68402700
H	3.65485900	0.32309300	-2.32535900
C	2.87208700	-3.49382000	-0.99031100
H	2.78633200	-4.43114400	-1.55260000
H	3.91079100	-3.16597900	-1.06964600
H	2.67659100	-3.74280500	0.05863600
Co	1.04311200	-0.88232400	-0.61243400

Zero-point correction= 0.650196 (Hartree/Particle)

Thermal correction to Energy= 0.692075

Thermal correction to Enthalpy= 0.693019

Thermal correction to Gibbs Free Energy= 0.576307

Sum of electronic and zero-point Energies= -2233.531917

Sum of electronic and thermal Energies= -2233.490038

Sum of electronic and thermal Enthalpies= -2233.489094

Sum of electronic and thermal Free Energies= -2233.605806

E(RM06L) = -2234.182114 A.U.

(S)A-8

1 1

Number of imaginary frequencies: 0

C	-1.77449300	1.40652900	0.02574400
C	-2.67222800	2.54270300	-0.21232300
C	-2.38088600	3.46222600	-1.24749300
C	-3.76848100	2.79899700	0.62454200
C	-3.14205900	4.62327500	-1.40385600
H	-1.66156400	3.18376200	-2.01530000

C	-4.51526600	3.95854300	0.46638000
H	-3.99442400	2.10343300	1.42761000
C	-4.19823700	4.87688200	-0.53945100
H	-2.92152100	5.30824900	-2.21633000
H	-5.34089600	4.16045000	1.14155900
H	-4.79091400	5.77875800	-0.65532900
C	-0.40371600	1.65306300	0.00913900
P	0.14255000	3.36896900	-0.03919900
C	1.95747800	0.48831500	0.15598300
C	3.23298800	0.96321100	0.60789900
C	3.36474600	2.22079300	1.23929700
C	4.37879300	0.15228200	0.49424800
C	4.60056800	2.65062500	1.70323700
H	2.48506100	2.83918400	1.40316900
C	5.61271000	0.59068900	0.95010700
H	4.26621800	-0.83027600	0.04308000
C	5.72884300	1.84501100	1.55090500
H	4.68318900	3.61630100	2.19257100
H	6.48671600	-0.04565900	0.84762900
H	6.69327800	2.18675000	1.91381200
C	0.69150100	0.78765300	-0.03353900
C	1.42130900	3.59387000	-1.30339700
H	2.39881800	3.28686900	-0.91375800
H	1.18545800	3.01549000	-2.19940600
H	1.47537100	4.65537500	-1.55186100
O	0.35325200	4.16812400	1.20670800
C	-3.82822900	-1.62817700	0.13289500

C	-2.64351900	-2.06059100	0.77772400
C	-2.48535900	-3.35641900	1.26699100
C	-3.53303000	-4.24169500	1.05497900
C	-4.70547300	-3.84705900	0.38166000
C	-4.86651000	-2.55271000	-0.07733400
C	-3.64270300	-0.26182600	-0.18147600
C	-2.37673900	0.12401300	0.24058400
H	-1.58306700	-3.66372900	1.79003400
H	-3.44712900	-5.26127400	1.41753800
H	-5.49740100	-4.57356400	0.23181900
H	-5.77723500	-2.25045300	-0.58531300
H	-4.32606900	0.38192100	-0.71822700
C	-0.69297200	-1.05317000	1.74807200
N	-0.99518300	-0.73314500	2.99681500
C	-0.04562700	-0.94719600	3.91383700
C	1.17621100	-1.53116600	3.59600900
C	1.41207800	-1.78908500	2.25444700
N	0.48866300	-1.52797500	1.31401100
H	-0.28410200	-0.64681400	4.93146600
H	1.92778100	-1.73711600	4.34834200
H	2.36292200	-2.17199000	1.89238000
N	-1.74122500	-1.00373500	0.79448100
C	0.05436100	-2.08970700	-2.05016400
C	0.77181100	-0.97421600	-2.57061500
C	2.17893200	-1.15793500	-2.29338800
C	2.33307200	-2.39335500	-1.58665300
C	1.01541900	-2.93498600	-1.40340400

C	0.71138500	-4.20628100	-0.69185400
H	-0.31340300	-4.22303600	-0.30981700
H	0.82133200	-5.06198800	-1.36799800
H	1.39160200	-4.37703500	0.14837300
C	-1.39857100	-2.35117000	-2.23043000
H	-1.99932100	-1.44566200	-2.09612200
H	-1.59974900	-2.72335300	-3.24242900
H	-1.77376400	-3.10280500	-1.53154700
C	0.16483600	0.17347400	-3.29739000
H	0.83558600	1.03684800	-3.32086400
H	-0.05383600	-0.09320800	-4.33800900
H	-0.78040100	0.48503800	-2.83773700
C	3.25966600	-0.24705900	-2.76203800
H	4.20820300	-0.43692800	-2.25515100
H	3.42877800	-0.36866700	-3.83791600
H	3.00763300	0.80473400	-2.59105600
C	3.60222200	-3.08026400	-1.21580000
H	3.76794800	-3.96170400	-1.84686100
H	4.47215000	-2.43153700	-1.34491900
H	3.60246300	-3.43563600	-0.17967700
Co	1.10538000	-1.04721400	-0.56077900

Zero-point correction= 0.649106 (Hartree/Particle)

Thermal correction to Energy= 0.691442

Thermal correction to Enthalpy= 0.692386

Thermal correction to Gibbs Free Energy= 0.574566

Sum of electronic and zero-point Energies= -2233.532214

Sum of electronic and thermal Energies= -2233.489878

Sum of electronic and thermal Enthalpies= -2233.488934

Sum of electronic and thermal Free Energies= -2233.606754

E(RM06L) = -2234.181320 A.U.

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1 3

Number of imaginary frequencies: 0

C	-2.06093400	1.08353600	0.03799600
C	-3.29542100	1.88060700	-0.09751900
C	-3.46347500	2.75377000	-1.18439500
C	-4.31599000	1.79226600	0.86061600
C	-4.61235600	3.52878100	-1.30231000
H	-2.70314700	2.77962500	-1.96312600
C	-5.45765000	2.57607200	0.74691400
H	-4.19055300	1.12421400	1.70874600
C	-5.60841600	3.44519400	-0.33294500
H	-4.73412500	4.18873300	-2.15559400
H	-6.23139000	2.51302100	1.50579300
H	-6.50461900	4.05136700	-0.42174600
C	-0.82941600	1.68528000	-0.12612100
P	-0.66273400	3.52713500	-0.10444100
C	1.70343400	1.03149400	0.02619800
C	2.98162600	1.48278500	0.48224700
C	3.14739700	2.83254900	0.85750200
C	4.07819200	0.60901100	0.58926900
C	4.38293900	3.27653100	1.30890700
H	2.29577800	3.50719400	0.81884400
C	5.30800600	1.06355900	1.04451300

H	3.94238800	-0.42903800	0.30119500
C	5.46583600	2.40206800	1.40099200
H	4.49943500	4.31677000	1.59746400
H	6.14582200	0.37604300	1.11806200
H	6.42760300	2.76158100	1.75353600
C	0.44135200	1.06904700	-0.12957500
C	0.12507000	3.93461000	-1.70358400
H	1.09322600	3.42472600	-1.77146300
H	-0.50174300	3.62962300	-2.54526900
H	0.29762100	5.01053800	-1.75827300
O	0.18066900	3.98470300	1.06865700
C	-3.11608700	-2.43348900	0.29425500
C	-1.80895000	-2.49395500	0.82470900
C	-1.25240100	-3.67072300	1.31017100
C	-2.01813500	-4.82715000	1.19589300
C	-3.30080300	-4.80133800	0.62544100
C	-3.86153300	-3.61542200	0.17723500
C	-3.37000500	-1.07084200	-0.02365100
C	-2.25936200	-0.32170900	0.29960400
H	-0.25761400	-3.69588900	1.74593200
H	-1.61343100	-5.76779600	1.55612200
H	-3.86488100	-5.72520800	0.54937600
H	-4.86170000	-3.59583600	-0.24460900
H	-4.25465800	-0.67049500	-0.49997000
C	-0.31432000	-0.88741900	1.80253000
N	-0.73604800	-0.37482300	2.94061300
C	0.20010900	-0.20582000	3.88508900

C	1.51942600	-0.60915300	3.70914600
C	1.86699700	-1.10363400	2.45995800
N	0.95468100	-1.21619300	1.48264900
H	-0.13208400	0.25599600	4.81145400
H	2.25782500	-0.50437200	4.49440200
H	2.88764600	-1.37518600	2.20607400
N	-1.25385700	-1.19727100	0.78309700
C	0.35007200	-1.94251300	-2.20271300
C	0.91477200	-0.69952600	-2.59265900
C	2.33755900	-0.71722000	-2.25672700
C	2.61045500	-1.93221800	-1.59482300
C	1.36740100	-2.67033900	-1.50815700
C	1.26238200	-4.04079600	-0.93980400
H	0.22716700	-4.34985900	-0.78448000
H	1.72703400	-4.76725500	-1.61714200
H	1.78652200	-4.12389000	0.01815100
C	-1.05341700	-2.37305400	-2.43812500
H	-1.76817200	-1.56708400	-2.24260900
H	-1.18873900	-2.67450000	-3.48299600
H	-1.33345700	-3.22481100	-1.81383700
C	0.22613000	0.39069200	-3.33303500
H	0.65624700	1.36756600	-3.09459700
H	0.31994200	0.24930900	-4.41627100
H	-0.84229500	0.42698000	-3.09755800
C	3.30100800	0.34017000	-2.65887400
H	4.25435900	0.25696000	-2.13330900
H	3.50307400	0.27221000	-3.73416700

H	2.90876300	1.34427900	-2.46968200
C	3.92846900	-2.46657200	-1.15146700
H	4.21167500	-3.33608300	-1.75581700
H	4.72822900	-1.72965500	-1.25344700
H	3.91264300	-2.80754200	-0.10976300
Co	1.09341000	-0.83517200	-0.53417800

Zero-point correction= 0.648827 (Hartree/Particle)

Thermal correction to Energy= 0.691367

Thermal correction to Enthalpy= 0.692311

Thermal correction to Gibbs Free Energy= 0.573410

Sum of electronic and zero-point Energies= -2233.538749

Sum of electronic and thermal Energies= -2233.496209

Sum of electronic and thermal Enthalpies= -2233.495264

Sum of electronic and thermal Free Energies= -2233.614166

E(RM06L) = -2234.187576 A.U.

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1 1

Number of imaginary frequencies: 0

C	-1.57619900	-0.29707500	1.04855400
C	-2.95110100	-0.58513200	1.45792900
C	-3.41106900	-1.89581000	1.67445300
C	-3.86069600	0.47525400	1.62543300
C	-4.72947600	-2.12761300	2.04116500
H	-2.75598000	-2.74373800	1.50049300
C	-5.17897100	0.23746400	1.99269500
H	-3.52931700	1.50023900	1.47024400
C	-5.61945100	-1.06634500	2.20356700

H	-5.06803900	-3.14841900	2.19132100
H	-5.86070700	1.07304700	2.11906300
H	-6.64900600	-1.25554200	2.49175700
C	-0.51744100	-1.15239800	0.97173500
P	-0.26255000	-2.93561000	0.66793500
C	1.07366700	-2.08411200	-0.22050700
C	2.02263100	-2.52141600	-1.20791900
C	2.58148700	-1.60826300	-2.11986000
C	2.40777800	-3.87253900	-1.29006200
C	3.52577300	-2.02066400	-3.04967600
H	2.23720300	-0.57506000	-2.09651500
C	3.35353400	-4.28212200	-2.21931300
H	1.96377500	-4.59695900	-0.61089000
C	3.92015200	-3.35811800	-3.09776800
H	3.94402000	-1.30477100	-3.75238500
H	3.64755000	-5.32608800	-2.26585700
H	4.65077000	-3.68345700	-3.83180500
C	0.74625100	-0.84663900	0.30619500
C	0.43365300	-3.68930500	2.16842200
H	0.89647300	-4.64677400	1.91881400
H	1.17393000	-3.04599300	2.65054000
H	-0.37892100	-3.88552000	2.87221000
O	-1.28949000	-3.79804300	0.00636500
C	-0.41896700	2.98955700	-0.29893400
C	-1.42957600	2.59213100	-1.19478000
C	-1.82262400	3.35423600	-2.28671400
C	-1.18505100	4.57906100	-2.46099500

C	-0.20563300	5.01991900	-1.56478300
C	0.18240900	4.23461200	-0.48428900
C	-0.26338800	1.91897000	0.69099600
C	-1.28137700	0.97261200	0.38413700
H	-2.61524300	3.02442700	-2.94761700
H	-1.47062300	5.21054800	-3.29591400
H	0.25198700	5.99336200	-1.71059900
H	0.93583900	4.59439300	0.20894600
H	-0.09434300	2.13381700	1.74417000
C	-2.83949400	0.51522200	-1.46759400
N	-3.93636100	1.11992600	-1.90417400
C	-4.82203400	0.30300300	-2.48969200
C	-4.61250600	-1.06624800	-2.60473200
C	-3.39492500	-1.55593300	-2.14113600
N	-2.48064500	-0.75743100	-1.58229000
H	-5.72898000	0.77213000	-2.86474600
H	-5.35400100	-1.71753300	-3.05203300
H	-3.12595200	-2.60778500	-2.21142700
N	-1.91479400	1.34274500	-0.75599400
C	3.32141300	0.03848500	1.26332900
C	3.65854200	0.98599700	0.26625100
C	3.17851100	2.29612700	0.67849800
C	2.52594900	2.15287900	1.91079500
C	2.51320200	0.73513500	2.24099800
C	1.91295600	0.13936400	3.46039200
H	1.71970700	-0.92802600	3.32920900
H	2.58534900	0.25140400	4.31988700

H	0.96536000	0.61659300	3.72649700
C	3.78644600	-1.36861200	1.35068800
H	4.03745500	-1.78195700	0.37168400
H	4.68758300	-1.41367700	1.97315500
H	3.04038700	-2.02374600	1.80672600
C	4.49834600	0.77510000	-0.93970300
H	4.05485800	1.22363900	-1.83490000
H	5.46926100	1.26517900	-0.79572300
H	4.68034800	-0.28033400	-1.14290100
C	3.44680600	3.54355800	-0.08551800
H	3.12607600	4.43415600	0.45758600
H	4.52081300	3.64533000	-0.27579300
H	2.95019200	3.55039400	-1.06199300
C	1.94937300	3.22779400	2.75953300
H	2.70775400	3.58544500	3.46518400
H	1.61317400	4.09062100	2.18013900
H	1.10782700	2.87739800	3.36312200
Co	1.58247300	0.86949200	0.50321800

Zero-point correction= 0.650474 (Hartree/Particle)

Thermal correction to Energy= 0.692356

Thermal correction to Enthalpy= 0.693300

Thermal correction to Gibbs Free Energy= 0.576387

Sum of electronic and zero-point Energies= -2233.546879

Sum of electronic and thermal Energies= -2233.504998

Sum of electronic and thermal Enthalpies= -2233.504053

Sum of electronic and thermal Free Energies= -2233.620966

E(RM06L) = -2234.197353 A.U.

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1 3

Number of imaginary frequencies: 0

C	1.60423400	-0.31688000	-1.05794800
C	2.98537000	-0.59256500	-1.45553300
C	3.46329600	-1.90015300	-1.65207700
C	3.88188900	0.47765300	-1.63253800
C	4.78674600	-2.11959200	-2.00760300
H	2.81823600	-2.75432400	-1.47159700
C	5.20506600	0.25204900	-1.98899800
H	3.53611200	1.50033400	-1.49594800
C	5.66360800	-1.04882200	-2.17890800
H	5.13944100	-3.13767400	-2.14252400
H	5.87638500	1.09456300	-2.12416700
H	6.69718800	-1.22833600	-2.45874300
C	0.55388500	-1.18536700	-1.00242100
P	0.31119900	-2.97346700	-0.69721200
C	-1.04077700	-2.13662300	0.18896500
C	-1.99826500	-2.56511900	1.17102400
C	-2.56434600	-1.64017600	2.06789700
C	-2.38904600	-3.91333000	1.25941100
C	-3.52125500	-2.04132000	2.98971200
H	-2.21946900	-0.60655500	2.04148200
C	-3.34802700	-4.31091000	2.18037900
H	-1.94097300	-4.64475300	0.59068000
C	-3.92129000	-3.37696600	3.04374100
H	-3.94473200	-1.31771300	3.68107600

H	-3.64759300	-5.35298500	2.23186400
H	-4.66263500	-3.69297000	3.77102200
C	-0.70815800	-0.90578200	-0.33828300
C	-0.38334000	-3.73927300	-2.19054000
H	-0.81614900	-4.70912100	-1.93535100
H	-1.14699900	-3.11261500	-2.65657700
H	0.42440800	-3.91182700	-2.90577800
O	1.34510200	-3.81748700	-0.02422600
C	0.46152600	3.00746900	0.21090700
C	1.46026500	2.61971800	1.12710800
C	1.84507200	3.40564500	2.20601600
C	1.21801300	4.64036000	2.33985100
C	0.25553800	5.07157200	1.41922500
C	-0.12818100	4.26542100	0.35398900
C	0.30478400	1.91598800	-0.74761700
C	1.29897000	0.96057900	-0.41006800
H	2.62549600	3.08517600	2.88564700
H	1.50018800	5.28989300	3.16201300
H	-0.19005600	6.05458400	1.53434500
H	-0.86626400	4.61666100	-0.36000600
H	0.07708100	2.07803100	-1.79835800
C	2.84910300	0.53994900	1.45847300
N	3.93526400	1.15212300	1.91147100
C	4.81292800	0.34374900	2.52014100
C	4.60745100	-1.02561300	2.64152800
C	3.40135700	-1.52399800	2.15798000
N	2.49425500	-0.73393800	1.57585800

H	5.71046500	0.81983600	2.90876600
H	5.34292700	-1.67021000	3.10796200
H	3.13605400	-2.57659000	2.23088900
N	1.93608800	1.35798900	0.72349500
C	-3.39327400	0.06853700	-1.10192800
C	-3.71023800	1.09749000	-0.14380200
C	-3.21239700	2.32070800	-0.65246800
C	-2.60208900	2.07284600	-1.93620500
C	-2.70489600	0.69096700	-2.21591600
C	-2.22413200	-0.01624500	-3.43317100
H	-1.94102800	-1.04806700	-3.20633300
H	-2.99783700	-0.05497900	-4.20848900
H	-1.34953500	0.47252700	-3.87239700
C	-3.93005100	-1.31634000	-1.10994300
H	-4.21236100	-1.66369500	-0.11430500
H	-4.82823400	-1.34637600	-1.73871400
H	-3.22006800	-2.03546900	-1.52771400
C	-4.53957800	0.95492400	1.08546800
H	-4.10555600	1.48056500	1.94209000
H	-5.53572400	1.38353900	0.92332600
H	-4.67520400	-0.09021500	1.36882300
C	-3.40018500	3.64486600	0.00322100
H	-3.09887300	4.46905100	-0.64674200
H	-4.45583600	3.79424700	0.25377100
H	-2.83872500	3.73885500	0.93966500
C	-2.02686900	3.10886100	-2.83607600
H	-2.82086000	3.60951400	-3.40132900

H	-1.48707200	3.88914500	-2.29159000
H	-1.34123900	2.67841300	-3.57104600
Co	-1.55575000	0.84824300	-0.38768400

Zero-point correction= 0.650101 (Hartree/Particle)

Thermal correction to Energy= 0.692320

Thermal correction to Enthalpy= 0.693265

Thermal correction to Gibbs Free Energy= 0.574787

Sum of electronic and zero-point Energies= -2233.550378

Sum of electronic and thermal Energies= -2233.508159

Sum of electronic and thermal Enthalpies= -2233.507215

Sum of electronic and thermal Free Energies= -2233.625692

E(RM06L) = -2234.200479 A.U.

A-13a

1 1

Number of imaginary frequencies: 0

C	3.51120300	0.03095300	0.85709300
C	4.74264000	0.20918400	0.18023100
C	5.37174400	-0.88387200	-0.44442600
C	5.34477800	1.47946600	0.12566200
C	6.57659300	-0.70406900	-1.10882200
H	4.90881200	-1.86511900	-0.39053800
C	6.55011600	1.64537600	-0.54188300
H	4.86052900	2.31869600	0.61478400
C	7.16675500	0.55812800	-1.15918400
H	7.06092200	-1.55105800	-1.58457200
H	7.01320700	2.62635300	-0.57807700
H	8.11112300	0.69377800	-1.67723400

C	2.43863700	-0.12729400	1.42181800
P	0.97304600	-0.31251800	2.34721200
C	-0.78137200	1.22140000	0.58688300
C	-1.31994200	2.45851100	0.15047400
C	-1.47484300	2.77687300	-1.21094500
C	-1.71639500	3.38325500	1.13765900
C	-2.03484400	3.99504800	-1.57035100
H	-1.14948000	2.06470900	-1.96201600
C	-2.26145200	4.60212300	0.76058300
H	-1.58043900	3.13125200	2.18582400
C	-2.42991400	4.90606800	-0.59008400
H	-2.15614700	4.24161700	-2.62065400
H	-2.55926700	5.31567000	1.52207700
H	-2.86416700	5.85791100	-0.87983400
C	-0.28131800	0.23644400	1.17334500
O	0.84978600	0.49067100	3.59604800
C	-2.53283900	-2.06381400	-1.27359300
C	-2.37001500	-2.50443400	0.09044500
C	-2.81776400	-1.46095400	0.94952600
C	-3.32384600	-0.38711000	0.11906100
C	-3.16191700	-0.76772600	-1.24422300
O	0.39999500	-1.70781900	-0.62912100
C	0.63615300	-0.91360500	-1.60389500
O	-0.29727800	-0.08681600	-1.87972400
C	1.92635000	-0.92511700	-2.33154900
C	-3.48739100	0.05109700	-2.43700200
H	-2.68141000	0.01390100	-3.17520100

H	-4.39157200	-0.33299600	-2.92224900
H	-3.66479700	1.09714800	-2.17846300
C	-2.16311700	-2.83302400	-2.48888100
H	-1.31094200	-3.49128100	-2.30310300
H	-2.99721500	-3.46376300	-2.81618700
H	-1.90917400	-2.17186900	-3.32089900
C	-1.73508900	-3.78377800	0.48703100
H	-1.55501900	-3.84255600	1.56145800
H	-2.38084100	-4.62330900	0.20770200
H	-0.78026100	-3.92615300	-0.02845900
C	-2.85356300	-1.45435900	2.43484300
H	-2.35802500	-0.57159000	2.85285700
H	-3.89161000	-1.43445500	2.78409300
H	-2.38476800	-2.34205900	2.86207400
C	-3.99206400	0.83038000	0.63929300
H	-5.03908200	0.59716000	0.86611800
H	-3.53218000	1.18159600	1.56677000
H	-3.98454000	1.65467000	-0.07709300
H	1.79179400	-0.61081500	-3.36670500
H	2.60540100	-0.21495400	-1.84792400
H	2.38788600	-1.91182700	-2.28497300
Co	-1.32673100	-0.77273100	-0.31600800
C	0.77441200	-2.09207900	2.53204400
H	1.59194500	-2.46049900	3.15496200
H	-0.16478600	-2.29809900	3.04987000
H	0.79995100	-2.59725800	1.56508400

Zero-point correction= 0.522696 (Hartree/Particle)

Thermal correction to Energy= 0.559918

Thermal correction to Enthalpy= 0.560862

Thermal correction to Gibbs Free Energy= 0.451033

Sum of electronic and zero-point Energies= -1835.840848

Sum of electronic and thermal Energies= -1835.803626

Sum of electronic and thermal Enthalpies= -1835.802682

Sum of electronic and thermal Free Energies= -1835.912511

E(RM06L) = -1836.363544 A.U.

A-13b

1 1

Number of imaginary frequencies: 0

C	3.68526900	-0.90915200	-0.22403700
C	5.02899000	-1.25183000	0.05178000
C	5.75734900	-2.04952600	-0.84974400
C	5.64464900	-0.79313700	1.23102100
C	7.07593200	-2.37816500	-0.57130000
H	5.27894100	-2.40021300	-1.75884900
C	6.96373800	-1.13024700	1.49681900
H	5.07857200	-0.17695900	1.92233600
C	7.68000400	-1.92079300	0.59913600
H	7.63582200	-2.99279700	-1.26892600
H	7.43642400	-0.77483600	2.40685800
H	8.71231600	-2.18092600	0.81192800
C	2.52334100	-0.61109800	-0.45945500
P	0.88733800	-0.18259600	-0.80506600
C	0.68860300	2.72690300	-0.36744500
C	0.54726100	4.09822900	-0.05043700

C	1.01008000	5.09370000	-0.92871700
C	-0.07507300	4.46610400	1.15758600
C	0.85170000	6.43232500	-0.59786200
H	1.49118200	4.80488900	-1.85785900
C	-0.22747300	5.80829900	1.47433100
H	-0.42973200	3.68856500	1.82888400
C	0.23481700	6.79123700	0.59965000
H	1.21162000	7.19948700	-1.27598600
H	-0.70568000	6.09029800	2.40703000
H	0.11488500	7.84007700	0.85285700
C	0.77598200	1.53688600	-0.63272100
C	0.60675600	-0.58044300	-2.53623300
H	-0.42020800	-0.31601400	-2.79649500
H	1.30144200	-0.03060700	-3.17424600
H	0.76320300	-1.65180500	-2.68275800
O	-0.05525400	-0.92664100	0.14869600
C	-3.89459700	-1.72375100	0.22802700
C	-3.15243300	-2.49419300	-0.74212500
C	-2.01730600	-3.04906600	-0.08983500
C	-2.06822900	-2.66379100	1.30935000
C	-3.24115100	-1.88272000	1.50486700
O	-2.20029000	0.30682800	-1.36734700
C	-2.35427300	1.22523100	-0.48529200
O	-2.29149800	0.85572800	0.73065600
C	-2.63666000	2.62969000	-0.87766700
C	-3.66005200	-1.19980500	2.75269100
H	-3.88760300	-0.14660700	2.56723400

H	-4.56702400	-1.66725900	3.15115500
H	-2.89127400	-1.24662200	3.52508500
C	-5.13111700	-0.94116500	-0.03048700
H	-5.15936800	-0.56454900	-1.05633500
H	-6.02550600	-1.55707300	0.11592100
H	-5.21017900	-0.08639900	0.64641300
C	-3.46120900	-2.55043200	-2.19206500
H	-2.61121800	-2.90337900	-2.77952300
H	-4.29768500	-3.23345500	-2.37588500
H	-3.75093400	-1.56785900	-2.57364400
C	-0.92598900	-3.85247800	-0.69478100
H	0.05044600	-3.50876100	-0.34066500
H	-1.02414800	-4.90654800	-0.41258500
H	-0.93468900	-3.80349500	-1.78571700
C	-1.02668300	-3.00855600	2.30826400
H	-1.05546600	-4.07859400	2.54140200
H	-0.03006000	-2.77996600	1.91993500
H	-1.15619700	-2.46020600	3.24256900
H	-2.43281900	3.31526000	-0.05507600
H	-2.04683500	2.90529600	-1.75356100
H	-3.69266900	2.71821000	-1.15095600
Co	-2.03306200	-1.02167000	0.10516700

Zero-point correction= 0.522824 (Hartree/Particle)

Thermal correction to Energy= 0.560442

Thermal correction to Enthalpy= 0.561386

Thermal correction to Gibbs Free Energy= 0.447366

Sum of electronic and zero-point Energies= -1835.852098

Sum of electronic and thermal Energies= -1835.814480

Sum of electronic and thermal Enthalpies= -1835.813536

Sum of electronic and thermal Free Energies= -1835.927557

E(RM06L) = -1836.374922 A.U.

A-14a

1 1

Number of imaginary frequencies: 0

C	3.19394900	-0.57030900	0.69913400
C	4.40520300	-0.72744300	-0.01788900
C	4.72179800	0.13733400	-1.08157400
C	5.30200000	-1.75353700	0.33093400
C	5.90954900	-0.02458400	-1.77978400
H	4.03157600	0.93440800	-1.34766600
C	6.48708400	-1.90487600	-0.37511500
H	5.05739200	-2.41580300	1.15509600
C	6.79270200	-1.04459500	-1.42856300
H	6.15066600	0.64670400	-2.59796200
H	7.17705500	-2.69644200	-0.10103000
H	7.72219200	-1.16741900	-1.97568800
C	2.13529900	-0.44198000	1.29937000
P	0.75146800	-0.30329700	2.35602800
C	-1.68823200	-1.02315900	0.71134600
C	-2.82290100	-1.73855600	0.22012400
C	-4.11772000	-1.21109000	0.36586500
C	-2.64141500	-2.97628600	-0.42294200
C	-5.21132400	-1.91315700	-0.12031600
H	-4.25109900	-0.26664500	0.88658300

C	-3.74124200	-3.66041400	-0.92226200
H	-1.63943400	-3.38377000	-0.52237600
C	-5.02339200	-3.13180800	-0.77371400
H	-6.21224200	-1.51497600	0.01246700
H	-3.60010600	-4.61420300	-1.42027500
H	-5.87998500	-3.67600100	-1.15876000
C	-0.56388200	-0.88794800	1.29106500
O	0.89778300	-0.89519500	3.70716100
C	-1.17971000	2.74585300	-0.23084000
C	0.04828300	2.19575400	-0.70654100
C	-0.27734300	1.02265800	-1.48334700
C	-1.71202200	0.92464000	-1.58923600
C	-2.26097700	1.96213100	-0.79012300
C	-3.69951800	2.23055000	-0.54568600
H	-3.90397500	2.42336000	0.51206700
H	-4.00974800	3.13028800	-1.08986300
H	-4.33495900	1.40727800	-0.87670000
C	-1.34933000	3.94617100	0.62619300
H	-0.45471900	4.15759300	1.21544500
H	-1.55386400	4.83030200	0.01180400
H	-2.18791900	3.83622500	1.31880800
C	1.42539000	2.69823900	-0.47727300
H	2.09152900	1.90040500	-0.13023000
H	1.83896400	3.08798300	-1.41442200
H	1.45338400	3.50839600	0.25369300
C	0.71749300	0.10459800	-2.08545200
H	0.28310500	-0.86685400	-2.33083500

H	1.11859400	0.53464400	-3.01172900
H	1.56243600	-0.05972800	-1.40883900
C	-2.44745900	-0.04916000	-2.43393400
H	-2.48448100	0.31627600	-3.46617300
H	-1.96037700	-1.02731600	-2.45534700
H	-3.47626500	-0.20022200	-2.10007400
Co	-0.95961100	0.80918700	0.38798500
C	0.07637500	1.31607700	2.03429500
H	0.77673200	2.14654100	1.94467500
H	-0.73117900	1.54134400	2.74161300

Zero-point correction= 0.458995 (Hartree/Particle)

Thermal correction to Energy= 0.489906

Thermal correction to Enthalpy= 0.490850

Thermal correction to Gibbs Free Energy= 0.396411

Sum of electronic and zero-point Energies= -1606.756920

Sum of electronic and thermal Energies= -1606.726009

Sum of electronic and thermal Enthalpies= -1606.725065

Sum of electronic and thermal Free Energies= -1606.819504

E(RM06L) = -1607.215915 A.U.

A-14b

1 1

Number of imaginary frequencies: 0

C	-0.16954900	2.57245700	-0.06826900
C	0.06740400	3.96626500	-0.03811300
C	0.89612500	4.56436200	-1.00556600
C	-0.52153000	4.76215500	0.96175900
C	1.12664900	5.93177700	-0.96901500

H	1.34195000	3.94827900	-1.78091400
C	-0.28121200	6.12832100	0.98698000
H	-1.16078900	4.29692100	1.70532300
C	0.54059000	6.71428200	0.02515000
H	1.76272200	6.39080400	-1.71912800
H	-0.73755000	6.73972100	1.75883700
H	0.72336500	7.78410400	0.04898100
C	-0.36850900	1.36617000	-0.09436800
P	-0.59222300	-0.34523000	-0.10759600
C	-3.48849700	-0.85119800	-0.02991800
C	-4.87870800	-1.09727300	-0.03384300
C	-5.36775700	-2.41395600	-0.12517600
C	-5.78232900	-0.02116900	0.05221100
C	-6.73569000	-2.64241300	-0.12958100
H	-4.66688500	-3.24019000	-0.18945400
C	-7.14742700	-0.26512200	0.04577000
H	-5.39902500	0.99174800	0.12253300
C	-7.62529500	-1.57196800	-0.04488400
H	-7.11109400	-3.65829600	-0.19893200
H	-7.84251100	0.56568000	0.11200600
H	-8.69504400	-1.75705900	-0.04909800
C	-2.28600300	-0.62057100	-0.01470200
C	0.34243300	-1.05711800	-1.41976200
H	-0.08367700	-2.00257100	-1.77038600
H	0.61205300	-0.40230300	-2.24793100
O	0.17973300	-1.03989000	1.08055600
C	3.36291100	-1.47554300	-1.11027300

C	3.32870000	-0.40950200	-0.14181500
C	3.28162100	-0.99739800	1.19085600
C	3.19754400	-2.39488900	1.03987800
C	3.21966200	-2.69280400	-0.38855500
C	3.09745200	-4.05219400	-0.97075600
H	2.78556000	-4.02351200	-2.01678400
H	4.06338300	-4.56975400	-0.93066700
H	2.38614500	-4.67155100	-0.41751600
C	3.46855300	-1.32467400	-2.58431900
H	3.09422700	-0.35562800	-2.92187700
H	4.51433600	-1.39716100	-2.90195700
H	2.91160100	-2.10070000	-3.11487300
C	3.37456100	1.04362900	-0.43588000
H	2.82224600	1.62707400	0.30540700
H	4.41197600	1.40002100	-0.42430100
H	2.96191000	1.27110500	-1.42212600
C	3.17962000	-0.21578900	2.44833000
H	2.82665600	-0.82673100	3.28044500
H	4.15495600	0.19912400	2.72523300
H	2.48700100	0.62393500	2.33917900
C	3.02183100	-3.40807800	2.11110600
H	3.96839700	-3.91950100	2.31938600
H	2.67504800	-2.95959800	3.04357700
H	2.30127900	-4.17938800	1.82508900
Co	1.67475400	-1.46309500	-0.00200100

Zero-point correction= 0.458245 (Hartree/Particle)

Thermal correction to Energy= 0.490238

Thermal correction to Enthalpy= 0.491182

Thermal correction to Gibbs Free Energy= 0.389599

Sum of electronic and zero-point Energies= -1606.770690

Sum of electronic and thermal Energies= -1606.738698

Sum of electronic and thermal Enthalpies= -1606.737753

Sum of electronic and thermal Free Energies= -1606.839336

E(RM06L) = -1607.228936 A.U.

A-TSa1

1 1

Number of imaginary frequencies: 1

C	-0.62007300	-1.16478400	-1.81770800
C	-1.23377300	-2.11782800	-0.91625100
C	-2.51358800	-1.61765000	-0.55882200
C	-2.72186800	-0.36102600	-1.24168300
C	-1.57400900	-0.12302000	-2.05813100
O	-0.36411900	0.15495800	2.94786500
O	-2.12080600	0.18553000	1.55350900
C	-1.59378300	0.31642700	2.70927800
C	-3.47843800	-2.24132500	0.37907500
H	-4.28840000	-2.72320600	-0.18011200
H	-3.00858100	-3.00513900	1.00188500
H	-3.93015500	-1.49317100	1.03513300
C	-0.66983900	-3.42920300	-0.50221200
H	-0.83042400	-3.63154400	0.56023500
H	-1.16123100	-4.23497700	-1.05901600
H	0.40044900	-3.49398200	-0.70417200
C	0.70703600	-1.30408400	-2.47358700

H	1.41855600	-1.83491300	-1.83553600
H	0.62216700	-1.86400500	-3.41159800
H	1.14459100	-0.33180800	-2.71755800
C	-1.35878000	1.04093000	-2.95495400
H	-0.31470400	1.36703800	-2.96606600
H	-1.61915500	0.76759900	-3.98333000
H	-1.98134600	1.89690200	-2.68331000
C	-3.94218500	0.47776600	-1.11447000
H	-3.81946300	1.45772000	-1.58236100
H	-4.80118200	-0.00262300	-1.59547200
H	-4.20213300	0.62953900	-0.06212400
C	4.10549800	0.75070300	-0.20653700
C	2.96027300	0.06119000	0.18602700
C	2.99700000	-1.29595000	0.60466700
C	4.22555500	-1.97555700	0.63744100
C	5.36508600	-1.29726000	0.24364400
C	5.30169800	0.04471800	-0.17243400
H	4.06241400	1.78902100	-0.50957400
H	4.27401800	-3.00987600	0.96383200
H	6.32535800	-1.80227700	0.25865000
H	6.21595400	0.54878300	-0.46983700
C	0.80216800	-0.61078100	0.73890400
H	0.19102200	-0.27751500	1.81640800
C	1.66669500	-1.68076800	0.92857700
H	1.37470800	-2.63595500	1.34659000
N	1.63187400	0.45998200	0.26157400
C	1.03982600	1.65264300	-0.03605300

N	-0.31764400	1.57820000	-0.05764600
C	-0.99287800	2.72671600	-0.19072700
C	-0.33220600	3.92954300	-0.38084500
C	1.05958700	3.87185800	-0.45349000
N	1.75513000	2.74894200	-0.27063100
H	-2.07718800	2.64622300	-0.15732500
H	-0.87493300	4.85929400	-0.49249000
H	1.64605600	4.76445300	-0.65972700
Co	-1.05337900	-0.25122600	-0.04085900
C	-2.49879700	0.66818700	3.84915500
H	-2.56106300	-0.18365900	4.53092000
H	-2.07259200	1.49501400	4.41969000
H	-3.49886400	0.92374800	3.50219500

Zero-point correction= 0.459749 (Hartree/Particle)

Thermal correction to Energy= 0.489245

Thermal correction to Enthalpy= 0.490189

Thermal correction to Gibbs Free Energy= 0.400155

Sum of electronic and zero-point Energies= -1390.738562

Sum of electronic and thermal Energies= -1390.709065

Sum of electronic and thermal Enthalpies= -1390.708121

Sum of electronic and thermal Free Energies= -1390.798155

E(RM06L) = -1391.198310 A.U.

A-TSb1

1 1

Number of imaginary frequencies: 1

C	-1.07755800	-2.12163900	-1.05334300
C	-2.27678500	-1.34404300	-1.06256600

C	-2.00284000	-0.09153200	-1.69255000
C	-0.63368400	-0.12937800	-2.15054400
C	-0.06459300	-1.37498000	-1.76515600
O	-1.99285300	-0.16486800	1.41083400
O	-0.36751500	0.15601800	2.91483400
C	-1.58877500	0.08782000	2.59586100
C	-2.98530000	0.99976800	-1.92861900
H	-3.56999100	0.80772700	-2.83549800
H	-3.69839500	1.08814300	-1.10354400
H	-2.49940700	1.96999200	-2.06412200
C	-3.56598300	-1.74074800	-0.44899600
H	-3.42647700	-2.46238700	0.35796700
H	-4.10584000	-0.88277600	-0.04446400
H	-4.20441000	-2.21023800	-1.20633300
C	-0.95740000	-3.51798600	-0.55610700
H	-1.45053800	-3.65264900	0.41086900
H	-1.43380800	-4.21208300	-1.25805500
H	0.08542300	-3.82169000	-0.44710800
C	1.29643200	-1.86225100	-2.10365400
H	1.72686400	-2.46923200	-1.30246600
H	1.24985200	-2.48939800	-3.00127200
H	1.98770700	-1.04263500	-2.31482000
C	0.05480800	0.95462200	-2.89891300
H	1.13561500	0.94903400	-2.73321300
H	-0.10669400	0.82956400	-3.97538300
H	-0.32795000	1.94483500	-2.63425700
C	0.97787600	-0.88713100	0.94652000

C	2.08344700	-0.17306600	0.45797400
C	3.39704200	-0.68231900	0.37612900
C	3.62945300	-1.99246800	0.80736000
C	2.56545400	-2.73622200	1.31591000
C	1.27846700	-2.19627300	1.37884800
H	0.27271000	-0.29947700	1.87830000
H	4.62705200	-2.41920700	0.75929200
H	2.74239700	-3.74443400	1.67807300
H	0.47854600	-2.79247500	1.81374900
C	3.44553600	1.44003100	-0.39142400
H	3.67056500	2.42681200	-0.76339100
C	4.22886000	0.35367600	-0.17157600
H	5.28918300	0.29624300	-0.37090800
N	2.12394300	1.13578300	-0.02734900
C	1.09224200	2.04804800	-0.00585600
N	1.41908900	3.32906400	-0.17569200
C	0.43827500	4.22063800	-0.07944400
C	-0.87449700	3.86259700	0.22568500
C	-1.13048400	2.50816100	0.32873800
N	-0.16676900	1.58144400	0.17235600
H	0.71883900	5.25880700	-0.24364900
H	-1.66091400	4.59613500	0.34945400
H	-2.12425900	2.11334400	0.52344700
Co	-0.73309200	-0.33600300	-0.08455800
C	-2.62023000	0.33902500	3.64934200
H	-2.58344000	1.39177800	3.94249600
H	-3.62115100	0.10095200	3.29264400

H	-2.38745700	-0.24196400	4.54299500

Zero-point correction= 0.460441 (Hartree/Particle)

Thermal correction to Energy= 0.489427

Thermal correction to Enthalpy= 0.490371

Thermal correction to Gibbs Free Energy= 0.403224

Sum of electronic and zero-point Energies= -1390.732797

Sum of electronic and thermal Energies= -1390.703811

Sum of electronic and thermal Enthalpies= -1390.702867

Sum of electronic and thermal Free Energies= -1390.790014

E(RM06L) = -1391.193238 A.U.

A-TSc1

1 1

Number of imaginary frequencies: 1

C	2.04282400	1.17575600	-1.40256100
C	2.98506600	0.10787200	-1.14660900
C	2.39352700	-1.12372200	-1.57396700
C	1.06176300	-0.83728500	-2.00405400
C	0.84894700	0.59563100	-1.92471100
O	2.00711100	0.22228500	2.83740700
O	1.99689600	-1.38468500	1.26513400
C	2.35769700	-0.92053700	2.39642500
C	3.01192600	-2.46558600	-1.43896300
H	3.80155400	-2.59777700	-2.18613500
H	3.46378300	-2.59577900	-0.45182100
H	2.28431400	-3.26629600	-1.58106500
C	4.32677400	0.26409400	-0.53009800
H	4.66462600	-0.66676600	-0.06830400

H	5.07142500	0.54432600	-1.28398000
H	4.33404200	1.04694400	0.23402200
C	2.28862700	2.61201300	-1.12815200
H	2.82404700	2.75980600	-0.18574900
H	2.91261200	3.04099100	-1.92084100
H	1.36003000	3.18432000	-1.08748100
C	-0.38000900	1.31038000	-2.35195200
H	-0.46664800	2.29605000	-1.88861400
H	-0.37325300	1.45235200	-3.43859400
H	-1.28612900	0.74808200	-2.10797100
C	0.04265100	-1.82980400	-2.42628900
H	-0.97177500	-1.47015200	-2.23802300
H	0.12554300	-2.02623900	-3.50190800
H	0.16155700	-2.78424200	-1.90811000
C	-3.07768100	2.24009600	0.19862200
C	-2.02914600	1.38281000	0.53620500
C	-0.74089800	1.87737100	0.87407700
C	-0.51034800	3.25869100	0.88935200
C	-1.55035200	4.11389400	0.56225500
C	-2.81264600	3.60390600	0.21846400
H	-4.05586300	1.85587500	-0.05346000
H	0.46352700	3.64530900	1.17657000
H	-1.39562500	5.18797300	0.58116000
H	-3.61285800	4.29409300	-0.03016000
H	1.20103000	0.62494800	2.03181300
C	0.12273900	0.75629000	1.13223100
N	-1.95612500	-0.01916400	0.57126900

C	-2.97157200	-0.96173100	0.32697800
N	-2.58430700	-2.23938300	0.39474000
C	-3.54698100	-3.13742600	0.17902200
C	-4.85945100	-2.77694300	-0.10854000
C	-5.12198000	-1.41437800	-0.16976800
N	-4.18361700	-0.48745000	0.04739000
H	-3.24750100	-4.18198300	0.23829700
H	-5.63139200	-3.51704800	-0.27944700
H	-6.11712600	-1.03895700	-0.39919700
Co	1.28241400	-0.18526600	-0.11117000
C	-0.67513400	-0.38334200	0.96278200
H	-0.49450400	-1.42269100	1.20364900
C	3.26891800	-1.74572400	3.24168800
H	3.27167500	-2.78385500	2.91277800
H	4.28454200	-1.34804800	3.15309000
H	2.98789600	-1.67183100	4.29233000

Zero-point correction= 0.459502 (Hartree/Particle)

Thermal correction to Energy= 0.489243

Thermal correction to Enthalpy= 0.490188

Thermal correction to Gibbs Free Energy= 0.399140

Sum of electronic and zero-point Energies= -1390.699147

Sum of electronic and thermal Energies= -1390.669406

Sum of electronic and thermal Enthalpies= -1390.668462

Sum of electronic and thermal Free Energies= -1390.759509

E(RM06L) = -1391.158649 A.U.

A-TSd1

1 1

Number of imaginary frequencies: 1

C	-0.94935800	-0.13509500	-2.10769800
C	-1.63430000	-1.27484400	-1.54117800
C	-2.76643300	-0.78103100	-0.82605300
C	-2.79054100	0.65242800	-0.91481600
C	-1.69284500	1.04100900	-1.75093900
O	-1.39321800	-2.73223100	1.54103200
O	-1.14543600	-0.51858400	1.91439500
C	-1.63424900	-1.75143300	2.21567800
C	-3.77370800	-1.60029300	-0.10866000
H	-4.64614200	-1.73791500	-0.75888200
H	-3.39600200	-2.58792700	0.15776000
H	-4.13570400	-1.10524900	0.79716500
C	-1.27998000	-2.70584000	-1.72025100
H	-1.35236000	-3.25208600	-0.77621600
H	-1.96372700	-3.17726200	-2.43502500
H	-0.26651500	-2.82222000	-2.10914700
C	0.26484200	-0.17080700	-2.96390200
H	0.89811500	-1.02886200	-2.72742100
H	-0.01221200	-0.24022100	-4.02182700
H	0.87217900	0.73101800	-2.84766000
C	-1.34403700	2.42396400	-2.16379000
H	-0.26289300	2.58290100	-2.20528600
H	-1.73437100	2.61475200	-3.16957200
H	-1.77528400	3.17954800	-1.50301800
C	-3.82772700	1.53128600	-0.30822100
H	-3.56505200	2.58941600	-0.38287000

H	-4.79326400	1.40793700	-0.81102300
H	-3.98791800	1.29699800	0.74982700
C	4.28846200	0.46135700	0.10326200
C	3.05163800	-0.17756300	0.11289900
C	2.91741700	-1.58062400	-0.05974400
C	4.06605100	-2.36363300	-0.24640600
C	5.29894600	-1.73374600	-0.26712300
C	5.40467400	-0.34333400	-0.09462300
H	4.37236700	1.53076400	0.24871400
H	3.98436900	-3.43871700	-0.37337400
H	6.20049700	-2.31945000	-0.41423500
H	6.38697500	0.11834700	-0.11187900
C	0.81097900	-0.73946600	0.23319400
H	-0.10071700	-0.75292700	1.29056700
C	1.52701000	-1.89711600	0.01082500
H	1.09004100	-2.88663100	-0.03425700
N	1.76153400	0.32081100	0.28467000
C	1.30639000	1.57804100	0.55146600
N	-0.05407900	1.66116800	0.56640000
C	-0.58588700	2.82492300	0.96196500
C	0.20893200	3.91651000	1.26978300
C	1.58552200	3.74531500	1.12525100
N	2.14405600	2.58548900	0.78049200
H	-1.67149600	2.86001800	1.01429800
H	-0.22356400	4.85595500	1.58864600
H	2.27340800	4.56972300	1.29972000
Co	-0.99393500	0.04369300	-0.10113800

C	-2.45863200	-1.74437600	3.46334300
H	-1.82020700	-1.52603900	4.32341600
H	-3.20744000	-0.94927000	3.42565200
H	-2.93717600	-2.71184900	3.60674400

Zero-point correction= 0.459832 (Hartree/Particle)

Thermal correction to Energy= 0.489141

Thermal correction to Enthalpy= 0.490085

Thermal correction to Gibbs Free Energy= 0.402083

Sum of electronic and zero-point Energies= -1390.709194

Sum of electronic and thermal Energies= -1390.679886

Sum of electronic and thermal Enthalpies= -1390.678942

Sum of electronic and thermal Free Energies= -1390.766944

E(RM06L) = -1391.169026 A.U.

A-TSe1

1 1

Number of imaginary frequencies: 1

C	2.50041100	-0.61192200	-1.60072100
C	2.69224700	-1.62134300	-0.60132500
C	1.42859100	-2.26356700	-0.33908600
C	0.45175200	-1.66699900	-1.21859500
C	1.11973400	-0.65922100	-1.99401000
O	4.01590200	1.41405000	1.11136100
O	2.33659300	0.09737200	1.75240000
C	3.21177100	1.12992900	1.96801100
C	1.19121300	-3.34454200	0.65032700
H	1.47491000	-4.31847200	0.23520500
H	1.78249500	-3.19378000	1.55708500

H	0.14018700	-3.40195700	0.94128200
C	3.96908800	-1.89353100	0.10056100
H	3.80965800	-2.35091200	1.07846100
H	4.57195000	-2.58877700	-0.49537200
H	4.55134100	-0.97965800	0.23695000
C	3.54581100	0.31565700	-2.10555300
H	4.18135900	0.67225900	-1.29090700
H	4.18778200	-0.18407800	-2.83978200
H	3.10809700	1.18966900	-2.59316100
C	0.45834500	0.19627700	-3.00846800
H	1.06135300	1.06573300	-3.27339400
H	0.28804600	-0.38382500	-3.92282100
H	-0.51911600	0.55320500	-2.66829900
C	-0.97852800	-2.04125700	-1.36286300
H	-1.60663400	-1.16413200	-1.54968400
H	-1.10558100	-2.71185900	-2.22057000
H	-1.36430100	-2.55698700	-0.48068900
C	-1.98858600	2.25520000	-0.96004900
C	-1.59790600	1.29882700	-0.03596300
C	-0.25226100	1.21162200	0.43121300
C	0.72796900	2.08837200	-0.08979000
C	0.34074500	2.99998200	-1.07838500
C	-0.98775700	3.08437500	-1.48860200
H	-3.02350500	2.36305700	-1.25574100
H	1.74017400	2.13200300	0.30510900
H	1.07516500	3.68585700	-1.48955700
H	-1.27088900	3.83502400	-2.21982400

H	1.32545400	0.12841200	2.11385600
C	-0.13388200	0.10803200	1.37323600
N	-2.30514200	0.30065200	0.65522100
C	-3.67821100	-0.02113400	0.55249300
N	-4.06970800	-1.06381400	1.28504900
C	-5.36717200	-1.36258300	1.19944600
C	-6.24959700	-0.64380600	0.39894700
C	-5.70554700	0.40774900	-0.32657400
N	-4.40989700	0.73468300	-0.26096800
H	-5.70297700	-2.20905900	1.79486600
H	-7.30180400	-0.89381000	0.34148400
H	-6.31816600	1.01816200	-0.98655000
Co	1.27503800	-0.30884000	0.00375600
C	-1.41512700	-0.41502900	1.42586200
H	-1.79768000	-1.27755200	1.95478700
C	3.04807700	1.80138300	3.29086200
H	2.05694500	2.26453200	3.34843900
H	3.10386200	1.07382400	4.10390000
H	3.81205000	2.56495700	3.42248800

Zero-point correction= 0.459648 (Hartree/Particle)

Thermal correction to Energy= 0.489505

Thermal correction to Enthalpy= 0.490449

Thermal correction to Gibbs Free Energy= 0.399933

Sum of electronic and zero-point Energies= -1390.661888

Sum of electronic and thermal Energies= -1390.632031

Sum of electronic and thermal Enthalpies= -1390.631087

Sum of electronic and thermal Free Energies= -1390.721602

E(RM06L) = -1391.121536 A.U.

A-TSf1

1 1

Number of imaginary frequencies: 1

C	-1.72373400	-2.11734400	-0.40450800
C	-2.58727400	-0.98631200	-0.69776700
C	-1.98797600	-0.22673500	-1.72497900
C	-0.71835500	-0.85212900	-2.05485200
C	-0.62015400	-2.07220700	-1.31078600
O	-1.16136200	-0.18775300	1.92446000
O	-0.18366400	1.72268500	2.63678400
C	-1.13381400	0.96936600	2.63489500
C	-2.54045400	0.97455200	-2.40180700
H	-2.98159200	0.68244900	-3.36148500
H	-3.33060900	1.45832200	-1.82272800
H	-1.77114200	1.71911300	-2.62486800
C	-3.83429500	-0.68182700	0.04728200
H	-3.68289700	-0.81053600	1.12362600
H	-4.18815000	0.33637000	-0.13311300
H	-4.63821400	-1.36473300	-0.24872100
C	-2.02643100	-3.16225600	0.60835500
H	-2.21896000	-2.71884200	1.59053700
H	-2.92173000	-3.72706300	0.32632600
H	-1.20876400	-3.87788600	0.71341200
C	0.45377700	-3.08254700	-1.48089400
H	0.48559700	-3.79931200	-0.65967800
H	0.27385100	-3.64015100	-2.40717200

H	1.44318800	-2.62452300	-1.56305200
C	0.24431700	-0.37902600	-3.08404500
H	1.26709400	-0.69027800	-2.85391000
H	-0.00594000	-0.78824000	-4.06987100
H	0.23662000	0.71051100	-3.17776700
C	1.05031300	-0.93084900	0.78896700
C	2.15902400	-0.23156800	0.30065300
C	3.48049700	-0.73071600	0.34143000
C	3.70833800	-1.98004900	0.92738500
C	2.63268400	-2.68578300	1.45892800
C	1.33307900	-2.18046500	1.37207800
H	0.03557800	-0.43772600	1.56399400
H	4.71421200	-2.38606900	0.98026500
H	2.80360100	-3.64213600	1.94333700
H	0.51148400	-2.75394000	1.79727200
C	3.55583700	1.31300800	-0.60969100
H	3.79434000	2.26563300	-1.05410700
C	4.33356500	0.26151200	-0.25045400
H	5.40433400	0.20071600	-0.38008300
N	2.21767500	1.02743800	-0.29584600
C	1.19379500	1.94246700	-0.38598600
N	1.54580900	3.20439900	-0.63495500
C	0.58506000	4.11926600	-0.61147100
C	-0.73971500	3.80592400	-0.30849100
C	-1.01899600	2.46724500	-0.13214100
N	-0.07647400	1.50806700	-0.22012600
H	0.89056000	5.14002000	-0.83079000

H	-1.51328700	4.55910300	-0.23452500
H	-2.02732200	2.11372100	0.07239700
Co	-0.68946100	-0.38850100	-0.09136400
C	-2.40177400	1.18334000	3.40668000
H	-3.24077800	1.31250700	2.71493100
H	-2.63283500	0.30754100	4.01694000
H	-2.31556000	2.06497500	4.03950400

Zero-point correction= 0.459948 (Hartree/Particle)

Thermal correction to Energy= 0.489131

Thermal correction to Enthalpy= 0.490075

Thermal correction to Gibbs Free Energy= 0.402476

Sum of electronic and zero-point Energies= -1390.701455

Sum of electronic and thermal Energies= -1390.672273

Sum of electronic and thermal Enthalpies= -1390.671328

Sum of electronic and thermal Free Energies= -1390.758928

E(RM06L) = -1391.161404 A.U.

A-TSa2

1 1

Number of imaginary frequencies: 1

C	-4.16991200	-0.45693700	-1.03568800
C	-5.40367800	0.05459700	-0.56841700
C	-5.85735600	1.31591800	-0.99601600
C	-6.17258800	-0.68608700	0.34777700
C	-7.05841400	1.81841000	-0.51543200
H	-5.25989800	1.88364000	-1.70346600
C	-7.37182200	-0.17197100	0.82013100
H	-5.81928200	-1.66089500	0.67142200

C	-7.81653000	1.07763400	0.39060100
H	-7.40853900	2.78933500	-0.85183900
H	-7.96474000	-0.74861300	1.52308700
H	-8.75716900	1.47390300	0.76045000
C	-3.09391400	-0.89247400	-1.41986800
P	-1.47687300	-1.44389200	-1.76918900
C	-0.09575400	0.68986000	-0.29033000
C	-0.63668400	2.03491800	-0.19270700
C	0.06212100	3.18102200	-0.59922400
C	-1.97623800	2.15722800	0.21647500
C	-0.56664900	4.41921800	-0.58738500
H	1.08895000	3.09390900	-0.93986800
C	-2.59309700	3.40232900	0.24239600
H	-2.52382100	1.26186400	0.50301900
C	-1.88847100	4.53530300	-0.15745300
H	-0.02319800	5.29899000	-0.91752000
H	-3.62423300	3.48408800	0.57362600
H	-2.36886400	5.50882400	-0.13906300
C	-0.47532000	-0.48498000	-0.65379200
C	-1.07448400	-0.75381500	-3.38915400
H	-1.25048600	0.32455000	-3.40705100
H	-0.02191900	-0.94914600	-3.61161200
H	-1.69110900	-1.23373300	-4.15185800
O	-1.25287800	-2.91886400	-1.62319200
C	3.32272400	2.42797200	0.60460500
C	3.76583000	1.60406500	-0.45996900
C	4.91252800	1.88379300	-1.19654300

C	5.62086400	3.02858300	-0.84417700
C	5.19849500	3.86499700	0.19988300
C	4.05400200	3.57830400	0.92868500
C	2.12483600	1.85320800	1.13211200
C	1.82966800	0.70375100	0.43703900
H	5.23082100	1.24168100	-2.00763700
H	6.52034800	3.28037800	-1.39703800
H	5.77876100	4.75086000	0.43821200
H	3.72971000	4.22719800	1.73689000
H	1.50322400	2.29188000	1.90189100
C	2.89312500	-0.59949200	-1.27902400
N	3.76650000	-0.74769300	-2.27251300
C	3.69371400	-1.89499400	-2.94723800
C	2.74519000	-2.87896000	-2.67620100
C	1.87954200	-2.64079200	-1.61983700
N	1.97182700	-1.51880800	-0.88894700
H	4.41930200	-2.02017100	-3.74830000
H	2.67648700	-3.78868800	-3.25882200
H	1.07430100	-3.32000300	-1.35490800
N	2.84633500	0.55155600	-0.54927800
C	1.49929700	-1.10999700	2.68344000
C	0.09123000	-0.81576500	2.57602500
C	-0.54373300	-1.91978500	1.90768200
C	0.46563700	-2.84602200	1.52558700
C	1.73591800	-2.32905300	1.99921900
C	3.06231900	-2.97442600	1.81811000
H	3.86319800	-2.23312800	1.74262800

H	3.29811700	-3.62113700	2.67069200
H	3.09449400	-3.59973800	0.92206400
C	2.52677600	-0.31451700	3.40253000
H	2.77257700	-0.80375800	4.35168800
H	3.45359500	-0.22485400	2.82910600
H	2.18248100	0.69502900	3.63143600
C	-0.61095400	0.35469600	3.16406400
H	-1.44893600	0.68064700	2.54168900
H	-1.01817300	0.10462500	4.15051800
H	0.05674100	1.20931400	3.29675200
C	-2.00125400	-2.05572000	1.65459600
H	-2.20293900	-2.72507900	0.81413200
H	-2.50001500	-2.46398900	2.54131700
H	-2.46718300	-1.08863900	1.43860800
C	0.23824200	-4.17887800	0.90647700
H	-0.13580800	-4.87697000	1.66442200
H	-0.49715600	-4.13272800	0.09846900
H	1.16338600	-4.60981600	0.51557800
Co	0.86182300	-0.97676200	0.68503500

Zero-point correction= 0.648182 (Hartree/Particle)

Thermal correction to Energy= 0.690459

Thermal correction to Enthalpy= 0.691403

Thermal correction to Gibbs Free Energy= 0.573025

Sum of electronic and zero-point Energies= -2233.530450

Sum of electronic and thermal Energies= -2233.488174

Sum of electronic and thermal Enthalpies= -2233.487229

Sum of electronic and thermal Free Energies= -2233.605607

E(RM06L) = -2234.178632 A.U.

A-TSb2

1 1

Number of imaginary frequencies: 1

C	-3.24218400	1.90045200	0.24507400
C	-4.60990600	1.82787200	-0.10951600
C	-5.55714200	1.40933300	0.84094000
C	-5.02367800	2.12340300	-1.42015300
C	-6.89124700	1.28602300	0.47916500
H	-5.22844900	1.17178800	1.84804000
C	-6.36030800	1.99408100	-1.77022400
H	-4.28593900	2.44296100	-2.15072900
C	-7.29468000	1.57515700	-0.82367100
H	-7.62004600	0.96142200	1.21542500
H	-6.67674600	2.22275300	-2.78328800
H	-8.33977300	1.47712300	-1.10155600
C	-2.05495800	1.92172000	0.53248100
P	-0.45924000	1.88861400	1.20966800
C	1.94893300	1.24416400	-0.08198000
C	3.13542700	2.03678400	0.05164200
C	3.28375500	3.21138000	-0.70790700
C	4.15237300	1.67162700	0.94975100
C	4.42657400	3.98947100	-0.57366500
H	2.49783600	3.49483900	-1.40350500
C	5.28629100	2.46162700	1.08531300
H	4.03042900	0.77571000	1.55228900
C	5.43129100	3.61704100	0.31793600

H	4.53281200	4.89227900	-1.16711400
H	6.05903700	2.17742400	1.79301900
H	6.32226600	4.22833300	0.41927100
C	0.67398700	1.17150800	-0.01113300
C	0.10431600	3.60453600	1.23232500
H	1.14755600	3.64673700	1.55370000
H	0.00350000	4.07183000	0.25026600
H	-0.50681500	4.15364200	1.95149500
O	-0.34936200	1.15811800	2.51191700
C	-2.59376200	-1.06260900	-0.92759700
C	-2.30311000	-1.52962100	0.37770100
C	-3.26299400	-2.10412100	1.20133800
C	-4.54839000	-2.22693600	0.67685200
C	-4.85806000	-1.79039000	-0.61784000
C	-3.89278300	-1.20523900	-1.42668500
C	-1.39373800	-0.49313800	-1.47111500
C	-0.38511900	-0.65971400	-0.55880200
H	-3.01762300	-2.43681300	2.20198300
H	-5.32600000	-2.67172200	1.29026900
H	-5.87324200	-1.89801700	-0.98835200
H	-4.14257500	-0.85214600	-2.42340800
H	-1.30108500	-0.00013400	-2.42950200
C	-0.12593900	-1.52561000	1.65308200
N	-0.61654900	-2.02153800	2.78418700
C	0.24085800	-2.12592800	3.79516400
C	1.58133500	-1.75261800	3.70135400
C	2.01215700	-1.31298200	2.46216100

N	1.17986300	-1.22154300	1.41989500
H	-0.16278900	-2.52923700	4.72146400
H	2.25872700	-1.82002200	4.54267800
H	3.04723300	-1.03776400	2.27245600
N	-0.93757900	-1.27987400	0.58429400
C	1.43362300	-2.25541100	-1.91744800
C	1.87918200	-1.01886100	-2.50759700
C	3.13345700	-0.67200900	-1.90255300
C	3.40087300	-1.60451000	-0.85731900
C	2.34646400	-2.59243500	-0.88294300
C	2.24817300	-3.78244500	0.00187800
H	1.20859600	-4.04983500	0.21202500
H	2.71377900	-4.65155800	-0.47649200
H	2.75792000	-3.62875200	0.95651500
C	0.26985100	-3.08096400	-2.33013400
H	-0.43431600	-2.52373100	-2.94861800
H	0.61961200	-3.94394900	-2.90785800
H	-0.28523300	-3.46845800	-1.47108700
C	1.26571700	-0.29566200	-3.65356300
H	1.15699800	0.77367400	-3.44264700
H	1.88843200	-0.38501300	-4.55081600
H	0.27856700	-0.69060400	-3.89941200
C	4.03760300	0.39843400	-2.39018500
H	4.75498500	0.72708800	-1.63534400
H	4.60922100	0.00956800	-3.24136100
H	3.49109600	1.27563400	-2.74566500
C	4.64032800	-1.67694700	-0.03791600

H	5.38926700	-2.30705400	-0.53191500
H	5.09262100	-0.69267500	0.10787500
H	4.46182900	-2.12216600	0.94531400
Co	1.55460200	-0.69575600	-0.48295100

Zero-point correction= 0.647390 (Hartree/Particle)

Thermal correction to Energy= 0.689836

Thermal correction to Enthalpy= 0.690780

Thermal correction to Gibbs Free Energy= 0.572586

Sum of electronic and zero-point Energies= -2233.519412

Sum of electronic and thermal Energies= -2233.476966

Sum of electronic and thermal Enthalpies= -2233.476021

Sum of electronic and thermal Free Energies= -2233.594215

E(RM06L) = -2234.166802 A.U.

A-TSc2

1 1

Number of imaginary frequencies: 1

C	-2.85681400	-1.08731400	-0.96230800
C	-4.15953600	-0.64584300	-1.22939000
C	-4.35239100	0.45809400	-2.09174900
C	-5.28013800	-1.29007000	-0.65984700
C	-5.63558700	0.90515700	-2.36139800
H	-3.48531400	0.93511500	-2.53951700
C	-6.55640800	-0.83040200	-0.93782000
H	-5.12794200	-2.14699600	-0.00906500
C	-6.73432900	0.26551300	-1.78520700
H	-5.78453100	1.74990800	-3.02589500
H	-7.41762000	-1.32496800	-0.50083400

H	-7.73763600	0.61928600	-2.00217100
C	-1.67404300	-1.38457200	-0.70948400
P	-0.25066100	-2.25461800	-1.37467700
C	0.93028500	-1.37212700	-0.33856300
C	3.29143100	-1.36778400	-1.50676700
C	3.70691700	-0.43170000	-2.47481200
C	4.02538300	-2.55674900	-1.32304300
C	4.82323700	-0.69431400	-3.25050800
H	3.13442800	0.48215200	-2.60307300
C	5.14216500	-2.80911600	-2.10790600
H	3.69692300	-3.27159000	-0.57249800
C	5.53995700	-1.87991300	-3.06808700
H	5.13802700	0.01949700	-4.00472700
H	5.70291100	-3.72833400	-1.97312500
H	6.41408800	-2.07977800	-3.68032200
C	2.11601100	-1.15163800	-0.75125000
C	-0.38905400	-3.92628200	-0.70267400
H	-0.56947600	-3.90855800	0.37262600
H	-1.21104800	-4.43910800	-1.20617900
H	0.53841900	-4.46535900	-0.91046300
O	-0.07559500	-2.17957800	-2.85058700
C	-0.87178200	3.13025500	-0.76447900
C	0.47608600	3.25077400	-0.36844000
C	1.19362100	4.42897500	-0.55520300
C	0.52156000	5.50636300	-1.12403000
C	-0.82279000	5.41109100	-1.50750500
C	-1.52484900	4.22688800	-1.33894900

C	-1.27530700	1.79057700	-0.47043000
C	-0.22069100	1.08064900	0.04445300
H	2.22837300	4.52360000	-0.25053400
H	1.05372200	6.44176400	-1.26647400
H	-1.31528500	6.27388100	-1.94554200
H	-2.56298100	4.14413100	-1.65118000
H	-2.27284700	1.39333000	-0.59790000
C	2.13913100	1.76392900	0.64529300
N	2.65181100	2.76765000	1.37670100
C	3.88118600	2.61034200	1.85782200
C	4.63539100	1.45777000	1.64816800
C	4.02183900	0.47368700	0.89150700
N	2.79305000	0.61315500	0.39107100
H	4.27134500	3.44049800	2.44453500
H	5.63643000	1.33783200	2.04324200
H	4.52555400	-0.46354900	0.64996600
N	0.88133100	1.97947200	0.10638600
C	-0.67349500	0.33588200	2.67754000
C	-1.85582700	-0.38399200	2.34843600
C	-1.52533400	-1.79691900	2.30647100
C	-0.14086600	-1.93335100	2.53667400
C	0.40903400	-0.61019100	2.73062200
C	1.79395100	-0.35382600	3.20201700
H	2.08907500	0.69212400	3.08993100
H	1.86951200	-0.59483400	4.26995700
H	2.52342500	-0.97958100	2.68026800
C	-0.59102800	1.79227500	2.96293900

H	-1.28796600	2.36363200	2.34468700
H	-0.84771700	1.97503900	4.01282800
H	0.40982000	2.19873500	2.79441300
C	-3.21421600	0.20034500	2.19468000
H	-3.89236700	-0.47974200	1.67190500
H	-3.66098100	0.41939000	3.17176200
H	-3.18249400	1.14123500	1.63540400
C	-2.52061900	-2.88417400	2.10924200
H	-2.05591800	-3.87214100	2.07541500
H	-3.23922600	-2.89033300	2.93599200
H	-3.09247500	-2.75167800	1.18482100
C	0.66279800	-3.18349400	2.63059000
H	1.11536700	-3.27293700	3.62421300
H	0.05963200	-4.08004200	2.47178100
H	1.48295700	-3.19633200	1.90322200
Co	-0.43237500	-0.65037400	0.86254300

Zero-point correction= 0.646809 (Hartree/Particle)

Thermal correction to Energy= 0.689304

Thermal correction to Enthalpy= 0.690249

Thermal correction to Gibbs Free Energy= 0.571492

Sum of electronic and zero-point Energies= -2233.478476

Sum of electronic and thermal Energies= -2233.435981

Sum of electronic and thermal Enthalpies= -2233.435037

Sum of electronic and thermal Free Energies= -2233.553793

E(RM06L) = -2234.125285 A.U.

A-TSd2

1 1

Number of imaginary frequencies: 1

C	-3.03047500	1.71592900	-0.99623400
C	-4.13918900	0.87013400	-1.23724200
C	-5.39116900	1.14775600	-0.66043700
C	-3.98703200	-0.25842800	-2.06235700
C	-6.46881700	0.31079000	-0.91500800
H	-5.50353900	2.02082100	-0.02520600
C	-5.07307600	-1.08467200	-2.30999400
H	-3.01254100	-0.47698400	-2.48994600
C	-6.31341400	-0.80207500	-1.74020500
H	-7.43548400	0.52990400	-0.47231100
H	-4.94883800	-1.95867200	-2.94201000
H	-7.16103700	-1.45135500	-1.93828100
C	-2.06706800	2.44388500	-0.80768000
P	-0.66544400	3.43445900	-0.54146500
C	1.47578700	1.35764900	-0.74732100
C	2.39794300	0.82485900	-1.71326500
C	2.03666300	-0.37145700	-2.38107000
C	3.62573100	1.45905100	-2.02603400
C	2.91067800	-0.92005900	-3.33285000
H	1.02627900	-0.75115500	-2.27824700
C	4.44649800	0.91299600	-2.99129800
H	3.88500800	2.38824900	-1.52804100
C	4.10066100	-0.28619100	-3.64070300
H	2.61420400	-1.82018300	-3.86415900
H	5.36821200	1.42204100	-3.25790400
H	4.75765700	-0.69495500	-4.40189100

C	0.61468700	2.18959600	-0.38568300
C	-0.21651400	4.10997600	-2.15712900
H	0.74415900	4.62411000	-2.08328800
H	-0.16477900	3.33234600	-2.92241800
H	-0.97816900	4.83923500	-2.44234300
O	-0.73007300	4.42076100	0.57303400
C	-1.61560300	-2.47506100	-0.46542000
C	-2.01025600	-1.60805000	0.57568800
C	-3.28319200	-1.66658300	1.13905100
C	-4.14424500	-2.65320900	0.67358100
C	-3.75941600	-3.54448600	-0.33864400
C	-2.50571000	-3.45575800	-0.92400000
C	-0.28586900	-2.09853700	-0.83479500
C	0.12654700	-1.02685000	-0.07389100
H	-3.58986900	-0.98903500	1.92651200
H	-5.13685600	-2.73197000	1.10676500
H	-4.45834400	-4.30571200	-0.67300500
H	-2.21400600	-4.13226400	-1.72292500
H	0.33247400	-2.61330600	-1.56117300
C	-0.96412400	0.23174600	1.82475100
N	-1.53438900	-0.16591600	2.97074100
C	-1.61007200	0.73008800	3.95469300
C	-1.09231800	2.01450000	3.84173700
C	-0.50588300	2.33023600	2.62443900
N	-0.45058000	1.45516900	1.61155000
H	-2.09327100	0.39047100	4.86948000
H	-1.15113700	2.73698300	4.64645900

H	-0.10361000	3.31765600	2.41559300
N	-0.94186600	-0.71352300	0.79967200
C	2.11362400	-1.69333600	1.70723400
C	2.92170700	-2.17287300	0.62633200
C	3.95536000	-1.18908000	0.37554600
C	3.72528800	-0.07528400	1.21124300
C	2.57601800	-0.37064600	2.03260900
C	2.11652000	0.47711600	3.15854600
H	1.13197500	0.18447500	3.52881500
H	2.82002200	0.37727500	3.99457300
H	2.08876900	1.53618600	2.88957200
C	1.06231200	-2.46977400	2.41194800
H	0.48486100	-3.09025400	1.72190100
H	1.53935700	-3.13649700	3.13960300
H	0.35841100	-1.83688800	2.95664700
C	2.80822500	-3.49804400	-0.03481800
H	3.07604500	-3.44705200	-1.09443500
H	3.48394300	-4.22353500	0.43430400
H	1.79299100	-3.89394100	0.03815800
C	5.07998300	-1.38004900	-0.57084700
H	5.53791700	-0.43771100	-0.87547100
H	5.85786600	-1.97984900	-0.08359700
H	4.77838000	-1.92142300	-1.47016100
C	4.51515500	1.18244700	1.27589700
H	5.16203700	1.19144300	2.16036300
H	5.15849700	1.30345400	0.40129400
H	3.86757000	2.06251300	1.34566100

Co	1.98219500	-0.46396300	0.07025400

Zero-point correction= 0.646288 (Hartree/Particle)

Thermal correction to Energy= 0.688932

Thermal correction to Enthalpy= 0.689876

Thermal correction to Gibbs Free Energy= 0.572708

Sum of electronic and zero-point Energies= -2233.457594

Sum of electronic and thermal Energies= -2233.414950

Sum of electronic and thermal Enthalpies= -2233.414006

Sum of electronic and thermal Free Energies= -2233.531173

E(RM06L) = -2234.103881 A.U.

A-TSa3

1 1

Number of imaginary frequencies: 1

C	1.36271100	1.33579900	-0.75405300
C	1.71514000	2.77013500	-0.73855000
C	0.86041000	3.73141000	-1.31390800
C	2.84771300	3.24767100	-0.03984600
C	1.15076200	5.08576500	-1.23358100
H	-0.01294200	3.41830500	-1.87308400
C	3.11766300	4.60536800	0.06055400
H	3.50032700	2.55611100	0.47809000
C	2.27484900	5.53420700	-0.54356700
H	0.48563000	5.79766400	-1.71224800
H	3.98467300	4.93652900	0.62382800
H	2.48571700	6.59646100	-0.46700500
C	0.05648800	0.80379500	-0.78256200
P	-1.09364900	1.06705800	-1.99423000

C	-3.42132800	-0.18272700	0.07358200
C	-2.21759300	-0.18891800	0.34538200
C	-1.94762300	-0.40261900	-2.61177800
H	-1.52486100	-0.57245100	-3.60633300
H	-1.82868900	-1.27367900	-1.97457400
H	-3.01254200	-0.18631800	-2.72172200
O	-1.02329500	2.08608600	-3.09189300
C	4.47420600	-0.63976700	-0.84558500
C	3.51619800	-1.64753800	-0.60378200
C	3.89159500	-2.97133700	-0.39003400
C	5.24762300	-3.26650500	-0.44486000
C	6.21391900	-2.27803000	-0.70616700
C	5.84084100	-0.96280900	-0.90469600
C	3.76847400	0.57759500	-0.94400300
C	2.41483600	0.35476600	-0.72872300
H	3.16318000	-3.75120200	-0.19676600
H	5.56821200	-4.29057800	-0.28145000
H	7.26182900	-2.55612800	-0.74300800
H	6.57987200	-0.18980400	-1.09045300
H	4.19910300	1.53892700	-1.17704500
C	1.13832800	-1.90722000	-0.83251100
N	0.01020700	-1.82573300	-0.09420200
C	-0.90049700	-2.80544000	-0.24131100
C	-0.71400100	-3.84764500	-1.13389400
C	0.42823900	-3.78205200	-1.92282700
N	1.34849200	-2.82944700	-1.76671600
H	-1.80347700	-2.68935600	0.35302000

H	-1.44853700	-4.63672300	-1.23763400
H	0.61992700	-4.50528300	-2.71246000
N	2.23889300	-1.05987300	-0.55833000
C	0.47796400	-0.97981100	2.65520500
C	1.04641700	0.29878900	2.38470500
C	-0.02787900	1.25788800	2.37322200
C	-1.23800000	0.57335600	2.68038500
C	-0.93833300	-0.83104100	2.81756800
C	-1.91820200	-1.89635000	3.15795300
H	-1.54991700	-2.88992400	2.88630900
H	-2.12103300	-1.91617100	4.23470400
H	-2.87083500	-1.73298600	2.64467500
C	1.24298500	-2.25190600	2.74512300
H	2.13297100	-2.23391600	2.10808000
H	1.58575500	-2.41843500	3.77248900
H	0.63725000	-3.11845600	2.46561700
C	2.50361100	0.59143500	2.38737800
H	2.71860900	1.57983400	1.98114900
H	2.87877700	0.57922900	3.41751000
H	3.08719500	-0.14588500	1.82814100
C	0.06921500	2.73075500	2.18458700
H	-0.56810800	3.07222000	1.36116000
H	-0.26416200	3.25464200	3.08694000
H	1.08774500	3.05648500	1.96711900
C	-2.54784000	1.22718800	2.92980400
H	-2.56318300	1.62327700	3.95261500
H	-2.71681000	2.06394200	2.24815300

H	-3.38165000	0.53224700	2.82049300
Co	-0.43130000	-0.22291000	0.91633200
C	-4.78602900	-0.22548200	-0.31777800
C	-5.69497000	0.76507900	0.09840900
C	-5.25495100	-1.26932900	-1.13965100
C	-7.02441900	0.70993000	-0.29733500
H	-5.34086900	1.57504300	0.73016600
C	-6.58623000	-1.31741800	-1.53020700
H	-4.55761700	-2.04082600	-1.46025500
C	-7.47474300	-0.32858400	-1.11131000
H	-7.71478100	1.48169600	0.02955500
H	-6.93368100	-2.12849700	-2.16320700
H	-8.51531100	-0.36705400	-1.41825500

Zero-point correction= 0.649601(Hartree/Particle)

Thermal correction to Energy= 0.691052

Thermal correction to Enthalpy= 0.691996

Thermal correction to Gibbs Free Energy= 0.577026

Sum of electronic and zero-point Energies= -2233.485670

Sum of electronic and thermal Energies= -2233.444219

Sum of electronic and thermal Enthalpies= -2233.443275

Sum of electronic and thermal Free Energies= -2233.558245

E(RM06L) = -2234.135271 A.U.

A-TSb3

1 1

Number of imaginary frequencies: 1

C	1.42348900	1.30997100	-0.27359700
C	2.09852600	2.64096800	-0.33535500

C	1.90110200	3.58107000	0.68339000
C	2.89316300	2.98900200	-1.43407500
C	2.46989500	4.84800200	0.60064200
H	1.30881500	3.30049000	1.55399500
C	3.44740000	4.26007200	-1.52322000
H	3.04891100	2.26623000	-2.23023500
C	3.23720200	5.19214100	-0.50888000
H	2.32045200	5.56288800	1.40455000
H	4.04182300	4.52671200	-2.39164800
H	3.67490000	6.18289500	-0.58125000
C	0.05955400	1.36798700	-0.06174300
P	-0.87677000	2.78236700	-0.61601000
C	-2.44334600	0.20601100	-0.43690400
C	-3.84885100	-0.00698900	-0.70689000
C	-4.68501100	1.10606600	-0.91837100
C	-4.41580400	-1.29004100	-0.76362000
C	-6.03945400	0.93424800	-1.16531000
H	-4.25721900	2.10463500	-0.87755600
C	-5.77055100	-1.45956600	-1.02284100
H	-3.78058300	-2.15730000	-0.60903300
C	-6.58673200	-0.34772800	-1.21853600
H	-6.67221800	1.80276900	-1.31968600
H	-6.19118200	-2.45940300	-1.07018200
H	-7.64637000	-0.47853900	-1.41418200
C	-1.61650000	1.19356800	-0.62554900
C	-1.65636700	3.79525600	0.66355100
H	-2.45905900	4.37058200	0.19743200

H	-2.06154700	3.19033000	1.47549900
H	-0.91992100	4.50057700	1.05665600
O	-0.52890500	3.53105400	-1.85624400
C	4.28803200	-0.95126400	0.05789300
C	3.30649800	-1.87413100	-0.35953600
C	3.57651300	-3.23801000	-0.45281600
C	4.85630600	-3.65987800	-0.11560100
C	5.84593000	-2.75474800	0.30265000
C	5.57364700	-1.40173500	0.39590000
C	3.67996000	0.32845400	0.05668300
C	2.35125000	0.20675400	-0.29682100
H	2.82951300	-3.94794700	-0.78793600
H	5.09471200	-4.71682300	-0.18015400
H	6.83364900	-3.12638400	0.55538300
H	6.33259700	-0.69773000	0.72285500
H	4.14306100	1.26107200	0.34579200
C	1.10126800	-1.68176400	-1.38466900
N	1.51984200	-2.47432900	-2.37041600
C	0.60947800	-2.97803100	-3.19609500
C	-0.74029200	-2.66894500	-3.07655000
C	-1.08982100	-1.86180400	-2.01174900
N	-0.19232800	-1.38098900	-1.12453500
H	0.98225000	-3.63186700	-3.98195100
H	-1.48942100	-3.04333000	-3.76294500
H	-2.12367900	-1.59415700	-1.83177300
N	2.09929700	-1.17207200	-0.55384700
C	0.25694900	-0.74071500	2.32106300

C	-0.91574300	0.05894700	2.56409300
C	-2.07621600	-0.71622500	2.25111100
C	-1.62676200	-1.97571500	1.73557600
C	-0.18609900	-1.98825800	1.81876500
C	0.64260900	-3.17302000	1.48070700
H	1.71005600	-2.94885700	1.45881400
H	0.48300700	-3.95497600	2.23213900
H	0.35986800	-3.61192300	0.51675000
C	1.63859800	-0.34994400	2.69987600
H	1.85741800	0.68736900	2.42868800
H	1.76335100	-0.43234800	3.78621500
H	2.39400600	-0.98738400	2.23372300
C	-0.89433200	1.40861200	3.18352700
H	-1.88130500	1.87553100	3.19203600
H	-0.56245100	1.33633300	4.22568900
H	-0.19507400	2.07749000	2.67073000
C	-3.48055800	-0.28688000	2.48349200
H	-4.19769200	-0.90031000	1.93476000
H	-3.72075600	-0.36225800	3.54979500
H	-3.64608300	0.75330900	2.18598600
C	-2.44793500	-3.17128300	1.39815800
H	-2.29395300	-3.96113000	2.14265600
H	-3.51529800	-2.94400000	1.38361700
H	-2.17769900	-3.60170200	0.42723800
Co	-0.90421300	-0.44947400	0.55330100

Zero-point correction= 0.649797 (Hartree/Particle)

Thermal correction to Energy= 0.690733

Thermal correction to Enthalpy= 0.691677

Thermal correction to Gibbs Free Energy= 0.578288

Sum of electronic and zero-point Energies= -2233.516972

Sum of electronic and thermal Energies= -2233.476036

Sum of electronic and thermal Enthalpies= -2233.475092

Sum of electronic and thermal Free Energies= -2233.588481

E(RM06L) = -2234.166769 A.U.

A-TS4

1 1

Number of imaginary frequencies: 1

C	-1.78954300	1.47263400	0.13589600
C	-2.65758600	2.64449400	-0.07359400
C	-2.35462400	3.58909700	-1.06934600
C	-3.78344200	2.86015300	0.73632000
C	-3.14197100	4.72262800	-1.23790000
H	-1.53472500	3.39428000	-1.75839200
C	-4.56288000	3.99832900	0.57048800
H	-4.02047400	2.14229000	1.51647900
C	-4.24379700	4.93335300	-0.41279700
H	-2.90579100	5.43249600	-2.02463300
H	-5.41841400	4.16132000	1.21847700
H	-4.85766700	5.81933200	-0.54101100
C	-0.41973800	1.68053200	0.15516700
P	0.54743200	3.11623700	0.15295300
C	2.00726900	0.45717800	0.26347900
C	3.34754200	0.80041900	0.66428600
C	3.69677500	2.05555600	1.20637600

C	4.35270700	-0.18026900	0.55578100
C	5.00717500	2.31498800	1.58456100
H	2.93838500	2.81610500	1.36470700
C	5.65917600	0.08318000	0.93860500
H	4.07194700	-1.15346900	0.16338900
C	5.99300000	1.33785400	1.44783400
H	5.25950200	3.28560400	2.00069700
H	6.41872100	-0.68727300	0.84391400
H	7.01424700	1.54916900	1.74976500
C	0.78991500	0.97363200	0.12970400
C	1.43054400	3.49560800	-1.37071900
H	2.50144700	3.33057700	-1.21677900
H	1.07033400	2.86882600	-2.18762500
H	1.27962300	4.54987200	-1.61399600
O	0.97081800	3.87560200	1.36364800
C	-3.92774900	-1.50161200	0.07809100
C	-2.75700100	-2.00246500	0.69799200
C	-2.64242200	-3.32455200	1.12388400
C	-3.71969400	-4.16326500	0.87291500
C	-4.87911100	-3.69867400	0.22224600
C	-4.99700200	-2.37936600	-0.17411000
C	-3.70180400	-0.12785400	-0.16468300
C	-2.42401300	0.19809400	0.27451900
H	-1.75144300	-3.68722500	1.63058100
H	-3.66742300	-5.20101800	1.18700100
H	-5.69493300	-4.39054700	0.04044400
H	-5.89725300	-2.02213700	-0.66467000

H	-4.36738800	0.56445500	-0.66124100
C	-0.78222300	-1.10149300	1.72253800
N	-1.12106400	-0.93864400	2.99339000
C	-0.18520400	-1.22184500	3.90413400
C	1.06773300	-1.71333200	3.55154100
C	1.34051800	-1.80492000	2.19664600
N	0.42390300	-1.47961200	1.26643000
H	-0.45864400	-1.05349900	4.94316700
H	1.81269000	-1.97479400	4.29311700
H	2.31297200	-2.10746800	1.81644400
N	-1.81908900	-0.97708600	0.76290800
C	-0.04482600	-1.83758600	-2.12308100
C	0.76058100	-0.76150800	-2.59650600
C	2.14665400	-1.04899800	-2.30655400
C	2.19972300	-2.31200400	-1.63613100
C	0.84149500	-2.76658600	-1.49250700
C	0.44568700	-4.03948900	-0.83226900
H	-0.59820100	-4.02284900	-0.50725300
H	0.55994600	-4.88164700	-1.52464100
H	1.07103600	-4.25911500	0.03894700
C	-1.50571900	-1.99722700	-2.35470900
H	-2.06063000	-1.07290800	-2.16394800
H	-1.69968000	-2.27883600	-3.39689400
H	-1.93968300	-2.77918600	-1.72665700
C	0.23887400	0.43471100	-3.31245200
H	1.02214500	1.17514800	-3.49320800
H	-0.16417200	0.15095700	-4.29134900

H	-0.58008500	0.91509200	-2.76221000
C	3.29950700	-0.20459600	-2.72375500
H	4.20745100	-0.44418900	-2.16569800
H	3.51787700	-0.34250600	-3.78876800
H	3.09972000	0.86082900	-2.56927100
C	3.40536300	-3.11785000	-1.29185700
H	3.48542900	-3.99158300	-1.94972000
H	4.32911100	-2.54645700	-1.41005800
H	3.37843300	-3.50381900	-0.26674000
Co	1.06822100	-0.92883300	-0.57944900

Zero-point correction= 0.648251 (Hartree/Particle)

Thermal correction to Energy= 0.690386

Thermal correction to Enthalpy= 0.691330

Thermal correction to Gibbs Free Energy= 0.573449

Sum of electronic and zero-point Energies= -2233.525114

Sum of electronic and thermal Energies= -2233.482979

Sum of electronic and thermal Enthalpies= -2233.482035

Sum of electronic and thermal Free Energies= -2233.599916

E(RM06L) = -2234.173365 A.U.

(S)A-TS5

1 1

Number of imaginary frequencies: 1

C	1.98137600	-1.23595500	0.02678200
C	3.04782400	-2.24111300	-0.10034000
C	2.96424200	-3.23764700	-1.08432000
C	4.16749200	-2.21974200	0.74568600
C	3.95715200	-4.19919400	-1.20756900

H	2.12742100	-3.22174700	-1.78100800
C	5.15582900	-3.18848300	0.62774400
H	4.23693600	-1.45387800	1.51370800
C	5.05214200	-4.18068100	-0.34550200
H	3.88539900	-4.95676700	-1.98173300
H	6.00712600	-3.17419400	1.30117400
H	5.82752300	-4.93495700	-0.43718300
C	0.65109700	-1.61412000	-0.03023700
P	-0.00026300	-3.28705400	0.20447300
C	-1.75379400	-1.16206100	0.24780500
C	-3.09573300	-1.43262100	0.62394600
C	-3.58594100	-2.75746900	0.66238800
C	-3.99354300	-0.39517300	0.96194100
C	-4.90160800	-3.02099600	1.01352300
H	-2.91225700	-3.57521800	0.42371200
C	-5.30810200	-0.66535800	1.31074200
H	-3.63690500	0.62988500	0.90919400
C	-5.77095500	-1.98034800	1.33752700
H	-5.25045000	-4.04869800	1.03869600
H	-5.97682900	0.15432500	1.55846400
H	-6.79958500	-2.19267500	1.61021900
C	-0.54268600	-0.82949000	-0.09044300
C	-0.79222900	-3.83380900	-1.34574500
H	-1.42793000	-4.69663400	-1.14057700
H	-1.38939400	-3.03104700	-1.78082200
H	-0.01241000	-4.14897700	-2.04721900
O	0.75942800	-4.36722400	0.90915600

C	3.57719800	2.07557300	-0.10684000
C	2.37556800	2.35769300	0.58642100
C	2.05928700	3.63005100	1.05294000
C	2.95818800	4.65051800	0.76160700
C	4.13821000	4.40434000	0.03803100
C	4.46024300	3.12887600	-0.39464400
C	3.57803900	0.68222700	-0.37151800
C	2.40913200	0.13427600	0.13445200
H	1.15092900	3.82361200	1.61834100
H	2.74380600	5.65856200	1.10262000
H	4.81093600	5.22935500	-0.17194700
H	5.38105000	2.94094200	-0.93835100
H	4.32155900	0.12046100	-0.92036200
C	0.67108800	1.07963800	1.70389400
N	1.08350600	0.75694000	2.91764400
C	0.18458900	0.85564900	3.90307900
C	-1.09736100	1.35061200	3.68749400
C	-1.45146000	1.60909900	2.37260100
N	-0.58692000	1.42770100	1.35840200
H	0.51700100	0.54605200	4.89098100
H	-1.80325900	1.49208600	4.49671300
H	-2.44856400	1.94252600	2.09772900
N	1.64105100	1.17533500	0.68117900
C	-0.46081500	1.96584300	-2.04507200
C	-1.09847500	0.77452300	-2.50731400
C	-2.47763400	0.82304800	-2.10491700
C	-2.71141000	2.06619600	-1.41805900

C	-1.46099900	2.74499700	-1.34658400
C	-1.22413000	4.05981300	-0.69303700
H	-0.18208100	4.17600700	-0.38203600
H	-1.45114300	4.87958400	-1.38404700
H	-1.85946600	4.19916500	0.18704900
C	0.94338400	2.35507500	-2.32932800
H	1.64491100	1.53549500	-2.13582500
H	1.05365600	2.62317000	-3.38731800
H	1.26443300	3.21574300	-1.73827400
C	-0.44277100	-0.30856900	-3.28842000
H	-0.97005800	-1.26022700	-3.18339200
H	-0.43009300	-0.06318800	-4.35675600
H	0.59461400	-0.46117700	-2.97450900
C	-3.49931100	-0.20851100	-2.42689700
H	-4.34701100	-0.18325700	-1.73776400
H	-3.88966400	-0.05209300	-3.43919700
H	-3.08105300	-1.21937100	-2.39527600
C	-4.02045800	2.57871300	-0.92768500
H	-4.46608000	3.26889400	-1.65391300
H	-4.74275300	1.77370400	-0.76740400
H	-3.92177400	3.13543800	0.01035600
Co	-1.23924000	0.90223600	-0.47665700

Zero-point correction= 0.648103 (Hartree/Particle)

Thermal correction to Energy= 0.690015

Thermal correction to Enthalpy= 0.690959

Thermal correction to Gibbs Free Energy= 0.574547

Sum of electronic and zero-point Energies= -2233.507101

Sum of electronic and thermal Energies= -2233.465189

Sum of electronic and thermal Enthalpies= -2233.464245

Sum of electronic and thermal Free Energies= -2233.580657

E(RM06L) = -2234.155204 A.U.

(T)A-TS5

1 3

Number of imaginary frequencies: 1

C	-2.05476500	1.11665800	-0.08323700
C	-3.23136700	1.99283900	-0.17913500
C	-3.28630500	3.01466500	-1.13796400
C	-4.31853100	1.82487400	0.69300400
C	-4.38819000	3.85456500	-1.21682900
H	-2.46765400	3.11598100	-1.84779100
C	-5.41587500	2.67292200	0.61979800
H	-4.27776900	1.04324900	1.44736800
C	-5.45347300	3.68864700	-0.33351700
H	-4.42218500	4.63360700	-1.97199000
H	-6.24252700	2.54559800	1.31186900
H	-6.31413400	4.34779100	-0.39209900
C	-0.77875100	1.62560400	-0.18202300
P	-0.23717300	3.34641500	0.01400200
C	1.61721700	1.46703300	0.16193700
C	2.96044000	1.76138700	0.49133200
C	3.45597100	3.07558900	0.34907900
C	3.84223000	0.76508400	0.96307200
C	4.77536100	3.36952300	0.65886000
H	2.78612300	3.85780800	0.00341000

C	5.16123600	1.06776900	1.26432600
H	3.47576700	-0.25407700	1.03786900
C	5.63510900	2.37106500	1.11525100
H	5.13603500	4.38674300	0.54363600
H	5.82576400	0.28149000	1.61195400
H	6.66733300	2.60682600	1.35286500
C	0.48856100	0.94159400	-0.19377100
C	0.37075900	3.91435100	-1.61238900
H	0.95006200	4.82995900	-1.48061000
H	0.99599500	3.15159500	-2.08107900
H	-0.48047300	4.14549000	-2.26002600
O	-1.07095700	4.35415300	0.74797500
C	-3.18614500	-2.39014700	-0.07144600
C	-1.94825700	-2.47969100	0.60246000
C	-1.45323400	-3.67373900	1.11087500
C	-2.20628000	-4.82035600	0.87711300
C	-3.41724400	-4.76579100	0.16768300
C	-3.91846700	-3.56304400	-0.30571000
C	-3.39326700	-1.01524400	-0.37978900
C	-2.31676100	-0.29281800	0.08235600
H	-0.51379400	-3.71723500	1.65513400
H	-1.84980400	-5.77475000	1.25207000
H	-3.97401200	-5.68219100	0.00086700
H	-4.86397100	-3.52475200	-0.83787800
H	-4.21849500	-0.58881800	-0.93409500
C	-0.57438800	-0.89486800	1.78013800
N	-1.13933900	-0.41617600	2.87088700

C	-0.33595500	-0.27900400	3.93395800
C	0.99596600	-0.68167300	3.91609500
C	1.50356200	-1.12800400	2.70515000
N	0.73034500	-1.19752300	1.60911000
H	-0.78727000	0.15035000	4.82490400
H	1.62392600	-0.61710500	4.79616700
H	2.54553900	-1.41035200	2.58434900
N	-1.37885100	-1.19123800	0.65016200
C	0.62425500	-2.22791100	-2.03876000
C	1.11590700	-0.95688900	-2.46389700
C	2.48888200	-0.81826000	-1.99550200
C	2.79101300	-1.94644200	-1.20438900
C	1.62031000	-2.80756400	-1.20376500
C	1.56983600	-4.13272000	-0.52955900
H	0.55777700	-4.54169100	-0.49782800
H	2.20318900	-4.85510700	-1.05797800
H	1.94625400	-4.08154700	0.49844100
C	-0.70500900	-2.79445200	-2.39328300
H	-1.50269700	-2.04864900	-2.30885600
H	-0.70610900	-3.14456200	-3.43198400
H	-0.97761300	-3.64273600	-1.76088400
C	0.40807600	-0.00819300	-3.36591500
H	0.75364300	1.01932400	-3.22255600
H	0.57876900	-0.26448800	-4.41846000
H	-0.67323800	-0.02260200	-3.19848300
C	3.39529500	0.29535600	-2.38189200
H	4.27888100	0.35690200	-1.74218900

H	3.73956500	0.15846700	-3.41377800
H	2.89130100	1.26670500	-2.34170800
C	4.09592000	-2.29792500	-0.57643500
H	4.58971900	-3.10636700	-1.12821400
H	4.78344000	-1.44873400	-0.56072600
H	3.97926900	-2.65476600	0.45384800
Co	1.08895200	-0.92522200	-0.38704300

Zero-point correction= 0.647873 (Hartree/Particle)

Thermal correction to Energy= 0.689919

Thermal correction to Enthalpy= 0.690863

Thermal correction to Gibbs Free Energy= 0.573037

Sum of electronic and zero-point Energies= -2233.517399

Sum of electronic and thermal Energies= -2233.475352

Sum of electronic and thermal Enthalpies= -2233.474408

Sum of electronic and thermal Free Energies= -2233.592235

E(RM06L) = -2234.165272 A.U.

(S)A-TS6

1 1

Number of imaginary frequencies: 1

C	-1.57534700	-0.74463800	0.89768900
C	-2.86087700	-1.27737700	1.36183000
C	-3.18393100	-2.64178900	1.27285300
C	-3.81638300	-0.39595900	1.89649300
C	-4.41765300	-3.10025900	1.71624800
H	-2.50014000	-3.33755700	0.79283100
C	-5.04909300	-0.86060700	2.33808200
H	-3.58651000	0.66517900	1.97374800

C	-5.35366600	-2.21659600	2.25233000
H	-4.65640100	-4.15602900	1.62778100
H	-5.77022700	-0.16286700	2.75289700
H	-6.31641100	-2.58260400	2.59588000
C	-0.42148700	-1.43825100	0.68813600
P	0.07589900	-3.16732700	0.36507900
C	1.37641100	-2.13956700	-0.39291600
C	2.45280200	-2.42820500	-1.28852500
C	3.20039700	-1.38684800	-1.87725200
C	2.77996500	-3.76120800	-1.60452100
C	4.24688600	-1.67278700	-2.73813800
H	2.94258100	-0.35602100	-1.64024400
C	3.82948000	-4.04166300	-2.46796200
H	2.18805600	-4.56972900	-1.18130200
C	4.56655300	-3.00132500	-3.03299600
H	4.81780700	-0.86415000	-3.18627400
H	4.07260400	-5.07188500	-2.70761500
H	5.38705500	-3.22348500	-3.70838500
C	0.79143900	-0.94388700	0.02842200
C	0.66971300	-3.97218100	1.87894300
H	1.21978500	-4.87622500	1.60724000
H	1.30726100	-3.33680700	2.49668200
H	-0.20214300	-4.27320000	2.46570900
O	-0.76348000	-4.07875200	-0.47222200
C	-0.89596600	2.84377600	0.18540800
C	-1.97511100	2.54608800	-0.66694000
C	-2.52115400	3.47483700	-1.54647400

C	-1.96062400	4.74879500	-1.54691900
C	-0.89044800	5.07367700	-0.70452700
C	-0.34972500	4.12690000	0.15756300
C	-0.54623300	1.62054000	0.90116700
C	-1.49116500	0.64762000	0.47078300
H	-3.36146200	3.22327100	-2.18074900
H	-2.36797600	5.50434900	-2.21113400
H	-0.47732300	6.07718800	-0.72830600
H	0.50018200	4.37763400	0.78574800
H	-0.34321700	1.62204400	1.96709700
C	-3.25701100	0.45551400	-1.24238700
N	-4.37923900	1.10068300	-1.54165200
C	-5.27616500	0.37555300	-2.22043200
C	-5.05665400	-0.95249200	-2.56588500
C	-3.82438400	-1.49237300	-2.21081100
N	-2.90214700	-0.78480500	-1.55524700
H	-6.20165600	0.88427200	-2.48168400
H	-5.80215000	-1.53288300	-3.09624400
H	-3.55102200	-2.51708400	-2.45569600
N	-2.31365800	1.18933300	-0.46511400
C	3.10338500	-0.02590000	1.69344900
C	3.58076700	1.09191500	0.95526700
C	2.90865700	2.27454800	1.44913900
C	2.02420700	1.87407300	2.47890000
C	2.06233400	0.43675800	2.57445600
C	1.30622800	-0.38433000	3.55758700
H	0.29651400	0.00336400	3.72455500

H	1.19717800	-1.41579500	3.21578500
H	1.81067400	-0.41018300	4.53064400
C	3.66961900	-1.39671800	1.65116300
H	4.09451300	-1.64487600	0.67622000
H	4.47808300	-1.46678500	2.38857400
H	2.93281000	-2.16124600	1.90349700
C	4.64933400	1.11874300	-0.07555100
H	4.31386100	1.65341700	-0.97068300
H	5.52987600	1.64868600	0.30553500
H	4.96710200	0.11677700	-0.36996100
C	3.17721700	3.65232500	0.96494500
H	2.62899600	4.40286600	1.53851400
H	4.24346000	3.88663300	1.05316100
H	2.90717000	3.75370700	-0.09155300
C	1.22502300	2.77894500	3.34748100
H	1.86265300	3.15872500	4.15373600
H	0.83261000	3.64694100	2.81197100
H	0.38626400	2.26805100	3.82689000
Co	1.53170500	0.91678700	0.63998300
O	0.21882600	0.55956300	-2.05111400
O	1.71378200	1.88729800	-1.05736400
C	0.94513700	1.59305200	-2.03390800
C	0.88661000	2.54871200	-3.18225900
H	1.83515600	3.07191700	-3.30377900
H	0.60414100	2.03793400	-4.10200400
H	0.11917200	3.29800000	-2.95690500
H	0.60432400	-0.11070700	-0.91777100

Zero-point correction= 0.710064(Hartree/Particle)

Thermal correction to Energy= 0.756529

Thermal correction to Enthalpy= 0.757473

Thermal correction to Gibbs Free Energy= 0.632584

Sum of electronic and zero-point Energies= -2462.591500

Sum of electronic and thermal Energies= -2462.545035

Sum of electronic and thermal Enthalpies= -2462.544091

Sum of electronic and thermal Free Energies= -2462.668980

E(RM06L) = -2463.301564 A.U.

(T)A-TS6

1 3

Number of imaginary frequencies: 1

C	-1.60359200	-0.89512600	0.87101800
C	-2.76264200	-1.60134400	1.42835500
C	-2.94839400	-2.98641800	1.27735700
C	-3.72421100	-0.86818300	2.14500100
C	-4.05023700	-3.61118300	1.84549300
H	-2.26642800	-3.56677000	0.66085000
C	-4.82151700	-1.50042800	2.71616200
H	-3.59579800	0.20487200	2.26760600
C	-4.98666300	-2.87545700	2.57177100
H	-4.18777300	-4.67957800	1.70766400
H	-5.54804100	-0.91827000	3.27481300
H	-5.84549300	-3.37111000	3.01425700
C	-0.38818300	-1.44822100	0.59496800
P	0.28032000	-3.11829600	0.27267700
C	1.45891400	-1.97036800	-0.52698100

C	2.57992700	-2.12783300	-1.39287600
C	3.18700300	-1.01305000	-2.01390400
C	3.11794200	-3.41071500	-1.62708500
C	4.30577500	-1.17745000	-2.81341500
H	2.76266300	-0.01911200	-1.86962500
C	4.23832400	-3.56876100	-2.42809000
H	2.63688900	-4.27696800	-1.17883100
C	4.83714100	-2.45441100	-3.01780300
H	4.76389400	-0.31596000	-3.29071800
H	4.64576000	-4.55944900	-2.60152300
H	5.71100600	-2.58047800	-3.64960800
C	0.75726300	-0.83735600	-0.09762000
C	1.01803600	-3.80464500	1.78040500
H	1.66997300	-4.64115400	1.51824600
H	1.58172400	-3.06295300	2.34909100
H	0.20935700	-4.18953700	2.40739500
O	-0.44921100	-4.13270600	-0.54789200
C	-1.53299700	2.79498400	0.52023700
C	-2.54870500	2.42673600	-0.39688600
C	-3.21330900	3.37628900	-1.17347600
C	-2.84642800	4.70727900	-1.01115700
C	-1.84987800	5.09333600	-0.10188200
C	-1.19122100	4.14572900	0.66610400
C	-1.04333700	1.58646900	1.10764900
C	-1.74387600	0.53353600	0.56451600
H	-3.99819300	3.08517700	-1.85781600
H	-3.35616600	5.46628800	-1.59649800

H	-1.59995700	6.14432600	0.00492900
H	-0.42238700	4.44868200	1.37256700
H	-0.37737600	1.48456200	1.95182700
C	-3.39788400	0.23506600	-1.26555700
N	-4.46409700	0.80047200	-1.83106200
C	-5.13474800	0.02076600	-2.68422400
C	-4.77085400	-1.29327200	-2.95211300
C	-3.63729300	-1.76121800	-2.29635400
N	-2.93301500	-0.99786400	-1.46160500
H	-6.00307400	0.47386900	-3.15899500
H	-5.33608000	-1.91519100	-3.63561800
H	-3.26320600	-2.77391900	-2.44071400
N	-2.67327600	1.02902700	-0.35150500
C	3.44623300	0.08687000	1.43473200
C	3.85431700	1.27383800	0.79026700
C	3.04753500	2.34777800	1.31917500
C	2.20897700	1.83801500	2.36092800
C	2.39259200	0.43663700	2.39845000
C	1.73326500	-0.50985500	3.33886400
H	0.80310600	-0.92422600	2.92597500
H	2.38925100	-1.35143300	3.57936700
H	1.47478700	-0.01730500	4.27939700
C	4.09209400	-1.24775800	1.34038400
H	4.62248900	-1.38697100	0.39516100
H	4.82606000	-1.35867700	2.14780500
H	3.37536700	-2.06723300	1.44241600
C	4.90299800	1.43452900	-0.25341700

H	4.52632500	1.98412600	-1.12338800
H	5.75770900	1.99977800	0.13387400
H	5.27438900	0.46958300	-0.60475800
C	3.11457800	3.76526300	0.89148100
H	2.13238300	4.24420100	0.92959600
H	3.78054800	4.32859800	1.55650900
H	3.49656600	3.86537200	-0.12573400
C	1.36169100	2.66346800	3.26382500
H	1.98401900	3.15967500	4.01726000
H	0.83091400	3.45377200	2.72578200
H	0.61759800	2.06953900	3.79940500
Co	1.75519900	0.89708300	0.39906000
O	-0.08520900	0.80779300	-1.98664700
O	1.36912800	2.19490600	-0.98521700
C	0.46137900	1.93642800	-1.85807700
C	0.05414100	3.05814900	-2.75705100
H	0.93490400	3.49472700	-3.23202500
H	-0.65358900	2.71775000	-3.51070200
H	-0.40796900	3.84265200	-2.14868200
H	0.42878600	0.02185800	-0.98913300

Zero-point correction= 0.708193 (Hartree/Particle)

Thermal correction to Energy= 0.755375

Thermal correction to Enthalpy= 0.756320

Thermal correction to Gibbs Free Energy= 0.628078

Sum of electronic and zero-point Energies= -2462.583789

Sum of electronic and thermal Energies= -2462.536607

Sum of electronic and thermal Enthalpies= -2462.535662

Sum of electronic and thermal Free Energies= -2462.663904

E(RM06L) = -2463.291982 A.U.

B-1-Co

1 1

Number of imaginary frequencies: 0

C	-0.35491500	-1.13967800	-1.58476900
C	-1.57910900	-1.69183500	-1.06878700
C	-2.58309800	-0.68351400	-1.11020800
C	-1.98259800	0.51351200	-1.67360300
C	-0.62406000	0.21363400	-1.99188100
O	-1.08990900	-1.00260900	1.79253400
O	-2.25931000	0.77475600	1.37089200
C	-1.94260000	-0.14540600	2.19884800
C	-3.98577100	-0.80037100	-0.63956000
H	-4.65043300	-1.03116300	-1.47942100
H	-4.10231800	-1.60055200	0.09554200
H	-4.33628000	0.12933500	-0.18615200
C	-1.70313600	-3.05586800	-0.50131300
H	-2.56513000	-3.15310500	0.16050200
H	-1.81768100	-3.78735200	-1.30928300
H	-0.80808800	-3.33001600	0.06378100
C	0.89054600	-1.91250400	-1.82492500
H	1.24045300	-2.42578500	-0.92356700
H	0.70497700	-2.68726300	-2.57767100
H	1.69646200	-1.28010800	-2.20051400
C	0.36991800	1.14468000	-2.58176800
H	1.39153300	0.94137500	-2.24261100

H	0.36593700	1.03898200	-3.67245400
H	0.13535200	2.18903700	-2.35974800
C	-2.68447800	1.80884100	-1.85822700
H	-1.98659400	2.63298900	-2.02227800
H	-3.34772400	1.76541700	-2.72938400
H	-3.30809600	2.05261300	-0.99268100
Co	-1.03215900	-0.04340900	0.02160300
C	-2.56206900	-0.22429800	3.54650700
H	-2.66765000	0.77176500	3.97841800
H	-3.56898400	-0.64170700	3.45189500
H	-1.98333300	-0.86820700	4.20747600
C	1.87473900	-1.03114800	1.48381300
C	2.47239300	-2.24836400	1.59315800
C	3.54853300	-2.56458100	0.72383500
C	3.95278900	-1.68524500	-0.23811600
C	3.31012400	-0.41622100	-0.43729800
C	1.72216400	1.17673000	0.51852300
C	-0.12239700	2.56988400	0.60274900
C	0.66977700	3.70166000	0.62458900
C	2.05402400	3.55013300	0.57743900
C	2.58436800	2.27255600	0.53427200
H	1.07745000	-0.70098000	2.13681800
H	2.14515500	-2.93233700	2.36574800
H	4.05639700	-3.51946800	0.82707100
H	4.76582700	-1.90909400	-0.91889500
H	-1.20405300	2.63164800	0.64309700
H	0.20544900	4.67960600	0.67751600

H	2.71109600	4.41337600	0.59135100
H	3.65252300	2.10016000	0.51029400
N	2.27367400	-0.13061300	0.52278600
N	0.38300800	1.31469300	0.52605800
O	3.53901800	0.38894600	-1.33588800

Zero-point correction= 0.441415(Hartree/Particle)

Thermal correction to Energy= 0.469865

Thermal correction to Enthalpy= 0.470810

Thermal correction to Gibbs Free Energy= 0.384917

Sum of electronic and zero-point Energies= -1334.443828

Sum of electronic and thermal Energies= -1334.415377

Sum of electronic and thermal Enthalpies= -1334.414433

Sum of electronic and thermal Free Energies= -1334.500326

E(RM06L) = -1334.885243 A.U.

B-2a-Co

1 1

Number of imaginary frequencies: 0

C	-0.80946800	-0.58869500	-2.05402400
C	-1.55210300	-1.56454200	-1.29066800
C	-2.56053700	-0.86633800	-0.57922100
C	-2.52322400	0.53184000	-0.96561300
C	-1.48211700	0.68243200	-1.91068300
C	-3.52148300	-1.44943200	0.39120400
H	-4.46137600	-1.70621000	-0.11065800
H	-3.13686000	-2.36477900	0.84815100
H	-3.76246100	-0.74235600	1.18884000
C	-1.36818000	-3.03678900	-1.34568900

H	-1.68043700	-3.53382300	-0.42397300
H	-1.98982300	-3.44402100	-2.15154800
H	-0.33560200	-3.32034500	-1.55606100
C	0.33134800	-0.87633500	-2.96365700
H	0.92816800	-1.71930300	-2.60418800
H	-0.02297500	-1.12937400	-3.96944200
H	0.99950500	-0.01658500	-3.06380900
C	-1.08230600	1.92510300	-2.61798300
H	0.00416500	2.02624900	-2.69392900
H	-1.47063000	1.90176100	-3.64227800
H	-1.47716100	2.82588300	-2.14341300
C	-3.43934300	1.57788900	-0.43823000
H	-3.15308200	2.57881900	-0.77033700
H	-4.46808200	1.40885900	-0.77373700
H	-3.45275000	1.57480200	0.65691500
N	2.06936700	-0.34394300	0.01324200
C	1.86961900	1.04189300	-0.04140400
N	0.56180700	1.38254700	0.04188500
C	0.20324400	2.67366300	0.15347900
C	1.12916800	3.69875000	0.13812700
C	2.47342700	3.35838400	-0.00739500
H	-0.86439200	2.85288900	0.25178200
H	0.80461800	4.72836900	0.23034700
H	3.23384700	4.13212100	-0.04042600
Co	-0.69922500	-0.07895200	-0.09940100
C	3.39863800	-0.92421200	-0.08796200
C	3.45495600	-2.31393900	0.28190800

H	4.44425100	-2.75530500	0.26562800
C	2.34597700	-3.02062600	0.62547200
C	1.05890500	-2.41500600	0.58815100
C	0.90402800	-1.09489100	0.25727900
O	4.35341300	-0.25270900	-0.44726700
H	2.43491600	-4.06581000	0.91060300
H	0.17683600	-3.01023300	0.80145400
C	2.86001000	2.02906100	-0.09632500
H	3.89429500	1.73747300	-0.19838500
O	0.08791800	-0.65182000	3.12142500
O	-1.40595200	0.33976100	1.75502500
C	-0.97556500	0.08265000	2.89053500
H	0.44918200	-0.98378000	2.26596200
C	-1.63917100	0.59259300	4.11777100
H	-2.53263700	1.15965300	3.86611800
H	-1.89477800	-0.24110500	4.77539500
H	-0.94385500	1.22505100	4.67504000

Zero-point correction= 0.440774 (Hartree/Particle)

Thermal correction to Energy= 0.469588

Thermal correction to Enthalpy= 0.470533

Thermal correction to Gibbs Free Energy= 0.381757

Sum of electronic and zero-point Energies= -1334.428917

Sum of electronic and thermal Energies= -1334.400102

Sum of electronic and thermal Enthalpies= -1334.399158

Sum of electronic and thermal Free Energies= -1334.487934

E(RM06L) = -1334.869691 A.U.

B-3a-Co

1 1

Number of imaginary frequencies: 0

C	1.83958800	-0.17102300	1.40631300
C	2.00554900	-1.37623900	0.62809200
C	2.42614100	-0.98045400	-0.66654300
C	2.64080900	0.46495400	-0.66099400
C	2.32858200	0.94647200	0.62417500
C	2.65307900	-1.85667000	-1.84338900
H	3.72669700	-2.00991800	-2.00459600
H	2.19642800	-2.84057600	-1.71925700
H	2.25630300	-1.41492600	-2.76204200
C	1.83400100	-2.75550400	1.15372300
H	1.84063000	-3.50810100	0.36317800
H	2.67024500	-2.98969000	1.82188200
H	0.91430400	-2.87320100	1.73151700
C	1.36822100	-0.10101700	2.81015000
H	0.68733200	-0.92044000	3.05058600
H	2.21784400	-0.16943800	3.50146600
H	0.85812800	0.84214600	3.02198400
C	2.44754400	2.33483900	1.14046100
H	1.54864800	2.66106200	1.67229400
H	3.27361100	2.38854800	1.85808200
H	2.66291000	3.05979200	0.35262400
C	3.09519700	1.24874300	-1.83853800
H	2.97314100	2.32423400	-1.69248500
H	4.15730100	1.06614500	-2.03797100
H	2.55404800	0.96884800	-2.74760200

N	-2.07305000	-0.42889600	-0.01684300
C	-1.93002600	0.96115400	-0.05773800
N	-0.63936500	1.34982600	-0.25106700
C	-0.36583300	2.65833800	-0.44518600
C	-1.33708700	3.63572600	-0.41462800
C	-2.65063300	3.24251600	-0.15636900
H	0.67510000	2.89349700	-0.63711100
H	-1.07110900	4.67208300	-0.58436700
H	-3.44469500	3.98053300	-0.10452800
Co	0.67328500	-0.05367300	-0.19921200
C	-3.37344100	-1.06217100	0.06232100
C	-3.35725500	-2.47852200	-0.21969100
H	-4.32947400	-2.95699400	-0.21138900
C	-2.20778400	-3.15885700	-0.47083200
C	-0.95815400	-2.48859600	-0.42018500
C	-0.87339100	-1.13784000	-0.19136400
O	-4.38209100	-0.43029600	0.33205600
H	-2.23884900	-4.22282100	-0.68894700
H	-0.04606300	-3.05192600	-0.57662000
C	-2.95994800	1.90354200	0.02325500
H	-3.96847800	1.56985400	0.21272800

Zero-point correction= 0.376160 (Hartree/Particle)

Thermal correction to Energy= 0.399685

Thermal correction to Enthalpy= 0.400629

Thermal correction to Gibbs Free Energy= 0.323901

Sum of electronic and zero-point Energies= -1105.378655

Sum of electronic and thermal Energies= -1105.355130

Sum of electronic and thermal Enthalpies= -1105.354186

Sum of electronic and thermal Free Energies= -1105.430914

E(RM06L) = -1105.754815 A.U.

B-4-Co

1 1

Number of imaginary frequencies: 0

C	3.87901900	-1.10161600	-0.71703100
C	5.15663300	-0.50622000	-0.57595800
C	5.85930000	-0.61876000	0.63795900
C	5.72815900	0.20846400	-1.64441400
C	7.10524600	-0.02324600	0.77498500
H	5.42109900	-1.18350300	1.45641600
C	6.97545200	0.79804300	-1.49502200
H	5.18864400	0.28239000	-2.58416500
C	7.66408900	0.68495700	-0.28798300
H	7.64626700	-0.11662000	1.71124600
H	7.41577400	1.34365900	-2.32359400
H	8.64099200	1.14521200	-0.17721600
C	2.74577000	-1.55409700	-0.80580600
P	1.25964600	-2.44928500	-1.05011300
C	-1.33990100	-1.55604600	-0.57908600
C	-2.65921300	-1.90668800	-0.95054100
C	-3.28517700	-1.24096400	-2.02243400
C	-3.34671000	-2.92713700	-0.26805500
C	-4.57236700	-1.59046000	-2.39796900
H	-2.75136100	-0.44568500	-2.53704800
C	-4.63791500	-3.26428500	-0.65045700

H	-2.85300900	-3.45375300	0.54295900
C	-5.25239000	-2.59586000	-1.70874300
H	-5.05186500	-1.07483500	-3.22388500
H	-5.16479500	-4.05593600	-0.12742500
H	-6.26258900	-2.86370100	-2.00272200
C	-0.09833500	-1.43270700	-0.42635000
C	1.00028800	-2.37512900	-2.83652800
H	0.04075500	-2.83994100	-3.07485600
H	1.00130800	-1.34206300	-3.19369200
H	1.79610700	-2.93151600	-3.33568200
O	1.24096500	-3.80704100	-0.43200500
C	-1.21854800	0.55881200	2.80069900
C	-0.83278500	-0.80377500	2.64276800
C	0.58178900	-0.83101400	2.32984800
C	1.02571300	0.50160000	2.17852300
C	-0.10694900	1.37219000	2.39963800
C	-0.08444300	2.85837200	2.36746700
H	-1.06732200	3.27233900	2.12682700
H	0.21069200	3.26508400	3.34158000
H	0.62874500	3.23725000	1.62966000
C	-2.47842300	1.06857000	3.39558300
H	-3.28503400	0.33498400	3.36629900
H	-2.28510700	1.29899600	4.45045100
H	-2.83278400	1.98483200	2.91935200
C	-1.66229600	-2.00602800	2.91696000
H	-1.33849500	-2.85392800	2.30648500
H	-1.57684200	-2.31328600	3.96582900

H	-2.72323800	-1.82751300	2.71772700
C	1.41558300	-2.05754300	2.30510100
H	2.37888000	-1.89350100	1.81691300
H	1.61832700	-2.36930000	3.33685800
H	0.93149300	-2.89850500	1.80297500
C	2.42498200	0.94985500	1.95679900
H	2.92590000	1.08489500	2.92275200
H	3.00520200	0.22007000	1.38716700
H	2.47724200	1.91018500	1.43753800
Co	-0.58593700	0.16620300	0.81608400
C	-2.29781800	0.91433500	0.27259300
C	-3.54620100	0.50379900	0.64408800
C	-4.70132900	1.19397000	0.21024200
C	-4.59896600	2.30524800	-0.57045300
C	-3.33566200	2.82499800	-1.00262100
C	-0.89068700	2.30037700	-1.02256800
C	1.30126200	1.49638300	-0.98788000
C	1.73581900	2.47675500	-1.85974900
C	0.80546400	3.41382600	-2.30160600
C	-0.51686300	3.33188800	-1.89315900
H	-3.64627100	-0.38678500	1.25565400
H	-5.68174000	0.82915700	0.50820200
H	-5.46426000	2.86323600	-0.90704000
H	1.96844600	0.72959900	-0.60991200
H	2.77394700	2.49968400	-2.17189000
H	1.10144200	4.21135700	-2.97589300
H	-1.26540100	4.03297600	-2.22780600

N	-2.18505900	2.03351900	-0.55889900
N	0.02917100	1.41873400	-0.56081900
O	-3.18520000	3.82770300	-1.68645600

Zero-point correction= 0.623466(Hartree/Particle)

Thermal correction to Energy= 0.665729

Thermal correction to Enthalpy= 0.666673

Thermal correction to Gibbs Free Energy= 0.547226

Sum of electronic and zero-point Energies= -2177.215241

Sum of electronic and thermal Energies= -2177.172979

Sum of electronic and thermal Enthalpies= -2177.172035

Sum of electronic and thermal Free Energies= -2177.291482

E(RM06L) = -2177.838708 A.U.

B-5a-Co

1 1

Number of imaginary frequencies: 0

C	-2.19764700	-0.83392800	-0.02621300
C	-2.97518300	-2.07577300	-0.22439900
C	-2.87835700	-3.12122200	0.70335400
C	-3.80784700	-2.23813300	-1.34020700
C	-3.56899600	-4.31171200	0.50729600
H	-2.28502900	-2.96987300	1.60343500
C	-4.49100900	-3.43093600	-1.54022400
H	-3.89836300	-1.42909900	-2.06197000
C	-4.37035500	-4.47138700	-0.62005500
H	-3.49377700	-5.10954400	1.24019500
H	-5.11896900	-3.55190100	-2.41766400
H	-4.91034800	-5.40005300	-0.77653400

C	-0.89647400	-0.84500200	0.35531000
P	0.24944500	-2.17452000	0.09447700
C	2.89318200	-1.05730200	-0.22139700
C	4.23947600	-1.01667200	-0.61318900
C	5.27299700	-1.20430300	0.33128900
C	4.57031500	-0.79263400	-1.96850400
C	6.59714900	-1.15619000	-0.07162600
H	5.01527300	-1.39103500	1.37045800
C	5.89903500	-0.74777100	-2.35824700
H	3.77026800	-0.67800200	-2.69443100
C	6.91044500	-0.92630200	-1.41277600
H	7.39003300	-1.30211100	0.65452300
H	6.15267900	-0.58158100	-3.40008500
H	7.94998900	-0.89289800	-1.72408000
C	1.68839200	-1.03206600	0.09828900
C	0.54992900	-3.14431900	1.59846600
H	1.55122400	-3.57859400	1.56107000
H	0.44962700	-2.53394500	2.49844200
H	-0.18174500	-3.95491400	1.62439900
O	0.16804400	-2.98195500	-1.15870000
C	-2.91737300	0.43260400	-0.20109600
C	-1.13553200	1.35384000	-1.66387200
C	-0.25826600	1.56435700	-3.89040900
C	1.01803300	1.41696600	-3.35649700
C	1.14524900	1.20291600	-1.99674800
N	0.09166000	1.15136000	-1.15450700
H	-0.40635100	1.71023600	-4.95509900

H	1.90444100	1.45623500	-3.97947700
H	2.11525900	1.05320000	-1.53433800
N	-2.27070200	1.50264400	-0.80680400
C	-0.06470100	0.78788900	2.70557500
C	1.33727900	0.58161600	2.57062900
C	1.88227700	1.64600200	1.74478500
C	0.81672000	2.49564100	1.38418800
C	-0.40394200	1.96214400	1.95343700
C	-1.70254100	2.67831700	2.02972800
H	-2.56265000	2.01378500	1.90779100
H	-1.79853200	3.13722300	3.02179600
H	-1.76830100	3.48375300	1.29682900
C	-1.02752700	-0.01145100	3.50858800
H	-0.66437200	-1.02333500	3.70631000
H	-1.20727100	0.46522100	4.47891100
H	-1.99267600	-0.09786900	3.00040600
C	2.15881400	-0.44539500	3.26443000
H	2.79864300	-1.00348900	2.57361600
H	2.81642600	0.04354300	3.99209900
H	1.54681100	-1.16208100	3.81553700
C	3.32296600	1.83376600	1.42147600
H	3.47530200	2.21578200	0.40699900
H	3.78432600	2.55596500	2.10484500
H	3.88347600	0.90003600	1.51222500
C	0.88935000	3.71155100	0.53355800
H	0.91920500	4.60894200	1.16205600
H	1.79049000	3.72184600	-0.08513400

H	0.01746400	3.80729100	-0.12341900
Co	0.41220700	0.53624300	0.70150200
C	-4.20207600	0.60736100	0.25341500
H	-4.69939600	-0.23691900	0.71630900
C	-2.83045300	2.83408400	-0.86481900
C	-4.17667400	2.93799500	-0.38199800
H	-4.63171000	3.91844300	-0.45992700
C	-4.83674800	1.86395300	0.14182200
H	-5.85630700	1.97790100	0.49953400
O	-2.13949400	3.74773100	-1.30776900
C	-1.34134600	1.54504700	-3.02796900
H	-2.35288500	1.70153700	-3.38476200

Zero-point correction= 0.625674 (Hartree/Particle)

Thermal correction to Energy= 0.666630

Thermal correction to Enthalpy= 0.667574

Thermal correction to Gibbs Free Energy= 0.553592

Sum of electronic and zero-point Energies= -2177.244796

Sum of electronic and thermal Energies= -2177.203840

Sum of electronic and thermal Enthalpies= -2177.202896

Sum of electronic and thermal Free Energies= -2177.316878

E(RM06L) = -2177.870470 A.U.

B-6-Co

1 1

Number of imaginary frequencies: 0

C	3.82574500	-0.11528700	-1.44675500
C	5.10077300	0.32789500	-1.02225700
C	5.97146900	-0.54428600	-0.34294200

C	5.51460200	1.65104000	-1.26120200
C	7.21221500	-0.09796000	0.08266000
H	5.66424000	-1.57142100	-0.16394600
C	6.75956000	2.08033700	-0.82964300
H	4.85323000	2.32696500	-1.79619000
C	7.63236500	1.21764300	-0.15360400
H	7.87636200	-0.78197800	0.60484800
H	7.06932800	3.10430500	-1.02293600
C	2.69330800	-0.47702500	-1.73829900
P	1.21794200	-1.07088600	-2.47369100
C	-1.32086000	-0.86023200	-1.40541700
C	-2.68291500	-0.70178700	-1.69555100
C	-3.18105700	0.58898200	-1.98119700
C	-3.57198000	-1.79481000	-1.69140600
C	-4.52629000	0.77266700	-2.23403000
H	-2.49709400	1.43451400	-1.98451700
C	-4.91822500	-1.58978300	-1.93732800
H	-3.19041600	-2.79144000	-1.49019500
C	-5.42206300	-0.30721400	-2.19991900
H	-4.90289800	1.77222500	-2.43562400
H	-5.60113300	-2.43504000	-1.92723400
C	-0.07884200	-0.92371600	-1.22496100
C	0.78163700	0.24686600	-3.63390000
H	-0.17908300	0.01049900	-4.09760800
H	0.70886000	1.20915900	-3.11833800
H	1.54463600	0.31059500	-4.41204800
O	1.30407000	-2.45046600	-3.03572300

C	-4.04309300	0.85070800	1.23528800
C	-3.18753700	1.93774800	0.94424700
C	-3.65757000	3.22751300	0.72257400
C	-5.03684500	3.41523200	0.78843000
C	-5.90576800	2.35342900	1.07033800
C	-5.42148300	1.07035700	1.30037700
C	-3.22716900	-0.32736700	1.36438700
C	-1.91888300	0.00334600	1.15256700
H	-2.98052900	4.04385800	0.50487100
H	-5.44246200	4.40799000	0.62000000
H	-6.97512100	2.53916800	1.11568400
H	-6.10030700	0.24936400	1.51674300
H	-3.60967600	-1.32396500	1.53900800
C	-0.69626900	1.99192500	0.64873900
N	-0.61771200	3.29905300	0.39579300
C	0.60371500	3.78713600	0.18935700
C	1.75221800	3.00034000	0.22645400
C	1.57035500	1.64717800	0.46655900
N	0.35589500	1.12200000	0.67450500
H	0.65956800	4.85460300	-0.01539100
H	2.74166400	3.41048500	0.06857300
H	2.40077700	0.95160200	0.47528100
N	-1.89111200	1.39974300	0.89956900
C	-0.61968600	-2.07357800	2.48080500
C	-0.24431000	-2.81022800	1.31993900
C	1.14114400	-2.49968000	1.02176200
C	1.56500800	-1.49531100	1.91532300

C	0.45200000	-1.16632300	2.78123800
C	0.46048500	-0.17426900	3.88829300
H	-0.53921300	0.23105100	4.06569500
H	0.80183800	-0.63069400	4.82488400
H	1.12767700	0.66513500	3.67502800
C	-1.82958700	-2.27788300	3.31419500
H	-2.61525300	-2.81725900	2.78271700
H	-1.54721400	-2.89130500	4.17813000
H	-2.24726500	-1.34369600	3.69212300
C	-1.06176700	-3.82346800	0.60322400
H	-0.84411500	-3.81826800	-0.46938600
H	-0.85264500	-4.83457100	0.97160500
H	-2.13204300	-3.64077800	0.73535800
C	1.97695900	-3.22909700	0.03615800
H	2.87516200	-2.67226600	-0.23968400
H	2.30103400	-4.17815100	0.48064600
H	1.44418000	-3.47025100	-0.88653900
C	2.94039100	-0.94445600	2.03174300
H	3.54062100	-1.58560500	2.68821900
H	3.45272700	-0.90454100	1.06646600
H	2.95350800	0.05444400	2.47518400
Co	-0.17413000	-0.79827000	0.88822800
C	-6.88114400	-0.07990900	-2.41763600
H	-7.06600800	0.48037200	-3.33888300
H	-7.44021300	-1.01581300	-2.46956500
H	-7.30106900	0.51851700	-1.60107900
C	8.98792600	1.67872100	0.27594900

H	9.72941000	1.48797800	-0.50795800
H	9.00731600	2.75223300	0.47759600
H	9.33074000	1.15435800	1.17100800

Zero-point correction= 0.703368 (Hartree/Particle)

Thermal correction to Energy= 0.750226

Thermal correction to Enthalpy= 0.751170

Thermal correction to Gibbs Free Energy= 0.620917

Sum of electronic and zero-point Energies= -2312.109778

Sum of electronic and thermal Energies= -2312.062920

Sum of electronic and thermal Enthalpies= -2312.061976

Sum of electronic and thermal Free Energies= -2312.192230

E(RM06L) = -2312.813147 A.U.

(S)B-7-Co

1 1

Number of imaginary frequencies: 0

C	-2.04919200	-0.59811700	-0.07339300
C	-3.19269400	-1.49853600	-0.35008800
C	-3.39976100	-2.64082400	0.43160600
C	-4.08493100	-1.24280700	-1.40208500
C	-4.44547000	-3.51475300	0.15612200
H	-2.75340300	-2.81617000	1.28926400
C	-5.11859300	-2.12336000	-1.67851200
H	-3.95028600	-0.35332700	-2.01234800
C	-5.31699500	-3.27942000	-0.91018900
H	-4.59919600	-4.38748800	0.78686700
H	-5.79011000	-1.91636100	-2.50851200
C	-0.81236200	-1.11020900	0.15261100

P	-0.16645700	-2.65947200	-0.43321700
C	2.54119100	-1.37450600	-0.26262900
C	3.86866700	-0.97132200	-0.57974700
C	4.88498200	-1.94353100	-0.63846800
C	4.20125800	0.36943900	-0.83611200
C	6.18409700	-1.57367700	-0.94624100
H	4.64060200	-2.98247900	-0.43847900
C	5.50583200	0.72291800	-1.14499200
H	3.42608900	1.12979000	-0.76908700
C	6.52265900	-0.23858300	-1.20757000
H	6.95818200	-2.33584100	-0.98468700
H	5.74748100	1.76550400	-1.33714100
C	1.47892100	-2.01080100	-0.11332500
C	-0.34187700	-4.04304800	0.72370100
H	0.48558800	-4.74119800	0.57603600
H	-0.35707300	-3.71628600	1.76570300
H	-1.27659000	-4.55806600	0.49227000
O	-0.38665700	-3.03478900	-1.86197500
C	-3.49629900	2.77783400	0.27138900
C	-2.25176700	3.08147000	-0.32092600
C	-1.85779100	4.39388800	-0.57200400
C	-2.74862300	5.40405300	-0.23226200
C	-3.99648400	5.12072600	0.34529200
C	-4.37803700	3.81548900	0.60527100
C	-3.55274900	1.36356600	0.42566100
C	-2.37050500	0.81615700	-0.00485500
H	-0.90327000	4.62404400	-1.03057100

H	-2.47117900	6.43612500	-0.42232000
H	-4.66614200	5.93818800	0.59274700
H	-5.33788100	3.59353300	1.06168700
H	-4.37562900	0.78039000	0.81760800
C	-0.47431700	1.74293400	-1.35368500
N	-0.49875800	2.56571100	-2.40088300
C	0.37582700	2.36885600	-3.37880600
C	1.23956800	1.28028400	-3.36757900
C	1.26964500	0.54154500	-2.20151100
N	0.49193300	0.81257400	-1.12831300
H	0.35137000	3.08178700	-4.20039300
H	1.88693700	1.03215800	-4.19915900
H	1.94839000	-0.29377800	-2.10250700
N	-1.53424800	1.87725100	-0.46375000
C	0.03692000	-0.00811700	2.62593500
C	1.26413800	-0.73183900	2.61750500
C	2.32306800	0.17581400	2.21445800
C	1.72804000	1.39916100	1.85199600
C	0.30849100	1.30174500	2.12241800
C	-0.59129200	2.47569700	2.24550500
H	-1.64786900	2.21575300	2.15473900
H	-0.44973000	2.90793400	3.24464600
H	-0.36729500	3.26470100	1.52560500
C	-1.26995200	-0.49309900	3.13748300
H	-1.38041300	-1.57329800	3.01040500
H	-1.35509400	-0.27460700	4.20826600
H	-2.10929500	-0.00942100	2.63077900

C	1.50180300	-2.10023000	3.14824300
H	2.06895000	-2.72271400	2.44824000
H	2.08328300	-2.04934700	4.07602900
H	0.56786600	-2.61404400	3.38405200
C	3.76839100	-0.12687300	2.37410200
H	4.41376600	0.52552400	1.78374400
H	4.03312900	0.01503100	3.42926000
H	4.01076800	-1.16276000	2.12404500
C	2.40832000	2.63927700	1.38867100
H	2.38886700	3.40798500	2.16948200
H	3.45484700	2.46008400	1.13114000
H	1.91142900	3.07111300	0.51201200
Co	0.81941900	-0.15189000	0.67583800
C	-6.42993300	-4.22689000	-1.22904600
H	-7.37653900	-3.70066300	-1.38250200
H	-6.22473200	-4.77757400	-2.15336500
H	-6.57712200	-4.96283000	-0.43563600
C	7.92498800	0.13977800	-1.55944800
H	8.65290800	-0.38236700	-0.93292600
H	8.15358000	-0.13053900	-2.59617100
H	8.09504100	1.21364100	-1.45875000

Zero-point correction= 0.705993 (Hartree/Particle)

Thermal correction to Energy= 0.751222

Thermal correction to Enthalpy= 0.752166

Thermal correction to Gibbs Free Energy= 0.628600

Sum of electronic and zero-point Energies= -2312.127685

Sum of electronic and thermal Energies= -2312.082457

Sum of electronic and thermal Enthalpies= -2312.081513

Sum of electronic and thermal Free Energies= -2312.205078

E(RM06L) = -2312.833679 A.U.

(T)B-7-Co

1 3

Number of imaginary frequencies: 0

C	-2.31050000	-0.12386000	-0.28716400
C	-3.62063600	0.43177000	-0.36599100
C	-3.66742700	1.80597300	-0.97782600
C	-4.79326300	-0.10482100	0.18448700
C	-4.85979400	2.62219900	-0.63533500
H	-3.65080000	1.67007900	-2.07662000
C	-5.93114900	0.66992300	0.32036300
H	-4.78262500	-1.11500900	0.58430400
C	-5.93984000	2.04917000	-0.05091600
H	-4.86405900	3.67263400	-0.91198600
H	-6.81428100	0.24109800	0.78365900
H	-6.82367300	2.64464800	0.15520100
C	-1.28137900	0.82302700	-0.45597300
P	-1.98001100	2.49986100	-0.64379000
C	1.23633600	1.33003600	-0.13442300
C	2.07353500	2.39329200	0.31967400
C	1.52384100	3.68204600	0.50338000
C	3.43197500	2.18537400	0.62638400
C	2.32849400	4.71766500	0.95605700
H	0.46196100	3.84407700	0.33257800
C	4.22539200	3.22880100	1.07938100

H	3.84743200	1.18880500	0.50404200
C	3.67788400	4.50188600	1.23790200
H	1.89471600	5.70268600	1.09917900
H	5.27174200	3.05219300	1.31022600
H	4.29835900	5.32043700	1.58923000
C	0.10354500	0.76964300	-0.36449000
C	-1.31975000	3.13911100	-2.20445600
H	-0.24271100	3.29675000	-2.09321900
H	-1.49082300	2.45046500	-3.03573800
H	-1.77735700	4.10409400	-2.43384100
O	-1.81089600	3.43655700	0.51046900
C	1.50183800	-2.29542200	-1.58144300
C	1.54973500	-1.08034200	-2.29567400
C	2.77811600	-0.38546000	-1.92879400
C	3.48118700	-1.20142400	-0.99702900
C	2.65785400	-2.33876600	-0.71253200
C	2.98641900	-3.43699200	0.23541700
H	2.09726000	-3.80569900	0.75606200
H	3.43678900	-4.28315600	-0.29676400
H	3.70742600	-3.11230200	0.99052300
C	0.51822200	-3.39066200	-1.77178400
H	-0.50931400	-3.02446400	-1.85460500
H	0.73883600	-3.92845200	-2.70143000
H	0.56536100	-4.11946000	-0.96115800
C	0.56019100	-0.59821200	-3.29452300
H	0.47113700	0.49190400	-3.27596900
H	0.86107700	-0.88160100	-4.30997600

H	-0.43239300	-1.02136700	-3.11367200
C	3.24746000	0.87805100	-2.55713800
H	4.01168700	1.38056000	-1.96023500
H	3.67653600	0.67239500	-3.54459300
H	2.42665900	1.58695100	-2.70141800
C	4.83313200	-0.95927900	-0.41881400
H	5.54070600	-1.70776100	-0.79234700
H	5.22816900	0.02165700	-0.69149500
H	4.84712100	-1.03990800	0.67348700
C	-2.14530600	-1.56453300	-0.06362900
C	-0.50916000	-1.27163300	1.77214400
C	-0.47555500	-0.29899100	3.95753400
C	0.88521400	-0.06682200	3.78936400
C	1.47427300	-0.42179400	2.58616000
N	0.79070400	-0.99853500	1.58056000
H	-0.97833200	-0.01380000	4.87559000
H	1.48280600	0.39507900	4.56635000
H	2.52539200	-0.21945100	2.39093700
N	-1.17288400	-2.06650700	0.78762600
C	-2.94625000	-2.45882000	-0.73900200
H	-3.67275200	-2.06798900	-1.44068600
C	-0.94722200	-3.48242200	1.00010600
C	-1.87362000	-4.34332700	0.32188000
H	-1.75767100	-5.40406300	0.51190000
C	-2.82858800	-3.84811000	-0.51565800
H	-3.50374700	-4.52605600	-1.03033500
O	-0.02709400	-3.83112600	1.73027600

C	-1.17924400	-0.92835900	2.93776400
H	-2.23219800	-1.17160400	3.03482500
Co	1.57574600	-0.62770200	-0.24558600

Zero-point correction= 0.624244 (Hartree/Particle)

Thermal correction to Energy= 0.665000

Thermal correction to Enthalpy= 0.665944

Thermal correction to Gibbs Free Energy= 0.552354

Sum of electronic and zero-point Energies= -2177.234329

Sum of electronic and thermal Energies= -2177.193573

Sum of electronic and thermal Enthalpies= -2177.192629

Sum of electronic and thermal Free Energies= -2177.306219

E(RM06L) = -2177.858573 A.U.

B-8-Co

1 1

Number of imaginary frequencies: 0

C	-2.25530500	0.16781600	-0.11978900
C	-3.52716200	0.90901100	-0.24463400
C	-3.75978900	1.73287100	-1.35468000
C	-4.49866900	0.84126100	0.76535300
C	-4.92509400	2.48544800	-1.44747600
H	-3.03029300	1.74425800	-2.16277800
C	-5.65612000	1.60273400	0.67635100
H	-4.31924000	0.21269900	1.63415200
C	-5.87193700	2.42690900	-0.42778900
H	-5.09990400	3.10868800	-2.31956300
H	-6.39095800	1.56074000	1.47433600
H	-6.78018600	3.01767700	-0.49533200

C	-1.10773900	0.88212100	-0.33021900
P	-0.81193100	2.68612300	-0.22042600
C	0.82319100	1.92816000	-0.02231500
C	2.11041300	2.45784100	0.33272100
C	3.24273200	1.63433100	0.48374800
C	2.26325600	3.83468200	0.58586200
C	4.47322000	2.15105800	0.85818000
H	3.13574900	0.56109300	0.30994900
C	3.49556300	4.35545300	0.95886800
H	1.39476000	4.48592100	0.51696600
C	4.60439000	3.52113600	1.09359800
H	5.33189000	1.49349000	0.96937000
H	3.59184600	5.41901800	1.15336800
H	5.56565100	3.93264100	1.38456800
C	0.31890800	0.65004100	-0.22384600
C	-0.84455000	3.47391000	-1.85927600
H	-0.15054500	4.31821400	-1.86023000
H	-0.55977700	2.77994600	-2.65433700
H	-1.84751600	3.85941000	-2.05179400
O	-1.41519000	3.51937100	0.86251900
C	2.30948000	-0.67053600	-2.06058500
C	3.12999700	-1.57111300	-1.26304100
C	2.35931400	-2.69743200	-0.90590700
C	1.04361400	-2.51272500	-1.46567000
C	1.02282500	-1.27636300	-2.20991600
C	-0.11345000	-0.77930400	-3.02649000
H	-0.08953200	0.30767600	-3.13379000

H	-0.07134200	-1.21443400	-4.03163400
H	-1.07848100	-1.05056600	-2.58853000
C	2.76098500	0.59270100	-2.69783200
H	3.53449600	1.09890100	-2.11587400
H	3.17905000	0.38473800	-3.68982100
H	1.93385200	1.29478900	-2.82810800
C	4.54545100	-1.33386800	-0.87734800
H	4.74550200	-1.61989400	0.16021700
H	5.20597700	-1.94621900	-1.50219100
H	4.84390900	-0.29233100	-1.01260100
C	2.81307900	-3.86080000	-0.09728700
H	1.98195000	-4.37393400	0.39525000
H	3.31199100	-4.60191400	-0.73133000
H	3.53153800	-3.56807700	0.67419000
C	-0.06200600	-3.49397800	-1.41004000
H	0.00549100	-4.15018700	-2.28751800
H	-0.00741600	-4.13290100	-0.52625000
H	-1.04638300	-3.01800900	-1.44798700
C	-2.38974400	-1.25879700	0.22092300
C	-0.45704000	-1.23609700	1.70737300
C	1.85628500	-0.87396400	2.28265300
C	1.46468400	0.33048800	2.85405000
C	0.09807000	0.62567100	2.90117000
N	-0.84596400	-0.14273300	2.35080400
H	2.89075100	-1.20599900	2.33731700
H	2.18761300	1.00495200	3.30004600
H	-0.26011500	1.51219200	3.41993500

N	-1.47617000	-1.94836700	1.02024200
C	-3.45507000	-1.96397900	-0.29717200
H	-4.15438700	-1.43714900	-0.93411600
C	-1.58042500	-3.36244800	1.31330500
C	-2.73847300	-4.00569800	0.76593800
H	-2.84832100	-5.05587700	1.00921600
C	-3.63413000	-3.33330500	-0.01117600
H	-4.49492100	-3.85262400	-0.42274600
O	-0.70964400	-3.91702400	1.97779100
C	0.88529800	-1.70496100	1.68226100
H	1.08667700	-2.74446100	1.46239900
Co	1.39773700	-0.90055800	-0.26656900

Zero-point correction= 0.625235 (Hartree/Particle)

Thermal correction to Energy= 0.665761

Thermal correction to Enthalpy= 0.666706

Thermal correction to Gibbs Free Energy= 0.553672

Sum of electronic and zero-point Energies= -2177.232632

Sum of electronic and thermal Energies= -2177.192105

Sum of electronic and thermal Enthalpies= -2177.191161

Sum of electronic and thermal Free Energies= -2177.304195

E(RM06L) = -2177.857866 A.U.

(T)B-8-Co

1 3

Number of imaginary frequencies: 0

C	2.24417200	0.10249100	0.15311800
C	3.55703300	0.76587000	0.27150500
C	3.83975900	1.57389500	1.38185600

C	4.52050600	0.64345000	-0.74090500
C	5.04592200	2.25928900	1.47181400
H	3.11589700	1.62270000	2.19331700
C	5.72030800	1.33700000	-0.65332000
H	4.30355600	0.02731200	-1.60989400
C	5.98565100	2.14716400	0.45030700
H	5.25833100	2.87027600	2.34418600
H	6.45016300	1.25239800	-1.45256500
H	6.92708300	2.68362400	0.51638900
C	1.13701900	0.86294300	0.39762800
P	0.90645500	2.67702700	0.28633300
C	-0.76993800	1.98735200	0.12747200
C	-2.04496300	2.56896400	-0.18647900
C	-3.16950500	1.78139600	-0.50455000
C	-2.19020500	3.96972500	-0.20933300
C	-4.39376000	2.36371800	-0.79375300
H	-3.06374900	0.69711200	-0.53048500
C	-3.41518200	4.55249200	-0.50310700
H	-1.32618400	4.59771600	-0.00519000
C	-4.52159400	3.75424500	-0.79070700
H	-5.24897400	1.73905800	-1.03855200
H	-3.50831300	5.63377300	-0.51485900
H	-5.47679700	4.21228200	-1.02741000
C	-0.30250200	0.69741100	0.31062300
C	0.99831100	3.45968400	1.92414900
H	0.36863500	4.35249500	1.93413300
H	0.66855500	2.78153900	2.71528900

H	2.02851700	3.76881500	2.11106700
O	1.53356100	3.46465600	-0.81623200
C	-2.40016100	-0.73228500	1.93509800
C	-3.15781300	-1.57553800	1.07849100
C	-2.37031400	-2.74906600	0.81353200
C	-1.14132800	-2.66309600	1.53353300
C	-1.12203600	-1.40435000	2.19871700
C	-0.05994100	-0.91711100	3.11687000
H	-0.06446400	0.17261000	3.20072100
H	-0.20638600	-1.32713300	4.12314000
H	0.93643200	-1.22341200	2.78277200
C	-2.83782100	0.53027100	2.58459200
H	-3.68251000	0.99052900	2.06775800
H	-3.14897800	0.33171500	3.61687200
H	-2.03235200	1.26962000	2.62434600
C	-4.53790500	-1.32985600	0.57117700
H	-4.62960100	-1.53353900	-0.50165600
H	-5.26244900	-1.97807800	1.07592200
H	-4.85219500	-0.29729400	0.74125400
C	-2.78438400	-3.87886700	-0.05994100
H	-1.93192700	-4.34067500	-0.56685800
H	-3.27330700	-4.65950000	0.53451200
H	-3.50695900	-3.56353300	-0.81835300
C	-0.08903600	-3.70972100	1.63203000
H	-0.18930500	-4.26274400	2.57305300
H	-0.15629800	-4.43500100	0.81852500
H	0.91907400	-3.28119900	1.62572600

C	2.27063100	-1.31994000	-0.22529500
C	0.42778500	-1.08835000	-1.81068500
C	-1.72504600	-0.42522000	-2.67666000
C	-1.11978400	0.71900900	-3.16597200
C	0.26698700	0.83986900	-3.01998100
N	1.02749000	-0.04499000	-2.37185900
H	-2.78296700	-0.61378300	-2.84118000
H	-1.68527400	1.48124600	-3.69018400
H	0.79891900	1.68298300	-3.45528700
N	1.26139900	-1.91111500	-1.00003700
C	3.28903800	-2.12009800	0.23542400
H	4.05105400	-1.66673300	0.85726500
C	1.18265100	-3.34483000	-1.21554300
C	2.32903800	-4.08528700	-0.77524600
H	2.31774400	-5.14310500	-1.00999000
C	3.33834800	-3.49685200	-0.07532400
H	4.17867400	-4.09072300	0.27219800
O	0.19227800	-3.83835100	-1.74706400
C	-0.95856600	-1.36375100	-1.95781900
H	-1.33821900	-2.35996300	-1.74077600
Co	-1.28257200	-0.93098600	0.18331700

Zero-point correction= 0.624056 (Hartree/Particle)

Thermal correction to Energy= 0.665178

Thermal correction to Enthalpy= 0.666122

Thermal correction to Gibbs Free Energy= 0.550715

Sum of electronic and zero-point Energies= -2177.238169

Sum of electronic and thermal Energies= -2177.197048

Sum of electronic and thermal Enthalpies= -2177.196104

Sum of electronic and thermal Free Energies= -2177.311510

E(RM06L) = -2177.862226 A.U.

B-1-Rh

1 1

Number of imaginary frequencies: 0

C	-0.53271500	-1.83671600	-1.01326400
C	-1.75520400	-1.99574000	-0.24630400
C	-2.70493600	-1.03341500	-0.70833500
C	-2.07115800	-0.26388500	-1.77527400
C	-0.74740900	-0.78608000	-1.97634000
O	-0.83990500	0.12142800	2.27562100
O	-2.04248000	1.58071600	1.17791900
C	-1.58506800	1.15575100	2.29298000
C	-4.10192000	-0.82500700	-0.21848800
H	-4.81694500	-1.20835700	-0.95550800
H	-4.27775200	-1.34288700	0.72533100
H	-4.30728600	0.23755300	-0.06662100
C	-1.93943800	-2.99352000	0.84933300
H	-2.72619200	-2.69418400	1.54294900
H	-2.21173000	-3.96537000	0.42016600
H	-1.01453000	-3.12354600	1.41569500
C	0.65680400	-2.73599900	-0.91813600
H	1.01905900	-2.81324300	0.10976000
H	0.38033200	-3.74383000	-1.24979000
H	1.47369300	-2.38556600	-1.54779200
C	0.24595800	-0.31563600	-2.98932800

H	1.27111800	-0.35689200	-2.61189000
H	0.18667100	-0.95772900	-3.87639000
H	0.03688000	0.70773100	-3.30660900
C	-2.73515300	0.82617400	-2.55275100
H	-2.00551800	1.50455900	-2.99853100
H	-3.33198200	0.39440500	-3.36525300
H	-3.40735100	1.40909500	-1.91868600
C	-1.88521100	1.87791300	3.57290600
H	-1.17198400	2.70134300	3.69037400
H	-2.88920600	2.30480700	3.53775000
H	-1.78115000	1.20360400	4.42398300
C	2.10044800	-0.41142500	1.73169500
C	2.63901400	-1.54085000	2.26656800
C	3.54786400	-2.31080800	1.48170400
C	3.83598400	-1.95559300	0.19513100
C	3.22918100	-0.80568600	-0.43345200
C	1.95065900	1.23577300	-0.04648700
C	0.22385000	2.73582000	-0.43199000
C	1.10843000	3.72225600	-0.83966200
C	2.47461700	3.43195200	-0.86321200
C	2.90049600	2.17662200	-0.44967800
H	1.41471300	0.22969300	2.26861500
H	2.39558200	-1.81742800	3.28457800
H	4.01178800	-3.19231700	1.91486000
H	4.51154600	-2.52760400	-0.42972000
H	-0.84282600	2.91420700	-0.37806700
H	0.72954700	4.69511500	-1.13156200

H	3.19673400	4.17664300	-1.18127500
H	3.94836600	1.90619000	-0.43476800
N	2.39454300	-0.03197100	0.43564000
N	0.63163400	1.49635300	-0.06627200
O	3.35046000	-0.47496700	-1.61377000
Rh	-0.97444400	0.03476700	0.07219900

Zero-point correction= 0.440166(Hartree/Particle)

Thermal correction to Energy= 0.469707

Thermal correction to Enthalpy= 0.470651

Thermal correction to Gibbs Free Energy= 0.380203

Sum of electronic and zero-point Energies= -1298.230269

Sum of electronic and thermal Energies= -1298.200728

Sum of electronic and thermal Enthalpies= -1298.199784

Sum of electronic and thermal Free Energies= -1298.290232

E(RB3LYP) = -1298.670435 A.U.

B-2a-Rh

1 1

Number of imaginary frequencies: 0

C	-1.56190900	0.55923400	-1.91183900
C	-1.87043900	-0.83976700	-1.70111200
C	-2.61263900	-0.92940700	-0.49175900
C	-2.94326500	0.43745600	-0.05199600
C	-2.33390900	1.33909700	-0.93473800
C	-3.15048200	-2.16848900	0.15429300
H	-4.18932700	-2.33977200	-0.15251700
H	-2.57114700	-3.05222300	-0.12089000
H	-3.13876800	-2.07715000	1.24328300

C	-1.49584200	-1.95483200	-2.62441600
H	-1.57761900	-2.93040500	-2.14285900
H	-2.17938800	-1.95156500	-3.48170600
H	-0.47856300	-1.84451500	-3.00382100
C	-0.84667800	1.12780800	-3.09800600
H	-0.08703600	0.43753800	-3.47034500
H	-1.55498900	1.32276300	-3.91245900
H	-0.35521800	2.07145900	-2.85094400
C	-2.41248200	2.83340200	-0.92317900
H	-1.44517300	3.28821300	-1.15186500
H	-3.11890000	3.17469000	-1.68893200
H	-2.75557500	3.21875200	0.03922300
C	-3.75592700	0.73625400	1.16796100
H	-3.85105500	1.80922300	1.34186200
H	-4.76350400	0.31756200	1.06965600
H	-3.29273100	0.28704300	2.05275100
N	2.20997700	-0.28246500	-0.45718800
C	2.10530100	1.06112200	-0.03512000
N	0.84604800	1.43147000	0.30046900
C	0.60555200	2.65594800	0.80668600
C	1.60927200	3.59460600	0.97627800
C	2.90662900	3.23590100	0.60270300
H	-0.42378600	2.86138000	1.07445300
H	1.37849300	4.57126100	1.38533900
H	3.72446600	3.94112600	0.71022700
C	3.48343000	-0.85425800	-0.86893200
C	3.46458800	-2.28901800	-1.06547300

H	4.42107200	-2.72332100	-1.32973000
C	2.33149800	-3.02497900	-0.93290500
C	1.09050000	-2.39062600	-0.60934000
C	1.02520900	-1.03869600	-0.39680000
O	4.47878400	-0.15981100	-1.01786100
H	2.35559800	-4.10039400	-1.08560000
H	0.18086200	-2.97721600	-0.56631800
C	3.16883000	1.96798600	0.09615900
H	4.16028500	1.66323100	-0.19768100
O	0.80748900	-1.99136100	2.51086300
O	-0.67480400	-0.31990900	2.18700200
C	-0.06844300	-1.10239200	2.93231100
H	0.90251500	-1.95496400	1.52976800
C	-0.27418700	-1.11234300	4.41736700
H	-1.03716100	-0.38751900	4.69630000
H	-0.56233900	-2.11671700	4.74038200
H	0.67192300	-0.87259700	4.91223200
Rh	-0.65521100	0.02279300	-0.02292600

Zero-point correction= 0.440282 (Hartree/Particle)

Thermal correction to Energy= 0.469746

Thermal correction to Enthalpy= 0.470691

Thermal correction to Gibbs Free Energy= 0.379925

Sum of electronic and zero-point Energies= -1298.225360

Sum of electronic and thermal Energies= -1298.195895

Sum of electronic and thermal Enthalpies= -1298.194951

Sum of electronic and thermal Free Energies= -1298.285717

E(RB3LYP) = -1298.665642 A.U.

B-3a-Rh

1 1

Number of imaginary frequencies: 0

C	1.96565300	0.00171500	1.39993900
C	2.13113800	-1.28282200	0.73078100
C	2.55875600	-1.00450500	-0.58794400
C	2.81714900	0.44839700	-0.69975900
C	2.49688300	1.04855700	0.52339800
C	2.85264400	-1.98976600	-1.67334200
H	3.93300600	-2.17180200	-1.73129300
H	2.35885500	-2.94655600	-1.49659000
H	2.53048600	-1.61492800	-2.64813600
C	1.94319500	-2.61841700	1.38020000
H	1.92360900	-3.42740600	0.64831400
H	2.78120300	-2.81181900	2.05987200
H	1.02067100	-2.66013300	1.96270600
C	1.57471600	0.18825000	2.82794700
H	0.89275600	-0.59635300	3.16045700
H	2.47121200	0.14735100	3.46088800
H	1.09741000	1.15679400	2.99043200
C	2.64325100	2.48625900	0.91403000
H	1.78500300	2.83564500	1.49424400
H	3.53266900	2.61494200	1.54174600
H	2.75928900	3.13629000	0.04417900
C	3.34829600	1.10189400	-1.93440100
H	3.27338000	2.18936500	-1.88679100
H	4.40523200	0.84238500	-2.07138800

H	2.81400300	0.75952500	-2.82538700
N	-2.27802800	-0.48811700	-0.04448700
C	-2.19977400	0.91600900	-0.08063300
N	-0.93340900	1.39206900	-0.22598100
C	-0.71564300	2.72333400	-0.31821700
C	-1.74075800	3.64760100	-0.26236100
C	-3.04394900	3.16746300	-0.09434700
H	0.31714300	3.02305600	-0.44366500
H	-1.52570700	4.70640900	-0.34547300
H	-3.87990000	3.85713400	-0.03666500
C	-3.54940300	-1.18167900	0.02558000
C	-3.46399200	-2.62310800	-0.12777000
H	-4.41816700	-3.13585100	-0.10757400
C	-2.28007200	-3.27076400	-0.27888100
C	-1.05649400	-2.53526400	-0.26559000
C	-1.05029000	-1.17105000	-0.15331300
O	-4.60537000	-0.58786400	0.19063200
H	-2.25556600	-4.35054300	-0.39479000
H	-0.11590800	-3.06272200	-0.34987800
C	-3.28555300	1.80297200	-0.00089100
H	-4.27924400	1.40579500	0.12959000
Rh	0.58282300	-0.01448400	-0.23851400

Zero-point correction= 0.376349 (Hartree/Particle)

Thermal correction to Energy= 0.400113

Thermal correction to Enthalpy= 0.401057

Thermal correction to Gibbs Free Energy= 0.323658

Sum of electronic and zero-point Energies= -1069.155076

Sum of electronic and thermal Energies= -1069.131312

Sum of electronic and thermal Enthalpies= -1069.130368

Sum of electronic and thermal Free Energies= -1069.207767

E(RB3LYP) = -1069.531425 A.U.

B-4-Rh

1 1

Number of imaginary frequencies: 0

C	3.41415800	0.75438600	-1.37180000
C	4.36313800	1.36647400	-0.50376400
C	5.41531400	0.61027600	0.05003900
C	4.22559300	2.72645200	-0.15799600
C	6.30391900	1.20615500	0.94177000
H	5.53142000	-0.43141100	-0.23141100
C	5.12141000	3.31094700	0.73352100
H	3.42158800	3.30851500	-0.59703100
C	6.15789100	2.55266700	1.28696700
H	7.11513200	0.62139100	1.36367600
H	5.01829800	4.36064900	0.99084500
H	6.85532500	3.01284000	1.97983300
C	2.56117100	0.22529200	-2.06133500
P	1.27617700	-0.56184900	-2.97109600
C	-1.15878900	0.45588500	-1.92985600
C	-2.28856400	1.29239800	-1.87647700
C	-2.15448100	2.60561500	-1.36589600
C	-3.55740700	0.81363500	-2.26944800
C	-3.27767200	3.40926900	-1.22891600
H	-1.17503900	2.96105600	-1.06401700

C	-4.67182900	1.63221600	-2.13101800
H	-3.64926700	-0.19614900	-2.65251000
C	-4.53444200	2.92163700	-1.60625800
H	-3.18358100	4.40764900	-0.81602200
H	-5.65091500	1.26497600	-2.41965300
H	-5.41163600	3.54893900	-1.48388300
C	-0.13102300	-0.24496200	-1.89262900
C	1.00187000	0.50134000	-4.42083200
H	0.12423700	0.13363700	-4.95853400
H	0.84814900	1.54026200	-4.11961800
H	1.87719900	0.42894000	-5.07120400
O	1.49194900	-2.00771000	-3.29338900
C	-0.49072500	-3.16748100	1.15578800
C	0.32726000	-3.28144300	-0.00023100
C	1.60696800	-2.60834900	0.27374200
C	1.50358900	-1.97774300	1.51861100
C	0.16181000	-2.23834500	2.05453900
C	-0.30306000	-1.87664200	3.43219900
H	-1.39334700	-1.86611100	3.49065100
H	0.06902700	-2.60280700	4.16531100
H	0.06083100	-0.88974000	3.72805000
C	-1.73534300	-3.93905700	1.45854500
H	-2.21714500	-4.31067500	0.55261300
H	-1.46759300	-4.81084700	2.06811600
H	-2.46152700	-3.34699300	2.01677200
C	0.06476000	-4.12546200	-1.20700000
H	0.44634500	-3.64172900	-2.10889700

H	0.57257500	-5.09267200	-1.10065900
H	-1.00206700	-4.32122800	-1.33406900
C	2.85031400	-2.77348200	-0.54022300
H	3.54873500	-1.95110100	-0.38103200
H	3.34835400	-3.70157700	-0.23003200
H	2.63630100	-2.84165200	-1.60643200
C	2.57147100	-1.20975300	2.23208500
H	3.10162700	-1.86980100	2.92970400
H	3.30979000	-0.79602500	1.54158500
H	2.15359500	-0.38822300	2.81891000
C	-2.23084000	-0.62572700	0.60701300
C	-3.29388800	-1.40410500	0.24729700
C	-4.62545400	-0.99836800	0.54435700
C	-4.86964600	0.19695500	1.14733000
C	-3.81034800	1.11328800	1.48929900
C	-1.33099100	1.40673200	1.47858900
C	0.98296400	1.54919900	1.10975600
C	1.06141400	2.79398700	1.71134800
C	-0.11304000	3.33836700	2.23782000
C	-1.31823300	2.65520700	2.12368000
H	-3.11396100	-2.33871300	-0.26642300
H	-5.45233000	-1.65047900	0.27473000
H	-5.86801700	0.54885600	1.37591300
H	1.84925900	1.06052500	0.68609000
H	2.01668600	3.30232000	1.77001600
H	-0.09787400	4.30215300	2.73688600
H	-2.24470400	3.05837400	2.49874400

N	-2.46750300	0.60974200	1.23604000
N	-0.17626100	0.87174100	1.01299200
O	-3.99731000	2.23659600	1.94608000
Rh	-0.28676300	-1.07537000	0.29846600

Zero-point correction= 0.624592(Hartree/Particle)

Thermal correction to Energy= 0.666917

Thermal correction to Enthalpy= 0.667861

Thermal correction to Gibbs Free Energy= 0.549394

Sum of electronic and zero-point Energies= -2141.123774

Sum of electronic and thermal Energies= -2141.081449

Sum of electronic and thermal Enthalpies= -2141.080504

Sum of electronic and thermal Free Energies= -2141.198972

E(RB3LYP) = -2141.748366 A.U.

B-5a-Rh

1 1

Number of imaginary frequencies: 0

C	-3.18451800	-0.66745800	1.27507700
C	-4.31381000	-1.21917700	0.60705400
C	-5.04395200	-0.44306300	-0.31390600
C	-4.67204000	-2.56561800	0.81890700
C	-6.10240800	-1.01209100	-1.01774300
H	-4.77338400	0.59704800	-0.45912300
C	-5.73180300	-3.12433400	0.10893500
H	-4.11651600	-3.15557500	1.54093700
C	-6.44527300	-2.35205400	-0.81302100
H	-6.66518300	-0.40967800	-1.72434800
H	-6.00680400	-4.16084200	0.27832500

H	-7.27199700	-2.79082200	-1.36311800
C	-2.19055400	-0.21345800	1.81288100
P	-0.59545700	0.27111700	2.38512400
C	-0.30592400	1.60486300	-0.12086400
C	-1.44329100	2.55614800	0.01642600
C	-2.59039400	2.39008500	-0.77685000
C	-1.37395400	3.64934300	0.89008600
C	-3.66013100	3.27529900	-0.66633600
H	-2.64337300	1.55269800	-1.46713600
C	-2.44492100	4.54008000	0.99736400
H	-0.47196400	3.80422500	1.47404600
C	-3.59181300	4.35048000	0.22571900
H	-4.54609800	3.13308000	-1.27842400
H	-2.37815900	5.38472400	1.67627200
H	-4.42416600	5.04230500	0.30828200
C	0.21080000	0.78769500	0.83061900
C	-0.87133400	1.66439400	3.52584000
H	0.08151100	2.16440900	3.71989600
H	-1.59082300	2.37803200	3.12409000
H	-1.24733000	1.24352100	4.46232100
O	0.15619300	-0.86258000	3.03431900
C	0.76561900	2.65595900	-2.14668000
C	0.33695300	1.55786600	-1.46114300
H	0.53293900	3.63748500	-1.75219600
C	-0.17894200	-0.86045600	-1.62485700
C	-2.06038300	-2.29246500	-1.88026300
C	-1.60743500	-3.01751800	-0.77861500

C	-0.44320400	-2.61177900	-0.12949900
N	0.25380700	-1.55522200	-0.56811700
H	-2.98218500	-2.57263000	-2.37856100
H	-2.16690900	-3.86534800	-0.40248300
H	-0.07032000	-3.09397000	0.76643400
N	0.65798400	0.27300000	-1.96000900
C	3.74023100	0.62780900	0.62373100
C	3.28920400	0.01919400	1.82830700
C	3.17083000	-1.40926300	1.56849600
C	3.71021900	-1.68160300	0.23926400
C	4.04165800	-0.44529000	-0.34261900
C	4.57726300	-0.23222900	-1.72128400
H	4.38320200	0.78256400	-2.07377400
H	5.66336200	-0.38482900	-1.72349700
H	4.13238300	-0.92990500	-2.43496500
C	4.00578900	2.08258600	0.39106000
H	3.49147900	2.70032900	1.12918100
H	5.07966500	2.29368600	0.45820700
H	3.66700900	2.39268600	-0.60153500
C	3.01597900	0.68022800	3.14022800
H	2.20308000	0.17314700	3.66154900
H	3.91692600	0.63734800	3.76446700
H	2.75058200	1.73174100	3.00999600
C	2.76740700	-2.43508600	2.57240000
H	2.55533700	-3.39519500	2.09748300
H	3.59154500	-2.58919500	3.28118200
H	1.88352700	-2.10266200	3.11915700

C	3.82315000	-3.03135400	-0.39912600
H	4.76018000	-3.51934600	-0.10654900
H	3.00184400	-3.68383700	-0.09305900
H	3.80255200	-2.95703600	-1.48817500
C	-1.32991400	-1.18566200	-2.32277600
H	-1.63778900	-0.59293100	-3.17615400
C	1.51803400	0.05870200	-3.10790500
C	1.96031600	1.27230500	-3.75733200
H	2.58419300	1.13770900	-4.63295700
C	1.57140300	2.50322300	-3.31481700
H	1.90219700	3.39299200	-3.84307700
O	1.78919700	-1.08811300	-3.43719700
Rh	1.83294500	-0.36265300	0.21355100

Zero-point correction= 0.625010 (Hartree/Particle)

Thermal correction to Energy= 0.667166

Thermal correction to Enthalpy= 0.668111

Thermal correction to Gibbs Free Energy= 0.548903

Sum of electronic and zero-point Energies= -2141.140949

Sum of electronic and thermal Energies= -2141.098793

Sum of electronic and thermal Enthalpies= -2141.097849

Sum of electronic and thermal Free Energies= -2141.217056

E(RB3LYP) = -2141.765960 A.U.

B-6-Rh

1 1

Number of imaginary frequencies: 0

C	-2.70512100	0.12432100	-0.49602700
C	-4.17443500	0.25663100	-0.41579100

C	-4.82314400	1.48484200	-0.64715200
C	-4.96745600	-0.85392100	-0.05953700
C	-6.20193900	1.60240900	-0.50956600
H	-4.24618800	2.34590200	-0.95848500
C	-6.34791800	-0.73352900	0.08238400
H	-4.50119900	-1.81984800	0.10779000
C	-6.97164800	0.49547200	-0.13961200
H	-6.67972400	2.55846500	-0.69952400
H	-6.93640400	-1.60071400	0.36586400
H	-8.04778600	0.58960900	-0.03371500
C	-1.86252900	1.17914200	-0.33670500
P	-1.65681700	2.94732600	-0.10790300
C	0.83475900	1.33209700	-0.19211600
C	1.76594200	2.47567900	-0.11137800
C	1.92901400	3.33426300	-1.21208100
C	2.48372800	2.74606700	1.06524200
C	2.81108100	4.41354300	-1.14677200
H	1.36939900	3.13670300	-2.12180900
C	3.35364600	3.83358000	1.13481100
H	2.33351300	2.11502600	1.93501500
C	3.52982700	4.66403700	0.02402100
H	2.93470600	5.06099500	-2.00980500
H	3.88755800	4.03945300	2.05781500
H	4.21241200	5.50629100	0.07601400
C	-0.48373600	1.61325200	-0.34271400
C	-1.98357600	3.87527400	-1.64350300
H	-1.26281400	4.69484700	-1.70628900

H	-1.88099300	3.22203700	-2.51268000
H	-2.98986100	4.30034200	-1.60930100
O	-1.86423500	3.69800400	1.17096300
C	2.63688300	-2.50130100	-0.89235900
C	2.86571100	-1.27483100	-1.68267800
C	3.55752100	-0.33407900	-0.87679600
C	3.54598500	-0.87161900	0.47303900
C	3.04019500	-2.25459500	0.41896200
C	2.96542500	-3.18203000	1.58970300
H	2.17695800	-3.92200500	1.45541100
H	3.92429300	-3.69565300	1.72947200
H	2.74914800	-2.63361400	2.51023000
C	2.09501000	-3.76974700	-1.45963700
H	1.28767600	-3.57484900	-2.17003000
H	2.88859100	-4.29529900	-2.00561900
H	1.71006700	-4.42464500	-0.67859500
C	2.57915400	-1.15676400	-3.14538100
H	2.59716100	-0.11660700	-3.47475100
H	3.33085900	-1.71063700	-3.72166900
H	1.60154000	-1.58038800	-3.39153900
C	4.26265300	0.89930200	-1.33971400
H	4.35122300	1.64533100	-0.55054000
H	5.27337600	0.62492300	-1.66646600
H	3.75133700	1.36783100	-2.18131200
C	4.23913600	-0.27275500	1.65161700
H	5.26933100	-0.65061400	1.69237900
H	4.28058000	0.81441400	1.58503200

H	3.75630900	-0.55579700	2.59008000
Rh	1.48652900	-0.57332500	-0.08285300
C	-2.17050700	-1.22574000	-0.80204900
C	-1.06786100	-1.26306100	1.39387100
C	-1.75558500	-0.74949600	3.62647500
C	-0.48348100	-0.22130000	3.84958700
C	0.43769000	-0.23240000	2.81027200
N	0.14844700	-0.73937400	1.59722400
H	-2.50428600	-0.74366300	4.41138400
H	-0.20874200	0.20601300	4.80699800
H	1.43014700	0.18436600	2.92860000
N	-1.30551900	-1.83948300	0.10054700
C	-2.52177800	-1.89390700	-1.94660300
H	-3.19254900	-1.41077000	-2.64523900
C	-0.82242000	-3.18765600	-0.05051800
C	-1.24150200	-3.83891400	-1.26613700
H	-0.90454200	-4.86008800	-1.39583800
C	-2.04779800	-3.21212300	-2.17441900
H	-2.35344100	-3.73460200	-3.07643300
O	-0.11506500	-3.67136900	0.83087000
C	-2.05001500	-1.29006800	2.37805100
H	-3.02079300	-1.71450500	2.15268100

Zero-point correction= 0.626281 (Hartree/Particle)

Thermal correction to Energy= 0.667500

Thermal correction to Enthalpy= 0.668444

Thermal correction to Gibbs Free Energy= 0.552792

Sum of electronic and zero-point Energies= -2141.124691

Sum of electronic and thermal Energies= -2141.083472

Sum of electronic and thermal Enthalpies= -2141.082528

Sum of electronic and thermal Free Energies= -2141.198179

E(RB3LYP) = -2141.750972 A.U.

B-7-Rh

1 1

Number of imaginary frequencies: 0

C	-2.35728300	0.03973300	-1.01939500
C	-3.68049800	0.45238100	-0.93566800
C	-3.86722700	1.94073000	-0.70720700
C	-4.83135400	-0.39670600	-0.90623200
C	-5.16797000	2.33225800	-0.08679900
H	-3.77725400	2.46280100	-1.67623700
C	-6.02373500	0.08007700	-0.44124300
H	-4.72535700	-1.43927200	-1.18735400
C	-6.17858400	1.44476400	0.01946000
H	-5.29655700	3.36548000	0.22180300
H	-6.87800400	-0.58744100	-0.37896900
H	-7.13352500	1.74834700	0.43651200
C	-1.39084200	1.04788800	-0.67996800
P	-2.27750900	2.41581200	0.17760800
C	1.10835600	1.46323800	-0.20002700
C	1.91920000	2.65784500	-0.30325500
C	1.81332700	3.51449400	-1.41707300
C	2.80469100	2.99091700	0.73732600
C	2.59309300	4.66568400	-1.49068800
H	1.13003600	3.25620300	-2.22045400

C	3.56057100	4.15880700	0.67224300
H	2.87218400	2.33207500	1.59677500
C	3.46428200	4.99231600	-0.44583500
H	2.51958300	5.31285000	-2.35927300
H	4.22842100	4.41766800	1.48802800
H	4.06397300	5.89535100	-0.50269100
C	-0.03776000	1.00837600	-0.65642800
C	-1.69306600	4.00470100	-0.49402800
H	-0.66288400	4.16266500	-0.16618600
H	-1.72877000	4.01244300	-1.58645700
H	-2.31384200	4.81239400	-0.09719700
O	-2.27896700	2.33273200	1.67489400
C	2.45752300	-2.52004600	-0.60225700
C	2.89664700	-1.42189800	-1.41520400
C	3.61582000	-0.48389100	-0.58277600
C	3.56145900	-0.97458600	0.76656500
C	2.79543200	-2.20593300	0.75119400
C	2.49214600	-3.06137400	1.94184700
H	1.51214200	-3.53292300	1.84148300
H	3.24964200	-3.84854400	2.03988300
H	2.50196600	-2.47690300	2.86469500
C	1.90458300	-3.81085300	-1.11458700
H	1.20734600	-3.65491900	-1.94026500
H	2.72738000	-4.43194900	-1.49221500
H	1.38931800	-4.36728700	-0.33237600
C	2.74552000	-1.33233900	-2.90041600
H	2.78026000	-0.29760900	-3.24673800

H	3.55964800	-1.87880100	-3.39338400
H	1.80202200	-1.77530800	-3.22799500
C	4.43126000	0.66311300	-1.09462600
H	4.66290700	1.38381400	-0.31074900
H	5.37703600	0.28623700	-1.50170500
H	3.91450300	1.20210400	-1.89161100
C	4.25650600	-0.39927500	1.96059300
H	5.18985600	-0.94295800	2.15402100
H	4.50915100	0.65177700	1.81187100
H	3.64265400	-0.48140000	2.86144100
Rh	1.47682200	-0.49037000	0.06959700
C	-1.98966900	-1.37996100	-1.19722200
C	-1.32186000	-1.37385400	1.17191700
C	-2.30330000	-0.72238900	3.25861700
C	-1.08458000	-0.14281700	3.60066600
C	-0.03553300	-0.20600800	2.69279100
N	-0.14780400	-0.80086300	1.48844900
H	-3.15026400	-0.67680000	3.93448000
H	-0.94668400	0.37118000	4.54454800
H	0.92371100	0.24853800	2.90825300
N	-1.43773100	-2.03327500	-0.09922700
C	-2.22305800	-2.08062600	-2.34860100
H	-2.64247600	-1.56260900	-3.20164200
C	-1.11043800	-3.42032300	-0.08536700
C	-1.41103200	-4.11960700	-1.31489100
H	-1.19427400	-5.18109100	-1.31841200
C	-1.93565100	-3.47455400	-2.39646700

H	-2.14649500	-4.02732400	-3.30753700
O	-0.61855200	-3.91697400	0.92761400
C	-2.41764700	-1.36050800	2.02704500
H	-3.33881300	-1.83507200	1.71104000

Zero-point correction= 0.626018 (Hartree/Particle)

Thermal correction to Energy= 0.666925

Thermal correction to Enthalpy= 0.667869

Thermal correction to Gibbs Free Energy= 0.553511

Sum of electronic and zero-point Energies= -2141.138429

Sum of electronic and thermal Energies= -2141.097522

Sum of electronic and thermal Enthalpies= -2141.096578

Sum of electronic and thermal Free Energies= -2141.210937

E(RB3LYP) = -2141.764447 A.U.

B-8-Rh

1 1

Number of imaginary frequencies: 0

C	-2.34813300	0.01307900	-0.15027600
C	-3.70366900	0.60953300	-0.32860900
C	-4.06484900	1.21396500	-1.54170800
C	-4.62085000	0.60172500	0.73438400
C	-5.31630100	1.81490600	-1.68736300
H	-3.36736400	1.19141400	-2.37412100
C	-5.86461800	1.21094700	0.58983300
H	-4.33694000	0.14148700	1.67565400
C	-6.21523600	1.81856700	-0.61990100
H	-5.59027700	2.27210100	-2.63345900
H	-6.56049000	1.21856000	1.42306900

H	-7.18729100	2.28931100	-0.72954800
C	-1.28771000	0.84493700	-0.32637600
P	-1.20800900	2.69217300	-0.26804800
C	0.52196900	2.13254500	-0.03915800
C	1.75686800	2.82287400	0.27409300
C	2.91852900	2.13899300	0.69031100
C	1.81752900	4.22926600	0.18901200
C	4.09486700	2.82004600	0.98350100
H	2.88971500	1.05473000	0.79524700
C	2.99461100	4.91319500	0.48205300
H	0.93069200	4.78594400	-0.09825800
C	4.13852700	4.21402600	0.87629600
H	4.97588500	2.27126000	1.30467700
H	3.01873600	5.99591800	0.40886600
H	5.05350200	4.74984200	1.10825800
C	0.16550400	0.80632800	-0.16359500
C	-1.37237700	3.40981400	-1.94314600
H	-0.88835800	4.38990600	-1.95874300
H	-0.91302500	2.76182300	-2.69391000
H	-2.43436400	3.53937500	-2.16070500
O	-1.91408500	3.46062500	0.80351600
C	2.86720300	-0.65715800	-1.75487000
C	3.33880300	-1.83162000	-0.98248800
C	2.31291500	-2.77287500	-0.94760900
C	1.15966200	-2.19655000	-1.66851300
C	1.56225800	-0.94023800	-2.26224300
C	0.76973400	-0.13310800	-3.24235900

H	1.06552000	0.91703600	-3.21978500
H	0.93216800	-0.51333600	-4.25764000
H	-0.29880700	-0.18789500	-3.02325000
C	3.71734000	0.51458200	-2.12151400
H	4.43247900	0.76049200	-1.33581900
H	4.28330700	0.27652100	-3.03157200
H	3.11507900	1.40332000	-2.31597800
C	4.69431300	-1.91556000	-0.35690400
H	4.77165100	-2.75596700	0.33427300
H	5.46131800	-2.04061500	-1.13052100
H	4.93580700	-0.99838400	0.18897600
C	2.29582900	-4.11639400	-0.29157600
H	1.41259600	-4.24659500	0.34256100
H	2.27053900	-4.90304700	-1.05503300
H	3.18282100	-4.27712400	0.32339500
C	-0.10049800	-2.92671800	-1.98029100
H	0.01980500	-3.43826300	-2.94484600
H	-0.33003400	-3.68407100	-1.23180900
H	-0.95103500	-2.24871100	-2.06670400
Rh	1.43052400	-0.73357100	-0.09763600
C	-2.34228200	-1.42931000	0.20007400
C	-0.55684200	-1.17740200	1.85710200
C	1.56987600	-0.48619400	2.77851900
C	0.94527500	0.66883900	3.23176300
C	-0.44223900	0.77606500	3.05513200
N	-1.17232100	-0.13294200	2.40477900
H	2.61684000	-0.67535000	2.99465500

H	1.49368500	1.44377500	3.75439000
H	-0.99196900	1.62054800	3.46160300
N	-1.38450500	-2.01458600	1.04363600
C	-3.29768000	-2.24142700	-0.36637000
H	-4.03388100	-1.79177100	-1.01861500
C	-1.28641600	-3.43888100	1.23614500
C	-2.34167600	-4.21712600	0.63806600
H	-2.30448300	-5.28108500	0.83839100
C	-3.31128100	-3.63782500	-0.12529600
H	-4.09298700	-4.24571800	-0.57110800
O	-0.35157500	-3.92422800	1.87691900
C	0.82810000	-1.45151300	2.05506100
H	1.20644900	-2.45182300	1.90230100

Zero-point correction= 0.625794 (Hartree/Particle)

Thermal correction to Energy= 0.666791

Thermal correction to Enthalpy= 0.667735

Thermal correction to Gibbs Free Energy= 0.552265

Sum of electronic and zero-point Energies= -2141.136682

Sum of electronic and thermal Energies= -2141.095685

Sum of electronic and thermal Enthalpies= -2141.094741

Sum of electronic and thermal Free Energies= -2141.210211

E(RB3LYP) = -2141.762476 A.U.

B-TSa1-Co

1 1

Number of imaginary frequencies: 1

C	-0.46145300	-1.48721700	-1.53159200
C	-1.42333200	-2.02431000	-0.59059800

C	-2.51240100	-1.11963200	-0.51433300
C	-2.25312400	-0.01766100	-1.41339500
C	-1.01493100	-0.28737800	-2.08006100
O	-0.07936700	0.88982100	2.76828700
O	-1.78420700	0.87768600	1.31689000
C	-1.24927200	1.22099900	2.42567000
C	-3.71104200	-1.24004400	0.34995000
H	-4.57524000	-1.55032600	-0.24814700
H	-3.57461900	-1.97978900	1.14098900
H	-3.95872700	-0.28247900	0.81436700
C	-1.34427000	-3.34475400	0.08716100
H	-1.71300000	-3.30931800	1.11561200
H	-1.97143400	-4.06585200	-0.44958700
H	-0.32764300	-3.74125100	0.10022500
C	0.81069600	-2.13318400	-1.94850200
H	1.27497000	-2.68362000	-1.12517600
H	0.63345900	-2.84943800	-2.75852900
H	1.53875500	-1.40460800	-2.31577700
C	-0.37122400	0.56170200	-3.11354000
H	0.71870600	0.56541800	-3.02597900
H	-0.61307200	0.17467000	-4.10949500
H	-0.71883800	1.59657000	-3.07527100
C	-3.16503900	1.13698100	-1.62001100
H	-2.69955300	1.93015400	-2.20972500
H	-4.06920200	0.82684600	-2.15543900
H	-3.48562200	1.56004400	-0.66296100
Co	-0.75974700	-0.12525500	-0.02061800

C	-2.05444400	2.07094600	3.35669100
H	-3.08575500	2.16516200	3.02056200
H	-2.02024700	1.65168600	4.36342100
H	-1.60197500	3.06417100	3.41476100
C	0.92105200	-0.78136700	1.02867600
C	1.12119800	-2.01427200	1.60275100
C	2.37339700	-2.67089600	1.51965300
C	3.39953800	-2.10056200	0.82711200
C	3.28418200	-0.81638200	0.17194100
C	1.76963300	1.11950200	-0.10488200
C	0.05683600	2.62819900	-0.59112900
C	0.96102800	3.64199500	-0.84938700
C	2.32131900	3.35572300	-0.73794100
C	2.74170800	2.09013100	-0.35572100
H	0.33398200	0.02866200	1.83151200
H	0.30466700	-2.45633200	2.16358100
H	2.51357100	-3.63195600	2.00714000
H	4.36476700	-2.58286300	0.72307400
H	-1.01865000	2.77352900	-0.64819400
H	0.60691800	4.62749400	-1.12777100
H	3.06110800	4.12555100	-0.93203600
H	3.78735300	1.84165800	-0.24859000
N	2.01625400	-0.17409400	0.37900200
N	0.45474200	1.39001200	-0.25360500
O	4.15247200	-0.29931300	-0.51452000

Zero-point correction= 0.435082 (Hartree/Particle)

Thermal correction to Energy= 0.463460

Thermal correction to Enthalpy= 0.464404

Thermal correction to Gibbs Free Energy= 0.378310

Sum of electronic and zero-point Energies= -1334.416827

Sum of electronic and thermal Energies= -1334.388449

Sum of electronic and thermal Enthalpies= -1334.387504

Sum of electronic and thermal Free Energies= -1334.473599

E(RM06L) = -1334.851908 A.U.

B-TSa2-Co

1 1

Number of imaginary frequencies: 1

C	-3.22816400	-0.07605000	1.47170200
C	-4.47934700	0.11239000	0.83610000
C	-4.71717900	1.25562100	0.05224500
C	-5.47374300	-0.87740000	0.93840000
C	-5.92414400	1.39782500	-0.61810800
H	-3.94599700	2.01660100	-0.02537200
C	-6.67778300	-0.72232600	0.26485400
H	-5.28645800	-1.75707500	1.54705400
C	-6.90428000	0.41108700	-0.51492400
H	-6.10349900	2.28192700	-1.22189300
H	-7.44380900	-1.48675600	0.34973000
H	-7.84733000	0.52786800	-1.03993400
C	-2.14247500	-0.26893200	1.99937500
P	-0.56416200	-0.72403000	2.58944000
C	0.84938300	1.01459400	0.67631800
C	1.10983500	2.40693600	1.01896600
C	0.64024100	3.47626300	0.24154800

C	1.77600700	2.67816700	2.22550000
C	0.82432500	4.78303400	0.67050200
H	0.11646500	3.27563600	-0.68910100
C	1.97353500	3.99077700	2.64060200
H	2.14015300	1.84679900	2.82548000
C	1.49627300	5.04397400	1.86545500
H	0.44213200	5.60372700	0.07167800
H	2.50132600	4.18915000	3.56825400
H	1.64716000	6.06877100	2.19002500
C	0.47866200	-0.05795900	1.29905000
C	-0.26524700	0.29773000	4.04681000
H	0.74189500	0.10437600	4.42450300
H	-0.37136500	1.36049800	3.81469900
H	-0.98459200	0.02607000	4.82255100
O	-0.37174600	-2.19522000	2.79249800
C	2.20504700	1.66843000	-1.60032900
C	1.20920500	0.78612500	-1.23825300
H	3.05041300	1.79230700	-0.93439800
C	-0.85698400	-0.28992700	-1.72337600
C	-2.95999200	-1.43297900	-1.76303900
C	-2.42796200	-2.40217800	-0.91860500
C	-1.12576400	-2.24497800	-0.48130800
N	-0.34587600	-1.22940900	-0.89597100
H	-3.99307300	-1.49342400	-2.09298300
H	-3.01575800	-3.24185000	-0.56583300
H	-0.68560500	-2.90831600	0.25497900
N	0.06146900	0.71953400	-2.04706000

C	3.49398000	-0.91180700	0.17229600
C	2.83192700	-1.79902600	1.08628200
C	2.12644400	-2.77426100	0.32759300
C	2.37346300	-2.49616800	-1.07426300
C	3.24452900	-1.38083100	-1.16835600
C	3.81281200	-0.84771500	-2.43425900
H	4.30397300	0.11667900	-2.29603300
H	4.55942200	-1.54561100	-2.82859500
H	3.04762200	-0.71997000	-3.20619900
C	4.38687800	0.20504600	0.58980400
H	3.85267900	0.96718800	1.17014500
H	5.19316600	-0.17023900	1.22889100
H	4.85328900	0.70010000	-0.26419100
C	2.89497500	-1.70498800	2.56721000
H	2.03760900	-2.19362100	3.03623500
H	3.80909200	-2.18329800	2.93766400
H	2.92806300	-0.66097600	2.89762800
C	1.43789700	-3.97362300	0.87466900
H	0.84191600	-4.48488600	0.11498600
H	2.18841400	-4.69403500	1.22057200
H	0.79693300	-3.72572200	1.72519900
C	1.82473900	-3.26747800	-2.21902700
H	2.49112300	-4.09789500	-2.47839200
H	0.84705100	-3.69866000	-1.98783900
H	1.71613700	-2.64467800	-3.11104100
Co	1.45581800	-0.86031000	-0.17389100
C	-2.18389300	-0.35369900	-2.15921400

H	-2.57491900	0.42342200	-2.79630500
C	-0.12288300	1.53249500	-3.24700300
C	0.99383600	2.37814600	-3.55887800
H	0.88744400	2.96467100	-4.46341300
C	2.10847300	2.43858100	-2.77354800
H	2.92828800	3.09869300	-3.04514400
O	-1.14561900	1.44910800	-3.90945700

Zero-point correction= 0.623427 (Hartree/Particle)

Thermal correction to Energy= 0.664412

Thermal correction to Enthalpy= 0.665356

Thermal correction to Gibbs Free Energy= 0.550786

Sum of electronic and zero-point Energies= -2177.211652

Sum of electronic and thermal Energies= -2177.170667

Sum of electronic and thermal Enthalpies= -2177.169723

Sum of electronic and thermal Free Energies= -2177.284293

E(RM06L) = -2177.835079 A.U.

B-TS3-Co

1 1

Number of imaginary frequencies: 1

C	-2.01961100	0.51353200	0.19204200
C	-3.07621900	1.56294700	0.21493000
C	-3.14709900	2.52367800	-0.80209700
C	-3.98399800	1.63583100	1.27865000
C	-4.08782500	3.54703700	-0.74859100
H	-2.46565100	2.44607200	-1.64940000
C	-4.91228900	2.66739100	1.33964900
H	-3.93626400	0.89552100	2.07323700

C	-4.96603500	3.62543100	0.32888300
H	-4.14111200	4.27715100	-1.55084000
H	-5.59404900	2.72778800	2.18228000
H	-5.69600000	4.42727200	0.37797600
C	-0.73203200	0.96666900	-0.02184700
P	-0.30449400	2.62001800	0.52960900
C	2.02759600	0.73927500	0.35526000
C	3.41187400	1.02114700	0.65974900
C	3.76521200	2.30552200	1.11866500
C	4.42172600	0.05462900	0.53272500
C	5.08407300	2.60620800	1.42576800
H	2.99151600	3.06086500	1.23052000
C	5.73980400	0.35453600	0.85123400
H	4.15736800	-0.93976500	0.18264200
C	6.07447200	1.63261200	1.29449900
H	5.34182200	3.60142200	1.77430800
H	6.50736500	-0.40693500	0.75358100
H	7.10481800	1.86971900	1.54038700
C	0.90066400	1.34842300	0.59357200
C	0.17658600	3.83315800	-0.72160400
H	0.71478200	4.63555200	-0.21231600
H	0.81155300	3.39996700	-1.49439200
H	-0.72158500	4.26351000	-1.17135500
O	-0.92583000	3.21601000	1.74534400
C	-0.20696700	-0.96529700	-2.43071800
C	0.73869900	0.10671100	-2.62934600
C	2.04823100	-0.37442600	-2.31410800

C	1.90298800	-1.70003000	-1.79686800
C	0.50612900	-2.07036900	-1.91969900
C	-0.01069400	-3.42608500	-1.61350500
H	-1.09167000	-3.49508100	-1.74732600
H	0.45121400	-4.15316800	-2.29122500
H	0.22033700	-3.74846100	-0.59416600
C	-1.63165900	-0.90649300	-2.84307000
H	-2.12335100	0.00678700	-2.49138700
H	-1.69842000	-0.90524800	-3.93741500
H	-2.20394400	-1.76135200	-2.47839600
C	0.40141000	1.41054100	-3.25489000
H	1.22123200	2.12844200	-3.18337300
H	0.18669500	1.27282600	-4.32128100
H	-0.49300400	1.85459100	-2.80480800
C	3.30607500	0.37901100	-2.55828200
H	4.17090700	-0.08416100	-2.08199500
H	3.50104900	0.42007700	-3.63576600
H	3.24863100	1.41168600	-2.20085200
C	2.97268500	-2.65945700	-1.40691500
H	2.97163300	-3.52449600	-2.07964700
H	3.96702900	-2.21223200	-1.46269200
H	2.82775700	-3.05580200	-0.39576500
C	-2.52981200	-0.85657200	0.23574500
C	-0.67288600	-1.76043400	1.59685900
C	0.19829400	-2.10691600	3.80364400
C	1.47128500	-1.91915300	3.27531600
C	1.59114800	-1.59594100	1.93616500

N	0.53924800	-1.48668300	1.09600300
H	0.05416800	-2.32644000	4.85625900
H	2.36151400	-1.99838300	3.88825700
H	2.56158200	-1.39280200	1.49971000
N	-1.77781200	-1.92111200	0.70797900
C	-3.77641700	-1.12913500	-0.29162800
H	-4.36285000	-0.30705600	-0.68008500
C	-2.21148500	-3.30537100	0.64625400
C	-3.48768200	-3.50523700	0.02262400
H	-3.82484700	-4.53300800	-0.04379300
C	-4.24600100	-2.45336300	-0.40172100
H	-5.22311500	-2.63153800	-0.84199700
O	-1.48891300	-4.17553700	1.11488600
C	-0.88476500	-2.04211900	2.94346600
H	-1.89466000	-2.24276600	3.28254200
Co	0.80444500	-0.41101400	-0.63296800

Zero-point correction= 0.624744 (Hartree/Particle)

Thermal correction to Energy= 0.664832

Thermal correction to Enthalpy= 0.665776

Thermal correction to Gibbs Free Energy= 0.554157

Sum of electronic and zero-point Energies= -2177.195677

Sum of electronic and thermal Energies= -2177.155589

Sum of electronic and thermal Enthalpies= -2177.154645

Sum of electronic and thermal Free Energies= -2177.266263

E(RM06L) = -2177.820420 A.U.

B-TS4-Co

1 1

Number of imaginary frequencies: 1

C	-2.34776400	0.40597600	0.04927700
C	-3.59500900	1.17750100	-0.11866800
C	-3.73680800	2.11231500	-1.15783500
C	-4.65361800	1.01851300	0.78870200
C	-4.88849100	2.88691300	-1.26638100
H	-2.97121800	2.17223800	-1.92938300
C	-5.79732600	1.79929600	0.68414200
H	-4.55916200	0.29448800	1.59425200
C	-5.91580100	2.73931500	-0.33919500
H	-4.99033200	3.59078600	-2.08660100
H	-6.59774300	1.67955400	1.40752600
H	-6.81299500	3.34456900	-0.42077400
C	-1.16003200	1.11240700	0.02839000
P	-0.88245500	2.82391400	-0.17079600
C	1.54004100	0.98847000	0.19419500
C	2.62282200	1.87615300	0.52832100
C	2.47942600	3.26914500	0.69864600
C	3.89903600	1.31088200	0.72202300
C	3.58007000	4.05318000	1.01472400
H	1.50424100	3.73690400	0.62279700
C	4.99394100	2.09690700	1.04585200
H	3.99958900	0.23583300	0.61392200
C	4.83853200	3.47586800	1.18421400
H	3.45316200	5.12374000	1.14273200
H	5.96752500	1.63866600	1.19202500
H	5.69222200	4.09763700	1.43609400

C	0.22506400	0.95510600	-0.03187700
C	-0.33759600	3.34150700	-1.81048600
H	0.72223000	3.61114400	-1.77832900
H	-0.49293000	2.53739900	-2.53190900
H	-0.90558700	4.22499000	-2.11160700
O	-0.69188000	3.79617400	0.94276700
C	0.79173100	-2.23875200	-1.85246100
C	1.04440500	-0.98473400	-2.47323900
C	2.38941900	-0.56799800	-2.14428400
C	2.97324500	-1.58232400	-1.31739700
C	1.96598200	-2.58082200	-1.10147100
C	2.13792600	-3.80296300	-0.27265800
H	1.22951700	-4.05684800	0.28092700
H	2.39095600	-4.65839000	-0.91013400
H	2.95165200	-3.68999700	0.44850300
C	-0.40789400	-3.09156100	-2.06287600
H	-1.34475800	-2.52964900	-1.98239300
H	-0.38993000	-3.53509700	-3.06585700
H	-0.44088100	-3.91790900	-1.34992200
C	0.07712600	-0.24565500	-3.33011400
H	0.41744300	0.77128600	-3.54185400
H	-0.04683900	-0.74900300	-4.29590600
H	-0.91752000	-0.19271200	-2.86985000
C	3.06754300	0.65169600	-2.66134300
H	3.89558300	0.96114300	-2.01834400
H	3.47323900	0.47701600	-3.66413900
H	2.37953000	1.50019900	-2.73389800

C	4.39800900	-1.70107900	-0.89728200
H	4.90107000	-2.48121600	-1.48084400
H	4.95296500	-0.77367600	-1.05643300
H	4.50641800	-1.98426300	0.15505000
C	-2.47427400	-1.03887700	0.17322000
C	-0.58919900	-1.34294700	1.77860000
C	-0.09459400	-0.86201500	4.06870100
C	1.25498000	-0.88003900	3.73348200
C	1.60640700	-1.08194800	2.40761700
N	0.70384200	-1.28461000	1.43160400
H	-0.41237400	-0.68001500	5.09013900
H	2.02646600	-0.71972100	4.47756400
H	2.64317300	-1.05235300	2.08437600
N	-1.52433400	-1.82983600	0.80677700
C	-3.55027200	-1.66659900	-0.43042200
H	-4.26971100	-1.05737500	-0.96140200
C	-1.60139200	-3.27433600	0.85461200
C	-2.76193500	-3.84437700	0.22851800
H	-2.84728800	-4.92308100	0.29123600
C	-3.69913600	-3.06683600	-0.38370200
H	-4.56715200	-3.52284400	-0.85086900
O	-0.71798400	-3.89833900	1.42911400
C	-1.03172500	-1.11782100	3.07582500
H	-2.09312100	-1.17589700	3.29360000
Co	1.27239700	-0.73461500	-0.45245500

Zero-point correction= 0.624188 (Hartree/Particle)

Thermal correction to Energy= 0.664882

Thermal correction to Enthalpy= 0.665826

Thermal correction to Gibbs Free Energy= 0.551977

Sum of electronic and zero-point Energies= -2177.204239

Sum of electronic and thermal Energies= -2177.163545

Sum of electronic and thermal Enthalpies= -2177.162601

Sum of electronic and thermal Free Energies= -2177.276450

E(RM06L) = -2177.828427 A.U.

(S)B-TS5-Co

1 1

Number of imaginary frequencies: 1

C	-2.26519100	0.42290900	-0.59416600
C	-3.55760900	1.11106400	-0.62993400
C	-3.65331500	2.43468000	-1.09594900
C	-4.73328300	0.48241300	-0.18190300
C	-4.86528600	3.10886200	-1.09615500
H	-2.76715900	2.91463900	-1.50623600
C	-5.94542900	1.15891200	-0.17799400
H	-4.68787000	-0.54254200	0.17774800
C	-6.01634400	2.47468900	-0.63122600
H	-4.91847800	4.12501600	-1.47469700
H	-6.83891000	0.65960500	0.18389400
H	-6.96595100	3.00056300	-0.63222100
C	-1.09663700	1.12367400	-0.35016400
P	-1.04594000	2.53294300	0.79617400
C	1.43401100	1.15723600	-0.09260500
C	2.40388500	2.21079800	-0.11042900
C	3.32296800	2.35918700	0.94496300

C	2.47427400	3.10015900	-1.20124500
C	4.26915600	3.37426700	0.91747400
H	3.26476400	1.67815900	1.79081700
C	3.44293200	4.09525000	-1.23524500
H	1.77207500	2.98221100	-2.02400000
C	4.33919300	4.23800900	-0.17666900
H	4.96032500	3.49059800	1.74662800
H	3.49770300	4.76463500	-2.08837500
H	5.09035300	5.02101000	-0.20285800
C	0.25127300	0.70116700	-0.46909900
C	-0.52350500	4.10185500	0.02487700
H	-1.04321900	4.90335900	0.55240500
H	0.55530600	4.25549300	0.10436000
H	-0.79724200	4.11248900	-1.03366200
O	-2.16897700	2.65827300	1.78386000
C	3.25978800	-0.84196100	-1.11560700
C	3.36911100	-1.53853800	0.13238000
C	2.40652400	-2.59525300	0.11419100
C	1.71678700	-2.57578400	-1.15009500
C	2.22352600	-1.47107800	-1.89291700
C	1.78999500	-1.06671100	-3.25571600
H	1.90953100	0.00775200	-3.41896900
H	2.38413100	-1.58052900	-4.02090300
H	0.74110200	-1.32020400	-3.43252100
C	4.18954400	0.19909800	-1.62177800
H	4.63291800	0.79893100	-0.82366800
H	5.01091000	-0.29251800	-2.15648000

H	3.71044900	0.88064900	-2.32849200
C	4.35943800	-1.25713300	1.20598100
H	3.98791100	-1.54399500	2.19414200
H	5.28459200	-1.82303500	1.04408100
H	4.63340100	-0.19864600	1.23822000
C	2.16958800	-3.57492800	1.20557200
H	1.11663600	-3.86271900	1.27484900
H	2.75387400	-4.48425100	1.02347100
H	2.48356800	-3.18394500	2.17744400
C	0.78290900	-3.60532100	-1.67364200
H	1.30504300	-4.24177800	-2.39869600
H	0.40329500	-4.25315600	-0.88224400
H	-0.06922500	-3.16329200	-2.19814000
C	-2.28234600	-1.03155200	-0.77729700
C	-1.11002700	-1.32853300	1.37075600
C	-1.43607900	-0.74973600	3.67215400
C	-0.06312100	-0.54502000	3.77197900
C	0.71693300	-0.72117700	2.64193000
N	0.20964200	-1.09326000	1.44981600
H	-2.08532200	-0.60068900	4.52826500
H	0.39949000	-0.24077200	4.70363200
H	1.78947500	-0.54397000	2.65491200
N	-1.63725900	-1.84584600	0.14606000
C	-2.98929400	-1.62696800	-1.79520300
H	-3.48720100	-0.98953300	-2.51577800
C	-1.71209600	-3.28122700	0.13691900
C	-2.47834100	-3.83116400	-0.94397300

H	-2.55676800	-4.91196300	-0.96706800
C	-3.08422700	-3.03330700	-1.87186700
H	-3.65968800	-3.48186200	-2.67697000
O	-1.14096300	-3.90888600	1.02559200
C	-1.96141800	-1.16133700	2.45622200
H	-3.01937600	-1.36441700	2.33193900
Co	1.42525000	-0.75895600	-0.12078900

Zero-point correction= 0.624163 (Hartree/Particle)

Thermal correction to Energy= 0.664709

Thermal correction to Enthalpy= 0.665654

Thermal correction to Gibbs Free Energy= 0.552505

Sum of electronic and zero-point Energies= -2177.202390

Sum of electronic and thermal Energies= -2177.161844

Sum of electronic and thermal Enthalpies= -2177.160900

Sum of electronic and thermal Free Energies= -2177.274049

E(RM06L) = -2177.826554 A.U.

(T)B-TS5-Co

1 3

Number of imaginary frequencies: 1

C	-2.25953100	0.38572500	-0.47815900
C	-3.55659900	1.03316800	-0.67791500
C	-3.62114600	2.33529300	-1.20753200
C	-4.76155100	0.39156400	-0.33670600
C	-4.83827700	2.97643800	-1.37424600
H	-2.69824200	2.82040000	-1.51814800
C	-5.97828300	1.03914100	-0.49341200
H	-4.73349100	-0.61099200	0.08257900

C	-6.02099200	2.33274800	-1.01089500
H	-4.87075300	3.97506600	-1.79865700
H	-6.89697000	0.53799100	-0.20519700
H	-6.97449800	2.83594700	-1.13806400
C	-1.15747300	1.15312500	-0.07404100
P	-1.41042400	2.45314100	1.15219900
C	1.43036200	1.23330400	-0.14358200
C	2.42087300	2.27170900	-0.18538300
C	3.38164600	2.38543300	0.83366200
C	2.43676300	3.19828800	-1.24408300
C	4.32812700	3.40167500	0.79712400
H	3.36446200	1.67349300	1.65578300
C	3.39545900	4.20301800	-1.28171700
H	1.69588600	3.10744100	-2.03531900
C	4.34277900	4.30670700	-0.26399600
H	5.05844200	3.48820700	1.59587600
H	3.40404500	4.90850100	-2.10690300
H	5.08956900	5.09375800	-0.29545500
C	0.21405400	0.82867000	-0.28714800
C	-0.61798900	3.99704200	0.61345300
H	-0.53539100	4.67455400	1.46420800
H	0.37336500	3.81707300	0.19548600
H	-1.25323900	4.47058100	-0.14186500
O	-2.78622500	2.60646500	1.73917400
C	3.23014500	-0.74331700	-1.22321400
C	3.44599700	-1.44562200	-0.00171200
C	2.50056100	-2.51881000	0.03947100

C	1.74954900	-2.52717300	-1.19777400
C	2.16125400	-1.40849700	-1.94858300
C	1.63577600	-1.00381000	-3.28345800
H	2.37461000	-0.43236300	-3.85059100
H	1.36515500	-1.88040500	-3.87814800
H	0.73724400	-0.38207300	-3.20018600
C	4.10011300	0.31162100	-1.80114700
H	4.62408300	0.89556600	-1.04129100
H	4.86124500	-0.16693500	-2.42930700
H	3.54855500	1.00764700	-2.43739800
C	4.49158100	-1.14903000	1.01548300
H	4.15183400	-1.36660800	2.03293200
H	5.38569900	-1.76096000	0.84869400
H	4.80657500	-0.10253800	0.98013900
C	2.36007500	-3.51937900	1.12910300
H	1.32078900	-3.83557600	1.26115600
H	2.95183100	-4.41251000	0.89651500
H	2.72768000	-3.13468100	2.08460500
C	0.84294100	-3.60136500	-1.67859800
H	1.36987300	-4.22254100	-2.41341100
H	0.51936300	-4.25923700	-0.87069800
H	-0.04418800	-3.20348400	-2.17840700
C	-2.21162200	-1.05501300	-0.70309100
C	-1.03059400	-1.37114200	1.43875600
C	-1.34956400	-0.82357700	3.74583500
C	0.02066800	-0.59355800	3.83653000
C	0.79657000	-0.74927100	2.69999400

N	0.28517400	-1.12097900	1.51019600
H	-1.99412300	-0.69379400	4.60864300
H	0.48389800	-0.28751200	4.76727000
H	1.86670400	-0.55540000	2.70852600
N	-1.54704300	-1.87356900	0.20335000
C	-2.90044600	-1.65143400	-1.73842300
H	-3.40898800	-1.01251300	-2.44982300
C	-1.59158400	-3.30816300	0.16854300
C	-2.34917100	-3.85600400	-0.92205300
H	-2.40566400	-4.93784100	-0.96201400
C	-2.96630500	-3.05611100	-1.84143300
H	-3.52876500	-3.50235200	-2.65670600
O	-1.00546700	-3.94081300	1.04225200
C	-1.87870700	-1.23304000	2.53017400
H	-2.93523700	-1.44700600	2.41009800
Co	1.45736600	-0.71413000	-0.08196800

Zero-point correction= 0.623656 (Hartree/Particle)

Thermal correction to Energy= 0.664534

Thermal correction to Enthalpy= 0.665479

Thermal correction to Gibbs Free Energy= 0.549471

Sum of electronic and zero-point Energies= -2177.216534

Sum of electronic and thermal Energies= -2177.175656

Sum of electronic and thermal Enthalpies= -2177.174712

Sum of electronic and thermal Free Energies= -2177.290719

E(RM06L) = -2177.840191 A.U.

(S)B-TS6-Co

1 1

Number of imaginary frequencies: 1

C	-2.40242400	0.38711500	0.07155200
C	-3.59682000	1.29342600	0.07989400
C	-4.10066800	1.83941500	-1.10572300
C	-4.19778100	1.63462900	1.29459700
C	-5.18205500	2.71625900	-1.07688200
H	-3.63918800	1.57010200	-2.05521700
C	-5.27351100	2.51593900	1.32360300
H	-3.79797800	1.22789200	2.22054200
C	-5.76755900	3.05721400	0.13945600
H	-5.56507600	3.13307700	-2.00386800
H	-5.72136100	2.78701100	2.27458400
H	-6.60621400	3.74600500	0.16471100
C	-1.19750900	1.01794700	0.08008000
P	-0.96496700	2.82933300	0.01401900
C	0.71173000	2.13539500	-0.01668500
C	1.95780700	2.83903700	0.04919300
C	3.20257900	2.22718900	-0.19034900
C	1.93543800	4.21767400	0.35995600
C	4.37993100	2.95382200	-0.11583200
H	3.21956200	1.17469700	-0.43851300
C	3.11691500	4.93951200	0.44138900
H	0.98350800	4.69671600	0.57974400
C	4.34054600	4.31318500	0.20251700
H	5.33188400	2.46528100	-0.30858000
H	3.08758600	5.99440700	0.69484200
H	5.26249400	4.88375000	0.26144200

C	0.27869600	0.79790800	0.08525600
C	-1.31187400	3.47732200	-1.64923900
H	-0.60532800	4.28427500	-1.86278900
H	-1.22216000	2.71081300	-2.42395900
H	-2.32299600	3.88817300	-1.66558500
O	-1.38145600	3.74578000	1.11818900
C	2.75939900	-1.06703400	-1.91856300
C	2.41972600	-2.39394100	-1.47152800
C	1.04319600	-2.61479000	-1.77263900
C	0.48343900	-1.38460600	-2.24285900
C	1.56854900	-0.43332200	-2.36402400
C	1.46195200	0.90988400	-2.98822300
H	2.17786600	1.62408200	-2.57337100
H	1.65878400	0.83386800	-4.06414100
H	0.45984500	1.32739700	-2.86841100
C	4.14091100	-0.52523700	-1.92228000
H	4.57182000	-0.52930900	-0.91479300
H	4.77693600	-1.16479500	-2.54398300
H	4.19267500	0.48827700	-2.32447500
C	3.37206100	-3.38609100	-0.90951900
H	2.85269400	-4.17085200	-0.35362700
H	3.94518700	-3.87731300	-1.70485500
H	4.09064800	-2.90654400	-0.23899900
C	0.36465600	-3.92250700	-1.63060500
H	0.40281800	-4.31529000	-0.61164600
H	-0.68438600	-3.87893000	-1.92698300
H	0.86653900	-4.64824700	-2.28023800

C	-0.89250700	-1.17713000	-2.76403800
H	-0.88844900	-1.19245800	-3.86041000
H	-1.57773900	-1.95849500	-2.42662800
H	-1.30550400	-0.21175700	-2.45389000
C	-2.70367700	-1.03325800	-0.07772100
C	-0.91750200	-1.86780900	1.43997300
C	-0.57382200	-2.21246100	3.78407400
C	0.73219000	-2.57834600	3.48600000
C	1.17898100	-2.43765700	2.18189200
N	0.39439100	-2.01701400	1.17163900
H	-0.94753800	-2.24728900	4.80213900
H	1.41258600	-2.93493500	4.25079900
H	2.21601400	-2.61978200	1.92264000
N	-1.83633700	-2.02464400	0.35618800
C	-3.82649300	-1.41133000	-0.78682300
H	-4.49962900	-0.64132800	-1.13769500
C	-2.11850600	-3.44859300	0.18994900
C	-3.22009200	-3.74448400	-0.67590600
H	-3.39986400	-4.79599700	-0.86788200
C	-4.06188800	-2.76128600	-1.10960100
H	-4.93316600	-3.01714500	-1.70622300
O	-1.42913400	-4.26477400	0.78803600
C	-1.42027900	-1.88359100	2.73313100
H	-2.48283900	-1.72231400	2.88450100
C	2.74051900	-0.02575300	1.89664900
O	2.87461900	-0.70530200	0.81993000
O	1.63521600	0.44045500	2.28246900

H	0.86892700	0.40377600	1.14059100
C	3.95511800	0.18641700	2.74419800
H	3.89351100	-0.46126200	3.62421700
H	4.86836700	-0.04870900	2.19772300
H	3.98024700	1.21585800	3.10484400
Co	1.32506800	-1.03299100	-0.37950100

Zero-point correction= 0.686527 (Hartree/Particle)

Thermal correction to Energy= 0.731185

Thermal correction to Enthalpy= 0.732129

Thermal correction to Gibbs Free Energy= 0.611851

Sum of electronic and zero-point Energies= -2406.259174

Sum of electronic and thermal Energies= -2406.214516

Sum of electronic and thermal Enthalpies= -2406.213572

Sum of electronic and thermal Free Energies= -2406.333850

E(RM06L) = -2406.945701 A.U.

(T)B-TS6-Co

1 3

Number of imaginary frequencies: 1

C	-2.39726900	0.39837300	0.06767500
C	-3.58389900	1.31576400	0.04127100
C	-4.06433000	1.84566200	-1.16182000
C	-4.19299800	1.69355900	1.24101500
C	-5.13456200	2.73623200	-1.16495800
H	-3.59123900	1.55499600	-2.09933000
C	-5.25802400	2.58863800	1.23764700
H	-3.80774600	1.30629500	2.18113900
C	-5.73155700	3.10951200	0.03640800

H	-5.49899600	3.13983200	-2.10514500
H	-5.71254500	2.88664400	2.17727700
H	-6.56159100	3.80905900	0.03640600
C	-1.19462600	1.02977400	0.13945700
P	-0.93306700	2.84164600	0.06600500
C	0.73767100	2.12463100	0.06093700
C	2.00776100	2.77786600	0.11441900
C	3.22774600	2.10522500	-0.09937100
C	2.03909800	4.16236500	0.39602000
C	4.43241200	2.78403500	-0.01999600
H	3.20628100	1.04806500	-0.33885600
C	3.24840100	4.83580400	0.47809200
H	1.10492800	4.68430900	0.59345000
C	4.44611900	4.15100700	0.27064800
H	5.36612800	2.25325400	-0.18780100
H	3.26178800	5.89605800	0.70907600
H	5.39123200	4.68208000	0.33189700
C	0.27761900	0.79992600	0.17762200
C	-1.23749000	3.47154300	-1.61187400
H	-0.54669500	4.29793500	-1.80124800
H	-1.09322200	2.70399500	-2.37783600
H	-2.25855200	3.85278400	-1.67120000
O	-1.35619300	3.77460000	1.15232700
C	2.89581700	-1.09681500	-1.95441000
C	2.36884300	-2.38984900	-1.55596900
C	0.99317800	-2.47732800	-1.94783800
C	0.61732900	-1.18300900	-2.39308300

C	1.82207600	-0.33760400	-2.42292200
C	1.85248700	1.02920100	-3.00107400
H	2.75762300	1.57696100	-2.73078100
H	1.81187000	0.97573700	-4.09582800
H	0.99272400	1.62594600	-2.68132700
C	4.32034000	-0.70171800	-1.81974600
H	4.64291000	-0.74252400	-0.77250600
H	4.96580100	-1.38611400	-2.38081100
H	4.50179700	0.30723700	-2.19718800
C	3.17129300	-3.48023300	-0.95342800
H	2.53990100	-4.21764100	-0.45150200
H	3.74113600	-4.01126200	-1.72629400
H	3.89312600	-3.08531100	-0.23304200
C	0.18408400	-3.72257200	-1.93274100
H	0.19752200	-4.22369000	-0.96126500
H	-0.86020200	-3.53102000	-2.18889100
H	0.57676300	-4.42797200	-2.67343100
C	-0.70081200	-0.76978200	-2.93962600
H	-0.65760500	-0.70287600	-4.03349400
H	-1.49016800	-1.48030100	-2.68206400
H	-1.00369200	0.21617400	-2.56930900
C	-2.70036800	-1.02290400	-0.11943600
C	-1.04117000	-1.90077400	1.51183000
C	-0.85285500	-2.03395500	3.88747800
C	0.46199900	-2.44737700	3.70936400
C	0.98377800	-2.46382900	2.42477800
N	0.26555300	-2.14971200	1.33507700

H	-1.28483600	-1.96070100	4.88027300
H	1.08569000	-2.72813800	4.55052100
H	2.02513000	-2.70992000	2.24108000
N	-1.87269400	-2.03522200	0.35262300
C	-3.78277200	-1.37458200	-0.89927700
H	-4.42368400	-0.59145800	-1.27958300
C	-2.15163000	-3.45456900	0.12769100
C	-3.22732400	-3.72008600	-0.78257600
H	-3.41151800	-4.76572900	-1.00034000
C	-4.02711700	-2.71891700	-1.24689300
H	-4.87265100	-2.95187300	-1.88822000
O	-1.48903800	-4.29321100	0.72019500
C	-1.62948300	-1.77994100	2.76290700
H	-2.68894700	-1.55627200	2.83693500
C	2.76708400	-0.20548600	1.93610700
O	2.83602000	-0.90078200	0.86575000
O	1.71401900	0.36567700	2.32914000
H	0.87905700	0.37550600	1.20690400
C	3.99737200	-0.10398400	2.78625300
H	4.89532700	-0.32874400	2.20994300
H	4.06628400	0.88731600	3.23520300
H	3.92354000	-0.82722900	3.60473900
Co	1.18072300	-1.04424600	-0.34423400

Zero-point correction= 0.683064 (Hartree/Particle)

Thermal correction to Energy= 0.729132

Thermal correction to Enthalpy= 0.730076

Thermal correction to Gibbs Free Energy= 0.604734

Sum of electronic and zero-point Energies= -2406.248854

Sum of electronic and thermal Energies= -2406.202786

Sum of electronic and thermal Enthalpies= -2406.201842

Sum of electronic and thermal Free Energies= -2406.327185

E(RM06L) = -2406.931918 A.U.

B-TSa1-Rh

1 1

Number of imaginary frequencies: 1

C	-0.96581700	-1.79835300	-1.20503000
C	-1.94500000	-1.84582400	-0.12439200
C	-2.80795900	-0.71808000	-0.26098300
C	-2.38217500	0.04448500	-1.41901000
C	-1.27207600	-0.65818000	-2.02017100
O	0.42651700	1.40518100	2.64508500
O	-1.36861800	1.58104300	1.30682700
C	-0.67314600	1.93747300	2.31927000
C	-3.94006400	-0.32819900	0.63430200
H	-4.88298400	-0.34849600	0.07707800
H	-4.03280800	-1.00228500	1.48675000
H	-3.78974800	0.68764300	1.01269700
C	-2.08755400	-2.94437400	0.88237200
H	-2.37988500	-2.55930400	1.86187200
H	-2.86614400	-3.64277500	0.55302800
H	-1.16070500	-3.50645300	0.99709100
C	0.07875100	-2.83221100	-1.48925200
H	0.48095000	-3.25695700	-0.56857700
H	-0.34956700	-3.64912700	-2.08162900

H	0.91385700	-2.41251000	-2.05369400
C	-0.55238400	-0.24647100	-3.26399000
H	0.48100300	-0.59745300	-3.26705900
H	-1.05673000	-0.67448300	-4.13832500
H	-0.54499000	0.83898300	-3.38301100
C	-3.06714300	1.26615000	-1.94382100
H	-2.40137500	1.86467400	-2.56955900
H	-3.93149500	0.98455200	-2.55746900
H	-3.42744000	1.89304800	-1.12485600
C	-1.21440300	3.05162100	3.18177200
H	-2.07963900	3.52280400	2.71620700
H	-1.49945100	2.63556900	4.15302000
H	-0.42600800	3.78638300	3.36130300
C	1.04187500	-0.68253000	1.18870000
C	1.02492400	-1.85918900	1.89604700
C	2.08687700	-2.80205800	1.77689900
C	3.12428000	-2.55433900	0.92886700
C	3.21844800	-1.33738000	0.13429000
C	2.10938500	0.82457700	-0.32466200
C	0.68608200	2.50128400	-1.12019700
C	1.75836300	3.28348300	-1.52088800
C	3.05117700	2.79480300	-1.30914500
C	3.23914000	1.55822000	-0.70102100
H	0.64126400	0.34529400	1.86568300
H	0.19926900	-2.03943800	2.57448500
H	2.06607000	-3.71738600	2.36183300
H	3.94533000	-3.24902400	0.79416400

H	-0.34280600	2.82199300	-1.23774700
H	1.58353800	4.24883400	-1.98151700
H	3.91482000	3.38159900	-1.60441700
H	4.22391100	1.15376000	-0.52115100
N	2.14921100	-0.41118300	0.35776000
N	0.86333500	1.29200400	-0.55657900
O	4.11233300	-1.10439400	-0.66828700
Rh	-0.72883100	0.02979400	0.02126200

Zero-point correction= 0.434754 (Hartree/Particle)

Thermal correction to Energy= 0.463838

Thermal correction to Enthalpy= 0.464782

Thermal correction to Gibbs Free Energy= 0.375239

Sum of electronic and zero-point Energies= -1298.205954

Sum of electronic and thermal Energies= -1298.176871

Sum of electronic and thermal Enthalpies= -1298.175927

Sum of electronic and thermal Free Energies= -1298.265470

E(RB3LYP) = -1298.640709 A.U.

B-TSa2-Rh

1 1

Number of imaginary frequencies: 1

C	-2.90374800	-1.47661500	1.35667000
C	-4.10496900	-1.43763800	0.59746200
C	-4.63326300	-0.19671000	0.18904500
C	-4.72569400	-2.63180400	0.18254500
C	-5.75659000	-0.15748200	-0.63165700
H	-4.15263000	0.71900400	0.51795400
C	-5.85051000	-2.57976700	-0.63705400

H	-4.31703700	-3.58428200	0.50373900
C	-6.36414300	-1.34613200	-1.04893000
H	-6.16136400	0.79920400	-0.94690200
H	-6.32958300	-3.50119300	-0.95305600
H	-7.24025600	-1.31078400	-1.68901200
C	-1.84905300	-1.49242300	1.96708800
P	-0.16416500	-1.42891100	2.45269600
C	-0.00985400	1.07392800	1.03965700
C	-0.81653600	2.21607500	1.40543800
C	-1.92487500	2.60380800	0.62684300
C	-0.52276700	2.90920900	2.59489200
C	-2.72638800	3.66263400	1.04252600
H	-2.16023300	2.06538100	-0.28352900
C	-1.33208400	3.96783700	3.00157500
H	0.33737000	2.61039700	3.18564300
C	-2.43131300	4.34691600	2.22654900
H	-3.58288000	3.95606400	0.44369000
H	-1.10481800	4.49775000	3.92118300
H	-3.05823900	5.17413000	2.54421300
C	0.41697100	-0.08989000	1.37886100
C	-0.12836500	-0.75560500	4.14047200
H	0.91266500	-0.59030200	4.43057900
H	-0.68159200	0.18641400	4.18507500
H	-0.57926900	-1.48123300	4.82238700
O	0.60445700	-2.70049000	2.24265200
C	1.33818700	2.71013300	-0.76365500
C	0.75442800	1.46405900	-0.80556100

H	2.03293500	2.92693300	0.03791700
C	-0.72624100	-0.13716300	-1.79596500
C	-2.33104900	-1.85501700	-2.27773900
C	-1.50488500	-2.77990000	-1.64112700
C	-0.31920800	-2.32564300	-1.08232500
N	0.06792900	-1.04016700	-1.17578800
H	-3.28788500	-2.15976200	-2.68778900
H	-1.78152900	-3.82313700	-1.54487300
H	0.32836700	-2.97360200	-0.50522900
N	-0.22810700	1.19102100	-1.77038800
C	3.87920800	0.22307400	0.37101900
C	3.58308800	-1.05861600	0.97024400
C	3.25987900	-1.96461200	-0.07576500
C	3.43612900	-1.25617000	-1.35149500
C	3.85554500	0.06794100	-1.07352100
C	4.21658600	1.13284200	-2.06178800
H	3.78557100	2.09767600	-1.78179200
H	5.30487000	1.25401300	-2.11006800
H	3.86124500	0.88937700	-3.06461600
C	4.35934500	1.43373000	1.11191400
H	3.80657400	1.57926200	2.04348100
H	5.41929900	1.32297800	1.37141400
H	4.26343100	2.33854700	0.50856100
C	3.63569800	-1.37812000	2.43179800
H	2.92771800	-2.16844800	2.68451800
H	4.64590300	-1.70883600	2.70221500
H	3.40643900	-0.49816500	3.03876100

C	2.96158400	-3.42341500	0.08428400
H	2.50591500	-3.83920900	-0.81748900
H	3.89070500	-3.97904800	0.26092800
H	2.28902700	-3.59111700	0.92825100
C	3.25116600	-1.88608400	-2.69635700
H	4.10644200	-2.52978300	-2.93348300
H	2.35401700	-2.51057700	-2.71881400
H	3.16120300	-1.13782500	-3.48562800
C	-1.95279300	-0.51780300	-2.35380000
H	-2.57494600	0.22134500	-2.83115100
C	-0.69195300	2.18986700	-2.70445700
C	0.01715500	3.45366800	-2.63494600
H	-0.30128600	4.18987200	-3.36326900
C	0.98934500	3.70477000	-1.71223900
H	1.48285300	4.67228200	-1.68652600
O	-1.60672000	1.96638900	-3.48695900
Rh	1.77788100	-0.27435800	-0.15917900

Zero-point correction= 0.623149 (Hartree/Particle)

Thermal correction to Energy= 0.665008

Thermal correction to Enthalpy= 0.665952

Thermal correction to Gibbs Free Energy= 0.547697

Sum of electronic and zero-point Energies= -2141.106055

Sum of electronic and thermal Energies= -2141.064196

Sum of electronic and thermal Enthalpies= -2141.063252

Sum of electronic and thermal Free Energies= -2141.181507

E(RB3LYP) = -2141.729204 A.U.

B-TS3-Rh

1 1

Number of imaginary frequencies: 1

C	-2.16848300	0.51036900	0.08718900
C	-3.37814900	1.38216700	-0.07449900
C	-3.58247800	2.09746600	-1.26415400
C	-4.30963400	1.50390000	0.96715100
C	-4.68964800	2.93561500	-1.40374200
H	-2.87941100	1.97737400	-2.08371900
C	-5.40621100	2.35213300	0.83133400
H	-4.15985600	0.94816600	1.88783800
C	-5.59847600	3.06951000	-0.35298800
H	-4.84498500	3.47673000	-2.33218500
H	-6.11068100	2.45659600	1.65053800
H	-6.45689700	3.72563100	-0.45699400
C	-0.96918300	1.13677400	-0.06612800
P	-0.61682400	2.87771800	0.10143800
C	1.86237100	1.11134000	0.26366200
C	3.23150200	1.50214000	0.54723600
C	3.56201200	2.86385700	0.70810100
C	4.24391100	0.53711200	0.69330800
C	4.87023000	3.24058900	0.99343000
H	2.78583900	3.61670800	0.60897400
C	5.55106000	0.91621700	0.98831200
H	3.98970000	-0.51067500	0.57527200
C	5.86757900	2.26917300	1.13458700
H	5.11445900	4.29160800	1.11158000
H	6.32185600	0.16045800	1.10369000

H	6.88645900	2.56726700	1.36120800
C	0.71965900	1.74286900	0.25748500
C	-0.47925900	3.76426400	-1.48510300
H	0.21296400	4.60050400	-1.35706000
H	-0.12412500	3.10193200	-2.27583800
H	-1.46635600	4.15927500	-1.73629800
O	-1.11155200	3.70406300	1.24153300
C	0.07602000	-1.60262100	-2.39236900
C	1.03460700	-0.53239500	-2.66857200
C	2.32041700	-0.93207800	-2.16999000
C	2.11702900	-2.12494100	-1.40148500
C	0.72952600	-2.56694200	-1.61037500
C	0.21081500	-3.88381400	-1.13218400
H	-0.86157500	-3.98340600	-1.30120000
H	0.71588600	-4.69050100	-1.67725700
H	0.39729900	-4.03441600	-0.06681800
C	-1.32599400	-1.62292300	-2.91227700
H	-1.84210500	-0.68383700	-2.69429400
H	-1.31965500	-1.75404400	-4.00091200
H	-1.90867900	-2.43207500	-2.47282000
C	0.76436300	0.64650300	-3.55009200
H	1.44471900	1.47249200	-3.33122800
H	0.89908500	0.37261000	-4.60371700
H	-0.26299700	0.99847600	-3.42989700
C	3.61149700	-0.23443300	-2.46538400
H	4.42106600	-0.57625100	-1.82170800
H	3.89728600	-0.43657800	-3.50442600

H	3.52613900	0.84795000	-2.34586500
C	3.15662100	-2.97049200	-0.73374200
H	3.40228800	-3.83236800	-1.36638200
H	4.08075400	-2.41827000	-0.55548700
H	2.79335400	-3.35867300	0.22136200
Rh	0.90321900	-0.53247400	-0.48115300
C	-2.47457400	-0.92177000	0.28686000
C	-0.74044800	-1.24400400	2.03105700
C	-0.21241400	-0.79958200	4.32686300
C	1.11419900	-0.62896500	3.93464200
C	1.43302800	-0.73221200	2.58701800
N	0.51938100	-1.01592500	1.63451600
H	-0.50545300	-0.70145400	5.36679600
H	1.89422100	-0.40229500	4.65243300
H	2.44469800	-0.56753700	2.24604600
N	-1.67916400	-1.74504700	1.07172400
C	-3.55962500	-1.47470900	-0.35263100
H	-4.18655600	-0.83868300	-0.96190500
C	-1.87762100	-3.16421700	1.19889700
C	-3.01881700	-3.68406500	0.47963600
H	-3.19592600	-4.74802700	0.58285000
C	-3.82937400	-2.86548900	-0.25009800
H	-4.69157500	-3.27412900	-0.76914500
O	-1.10298200	-3.81873100	1.88844200
C	-1.15266200	-1.12513500	3.35557000
H	-2.18939000	-1.31811300	3.60424400

Zero-point correction= 0.625149 (Hartree/Particle)

Thermal correction to Energy= 0.665789

Thermal correction to Enthalpy= 0.666733

Thermal correction to Gibbs Free Energy= 0.553338

Sum of electronic and zero-point Energies= -2141.088258

Sum of electronic and thermal Energies= -2141.047618

Sum of electronic and thermal Enthalpies= -2141.046674

Sum of electronic and thermal Free Energies= -2141.160068

E(RB3LYP) = -2141.713407 A.U.

B-TS4-Rh

1 1

Number of imaginary frequencies: 1

C	-2.69143200	0.00622000	-0.55778300
C	-4.12797100	0.27782200	-0.59172600
C	-4.63279600	1.51319100	-1.05283500
C	-5.04647100	-0.67583900	-0.09805300
C	-5.99505000	1.80530500	-0.96530500
H	-3.97183400	2.20602400	-1.56072400
C	-6.40130900	-0.38159200	-0.01775000
H	-4.68418000	-1.64243500	0.23776100
C	-6.88023800	0.86542100	-0.44053900
H	-6.36519000	2.75710600	-1.33340300
H	-7.09004300	-1.12100600	0.37908000
H	-7.94062000	1.08923100	-0.38024300
C	-1.77265100	0.99500600	-0.28768700
P	-1.96212300	2.68500400	0.32470400
C	0.85898600	1.36842800	-0.19433300
C	1.68784200	2.58048800	-0.23491300

C	1.78389200	3.35653000	-1.40244200
C	2.40331700	2.97536700	0.90732200
C	2.58731100	4.49760700	-1.42649300
H	1.23566700	3.04855000	-2.28809400
C	3.19219500	4.12471700	0.88438000
H	2.31969100	2.38454900	1.81424500
C	3.29291400	4.88462300	-0.28457700
H	2.66191700	5.08456800	-2.33709000
H	3.72754000	4.42923500	1.77864400
H	3.91458000	5.77413000	-0.30397900
C	-0.44244600	1.27167800	-0.38807000
C	-1.68756500	3.98777100	-0.93010300
H	-0.67714400	4.38970700	-0.82229200
H	-1.81438200	3.56490000	-1.92870200
H	-2.41456700	4.78673400	-0.76478100
O	-1.68810900	3.02821600	1.75813400
C	2.67126600	-2.42666200	-0.97121700
C	2.93691600	-1.15884700	-1.66827100
C	3.62569300	-0.27805200	-0.78244300
C	3.57225900	-0.89345400	0.52181200
C	3.04343900	-2.26216800	0.36492000
C	2.95064600	-3.25357300	1.47973800
H	2.26169700	-4.06213500	1.24298200
H	3.94281000	-3.67052500	1.69216000
H	2.59024900	-2.77768800	2.39578800
C	2.10621000	-3.64669100	-1.62365000
H	1.28487900	-3.39209500	-2.29932500

H	2.87750800	-4.14704400	-2.22223900
H	1.72624300	-4.35062800	-0.88342900
C	2.70149400	-0.93508200	-3.12861300
H	2.68861700	0.12865300	-3.37349700
H	3.49831500	-1.40871200	-3.71572400
H	1.75320800	-1.37487300	-3.44864000
C	4.34458100	0.97965400	-1.15115100
H	4.41286600	1.67358300	-0.31314200
H	5.36375600	0.73013900	-1.47107900
H	3.85320900	1.50456800	-1.97169500
C	4.20973900	-0.36204700	1.76522700
H	5.25645900	-0.68831800	1.82054500
H	4.19760400	0.72973700	1.78202100
H	3.70763700	-0.73380800	2.66174800
Rh	1.52840900	-0.52489600	-0.06970700
C	-2.21396800	-1.36955200	-0.79551400
C	-1.05646700	-1.34975600	1.38513000
C	-1.76955200	-0.80956700	3.60793000
C	-0.51491800	-0.24185900	3.82565300
C	0.41400000	-0.25906700	2.79273000
N	0.14867500	-0.79527200	1.58677200
H	-2.52336600	-0.80800900	4.38800400
H	-0.25824600	0.21807900	4.77284300
H	1.39613600	0.18297800	2.90955600
N	-1.31162300	-1.94751800	0.10201400
C	-2.62958600	-2.09348400	-1.88364000
H	-3.32075000	-1.63458400	-2.57874000

C	-0.80621800	-3.28176200	-0.04041200
C	-1.27163400	-3.98440400	-1.21449000
H	-0.90793100	-4.99814700	-1.33078600
C	-2.15038300	-3.41535800	-2.08929800
H	-2.49633700	-3.97507200	-2.95347500
O	-0.05344100	-3.73649700	0.81731500
C	-2.03955300	-1.38422500	2.36907800
H	-2.99444400	-1.84704000	2.15118200

Zero-point correction= 0.623982 (Hartree/Particle)

Thermal correction to Energy= 0.665433

Thermal correction to Enthalpy= 0.666377

Thermal correction to Gibbs Free Energy= 0.549693

Sum of electronic and zero-point Energies= -2141.096504

Sum of electronic and thermal Energies= -2141.055053

Sum of electronic and thermal Enthalpies= -2141.054109

Sum of electronic and thermal Free Energies= -2141.170793

E(RB3LYP) = -2141.720486 A.U.

B-TS5-Rh

1 1

Number of imaginary frequencies: 1

C	-2.42630300	0.27183300	-0.70901900
C	-3.82192600	0.73315300	-0.73154400
C	-4.15108700	2.02227900	-1.19574700
C	-4.86651100	-0.10220900	-0.28693600
C	-5.46733300	2.47282100	-1.18131900
H	-3.37077100	2.64939100	-1.61524100
C	-6.18160500	0.35147700	-0.26798000

H	-4.64227400	-1.10917200	0.05046200
C	-6.48666300	1.64218300	-0.70915600
H	-5.70208200	3.46539600	-1.55301900
H	-6.97140300	-0.30145700	0.09033700
H	-7.51395800	1.99255500	-0.69906200
C	-1.37896800	1.12710400	-0.44858900
P	-1.47950900	2.53772900	0.73601300
C	1.11233500	1.48014200	-0.13408700
C	2.03221900	2.58152300	-0.20319600
C	2.89499200	2.85740600	0.87586200
C	2.10731000	3.37824700	-1.36470300
C	3.79391500	3.91695400	0.80289100
H	2.83622600	2.23972200	1.76625200
C	3.02575300	4.42328200	-1.43807700
H	1.45829900	3.15309600	-2.20579400
C	3.86661900	4.69837100	-0.35588900
H	4.44380600	4.13268400	1.64527200
H	3.08551800	5.02442300	-2.34005100
H	4.57694200	5.51685400	-0.41479600
C	0.01783400	0.87769800	-0.53155600
C	-1.22201600	4.15692400	-0.09048100
H	-1.06571100	4.91671800	0.67838500
H	-0.35861300	4.11860200	-0.75520400
H	-2.12792400	4.40241900	-0.65555700
O	-2.60228000	2.51329000	1.73363400
C	3.48296000	-0.58973600	-0.89527200
C	3.58333000	-1.15478900	0.42861100

C	2.76688800	-2.33496800	0.45160000
C	2.24742500	-2.56470700	-0.87629000
C	2.65772200	-1.46392000	-1.69482100
C	2.37278600	-1.30963100	-3.15553000
H	2.38573500	-0.26093700	-3.45910300
H	3.13218300	-1.83779700	-3.74602700
H	1.39827100	-1.72969400	-3.41460800
C	4.27787100	0.56385800	-1.42062900
H	4.52537100	1.28210600	-0.63817800
H	5.21699200	0.19185300	-1.84792600
H	3.74363000	1.10012700	-2.20702500
C	4.42457500	-0.62591700	1.54754200
H	4.00894000	-0.89034600	2.52298700
H	5.43628300	-1.04840400	1.49998100
H	4.51967100	0.46123600	1.49711600
C	2.54630300	-3.24556100	1.62017200
H	1.52201500	-3.62607200	1.62506400
H	3.23170900	-4.09982500	1.56613800
H	2.73021300	-2.73308800	2.56719600
C	1.57578400	-3.80940500	-1.35966300
H	2.32641700	-4.47278100	-1.80961900
H	1.09177400	-4.34839400	-0.54577000
H	0.82607800	-3.59515200	-2.12404500
Rh	1.40486100	-0.58501300	-0.01626200
C	-2.19795700	-1.17534200	-0.93189700
C	-1.28816300	-1.33988100	1.35190600
C	-1.96472700	-0.75319900	3.57516500

C	-0.65936800	-0.32531200	3.81377200
C	0.27111200	-0.41473000	2.78602300
N	-0.03637200	-0.90275400	1.56749800
H	-2.72387700	-0.68010100	4.34633100
H	-0.36421700	0.08478600	4.77273200
H	1.29257800	-0.07667600	2.91578400
N	-1.58303800	-1.91459700	0.07380800
C	-2.62208800	-1.81856700	-2.06478200
H	-3.11340000	-1.24251700	-2.83835900
C	-1.32643900	-3.31657400	-0.00985900
C	-1.80193400	-3.94047200	-1.22179200
H	-1.64403200	-5.00966100	-1.29653000
C	-2.42069100	-3.21860000	-2.20223800
H	-2.76959900	-3.71642000	-3.10246600
O	-0.74951400	-3.88044100	0.92065900
C	-2.27809900	-1.28331800	2.32706300
H	-3.27177700	-1.64566400	2.09511000

Zero-point correction= 0.623953 (Hartree/Particle)

Thermal correction to Energy= 0.665137

Thermal correction to Enthalpy= 0.666081

Thermal correction to Gibbs Free Energy= 0.550587

Sum of electronic and zero-point Energies= -2141.093579

Sum of electronic and thermal Energies= -2141.052395

Sum of electronic and thermal Enthalpies= -2141.051451

Sum of electronic and thermal Free Energies= -2141.166944

E(RB3LYP) = -2141.717532 A.U.

B-TS6-Rh

1 1

Number of imaginary frequencies: 1

C	-2.54418300	0.24542000	0.08194700
C	-3.82299800	1.04827500	0.10373100
C	-4.41717200	1.54035500	-1.06902800
C	-4.40609400	1.35516800	1.34003000
C	-5.57697900	2.31377400	-1.00628100
H	-3.95916000	1.32948600	-2.03177700
C	-5.56410400	2.13138900	1.40287900
H	-3.93487200	1.00366400	2.25251400
C	-6.15345000	2.60884100	0.23145200
H	-6.02487200	2.69003900	-1.92115800
H	-5.99816000	2.37103300	2.36839600
H	-7.05283100	3.21457000	0.28175500
C	-1.41868600	0.97531000	0.29351600
P	-1.31985100	2.82245900	0.31430600
C	0.42110100	2.23536400	0.22872300
C	1.65541900	3.00058500	0.14377500
C	2.75427300	2.81115000	1.00092500
C	1.74243500	4.00857900	-0.84156100
C	3.91223400	3.56863900	0.84913700
H	2.66352000	2.12300500	1.82461600
C	2.91466100	4.74126600	-1.01250400
H	0.89609500	4.19775500	-1.49353400
C	4.00735000	4.51958300	-0.17032900
H	4.74101500	3.42301300	1.53537700
H	2.96911500	5.49662800	-1.79019400

H	4.91602000	5.10068500	-0.29204700
C	0.07710000	0.89587400	0.40792100
C	-1.84961800	3.58604600	-1.25951400
H	-1.39446000	4.57872000	-1.31474200
H	-1.55363600	2.99054700	-2.12671300
H	-2.93416200	3.70258600	-1.24342200
O	-1.72749200	3.60406900	1.52232000
C	2.70671900	-0.15048600	-1.86058900
C	3.05881300	-1.53020900	-1.55572100
C	1.92773100	-2.35252100	-1.83182100
C	0.86223500	-1.49218700	-2.32775900
C	1.36854900	-0.15192800	-2.38515400
C	0.62477800	1.01003300	-2.95736600
H	1.01853700	1.95952600	-2.59568200
H	0.71892500	0.99420200	-4.05015600
H	-0.43772800	0.94956100	-2.71193700
C	3.67283200	0.98801500	-1.80097300
H	4.20469300	0.99399100	-0.84741900
H	4.41423000	0.88094900	-2.60212500
H	3.18141500	1.95310300	-1.91576000
C	4.39014300	-1.94687300	-1.02338500
H	4.41583900	-3.00895800	-0.77705300
H	5.16660800	-1.74856800	-1.77100300
H	4.63166100	-1.37494400	-0.12273900
C	1.83638600	-3.83637100	-1.69514200
H	0.90635300	-4.13442200	-1.20443000
H	1.86136600	-4.29465400	-2.69151900

H	2.67180400	-4.23837900	-1.11999900
C	-0.41959200	-1.94962900	-2.94631900
H	-0.34138100	-1.87483600	-4.03803500
H	-0.63083300	-2.98854500	-2.70064100
H	-1.26924300	-1.33937400	-2.63287300
Rh	1.39305900	-0.84640500	-0.25306100
C	-2.69721600	-1.17968300	-0.28011500
C	-1.01909400	-2.11341000	1.30127300
C	-0.97949900	-2.71206500	3.62277800
C	0.39640800	-2.88875100	3.49986500
C	1.00549600	-2.56395100	2.29391500
N	0.32124900	-2.11999300	1.22371400
H	-1.48732000	-2.90777400	4.56140400
H	0.99898700	-3.24568300	4.32713800
H	2.07947500	-2.62218300	2.17433600
N	-1.75784900	-2.14554900	0.07484200
C	-3.74044100	-1.56339100	-1.09773300
H	-4.48631800	-0.83679400	-1.37764300
C	-1.78905100	-3.50473600	-0.43485200
C	-2.89022000	-3.81799200	-1.30699900
H	-2.93229100	-4.83970400	-1.66473900
C	-3.83967000	-2.88576400	-1.59799600
H	-4.68413500	-3.14451600	-2.23015400
O	-0.92588900	-4.30302900	-0.07801700
C	-1.70352100	-2.34566200	2.49080400
H	-2.78660900	-2.29903900	2.49410600
C	2.46541400	-0.05710800	2.43968800

O	2.82593700	-0.54042000	1.30974000
O	1.28996700	0.32249100	2.68736700
H	0.65262500	0.41467000	1.42016800
C	3.51963700	0.02580400	3.51813100
H	3.20691500	0.71338500	4.30395000
H	3.65531500	-0.97063400	3.95250200
H	4.47486800	0.33259500	3.08710900

Zero-point correction= 0.686276 (Hartree/Particle)

Thermal correction to Energy= 0.731936

Thermal correction to Enthalpy= 0.732880

Thermal correction to Gibbs Free Energy= 0.607622

Sum of electronic and zero-point Energies= -2370.177836

Sum of electronic and thermal Energies= -2370.132176

Sum of electronic and thermal Enthalpies= -2370.131232

Sum of electronic and thermal Free Energies= -2370.256491

E(RB3LYP) = -2370.864113 A.U.

C-1

0 1

Number of imaginary frequencies: 0

C	-0.42020500	-0.83158900	-1.65436200
C	-1.20041800	-1.85556200	-1.04948300
C	-2.57256700	-1.41117100	-1.00268700
C	-2.63881600	-0.12706500	-1.65243500
C	-1.31335400	0.25619700	-2.00781700
O	-1.62938700	-0.93884400	1.82799500
O	-2.85817100	0.70617700	1.14305000
C	-2.57158200	-0.11808600	2.07814400

C	-3.71421100	-2.16674300	-0.42555600
H	-4.14903700	-2.84445400	-1.16855400
H	-3.39891200	-2.77560900	0.42569800
H	-4.51120500	-1.49794000	-0.09056100
C	-0.70272400	-3.12207100	-0.46084400
H	-1.08630300	-3.26102800	0.55480200
H	-1.04847600	-3.97399000	-1.05677100
H	0.38710400	-3.15184500	-0.41917900
C	1.02367700	-0.89512300	-1.99273900
H	1.58695600	-1.54002500	-1.31405500
H	1.13802400	-1.30033300	-3.00503900
H	1.49708100	0.09003900	-1.99323800
C	-0.89819600	1.51845900	-2.67250500
H	0.09689600	1.83778600	-2.34957900
H	-0.85277300	1.38206400	-3.75870600
H	-1.59515400	2.33696100	-2.47708700
C	-3.86276500	0.69895500	-1.78196900
H	-3.63302300	1.74458600	-1.99614200
H	-4.48242200	0.32225300	-2.60312300
H	-4.46635100	0.66278600	-0.87173000
C	4.18082400	0.74805400	-0.34393400
C	3.24175600	-0.02210700	0.33815900
C	3.50605300	-1.36019400	0.71309500
C	4.74712200	-1.93160400	0.41620200
C	5.69034300	-1.16641400	-0.25365700
C	5.40517400	0.15180300	-0.63043400
H	3.98218500	1.77469700	-0.61874200

H	4.96208700	-2.95584100	0.70584800
H	6.66097500	-1.59112700	-0.48908400
H	6.15957000	0.73283700	-1.15149400
C	1.38767200	-0.89391300	1.34800100
H	0.40593100	-0.86465000	1.79126200
C	2.33014300	-1.87077800	1.35812500
H	2.21325100	-2.84492300	1.81293800
N	1.90879100	0.25109200	0.72765000
C	1.21675700	1.42308800	0.53558000
N	-0.14822300	1.39580000	0.53583800
C	-0.76034000	2.60124300	0.52655100
C	-0.07001700	3.79328000	0.43540200
C	1.31126100	3.68878700	0.28528000
N	1.94643000	2.52650900	0.35069000
H	-1.84491400	2.57069700	0.56921300
H	-0.58721000	4.74419300	0.43284400
H	1.93337700	4.56491100	0.11244700
Co	-1.43706300	-0.10325500	0.00299700
C	-3.32213800	-0.14424800	3.35795600
H	-3.75893500	0.83027600	3.57457100
H	-4.13882100	-0.86818800	3.27457700
H	-2.67842600	-0.46790800	4.17592200

Zero-point correction= 0.465277 (Hartree/Particle)

Thermal correction to Energy= 0.495196

Thermal correction to Enthalpy= 0.496140

Thermal correction to Gibbs Free Energy= 0.404774

Sum of electronic and zero-point Energies= -1390.756594

Sum of electronic and thermal Energies= -1390.726674

Sum of electronic and thermal Enthalpies= -1390.725730

Sum of electronic and thermal Free Energies= -1390.817097

E(RM06L) = -1391.221871 A.U.

C-2a

0 1

Number of imaginary frequencies: 0

C	-1.20142300	-0.29263200	-2.13655600
C	-1.59055100	-1.52786400	-1.49355800
C	-2.66594400	-1.22816600	-0.61476800
C	-3.00052500	0.17383400	-0.74045700
C	-2.12880700	0.72792400	-1.71342200
O	-0.13626000	-1.91822500	2.44101200
O	-1.52036100	-0.25280900	1.82199300
C	-1.13258300	-1.09372000	2.65151600
C	-3.34773500	-2.18769000	0.29140100
H	-4.19825400	-2.65107900	-0.22148800
H	-2.68459100	-2.99854500	0.60597900
H	-3.74023700	-1.69191400	1.18294900
C	-1.03795400	-2.88008500	-1.76268000
H	-0.95521000	-3.48185500	-0.85261100
H	-1.70304200	-3.42238200	-2.44414400
H	-0.05422600	-2.83220900	-2.23147200
C	-0.13057000	-0.13001800	-3.15471600
H	0.68870700	-0.83336200	-2.98688200
H	-0.52019500	-0.30058800	-4.16470500
H	0.29327400	0.87788900	-3.13696100

C	-2.10923600	2.13063000	-2.20003300
H	-1.09114500	2.51008400	-2.32222500
H	-2.58716300	2.18309800	-3.18449300
H	-2.65365000	2.81227100	-1.54284400
C	-4.07861700	0.86102500	0.02048000
H	-4.07042300	1.94149400	-0.14316100
H	-5.06829800	0.49962100	-0.27850900
H	-3.98068500	0.68292400	1.09673900
C	4.25039800	0.70661300	0.04917700
C	3.05963500	-0.00689400	-0.02992200
C	3.01866100	-1.40709800	-0.20966700
C	4.21744600	-2.11771600	-0.31437000
C	5.41422700	-1.41610800	-0.24128200
C	5.42848600	-0.02700800	-0.06242900
H	4.25699500	1.77971500	0.19155500
H	4.21146300	-3.19508500	-0.45105200
H	6.35497200	-1.95140400	-0.32274000
H	6.37929500	0.49373100	-0.00862800
C	0.83509600	-0.69351900	-0.08828100
H	0.29912900	-1.69238100	1.57749300
C	1.63239500	-1.80026600	-0.24941300
H	1.28347000	-2.81713600	-0.37741900
N	1.72232000	0.41139400	0.04485400
C	1.19078400	1.63802700	0.28778400
N	-0.17166000	1.63466500	0.29908300
C	-0.78409700	2.77247100	0.65012400
C	-0.06685300	3.92439100	0.92515500

C	1.32084400	3.83409300	0.80986500
N	1.95804400	2.70523600	0.50550100
H	-1.86992200	2.73176500	0.70227500
H	-0.56319200	4.84426600	1.20554200
H	1.95242300	4.70410200	0.97714100
Co	-1.00924500	-0.08897700	-0.13822200
C	-1.79241000	-1.25224900	3.97310900
H	-2.61406500	-0.54759400	4.08152100
H	-2.16323000	-2.27563900	4.07356800
H	-1.06453300	-1.10605100	4.77411800

Zero-point correction= 0.465701 (Hartree/Particle)

Thermal correction to Energy= 0.495361

Thermal correction to Enthalpy= 0.496306

Thermal correction to Gibbs Free Energy= 0.406161

Sum of electronic and zero-point Energies= -1390.745963

Sum of electronic and thermal Energies= -1390.716302

Sum of electronic and thermal Enthalpies= -1390.715358

Sum of electronic and thermal Free Energies= -1390.805503

E(RM06L) = -1391.211664 A.U.

C-3a

1 1

Number of imaginary frequencies: 0

C	-2.95519000	-1.44152600	-0.00007400
C	-2.98639900	-0.02086800	-0.00001100
C	-4.17320300	0.69674400	-0.00009800
C	-5.35337800	-0.04692300	-0.00024300
C	-5.35163400	-1.45116000	-0.00030400

C	-4.16168700	-2.15951300	-0.00023100
C	-1.59003200	-1.83999700	0.00007500
C	-0.76869400	-0.71820600	0.00015500
H	-4.18036000	1.77902100	-0.00005900
H	-6.30244500	0.48017300	-0.00030900
H	-6.29717100	-1.98315400	-0.00041000
H	-4.15613900	-3.24517300	-0.00027200
H	-1.24428200	-2.86537300	0.00009700
C	-1.10346900	1.63736800	-0.00009100
N	-1.86119300	2.72892300	-0.00008800
C	-1.21225300	3.89255400	-0.00017800
C	0.18020900	3.98841900	-0.00018900
C	0.88552500	2.79960800	-0.00026600
N	0.26469600	1.60678000	-0.00027500
H	-1.83492900	4.78442100	-0.00013700
H	0.68938700	4.94341600	-0.00017000
H	1.97163900	2.77093400	-0.00033800
N	-1.65093600	0.39161700	0.00009100
C	1.95635800	-1.98690700	-0.00027400
C	2.31819300	-1.21521900	-1.15332000
C	2.95892500	0.00241700	-0.70814500
C	2.95797300	0.00212300	0.70970000
C	2.31669700	-1.21575600	1.15358300
C	2.08633600	-1.59247500	2.56955400
H	1.22824400	-2.25866200	2.68033300
H	2.96306700	-2.11749500	2.96877800
H	1.92238400	-0.71710700	3.20274700

C	1.39093600	-3.36022100	-0.00100000
H	0.78045300	-3.55095400	-0.88690900
H	2.19951800	-4.09943800	-0.00144500
H	0.78058700	-3.55192300	0.88478700
C	2.08942700	-1.59112500	-2.56975700
H	1.92426400	-0.71549100	-3.20228900
H	2.96741500	-2.11409700	-2.96891000
H	1.23266900	-2.25882200	-2.68169100
C	3.47569600	1.05922700	-1.61867000
H	3.82462600	1.94029600	-1.07530800
H	4.32534000	0.68406300	-2.19902200
H	2.71971800	1.38538500	-2.34068400
C	3.47338700	1.05866000	1.62129800
H	4.32205100	0.68326400	2.20292900
H	3.82323200	1.93982500	1.07868400
H	2.71627900	1.38472200	2.34217100
Co	1.02793100	-0.19897800	-0.00036100

Zero-point correction= 0.400896 (Hartree/Particle)

Thermal correction to Energy= 0.425428

Thermal correction to Enthalpy= 0.426372

Thermal correction to Gibbs Free Energy= 0.347648

Sum of electronic and zero-point Energies= -1161.701802

Sum of electronic and thermal Energies= -1161.677269

Sum of electronic and thermal Enthalpies= -1161.676325

Sum of electronic and thermal Free Energies= -1161.755049

E(RM06L) = -1162.102697 A.U.

C-4

1 1

Number of imaginary frequencies: 0

C	3.82574500	-0.11528700	-1.44675500
C	5.10077300	0.32789500	-1.02225700
C	5.97146900	-0.54428600	-0.34294200
C	5.51460200	1.65104000	-1.26120200
C	7.21221500	-0.09796000	0.08266000
H	5.66424000	-1.57142100	-0.16394600
C	6.75956000	2.08033700	-0.82964300
H	4.85323000	2.32696500	-1.79619000
C	7.63236500	1.21764300	-0.15360400
H	7.87636200	-0.78197800	0.60484800
H	7.06932800	3.10430500	-1.02293600
C	2.69330800	-0.47702500	-1.73829900
P	1.21794200	-1.07088600	-2.47369100
C	-1.32086000	-0.86023200	-1.40541700
C	-2.68291500	-0.70178700	-1.69555100
C	-3.18105700	0.58898200	-1.98119700
C	-3.57198000	-1.79481000	-1.69140600
C	-4.52629000	0.77266700	-2.23403000
H	-2.49709400	1.43451400	-1.98451700
C	-4.91822500	-1.58978300	-1.93732800
H	-3.19041600	-2.79144000	-1.49019500
C	-5.42206300	-0.30721400	-2.19991900
H	-4.90289800	1.77222500	-2.43562400
H	-5.60113300	-2.43504000	-1.92723400
C	-0.07884200	-0.92371600	-1.22496100

C	0.78163700	0.24686600	-3.63390000
H	-0.17908300	0.01049900	-4.09760800
H	0.70886000	1.20915900	-3.11833800
H	1.54463600	0.31059500	-4.41204800
O	1.30407000	-2.45046600	-3.03572300
C	-4.04309300	0.85070800	1.23528800
C	-3.18753700	1.93774800	0.94424700
C	-3.65757000	3.22751300	0.72257400
C	-5.03684500	3.41523200	0.78843000
C	-5.90576800	2.35342900	1.07033800
C	-5.42148300	1.07035700	1.30037700
C	-3.22716900	-0.32736700	1.36438700
C	-1.91888300	0.00334600	1.15256700
H	-2.98052900	4.04385800	0.50487100
H	-5.44246200	4.40799000	0.62000000
H	-6.97512100	2.53916800	1.11568400
H	-6.10030700	0.24936400	1.51674300
H	-3.60967600	-1.32396500	1.53900800
C	-0.69626900	1.99192500	0.64873900
N	-0.61771200	3.29905300	0.39579300
C	0.60371500	3.78713600	0.18935700
C	1.75221800	3.00034000	0.22645400
C	1.57035500	1.64717800	0.46655900
N	0.35589500	1.12200000	0.67450500
H	0.65956800	4.85460300	-0.01539100
H	2.74166400	3.41048500	0.06857300
H	2.40077700	0.95160200	0.47528100

N	-1.89111200	1.39974300	0.89956900
C	-0.61968600	-2.07357800	2.48080500
C	-0.24431000	-2.81022800	1.31993900
C	1.14114400	-2.49968000	1.02176200
C	1.56500800	-1.49531100	1.91532300
C	0.45200000	-1.16632300	2.78123800
C	0.46048500	-0.17426900	3.88829300
H	-0.53921300	0.23105100	4.06569500
H	0.80183800	-0.63069400	4.82488400
H	1.12767700	0.66513500	3.67502800
C	-1.82958700	-2.27788300	3.31419500
H	-2.61525300	-2.81725900	2.78271700
H	-1.54721400	-2.89130500	4.17813000
H	-2.24726500	-1.34369600	3.69212300
C	-1.06176700	-3.82346800	0.60322400
H	-0.84411500	-3.81826800	-0.46938600
H	-0.85264500	-4.83457100	0.97160500
H	-2.13204300	-3.64077800	0.73535800
C	1.97695900	-3.22909700	0.03615800
H	2.87516200	-2.67226600	-0.23968400
H	2.30103400	-4.17815100	0.48064600
H	1.44418000	-3.47025100	-0.88653900
C	2.94039100	-0.94445600	2.03174300
H	3.54062100	-1.58560500	2.68821900
H	3.45272700	-0.90454100	1.06646600
H	2.95350800	0.05444400	2.47518400
Co	-0.17413000	-0.79827000	0.88822800

C	-6.88114400	-0.07990900	-2.41763600
H	-7.06600800	0.48037200	-3.33888300
H	-7.44021300	-1.01581300	-2.46956500
H	-7.30106900	0.51851700	-1.60107900
C	8.98792600	1.67872100	0.27594900
H	9.72941000	1.48797800	-0.50795800
H	9.00731600	2.75223300	0.47759600
H	9.33074000	1.15435800	1.17100800

Zero-point correction= 0.703368 (Hartree/Particle)

Thermal correction to Energy= 0.750226

Thermal correction to Enthalpy= 0.751170

Thermal correction to Gibbs Free Energy= 0.620917

Sum of electronic and zero-point Energies= -2312.109778

Sum of electronic and thermal Energies= -2312.062920

Sum of electronic and thermal Enthalpies= -2312.061976

Sum of electronic and thermal Free Energies= -2312.192230

E(RM06L) = -2312.813147 A.U.

(S)C-5a

1 1

Number of imaginary frequencies: 0

C	-2.04919200	-0.59811700	-0.07339300
C	-3.19269400	-1.49853600	-0.35008800
C	-3.39976100	-2.64082400	0.43160600
C	-4.08493100	-1.24280700	-1.40208500
C	-4.44547000	-3.51475300	0.15612200
H	-2.75340300	-2.81617000	1.28926400
C	-5.11859300	-2.12336000	-1.67851200

H	-3.95028600	-0.35332700	-2.01234800
C	-5.31699500	-3.27942000	-0.91018900
H	-4.59919600	-4.38748800	0.78686700
H	-5.79011000	-1.91636100	-2.50851200
C	-0.81236200	-1.11020900	0.15261100
P	-0.16645700	-2.65947200	-0.43321700
C	2.54119100	-1.37450600	-0.26262900
C	3.86866700	-0.97132200	-0.57974700
C	4.88498200	-1.94353100	-0.63846800
C	4.20125800	0.36943900	-0.83611200
C	6.18409700	-1.57367700	-0.94624100
H	4.64060200	-2.98247900	-0.43847900
C	5.50583200	0.72291800	-1.14499200
H	3.42608900	1.12979000	-0.76908700
C	6.52265900	-0.23858300	-1.20757000
H	6.95818200	-2.33584100	-0.98468700
H	5.74748100	1.76550400	-1.33714100
C	1.47892100	-2.01080100	-0.11332500
C	-0.34187700	-4.04304800	0.72370100
H	0.48558800	-4.74119800	0.57603600
H	-0.35707300	-3.71628600	1.76570300
H	-1.27659000	-4.55806600	0.49227000
O	-0.38665700	-3.03478900	-1.86197500
C	-3.49629900	2.77783400	0.27138900
C	-2.25176700	3.08147000	-0.32092600
C	-1.85779100	4.39388800	-0.57200400
C	-2.74862300	5.40405300	-0.23226200

C	-3.99648400	5.12072600	0.34529200
C	-4.37803700	3.81548900	0.60527100
C	-3.55274900	1.36356600	0.42566100
C	-2.37050500	0.81615700	-0.00485500
H	-0.90327000	4.62404400	-1.03057100
H	-2.47117900	6.43612500	-0.42232000
H	-4.66614200	5.93818800	0.59274700
H	-5.33788100	3.59353300	1.06168700
H	-4.37562900	0.78039000	0.81760800
C	-0.47431700	1.74293400	-1.35368500
N	-0.49875800	2.56571100	-2.40088300
C	0.37582700	2.36885600	-3.37880600
C	1.23956800	1.28028400	-3.36757900
C	1.26964500	0.54154500	-2.20151100
N	0.49193300	0.81257400	-1.12831300
H	0.35137000	3.08178700	-4.20039300
H	1.88693700	1.03215800	-4.19915900
H	1.94839000	-0.29377800	-2.10250700
N	-1.53424800	1.87725100	-0.46375000
C	0.03692000	-0.00811700	2.62593500
C	1.26413800	-0.73183900	2.61750500
C	2.32306800	0.17581400	2.21445800
C	1.72804000	1.39916100	1.85199600
C	0.30849100	1.30174500	2.12241800
C	-0.59129200	2.47569700	2.24550500
H	-1.64786900	2.21575300	2.15473900
H	-0.44973000	2.90793400	3.24464600

H	-0.36729500	3.26470100	1.52560500
C	-1.26995200	-0.49309900	3.13748300
H	-1.38041300	-1.57329800	3.01040500
H	-1.35509400	-0.27460700	4.20826600
H	-2.10929500	-0.00942100	2.63077900
C	1.50180300	-2.10023000	3.14824300
H	2.06895000	-2.72271400	2.44824000
H	2.08328300	-2.04934700	4.07602900
H	0.56786600	-2.61404400	3.38405200
C	3.76839100	-0.12687300	2.37410200
H	4.41376600	0.52552400	1.78374400
H	4.03312900	0.01503100	3.42926000
H	4.01076800	-1.16276000	2.12404500
C	2.40832000	2.63927700	1.38867100
H	2.38886700	3.40798500	2.16948200
H	3.45484700	2.46008400	1.13114000
H	1.91142900	3.07111300	0.51201200
Co	0.81941900	-0.15189000	0.67583800
C	-6.42993300	-4.22689000	-1.22904600
H	-7.37653900	-3.70066300	-1.38250200
H	-6.22473200	-4.77757400	-2.15336500
H	-6.57712200	-4.96283000	-0.43563600
C	7.92498800	0.13977800	-1.55944800
H	8.65290800	-0.38236700	-0.93292600
H	8.15358000	-0.13053900	-2.59617100
H	8.09504100	1.21364100	-1.45875000

Zero-point correction= 0.705993 (Hartree/Particle)

Thermal correction to Energy= 0.751222

Thermal correction to Enthalpy= 0.752166

Thermal correction to Gibbs Free Energy= 0.628600

Sum of electronic and zero-point Energies= -2312.127685

Sum of electronic and thermal Energies= -2312.082457

Sum of electronic and thermal Enthalpies= -2312.081513

Sum of electronic and thermal Free Energies= -2312.205078

E(RM06L) = -2312.833679 A.U.

(T)C-5a

1 3

Number of imaginary frequencies: 0

C	-1.97459600	-0.93900800	-0.04987600
C	-2.86486600	-2.07815100	-0.33909700
C	-2.90651700	-3.17374800	0.53391200
C	-3.68857100	-2.10066300	-1.47440600
C	-3.72281100	-4.26294900	0.27187800
H	-2.32038400	-3.13586700	1.45010300
C	-4.49234000	-3.19892300	-1.73872400
H	-3.67860500	-1.25714900	-2.15997000
C	-4.52107400	-4.30342600	-0.87737100
H	-3.75440900	-5.09481000	0.97136800
H	-5.11212800	-3.20677600	-2.63208900
C	-0.70117900	-1.10444500	0.42109000
P	0.32640900	-2.55356600	0.15680200
C	3.07954100	-1.48063400	-0.22770500
C	4.41190300	-1.12550500	-0.54630700
C	5.41064200	-1.08028000	0.44510800

C	4.76352000	-0.81300900	-1.87336900
C	6.70825700	-0.72643600	0.11432100
H	5.15480500	-1.33128500	1.47133800
C	6.06738900	-0.46186200	-2.18757800
H	4.00632400	-0.87531200	-2.65116500
C	7.06396700	-0.41209400	-1.20473000
H	7.46870000	-0.69694600	0.89060300
H	6.32631600	-0.23013700	-3.21769700
C	1.90552500	-1.73019800	0.03591000
C	0.50863500	-3.49207100	1.69758200
H	1.37907300	-4.14616300	1.61095100
H	0.63984700	-2.83658200	2.56118100
H	-0.37701600	-4.11431000	1.84132400
O	0.01171500	-3.38587500	-1.04262400
C	-3.99833000	2.14323400	-0.30093200
C	-2.75481500	2.59716500	-0.79156400
C	-2.54108200	3.92304800	-1.16270500
C	-3.60720300	4.80130500	-1.02224500
C	-4.85034700	4.37222800	-0.52641600
C	-5.05733800	3.05224800	-0.16337500
C	-3.85114700	0.75878600	-0.00740800
C	-2.55478700	0.38098600	-0.24599000
H	-1.58832200	4.25905700	-1.55892300
H	-3.47589500	5.84142100	-1.30308300
H	-5.65824700	5.09027000	-0.42925600
H	-6.01715200	2.72325700	0.22275900
H	-4.60622300	0.08866100	0.38179400

C	-0.70607700	1.52737500	-1.55494400
N	-0.82358200	2.03765600	-2.77510700
C	0.27471100	2.06807100	-3.52991300
C	1.50440100	1.58588200	-3.08768200
C	1.54607300	1.08375200	-1.80046700
N	0.44900300	1.06726800	-1.02262700
H	0.15679000	2.48851500	-4.52623800
H	2.39169800	1.60975600	-3.70846000
H	2.45630000	0.70033500	-1.34767600
N	-1.84210200	1.53303500	-0.73147500
C	-0.09836600	0.53947300	2.90985700
C	1.33093800	0.38144800	2.73679300
C	1.79159900	1.50002300	1.99808400
C	0.66660300	2.38420600	1.77452200
C	-0.48260900	1.81612800	2.37479600
C	-1.84093500	2.41360000	2.46838800
H	-2.62791600	1.67568200	2.28769100
H	-2.00957400	2.82153400	3.47193200
H	-1.98567000	3.23249500	1.75906800
C	-1.00701100	-0.37406900	3.65131800
H	-0.63656800	-1.40212900	3.66695200
H	-1.11544200	-0.04744900	4.69225400
H	-2.00733100	-0.38964200	3.20864400
C	2.18507200	-0.69544500	3.31288900
H	2.72416300	-1.26081700	2.54536900
H	2.93371200	-0.26349600	3.98586800
H	1.59975100	-1.40403800	3.90317300

C	3.19736900	1.75868500	1.58175800
H	3.25692000	2.24502800	0.60186500
H	3.70520500	2.42358100	2.29054800
H	3.77805300	0.83370400	1.52761700
C	0.72466900	3.67490700	1.03578800
H	1.07920000	4.48340700	1.68485300
H	1.41497100	3.62917800	0.18665000
H	-0.25925000	3.97117400	0.65886100
Co	0.34551100	0.44580300	0.83921900
C	-5.36942100	-5.49548400	-1.18521600
H	-6.28336500	-5.21800800	-1.71625600
H	-4.82989100	-6.20019700	-1.82802100
H	-5.65035900	-6.03958800	-0.28040300
C	8.47553600	-0.06717000	-1.55512100
H	8.96400400	0.49994200	-0.75882900
H	9.07078600	-0.97435200	-1.70761100
H	8.53569200	0.51426400	-2.47770700

Zero-point correction= 0.703210 (Hartree/Particle)

Thermal correction to Energy= 0.750076

Thermal correction to Enthalpy= 0.751020

Thermal correction to Gibbs Free Energy= 0.619961

Sum of electronic and zero-point Energies= -2312.123945

Sum of electronic and thermal Energies= -2312.077080

Sum of electronic and thermal Enthalpies= -2312.076135

Sum of electronic and thermal Free Energies= -2312.207195

E(RM06L) = -2312.827155 A.U.

（S）C-6

1 1

Number of imaginary frequencies: 0

C	1.84413400	1.06175600	-0.18627800
C	2.86755900	2.13241300	-0.11022600
C	2.79632500	3.12286700	0.87878200
C	3.91961400	2.20070100	-1.03640600
C	3.73069900	4.14848100	0.93257600
H	2.02417200	3.05568700	1.64194100
C	4.84077200	3.23677500	-0.98680900
H	3.99604600	1.44285200	-1.81156400
C	4.76415000	4.23387600	-0.00646700
H	3.66786200	4.89206200	1.72375400
H	5.63623800	3.27921100	-1.72697600
C	0.53551700	1.49850200	-0.12545300
P	-0.37325900	2.98237000	-0.10691700
C	-2.02530800	0.50544100	-0.08846200
C	-3.35876800	0.92370000	-0.42534300
C	-3.64706600	2.21038700	-0.93525800
C	-4.42262700	0.00733700	-0.32266100
C	-4.94353100	2.55590600	-1.27130100
H	-2.84487100	2.92705200	-1.09646800
C	-5.71632300	0.36077200	-0.67137100
H	-4.20251300	-0.99670800	0.03140900
C	-6.00671000	1.64722600	-1.14117600
H	-5.14341400	3.55172900	-1.65982800
H	-6.51915000	-0.36757300	-0.58404300
C	-0.87487000	1.23544900	-0.06570900

C	-0.60033500	3.75034100	1.51290500
H	-1.64778400	4.04356800	1.61926400
H	-0.32709900	3.06862500	2.31976500
H	0.01152800	4.65358000	1.56821900
O	-0.66246700	3.88038200	-1.26781900
C	3.87271500	-1.99327900	-0.09716600
C	2.70057500	-2.48602900	-0.71412200
C	2.58675600	-3.80858700	-1.13831600
C	3.67078200	-4.64502400	-0.90824800
C	4.83639100	-4.18190900	-0.27089600
C	4.94929700	-2.86572900	0.13760700
C	3.65344600	-0.61944100	0.15184400
C	2.37688000	-0.27348900	-0.26574800
H	1.69565700	-4.17384000	-1.63979000
H	3.61643400	-5.68011400	-1.23040900
H	5.65849600	-4.87065500	-0.10585900
H	5.85137900	-2.50569000	0.62264700
H	4.34070900	0.07182600	0.61833500
C	0.68611500	-1.55080200	-1.66432600
N	1.01003700	-1.84369200	-2.92016600
C	0.01127400	-2.03190400	-3.78200000
C	-1.32262300	-1.92662800	-3.40157200
C	-1.56602900	-1.59873000	-2.08134900
N	-0.56713200	-1.42050100	-1.18836200
H	0.29697800	-2.26349100	-4.80571100
H	-2.13733500	-2.07596400	-4.09942000
H	-2.57267100	-1.46744200	-1.69453300

N	1.75698400	-1.45380700	-0.75589500
C	-0.00446400	-1.80767200	2.24481500
C	-0.90407400	-0.78252500	2.70100300
C	-2.25252600	-1.14300800	2.36012700
C	-2.18493100	-2.35549900	1.60357700
C	-0.79013300	-2.75495600	1.54537000
C	-0.30869200	-3.98846400	0.87184000
H	0.77105100	-3.97185400	0.70743100
H	-0.53525200	-4.86794700	1.48563600
H	-0.80085800	-4.14545000	-0.09412500
C	1.45191100	-1.86840200	2.53564400
H	1.92151800	-0.88169300	2.48638500
H	1.62368800	-2.25667100	3.54660500
H	1.98467700	-2.52374800	1.84178000
C	-0.48933300	0.44173300	3.43441000
H	-1.27282500	1.20351100	3.42767700
H	-0.26657900	0.20776100	4.48209100
H	0.42258100	0.87354300	3.00504400
C	-3.46461300	-0.39585800	2.79421500
H	-4.37556800	-0.78134800	2.33328400
H	-3.58521100	-0.47129300	3.88047200
H	-3.40281700	0.66842500	2.54591000
C	-3.31093100	-3.19169500	1.10395200
H	-3.34411200	-4.14912000	1.63717400
H	-4.27944300	-2.70877400	1.25098400
H	-3.21363500	-3.43285900	0.03949100
Co	-1.10191900	-0.89107000	0.68383200

C	5.74790200	5.36000900	0.02375000
H	6.75376500	5.02664500	-0.24460300
H	5.47203400	6.13996500	-0.69462700
H	5.79614000	5.83143900	1.00794700
C	-7.39974600	2.04693600	-1.50364900
H	-7.78690600	2.79895300	-0.80762800
H	-7.44077200	2.49831200	-2.49945000
H	-8.08601900	1.19791800	-1.48704700

Zero-point correction= 0.705065 (Hartree/Particle)

Thermal correction to Energy= 0.750694

Thermal correction to Enthalpy= 0.751639

Thermal correction to Gibbs Free Energy= 0.625449

Sum of electronic and zero-point Energies= -2312.109443

Sum of electronic and thermal Energies= -2312.063813

Sum of electronic and thermal Enthalpies= -2312.062869

Sum of electronic and thermal Free Energies= -2312.189059

E(RM06L) = -2312.814508 A.U.

（T）C-6

1 3

Number of imaginary frequencies: 0

C	2.44851400	0.51830400	0.20245100
C	3.80673000	1.04538000	0.32536000
C	4.06914300	2.16402500	1.13774700
C	4.88294100	0.47865000	-0.38061100
C	5.34589000	2.68756200	1.23905400
H	3.25935700	2.58837000	1.72586200
C	6.15754900	1.01611800	-0.28172500

H	4.70238600	-0.36580400	-1.03948600
C	6.41728600	2.12900500	0.52592100
H	5.52827000	3.53859200	1.89100300
H	6.97095500	0.57224600	-0.85035600
C	1.38050500	1.39588800	0.25303000
P	0.91106300	3.03721800	-0.17159700
C	-1.29219800	1.03378500	0.20635500
C	-2.46626400	1.87236700	0.00382800
C	-2.54600500	3.18318600	0.51300500
C	-3.58822500	1.38635600	-0.69132500
C	-3.67962400	3.95703900	0.32620300
H	-1.71353700	3.57310600	1.09306900
C	-4.71898600	2.16743100	-0.88533200
H	-3.56796800	0.36684100	-1.07452000
C	-4.78813800	3.47174500	-0.38274800
H	-3.71674500	4.96068900	0.74366800
H	-5.56700800	1.76226600	-1.43359300
C	-0.03391400	1.55356300	0.18807300
C	0.96724700	4.20105000	1.21197200
H	0.22035400	4.98380900	1.06341500
H	0.78624700	3.69080400	2.16080500
H	1.94932100	4.67982300	1.23649300
O	1.06503100	3.64503400	-1.53004500
C	2.49759800	-3.16381400	0.03126700
C	1.33498300	-2.84382700	-0.70900900
C	0.56395500	-3.80970900	-1.34441800
C	0.94581900	-5.13713400	-1.17518800

C	2.06476600	-5.48461700	-0.40012700
C	2.84786100	-4.51190400	0.20058300
C	3.07607100	-1.93551700	0.45542600
C	2.29394600	-0.89893900	-0.00709400
H	-0.30884700	-3.54841900	-1.93451500
H	0.36385400	-5.91948600	-1.65327500
H	2.32599200	-6.53167200	-0.28602400
H	3.72520500	-4.78253300	0.78005900
H	3.95142300	-1.80685400	1.07743400
C	0.46827300	-0.80019200	-1.70507800
N	1.08276152	0.09285238	-2.45847691
C	0.36091504	0.63011434	-3.44727960
C	-0.92673341	0.19174456	-3.75173890
C	-1.49460732	-0.72748412	-2.88744352
N	-0.82507076	-1.18671969	-1.81148760
H	0.84334271	1.41880462	-4.01873868
H	-1.47881407	0.58130855	-4.59780547
H	-2.51555641	-1.08151223	-3.00507874
N	1.18725000	-1.44705700	-0.68791800
C	-1.36287125	-2.56248533	1.88622080
C	-1.62308725	-1.29724333	2.47872580
C	-2.94358725	-0.85819333	2.03430080
C	-3.44934025	-1.83837733	1.13461380
C	-2.46653625	-2.87069333	1.02698280
C	-2.62422925	-4.08893433	0.18756180
H	-1.70808325	-4.68096533	0.14525580
H	-3.41867425	-4.72871733	0.58880680

H	-2.91615825	-3.84256233	-0.84021020
C	-0.20548125	-3.43661933	2.22163880
H	0.72178875	-2.86666633	2.33018680
H	-0.38395125	-3.93591733	3.18142580
H	-0.03059425	-4.21571133	1.47639780
C	-0.76874925	-0.59809333	3.47644880
H	-0.91678625	0.48487167	3.44585580
H	-0.99700325	-0.93388233	4.49510380
H	0.29381975	-0.79226333	3.30207680
C	-3.68262725	0.29630867	2.60424080
H	-4.45994925	0.67102367	1.93393280
H	-4.16944825	-0.01261933	3.53714880
H	-3.02095525	1.13214367	2.84446480
C	-4.78005025	-1.83575133	0.46378280
H	-5.48389925	-2.50149833	0.97687680
H	-5.22757025	-0.83827533	0.45265080
H	-4.71840525	-2.18699733	-0.57236920
Co	-1.57389000	-0.88291700	0.24078800
C	7.78692700	2.72024400	0.61424600
H	8.55525500	2.01899600	0.28180500
H	7.86827800	3.61295300	-0.01610100
H	8.02695800	3.03394000	1.63373100
C	-5.99391600	4.32760800	-0.60301400
H	-6.25669200	4.89427300	0.29441000
H	-5.81419200	5.06256100	-1.39550800
H	-6.86368900	3.73745800	-0.89993000

Zero-point correction= 0.704316 (Hartree/Particle)

Thermal correction to Energy= 0.749205

Thermal correction to Enthalpy= 0.750149

Thermal correction to Gibbs Free Energy= 0.625958

Sum of electronic and zero-point Energies= -2312.116987

Sum of electronic and thermal Energies= -2312.072099

Sum of electronic and thermal Enthalpies= -2312.071154

Sum of electronic and thermal Free Energies= -2312.195345

E(RM06L) = -2312.821303 A.U.

(S)C-7

1 1

Number of imaginary frequencies: 0

C	-2.05070500	0.67117700	0.36708100
C	-3.25636500	1.52961100	0.30710700
C	-4.24169400	1.37230600	-0.67907500
C	-3.37059500	2.62693900	1.18552300
C	-5.28993200	2.27656200	-0.78378300
H	-4.15209500	0.56251600	-1.39978500
C	-4.43182000	3.52641900	1.07356800
H	-2.67509600	2.71487900	2.01633500
C	-5.40764800	3.37081200	0.08909500
H	-6.02843200	2.14588500	-1.57139200
H	-4.50541700	4.35339500	1.77498200
C	-0.82464100	1.31897000	0.17688000
P	-0.94185900	3.08096000	-0.17708500
C	1.78075500	0.85350700	0.06185700
C	3.01368200	1.47664200	0.44708700
C	3.06189400	2.79754000	0.94179400

C	4.21990700	0.75757000	0.36570500
C	4.26927200	3.35394300	1.32925400
H	2.14357800	3.37204600	1.00898500
C	5.42269800	1.32608000	0.75662000
H	4.18564700	-0.25955300	-0.02118500
C	5.47233700	2.63693800	1.24485800
H	4.28705600	4.37379100	1.70734300
H	6.34297200	0.75072400	0.68395200
C	0.48451400	0.83387900	0.05654900
C	-1.70509700	3.49260800	-1.77038500
H	-0.91755100	3.62520500	-2.51628000
H	-2.40947300	2.72283700	-2.08642800
H	-2.23462400	4.44217700	-1.66243200
O	0.16824800	4.00117200	0.21044900
C	-3.17756100	-2.81695000	0.60844100
C	-1.79893300	-2.93481400	0.90098500
C	-1.20874900	-4.15231600	1.22836000
C	-2.02218400	-5.27852800	1.19664100
C	-3.38602200	-5.19215500	0.86257000
C	-3.97433500	-3.97423000	0.57237300
C	-3.43647200	-1.43914100	0.42622200
C	-2.24543400	-0.73542900	0.56172000
H	-0.15590200	-4.22491500	1.48777800
H	-1.59409400	-6.24720300	1.43481200
H	-3.98404300	-6.09738700	0.84473000
H	-5.03131900	-3.90746800	0.33323900
H	-4.39375900	-0.99831500	0.19093600

C	-0.08968000	-1.46341000	1.67126600
N	-0.31970000	-1.25199800	2.95759500
C	0.75190000	-1.24914200	3.75857500
C	2.03350800	-1.51759500	3.28923600
C	2.17455000	-1.67163200	1.91822800
N	1.11611700	-1.61354200	1.09429800
H	0.56592300	-1.03556800	4.80864600
H	2.89089300	-1.55553100	3.94994600
H	3.14336000	-1.79779400	1.44180600
N	-1.21651300	-1.66602300	0.82728700
C	0.26625300	-1.72611300	-2.34745200
C	0.85335100	-0.46057700	-2.69424500
C	2.28070200	-0.54292300	-2.51281300
C	2.57777500	-1.83504900	-1.98745000
C	1.32623600	-2.55069900	-1.87416900
C	1.20743800	-3.94648200	-1.37235400
H	0.18775600	-4.18828200	-1.06259000
H	1.49409900	-4.66072100	-2.15290400
H	1.86934900	-4.12744500	-0.51893400
C	-1.17214200	-2.08623300	-2.46499600
H	-1.82522700	-1.25456700	-2.17773000
H	-1.43018000	-2.35728800	-3.49586500
H	-1.43267000	-2.93807100	-1.83024700
C	0.12020200	0.73122900	-3.19805300
H	0.61184700	1.65779200	-2.88365500
H	0.07576400	0.74151900	-4.29349000
H	-0.91082900	0.74932200	-2.82782200

C	3.24847700	0.53067600	-2.86555200
H	4.21833700	0.38617700	-2.38441400
H	3.41549800	0.55334900	-3.94862800
H	2.88653600	1.52044800	-2.57154400
C	3.92068900	-2.41669800	-1.71360200
H	4.21937000	-3.11159000	-2.50815000
H	4.69636000	-1.64869700	-1.65354300
H	3.94031000	-2.98909400	-0.77963200
Co	1.25578700	-0.82382400	-0.74945500
C	-6.55886100	4.31811300	-0.02622600
H	-7.48432800	3.85508500	0.33210200
H	-6.39920800	5.22499300	0.56009200
H	-6.73780100	4.61036500	-1.06473500
C	6.76550300	3.26408300	1.65747100
H	7.03069300	4.09646300	0.99686700
H	6.70566700	3.67883500	2.66844600
H	7.59074100	2.54916600	1.63465200

Zero-point correction= 0.703418 (Hartree/Particle)

Thermal correction to Energy= 0.749770

Thermal correction to Enthalpy= 0.750714

Thermal correction to Gibbs Free Energy= 0.621765

Sum of electronic and zero-point Energies= -2312.102810

Sum of electronic and thermal Energies= -2312.056458

Sum of electronic and thermal Enthalpies= -2312.055514

Sum of electronic and thermal Free Energies= -2312.184463

E(RM06L) = -2312.806228 A.U.

(T)C-7

1 3

Number of imaginary frequencies: 0

C	-2.11007900	-0.62252400	-0.36918600
C	-3.44270300	-1.27881700	-0.35459800
C	-4.38099400	-1.00372500	0.64792600
C	-3.75259900	-2.25455600	-1.30927900
C	-5.58710300	-1.69127100	0.69691800
H	-4.14173300	-0.27383600	1.41960600
C	-4.96331200	-2.93667800	-1.25589300
H	-3.03658800	-2.47519300	-2.09741100
C	-5.90295600	-2.66938400	-0.25416500
H	-6.29475500	-1.47690500	1.49440600
H	-5.18543400	-3.69159600	-2.00631000
C	-0.99691800	-1.38537800	-0.06711000
P	-1.09486100	-3.17936000	0.33662900
C	1.60644800	-1.06706100	-0.09361600
C	2.87333500	-1.63053600	-0.43347000
C	2.96791200	-3.00618000	-0.72934400
C	4.04279200	-0.85490100	-0.47148000
C	4.19371900	-3.55797900	-1.06167300
H	2.07587700	-3.61985700	-0.65549800
C	5.26348500	-1.42316800	-0.80713600
H	3.97834100	0.19748800	-0.20972800
C	5.36360000	-2.78488900	-1.11192100
H	4.25270900	-4.62182600	-1.27998200
H	6.15911300	-0.80600500	-0.82568600
C	0.34675200	-0.94482700	-0.04797100

C	-2.39663900	-3.47818700	1.58934600
H	-2.40933200	-2.68274600	2.33988000
H	-3.38944500	-3.56737200	1.14552900
H	-2.12829000	-4.41895800	2.07382300
O	0.25458900	-3.68248700	0.81442900
C	-2.69314100	2.99978600	-0.60241700
C	-1.30402400	2.92884900	-0.83233800
C	-0.52718800	4.05595200	-1.06200700
C	-1.16470300	5.29218300	-0.98605800
C	-2.53656200	5.39026600	-0.70909100
C	-3.31154800	4.25561900	-0.52263100
C	-3.16471700	1.66340600	-0.48922700
C	-2.09949800	0.79509300	-0.61911900
H	0.53601000	3.98473200	-1.27151600
H	-0.58576300	6.19671600	-1.14428100
H	-2.99726800	6.37121900	-0.65391600
H	-4.37707800	4.33328800	-0.32951500
H	-4.17999900	1.36143200	-0.27562400
C	0.08621200	1.25874000	-1.78210900
N	-0.26600800	0.92272900	-3.00616800
C	0.73791700	0.80091800	-3.88616900
C	2.05935200	1.07861000	-3.55479100
C	2.32631200	1.37651300	-2.22536000
N	1.34134700	1.43299100	-1.31762900
H	0.45990500	0.48769400	-4.88959100
H	2.85570200	1.02397400	-4.28667300
H	3.33579700	1.53924200	-1.85980900

N	-0.91401300	1.56389600	-0.81535100
C	0.37435100	1.78645900	2.34425400
C	0.70080900	0.43035300	2.61518300
C	2.14123800	0.26016300	2.44046600
C	2.67141200	1.48949600	1.99321200
C	1.56913700	2.42421800	1.88017300
C	1.73296800	3.85282500	1.49872400
H	0.78057000	4.33328000	1.26573500
H	2.19517600	4.41444700	2.31923200
H	2.39026500	3.96733400	0.63007200
C	-0.98037500	2.39353000	2.44798900
H	-1.75684400	1.72818200	2.05316800
H	-1.23383400	2.59551000	3.49471500
H	-1.04984300	3.34030700	1.90612800
C	-0.22325100	-0.62713400	3.10501200
H	0.07204300	-1.61758500	2.74206000
H	-0.22430800	-0.66717700	4.20073300
H	-1.25243400	-0.43796500	2.78225600
C	2.87305300	-0.99200800	2.76361200
H	3.87260300	-1.01272500	2.32366400
H	2.98212500	-1.09026700	3.85002900
H	2.33668600	-1.87935100	2.41097200
C	4.10095200	1.84308000	1.77129800
H	4.46084300	2.50923400	2.56419200
H	4.74579000	0.96128700	1.77035600
H	4.25555300	2.37643600	0.82621800
Co	1.17327700	0.79876200	0.63355900

C	-7.21498300	-3.38796000	-0.21507500
H	-7.96866400	-2.85949000	-0.80923800
H	-7.13690500	-4.39716000	-0.62640300
H	-7.60665100	-3.46312900	0.80214200
C	6.67496500	-3.40710600	-1.47124200
H	6.92334700	-4.23171700	-0.79575400
H	6.65152700	-3.83045400	-2.48068400
H	7.49305400	-2.68482400	-1.43202600

Zero-point correction= 0.704228 (Hartree/Particle)

Thermal correction to Energy= 0.750014

Thermal correction to Enthalpy= 0.750958

Thermal correction to Gibbs Free Energy= 0.624933

Sum of electronic and zero-point Energies= -2312.114813

Sum of electronic and thermal Energies= -2312.069028

Sum of electronic and thermal Enthalpies= -2312.068083

Sum of electronic and thermal Free Energies= -2312.194108

E(RM06L) = -2312.819041 A.U.

(S)C-8

1 1

Number of imaginary frequencies: 0

C	1.67469400	-0.14106500	-0.89199700
C	3.07895000	-0.47063200	-1.11586400
C	3.49889800	-1.76162700	-1.48426500
C	4.06974900	0.51173400	-0.94023900
C	4.84280200	-2.04556600	-1.65997100
H	2.77723700	-2.56575100	-1.58570400
C	5.41421900	0.21676900	-1.11820700

H	3.78478600	1.52395100	-0.65957700
C	5.83039200	-1.06605200	-1.48504900
H	5.13968600	-3.05638100	-1.93013900
H	6.15672700	0.99806400	-0.97449400
C	0.57808100	-0.93118100	-1.07443200
P	0.20177100	-2.71566000	-0.99906300
C	-1.21315400	-1.87849600	-0.22477100
C	-2.30636300	-2.35646000	0.57268200
C	-2.96596900	-1.50849700	1.47950300
C	-2.74692100	-3.69035500	0.47710100
C	-4.04509800	-1.96095200	2.22286900
H	-2.59538700	-0.49156700	1.60267400
C	-3.82652800	-4.13496700	1.22180000
H	-2.23855300	-4.37406100	-0.19936600
C	-4.49934700	-3.28179400	2.10883300
H	-4.53866100	-1.28938700	2.92304200
H	-4.15783700	-5.16593100	1.12427700
C	-0.75297400	-0.61604200	-0.56226200
C	-0.30331500	-3.27869800	-2.65235800
H	-0.84988800	-4.22095500	-2.57047600
H	-0.92825400	-2.54321600	-3.16496700
H	0.59178200	-3.46349400	-3.25126000
O	1.08020400	-3.69954200	-0.29330500
C	0.47894000	3.03791300	0.66785000
C	1.27688300	2.44798500	1.66691300
C	1.50344200	3.03406300	2.90490600
C	0.92184000	4.27884200	3.12746000

C	0.15894200	4.90968100	2.13887100
C	-0.06673800	4.29913700	0.90970300
C	0.44792500	2.11457600	-0.46962500
C	1.33297700	1.05807200	-0.12293800
H	2.13630500	2.55890600	3.64491700
H	1.08392400	4.77662300	4.07794700
H	-0.25500700	5.89452300	2.33137600
H	-0.65020100	4.80538900	0.14713100
H	0.46344800	2.46373900	-1.49946400
C	2.47795500	0.23826500	1.89725700
N	3.50073700	0.68387400	2.61528300
C	4.20495400	-0.27666400	3.22861600
C	3.90129000	-1.62649900	3.09580900
C	2.77267900	-1.94540700	2.34598100
N	2.03147500	-1.00343400	1.75560800
H	5.04443900	0.05937800	3.83341000
H	4.50350500	-2.39204700	3.57061600
H	2.43574400	-2.97000000	2.20218400
N	1.75983100	1.22660000	1.15420900
C	-3.10463700	0.53863300	-1.76194300
C	-3.53294200	1.39703500	-0.71917600
C	-2.93094300	2.70693800	-0.90932700
C	-2.11397600	2.64948400	-2.04763500
C	-2.13017800	1.27852400	-2.53459900
C	-1.38892600	0.77513900	-3.71754400
H	-1.28326700	-0.31195800	-3.68924700
H	-1.91342300	1.03386200	-4.64561400

H	-0.38413000	1.20264600	-3.78355000
C	-3.62368600	-0.81805200	-2.06886500
H	-4.01708900	-1.31913100	-1.18194200
H	-4.43883400	-0.73834500	-2.79736400
H	-2.85784000	-1.46531200	-2.50265800
C	-4.54941200	1.11788000	0.32669300
H	-4.21728300	1.43757300	1.32010400
H	-5.46194200	1.68577400	0.10665800
H	-4.81413200	0.06167300	0.38106100
C	-3.24129900	3.88310400	-0.05377500
H	-2.79547100	4.80080500	-0.44122100
H	-4.32457100	4.03974800	-0.00705400
H	-2.89474200	3.75303400	0.97730400
C	-1.36035800	3.76632900	-2.67480400
H	-1.98789500	4.25859600	-3.42636700
H	-1.05878600	4.52989300	-1.95387700
H	-0.46397900	3.42285200	-3.19807400
Co	-1.45575500	1.16313300	-0.68005500
C	7.27538300	-1.38322000	-1.70399300
H	7.54486900	-2.35457600	-1.27974900
H	7.51092100	-1.43323200	-2.77298000
H	7.92881500	-0.62630600	-1.26426700
C	-5.63525900	-3.78343300	2.94138900
H	-6.27138900	-4.47519400	2.38282700
H	-5.26855600	-4.33191700	3.81634000
H	-6.26002800	-2.96758100	3.31214900

Zero-point correction= 0.704952 (Hartree/Particle)

Thermal correction to Energy= 0.750794

Thermal correction to Enthalpy= 0.751738

Thermal correction to Gibbs Free Energy= 0.624781

Sum of electronic and zero-point Energies= -2312.123908

Sum of electronic and thermal Energies= -2312.078066

Sum of electronic and thermal Enthalpies= -2312.077122

Sum of electronic and thermal Free Energies= -2312.204080

E(RM06L) = -2312.828860 A.U.

(T)C-8

1 3

Number of imaginary frequencies: 0

C	1.69738900	-0.15891100	-0.90871900
C	3.10397800	-0.47976300	-1.12884000
C	3.53236000	-1.76947800	-1.49309800
C	4.08937700	0.50932900	-0.95658500
C	4.87780100	-2.04711300	-1.66442900
H	2.81599100	-2.57734300	-1.59848500
C	5.43543300	0.22080000	-1.12996700
H	3.79933800	1.52209700	-0.68433400
C	5.85963600	-1.06165000	-1.48995500
H	5.18055000	-3.05676700	-1.93202300
H	6.17311300	1.00715700	-0.98960500
C	0.61171500	-0.96631000	-1.09320200
P	0.25876000	-2.75745900	-0.98263900
C	-1.17047200	-1.93064400	-0.21525700
C	-2.26675100	-2.39360000	0.58566900
C	-2.92839700	-1.52559800	1.47319200

C	-2.71277000	-3.72589300	0.50818100
C	-4.01461700	-1.96107800	2.21634800
H	-2.55813200	-0.50617100	1.58243300
C	-3.80051600	-4.15244900	1.25169400
H	-2.20449100	-4.42234600	-0.15508000
C	-4.47500300	-3.28133200	2.11971700
H	-4.50964100	-1.27530100	2.90129800
H	-4.13740900	-5.18272000	1.16775400
C	-0.71519200	-0.67813200	-0.57652700
C	-0.25776200	-3.36305300	-2.61598100
H	-0.76490700	-4.32413500	-2.50528100
H	-0.92223900	-2.65938100	-3.12244800
H	0.63052200	-3.52322800	-3.23168900
O	1.15774700	-3.70711200	-0.25769000
C	0.51918400	3.06902800	0.56443700
C	1.31459900	2.50215000	1.58154200
C	1.53636400	3.12375200	2.80407400
C	0.95900900	4.37623600	2.98661700
C	0.20250200	4.98382900	1.97700100
C	-0.02207700	4.34115000	0.76541900
C	0.48554400	2.11455300	-0.54003400
C	1.35128600	1.05669300	-0.16534400
H	2.16375200	2.66810300	3.56078300
H	1.12020000	4.90104500	3.92263500
H	-0.20559500	5.97628300	2.14024800
H	-0.59930300	4.82768900	-0.01476700
H	0.43653600	2.40916900	-1.58492600

C	2.50776300	0.29880700	1.87426200
N	3.52046200	0.76492600	2.59379200
C	4.22530300	-0.17855400	3.23212600
C	3.93317100	-1.53299700	3.12170300
C	2.81479900	-1.87428000	2.36657900
N	2.07244000	-0.94908000	1.75151600
H	5.05624500	0.17511000	3.83862800
H	4.53621300	-2.28494100	3.61670000
H	2.48731300	-2.90403300	2.23847200
N	1.79166400	1.26730300	1.10541500
C	-3.19907400	0.51614500	-1.61070300
C	-3.61308000	1.46157700	-0.60495900
C	-2.99517800	2.69837800	-0.90391000
C	-2.21168200	2.54526600	-2.10644700
C	-2.33030900	1.20617000	-2.54443800
C	-1.70402300	0.59332700	-3.74666500
H	-1.46575100	-0.46057900	-3.57522000
H	-2.36997300	0.63885500	-4.61599000
H	-0.77292700	1.09574300	-4.02413100
C	-3.78077100	-0.83146500	-1.83757300
H	-4.20753000	-1.26295900	-0.93010400
H	-4.58593500	-0.75273100	-2.57821500
H	-3.04638800	-1.53897500	-2.23233900
C	-4.61992400	1.24412800	0.47115700
H	-4.29560400	1.65642500	1.43211900
H	-5.56259300	1.74256400	0.21547500
H	-4.83859200	0.18520300	0.61927100

C	-3.21894400	3.95909700	-0.14288400
H	-2.77808500	4.82307200	-0.64454400
H	-4.29226800	4.15199500	-0.04072600
H	-2.80833200	3.92029300	0.87243500
C	-1.46650200	3.63372200	-2.79527500
H	-2.14631600	4.23837100	-3.40583200
H	-0.97800800	4.31813900	-2.09511300
H	-0.70016400	3.24291500	-3.47013200
Co	-1.45340200	1.12175000	-0.57391700
C	7.30644800	-1.37113700	-1.70551400
H	7.57702500	-2.34690200	-1.29252000
H	7.54646300	-1.40668500	-2.77410200
H	7.95526500	-0.61728800	-1.25396200
C	-5.62048800	-3.76277800	2.95086800
H	-6.25050300	-4.46726500	2.40158200
H	-5.26339700	-4.29034600	3.84246700
H	-6.24869000	-2.93817800	3.29538500

Zero-point correction= 0.704413 (Hartree/Particle)

Thermal correction to Energy= 0.750602

Thermal correction to Enthalpy= 0.751547

Thermal correction to Gibbs Free Energy= 0.622546

Sum of electronic and zero-point Energies= -2312.127848

Sum of electronic and thermal Energies= -2312.081658

Sum of electronic and thermal Enthalpies= -2312.080714

Sum of electronic and thermal Free Energies= -2312.209715

E(RM06L) = -2312.832261 A.U.

C-TSa1

1 1

Number of imaginary frequencies: 1

C	-0.62007300	-1.16478400	-1.81770800
C	-1.23377300	-2.11782800	-0.91625100
C	-2.51358800	-1.61765000	-0.55882200
C	-2.72186800	-0.36102600	-1.24168300
C	-1.57400900	-0.12302000	-2.05813100
O	-0.36411900	0.15495800	2.94786500
O	-2.12080600	0.18553000	1.55350900
C	-1.59378300	0.31642700	2.70927800
C	-3.47843800	-2.24132500	0.37907500
H	-4.28840000	-2.72320600	-0.18011200
H	-3.00858100	-3.00513900	1.00188500
H	-3.93015500	-1.49317100	1.03513300
C	-0.66983900	-3.42920300	-0.50221200
H	-0.83042400	-3.63154400	0.56023500
H	-1.16123100	-4.23497700	-1.05901600
H	0.40044900	-3.49398200	-0.70417200
C	0.70703600	-1.30408400	-2.47358700
H	1.41855600	-1.83491300	-1.83553600
H	0.62216700	-1.86400500	-3.41159800
H	1.14459100	-0.33180800	-2.71755800
C	-1.35878000	1.04093000	-2.95495400
H	-0.31470400	1.36703800	-2.96606600
H	-1.61915500	0.76759900	-3.98333000
H	-1.98134600	1.89690200	-2.68331000
C	-3.94218500	0.47776600	-1.11447000

H	-3.81946300	1.45772000	-1.58236100
H	-4.80118200	-0.00262300	-1.59547200
H	-4.20213300	0.62953900	-0.06212400
C	4.10549800	0.75070300	-0.20653700
C	2.96027300	0.06119000	0.18602700
C	2.99700000	-1.29595000	0.60466700
C	4.22555500	-1.97555700	0.63744100
C	5.36508600	-1.29726000	0.24364400
C	5.30169800	0.04471800	-0.17243400
H	4.06241400	1.78902100	-0.50957400
H	4.27401800	-3.00987600	0.96383200
H	6.32535800	-1.80227700	0.25865000
H	6.21595400	0.54878300	-0.46983700
C	0.80216800	-0.61078100	0.73890400
H	0.19102200	-0.27751500	1.81640800
C	1.66669500	-1.68076800	0.92857700
H	1.37470800	-2.63595500	1.34659000
N	1.63187400	0.45998200	0.26157400
C	1.03982600	1.65264300	-0.03605300
N	-0.31764400	1.57820000	-0.05764600
C	-0.99287800	2.72671600	-0.19072700
C	-0.33220600	3.92954300	-0.38084500
C	1.05958700	3.87185800	-0.45349000
N	1.75513000	2.74894200	-0.27063100
H	-2.07718800	2.64622300	-0.15732500
H	-0.87493300	4.85929400	-0.49249000
H	1.64605600	4.76445300	-0.65972700

Co	-1.05337900	-0.25122600	-0.04085900
C	-2.49879700	0.66818700	3.84915500
H	-2.56106300	-0.18365900	4.53092000
H	-2.07259200	1.49501400	4.41969000
H	-3.49886400	0.92374800	3.50219500

Zero-point correction= 0.459749 (Hartree/Particle)

Thermal correction to Energy= 0.489245

Thermal correction to Enthalpy= 0.490189

Thermal correction to Gibbs Free Energy= 0.400155

Sum of electronic and zero-point Energies= -1390.738562

Sum of electronic and thermal Energies= -1390.709065

Sum of electronic and thermal Enthalpies= -1390.708121

Sum of electronic and thermal Free Energies= -1390.798155

E(RM06L) = -1391.198310 A.U.

C-TSb1

1 1

Number of imaginary frequencies: 1

C	2.04282400	1.17575600	-1.40256100
C	2.98506600	0.10787200	-1.14660900
C	2.39352700	-1.12372200	-1.57396700
C	1.06176300	-0.83728500	-2.00405400
C	0.84894700	0.59563100	-1.92471100
O	2.00711100	0.22228500	2.83740700
O	1.99689600	-1.38468500	1.26513400
C	2.35769700	-0.92053700	2.39642500
C	3.01192600	-2.46558600	-1.43896300
H	3.80155400	-2.59777700	-2.18613500

H	3.46378300	-2.59577900	-0.45182100
H	2.28431400	-3.26629600	-1.58106500
C	4.32677400	0.26409400	-0.53009800
H	4.66462600	-0.66676600	-0.06830400
H	5.07142500	0.54432600	-1.28398000
H	4.33404200	1.04694400	0.23402200
C	2.28862700	2.61201300	-1.12815200
H	2.82404700	2.75980600	-0.18574900
H	2.91261200	3.04099100	-1.92084100
H	1.36003000	3.18432000	-1.08748100
C	-0.38000900	1.31038000	-2.35195200
H	-0.46664800	2.29605000	-1.88861400
H	-0.37325300	1.45235200	-3.43859400
H	-1.28612900	0.74808200	-2.10797100
C	0.04265100	-1.82980400	-2.42628900
H	-0.97177500	-1.47015200	-2.23802300
H	0.12554300	-2.02623900	-3.50190800
H	0.16155700	-2.78424200	-1.90811000
C	-3.07768100	2.24009600	0.19862200
C	-2.02914600	1.38281000	0.53620500
C	-0.74089800	1.87737100	0.87407700
C	-0.51034800	3.25869100	0.88935200
C	-1.55035200	4.11389400	0.56225500
C	-2.81264600	3.60390600	0.21846400
H	-4.05586300	1.85587500	-0.05346000
H	0.46352700	3.64530900	1.17657000
H	-1.39562500	5.18797300	0.58116000

H	-3.61285800	4.29409300	-0.03016000
H	1.20103000	0.62494800	2.03181300
C	0.12273900	0.75629000	1.13223100
N	-1.95612500	-0.01916400	0.57126900
C	-2.97157200	-0.96173100	0.32697800
N	-2.58430700	-2.23938300	0.39474000
C	-3.54698100	-3.13742600	0.17902200
C	-4.85945100	-2.77694300	-0.10854000
C	-5.12198000	-1.41437800	-0.16976800
N	-4.18361700	-0.48745000	0.04739000
H	-3.24750100	-4.18198300	0.23829700
H	-5.63139200	-3.51704800	-0.27944700
H	-6.11712600	-1.03895700	-0.39919700
Co	1.28241400	-0.18526600	-0.11117000
C	-0.67513400	-0.38334200	0.96278200
H	-0.49450400	-1.42269100	1.20364900
C	3.26891800	-1.74572400	3.24168800
H	3.27167500	-2.78385500	2.91277800
H	4.28454200	-1.34804800	3.15309000
H	2.98789600	-1.67183100	4.29233000

Zero-point correction= 0.459502 (Hartree/Particle)

Thermal correction to Energy= 0.489243

Thermal correction to Enthalpy= 0.490188

Thermal correction to Gibbs Free Energy= 0.399140

Sum of electronic and zero-point Energies= -1390.699147

Sum of electronic and thermal Energies= -1390.669406

Sum of electronic and thermal Enthalpies= -1390.668462

Sum of electronic and thermal Free Energies= -1390.759509

E(RM06L) = -1391.158649 A.U.

C-TSc1

1 1

Number of imaginary frequencies: 1

C	-1.07755800	-2.12163900	-1.05334300
C	-2.27678500	-1.34404300	-1.06256600
C	-2.00284000	-0.09153200	-1.69255000
C	-0.63368400	-0.12937800	-2.15054400
C	-0.06459300	-1.37498000	-1.76515600
O	-1.99285300	-0.16486800	1.41083400
O	-0.36751500	0.15601800	2.91483400
C	-1.58877500	0.08782000	2.59586100
C	-2.98530000	0.99976800	-1.92861900
H	-3.56999100	0.80772700	-2.83549800
H	-3.69839500	1.08814300	-1.10354400
H	-2.49940700	1.96999200	-2.06412200
C	-3.56598300	-1.74074800	-0.44899600
H	-3.42647700	-2.46238700	0.35796700
H	-4.10584000	-0.88277600	-0.04446400
H	-4.20441000	-2.21023800	-1.20633300
C	-0.95740000	-3.51798600	-0.55610700
H	-1.45053800	-3.65264900	0.41086900
H	-1.43380800	-4.21208300	-1.25805500
H	0.08542300	-3.82169000	-0.44710800
C	1.29643200	-1.86225100	-2.10365400
H	1.72686400	-2.46923200	-1.30246600

H	1.24985200	-2.48939800	-3.00127200
H	1.98770700	-1.04263500	-2.31482000
C	0.05480800	0.95462200	-2.89891300
H	1.13561500	0.94903400	-2.73321300
H	-0.10669400	0.82956400	-3.97538300
H	-0.32795000	1.94483500	-2.63425700
C	0.97787600	-0.88713100	0.94652000
C	2.08344700	-0.17306600	0.45797400
C	3.39704200	-0.68231900	0.37612900
C	3.62945300	-1.99246800	0.80736000
C	2.56545400	-2.73622200	1.31591000
C	1.27846700	-2.19627300	1.37884800
H	0.27271000	-0.29947700	1.87830000
H	4.62705200	-2.41920700	0.75929200
H	2.74239700	-3.74443400	1.67807300
H	0.47854600	-2.79247500	1.81374900
C	3.44553600	1.44003100	-0.39142400
H	3.67056500	2.42681200	-0.76339100
C	4.22886000	0.35367600	-0.17157600
H	5.28918300	0.29624300	-0.37090800
N	2.12394300	1.13578300	-0.02734900
C	1.09224200	2.04804800	-0.00585600
N	1.41908900	3.32906400	-0.17569200
C	0.43827500	4.22063800	-0.07944400
C	-0.87449700	3.86259700	0.22568500
C	-1.13048400	2.50816100	0.32873800
N	-0.16676900	1.58144400	0.17235600

H	0.71883900	5.25880700	-0.24364900
H	-1.66091400	4.59613500	0.34945400
H	-2.12425900	2.11334400	0.52344700
Co	-0.73309200	-0.33600300	-0.08455800
C	-2.62023000	0.33902500	3.64934200
H	-2.58344000	1.39177800	3.94249600
H	-3.62115100	0.10095200	3.29264400
H	-2.38745700	-0.24196400	4.54299500

Zero-point correction= 0.460441 (Hartree/Particle)

Thermal correction to Energy= 0.489427

Thermal correction to Enthalpy= 0.490371

Thermal correction to Gibbs Free Energy= 0.403224

Sum of electronic and zero-point Energies= -1390.732797

Sum of electronic and thermal Energies= -1390.703811

Sum of electronic and thermal Enthalpies= -1390.702867

Sum of electronic and thermal Free Energies= -1390.790014

E(RM06L) = -1391.193238 A.U.

C-TSa2

1 1

Number of imaginary frequencies: 1

C	-3.82186600	-1.02229400	-1.07281200
C	-5.10855200	-0.61778400	-0.65045900
C	-5.64724000	0.60639400	-1.08623000
C	-5.85924500	-1.41798600	0.23011000
C	-6.90101400	1.00771700	-0.65290800
H	-5.07059500	1.23012400	-1.76340700
C	-7.11132000	-1.00106800	0.65171200

H	-5.44788100	-2.36374400	0.57096300
C	-7.65848700	0.21362000	0.21751100
H	-7.30873400	1.95480500	-0.99774800
H	-7.68296500	-1.62863900	1.33089100
C	-2.70124800	-1.35848300	-1.42993500
P	-1.03497300	-1.73675000	-1.76928700
C	0.11364300	0.52136500	-0.28750800
C	-0.55341000	1.80509800	-0.19499200
C	0.03463200	3.01732900	-0.58967600
C	-1.90392600	1.80575300	0.19267600
C	-0.70841300	4.18604700	-0.58725500
H	1.06980800	3.03335700	-0.91605000
C	-2.63307100	2.98780500	0.20719900
H	-2.37473900	0.86529600	0.47151800
C	-2.05074000	4.19900600	-0.17835400
H	-0.24312700	5.11366900	-0.91162200
H	-3.67434400	2.96922500	0.52097200
C	-0.13993700	-0.69065300	-0.64025400
C	-0.69706600	-0.99045400	-3.38002600
H	-0.97974000	0.06518000	-3.38530900
H	0.37070600	-1.07671100	-3.59913200
H	-1.25969900	-1.51977600	-4.15167400
O	-0.65733600	-3.18195200	-1.63904500
C	3.32671900	2.59536600	0.65809400
C	3.85796800	1.83664300	-0.41451800
C	4.97313800	2.24233500	-1.14050000
C	5.55952200	3.44822300	-0.76847600

C	5.04876900	4.22182500	0.28439700
C	3.93561700	3.80967000	1.00183800
C	2.19231200	1.89173100	1.16968200
C	2.02190100	0.72681900	0.45800000
H	5.35851500	1.64691900	-1.95818600
H	6.43131300	3.79852400	-1.31201900
H	5.53444700	5.15865800	0.53898200
H	3.54305400	4.41082500	1.81669400
H	1.52315900	2.25194100	1.94052900
C	3.22465700	-0.43257200	-1.27022400
N	4.11191200	-0.47032700	-2.26193000
C	4.16393600	-1.60743200	-2.95548300
C	3.32423600	-2.69052600	-2.70537600
C	2.43521500	-2.56352600	-1.64902500
N	2.40607200	-1.45111300	-0.89840400
H	4.90161900	-1.64141500	-3.75460600
H	3.35374500	-3.59237800	-3.30337300
H	1.70575500	-3.32885100	-1.39934000
N	3.05372100	0.69568000	-0.52381600
C	1.89466100	-1.14190100	2.68126500
C	0.46252800	-1.00388200	2.57217300
C	-0.04507600	-2.16463900	1.89104700
C	1.06191800	-2.96744300	1.50001800
C	2.26620000	-2.31847200	1.98341100
C	3.65628200	-2.80967500	1.79528900
H	4.37067100	-1.98305100	1.74079200
H	3.95971800	-3.44663400	2.63371900

H	3.75930700	-3.40619200	0.88491000
C	2.82720500	-0.24581900	3.41144400
H	3.12284400	-0.71406800	4.35696800
H	3.74001800	-0.04992800	2.84192600
H	2.37441500	0.71805600	3.64813700
C	-0.36735100	0.07781700	3.16430100
H	-1.21883500	0.33096100	2.52619600
H	-0.77081300	-0.23089400	4.13554500
H	0.20817500	0.99202500	3.32775700
C	-1.47817000	-2.46170300	1.63546100
H	-1.60369400	-3.13274000	0.78171500
H	-1.92343800	-2.94322700	2.51387300
H	-2.05343100	-1.55089800	1.44037700
C	0.98646500	-4.30778400	0.86014800
H	0.69546900	-5.05643800	1.60618400
H	0.24921300	-4.33165600	0.05283000
H	1.95407700	-4.62385000	0.46210700
Co	1.24702700	-1.05635900	0.68440000
C	-2.82722600	5.47671800	-0.15611600
H	-2.43045000	6.16815900	0.59461800
H	-2.76992400	5.99630700	-1.11731400
H	-3.88100900	5.30842700	0.07492800
C	-9.02579200	0.63572700	0.65109200
H	-9.24434700	0.31539500	1.67286700
H	-9.15358800	1.71923300	0.59642700
H	-9.79329400	0.18943800	0.00881500

Zero-point correction= 0.703239 (Hartree/Particle)

Thermal correction to Energy= 0.749212

Thermal correction to Enthalpy= 0.750156

Thermal correction to Gibbs Free Energy= 0.621141

Sum of electronic and zero-point Energies= -2312.107506

Sum of electronic and thermal Energies= -2312.061534

Sum of electronic and thermal Enthalpies= -2312.060590

Sum of electronic and thermal Free Energies= -2312.189605

E(RM06L) = -2312.810746 A.U.

C-TSa3

1 1

Number of imaginary frequencies: 1

C	-1.77720800	0.82909900	0.43839000
C	-1.85491700	2.11171100	1.22315000
C	-1.81004200	2.12856800	2.61764600
C	-1.98237100	3.33672300	0.55085200
C	-1.86228400	3.33288500	3.31337600
H	-1.72461000	1.19591100	3.16318800
C	-2.02779500	4.53353300	1.24745800
H	-2.02057000	3.34810200	-0.53647000
C	-1.96134700	4.55506400	2.64640000
H	-1.81701200	3.31983600	4.39974500
H	-2.09385400	5.47143300	0.69873200
C	-0.55266100	0.17630700	0.28293400
P	0.89665500	0.90651600	1.18438500
C	1.11818800	3.74928200	0.33555200
C	1.12057100	5.12622800	0.00773900
C	1.11447900	6.09994300	1.02275800

C	1.06570200	5.54526400	-1.33185500
C	1.05531200	7.44566300	0.69766400
H	1.14272200	5.78045900	2.06074500
C	1.00670800	6.89676000	-1.64048700
H	1.06483900	4.79984100	-2.12363200
C	1.00238600	7.87151800	-0.63650600
H	1.04761800	8.18759200	1.49322600
H	0.96104100	7.20734200	-2.68163300
C	1.04656900	2.55784800	0.59771200
C	2.45286600	0.12467800	0.67613600
H	3.23390300	0.88870100	0.69926000
H	2.68208800	-0.62756900	1.43266400
H	2.44189800	-0.36120300	-0.29641900
O	0.81062800	0.86423800	2.68688800
C	-5.14659600	0.94960800	-1.02314900
C	-4.71975500	-0.28997500	-1.53349000
C	-5.47916600	-0.99254700	-2.46738900
C	-6.68321700	-0.42878100	-2.86711300
C	-7.13225600	0.80040000	-2.35267000
C	-6.37200600	1.49965300	-1.43444300
C	-4.12650300	1.40868200	-0.16262700
C	-3.05236700	0.52705500	-0.17666900
H	-5.15601400	-1.94438700	-2.87321000
H	-7.29094900	-0.95274100	-3.59826100
H	-8.08189800	1.20301700	-2.68988300
H	-6.70166400	2.45710400	-1.04292400
H	-4.14795800	2.33238700	0.39242100

C	-3.06953200	-1.92362100	-0.94340200
N	-4.07195500	-2.78609900	-0.75707700
C	-3.81663100	-4.08130700	-0.91112600
C	-2.54912900	-4.54867700	-1.23760100
C	-1.54432800	-3.59893000	-1.29695700
N	-1.78946600	-2.27924500	-1.15328500
H	-4.65646400	-4.75634000	-0.75422500
H	-2.32896000	-5.59804900	-1.39223800
H	-0.50294900	-3.88385400	-1.44787500
N	-3.44215700	-0.57517600	-1.01174200
C	-0.27065800	0.47958500	-2.77438900
C	1.11082900	0.19802200	-2.47457300
C	1.36930000	-1.16861200	-2.81721900
C	0.16516400	-1.74214600	-3.29393500
C	-0.84376800	-0.69910400	-3.30450700
C	-2.19943700	-0.84716800	-3.89365000
H	-2.87830200	-0.04576800	-3.59617600
H	-2.12187400	-0.82518600	-4.98719300
H	-2.66674400	-1.80527300	-3.63929300
C	-0.90916700	1.81453700	-2.63873000
H	-0.49283000	2.35971200	-1.78477200
H	-0.73335100	2.42181100	-3.53537600
H	-1.99258300	1.74181800	-2.49906700
C	2.15580700	1.23932400	-2.27283000
H	3.12366000	0.81270700	-2.00335400
H	2.29602800	1.77662200	-3.21990800
H	1.89070100	1.98515900	-1.52116400

C	2.69745700	-1.83329100	-2.80585200
H	2.61726000	-2.90279800	-2.59428400
H	3.16457300	-1.72175700	-3.79254700
H	3.37727800	-1.39038900	-2.07400100
C	0.02744100	-3.09723900	-3.89332800
H	0.35209700	-3.07969200	-4.94117800
H	0.64158000	-3.83514300	-3.36864600
H	-1.00960000	-3.44619900	-3.89440200
Co	-0.17572500	-1.05968600	-1.31630700
C	-2.01444100	5.84974500	3.39600300
H	-1.52144100	5.77538700	4.36862900
H	-1.53983300	6.65888800	2.83262300
H	-3.04870600	6.15966400	3.58407200
C	0.96509700	9.32862000	-0.97401300
H	0.60104300	9.50142400	-1.98938100
H	0.32734800	9.88771800	-0.28386700
H	1.96433300	9.77354900	-0.90861800
C	-0.15270200	-1.77882900	1.06041900
C	-1.02069100	-2.07565200	2.15619800
C	-1.84367500	-3.21637100	2.05411200
C	-1.06541200	-1.33135500	3.35763600
C	-2.68528000	-3.60409400	3.08332700
H	-1.80230500	-3.82052100	1.15390000
C	-1.89381200	-1.71688300	4.38775500
H	-0.41398800	-0.46593400	3.45485400
C	-2.72125700	-2.84661500	4.26261200
H	-3.30147500	-4.48887300	2.96702800

H	-1.92395500	-1.16017800	5.31884000
C	0.63893500	-2.19410400	0.12093100
P	1.70267900	-3.64402700	0.08844500
C	4.46761100	-2.59692100	0.22062100
C	5.76553400	-2.04352700	0.20483600
C	6.27465500	-1.35945900	1.32136800
C	6.57255700	-2.15392200	-0.94807600
C	7.54442300	-0.80272100	1.29866800
H	5.66204900	-1.26764100	2.21354700
C	7.83584300	-1.60243700	-0.97567600
H	6.19057800	-2.68576700	-1.81475000
C	8.33415700	-0.92286700	0.14741400
H	7.91424600	-0.28148800	2.17409300
H	8.46880200	-1.68361500	-1.85280400
C	3.33265200	-3.05244900	0.20234100
C	1.43686200	-4.51447100	1.65087200
H	2.14488500	-5.34295900	1.71632200
H	1.58528900	-3.84686400	2.50360500
H	0.42095900	-4.91485700	1.68562700
O	1.42449400	-4.46908500	-1.14139800
C	-4.35415900	-4.25466900	5.24268400
H	-4.89037200	-4.29084600	6.18901000
H	-5.07098800	-4.15465600	4.41986600
H	-3.77846000	-5.17820500	5.11388200
C	10.13170900	0.26007500	1.13487900
H	9.53754000	1.14301500	1.39825600
H	10.20750000	-0.39774200	2.00842700

H	11.12881500	0.57295400	0.83007300
O	9.57882300	-0.42223700	0.02029200
O	-3.49979900	-3.12212100	5.32151600

Zero-point correction= 1.018794 (Hartree/Particle)

Thermal correction to Energy= 1.086784

Thermal correction to Enthalpy= 1.087728

Thermal correction to Gibbs Free Energy= 0.913499

Sum of electronic and zero-point Energies= -3612.873568

Sum of electronic and thermal Energies= -3612.805578

Sum of electronic and thermal Enthalpies= -3612.804634

Sum of electronic and thermal Free Energies= -3612.978864

E(RM06L) = -3613.892362 A.U.

C-TSb3

1 1

Number of imaginary frequencies: 1

C	1.69841300	0.89693000	-0.24813100
C	2.58864700	2.09246700	-0.29460500
C	2.56210200	3.03852900	0.73572300
C	3.42820600	2.32684200	-1.39125700
C	3.33330100	4.19307600	0.66482700
H	1.94216800	2.84982700	1.61194100
C	4.18329900	3.48762500	-1.46325400
H	3.46293900	1.60335000	-2.20134800
C	4.14790200	4.44605900	-0.44202100
H	3.31052800	4.90822800	1.48408300
H	4.81123400	3.66212400	-2.33372300
C	0.36904800	1.17739000	0.00627800

P	-0.32585600	2.74361800	-0.49180100
C	-2.30633600	0.47472100	-0.31785000
C	-3.73162400	0.51012600	-0.54972900
C	-4.36921100	1.75014600	-0.75614100
C	-4.52330800	-0.64736900	-0.57952300
C	-5.73505500	1.81694600	-0.96855300
H	-3.77493000	2.66049900	-0.73842900
C	-5.89153200	-0.57303800	-0.80568200
H	-4.05410300	-1.61567100	-0.43094500
C	-6.52602000	0.65811000	-0.99943400
H	-6.20576700	2.78579000	-1.11757700
H	-6.48280100	-1.48516500	-0.83118900
C	-1.32446600	1.30520700	-0.52345300
C	-0.90363800	3.83820600	0.82800100
H	-1.60001400	4.55669500	0.39039100
H	-1.39943800	3.28758900	1.62831600
H	-0.05265600	4.39388800	1.22986100
O	0.12132900	3.45966400	-1.71977800
C	4.13181300	-1.83827300	-0.05990200
C	2.99222300	-2.56269900	-0.46696900
C	3.01421900	-3.94948700	-0.60003100
C	4.20797100	-4.59942100	-0.31367600
C	5.35268700	-3.89424500	0.09354000
C	5.32623400	-2.51749000	0.22654900
C	3.75770900	-0.47218900	-0.01152200
C	2.41952500	-0.34960600	-0.32601000
H	2.14408200	-4.50661100	-0.92731900

H	4.25431200	-5.67957000	-0.41019000
H	6.26592300	-4.44055400	0.30615200
H	6.20640300	-1.96767100	0.54531600
H	4.38396900	0.35687500	0.28540800
C	0.82705300	-1.96326200	-1.41336100
N	1.07656000	-2.77838700	-2.43757200
C	0.06657800	-3.10494400	-3.23608600
C	-1.21258400	-2.59562200	-3.04720600
C	-1.38753600	-1.77456100	-1.95039400
N	-0.39009100	-1.46555200	-1.09413700
H	0.30119300	-3.78044200	-4.05630400
H	-2.03869600	-2.82891500	-3.70721800
H	-2.35811000	-1.35345500	-1.71868800
N	1.92263300	-1.65525300	-0.60610500
C	0.26743000	-0.97182000	2.34517000
C	-0.74832000	0.00739500	2.63473800
C	-2.03001700	-0.55785500	2.34595200
C	-1.81124200	-1.86367800	1.79802200
C	-0.39088400	-2.11766700	1.83795100
C	0.21803500	-3.41799200	1.45963500
H	1.30747700	-3.37838200	1.42255900
H	-0.06134900	-4.17902300	2.19745900
H	-0.14933900	-3.77980700	0.49221000
C	1.70552600	-0.82197100	2.68396800
H	2.08547600	0.16924400	2.41731100
H	1.84762200	-0.94205100	3.76466200
H	2.32988900	-1.56764700	2.18542700

C	-0.48458300	1.32081500	3.27630500
H	-1.37943100	1.94445300	3.32578700
H	-0.13803600	1.17114200	4.30540600
H	0.29987000	1.87675000	2.75200300
C	-3.33573200	0.09495500	2.62831500
H	-4.16158400	-0.38331300	2.09834900
H	-3.55117700	0.04635900	3.70149500
H	-3.33563300	1.15188900	2.34406500
C	-2.82756300	-2.90153300	1.46933500
H	-2.76961600	-3.73077400	2.18406300
H	-3.84419300	-2.50710800	1.51378800
H	-2.67379200	-3.33659000	0.47522900
Co	-0.87592400	-0.45571900	0.61687500
C	4.95181200	5.70358100	-0.54443600
H	4.52304400	6.38331100	-1.28858300
H	4.98926100	6.24076400	0.40578300
H	5.97934000	5.50175900	-0.86022500
C	-7.99885100	0.74601800	-1.23900000
H	-8.48421400	1.39764900	-0.50588600
H	-8.21490200	1.17234100	-2.22391400
H	-8.47890100	-0.23313500	-1.18776200

Zero-point correction= 0.704917 (Hartree/Particle)

Thermal correction to Energy= 0.749386

Thermal correction to Enthalpy= 0.750330

Thermal correction to Gibbs Free Energy= 0.628952

Sum of electronic and zero-point Energies= -2312.093820

Sum of electronic and thermal Energies= -2312.049351

Sum of electronic and thermal Enthalpies= -2312.048406

Sum of electronic and thermal Free Energies= -2312.169784

E(RM06L) = -2312.798736 A.U.

(S)C-TS4

1 1

Number of imaginary frequencies: 1

C	2.01586000	0.99797300	-0.18659800
C	3.06401600	2.01797400	-0.02994100
C	4.17059000	2.05544400	-0.89428500
C	2.97097000	3.00495200	0.96510800
C	5.12192900	3.05732400	-0.78219300
H	4.25825000	1.30621800	-1.67618400
C	3.93466600	3.99983300	1.07636800
H	2.17506600	2.94556800	1.70548600
C	5.02223100	4.05303000	0.19931600
H	5.95910900	3.07732800	-1.47569700
H	3.85462100	4.73868300	1.86992100
C	0.69445800	1.41287900	-0.13313300
P	-0.03716300	2.97984200	-0.06445900
C	-1.89528500	0.58403200	-0.12112300
C	-3.18458000	1.12976600	-0.44696100
C	-3.37898100	2.43981400	-0.93720800
C	-4.31849700	0.30453300	-0.32289900
C	-4.65096200	2.89295600	-1.24479100
H	-2.52922100	3.09239900	-1.11279500
C	-5.58594900	0.76618000	-0.63834400
H	-4.17087100	-0.71398600	0.02575900

C	-5.78115500	2.07496900	-1.09645600
H	-4.77562800	3.90454000	-1.62412800
H	-6.44356300	0.10551600	-0.53352600
C	-0.60642400	0.90105500	-0.03488900
C	-0.75312400	3.47253300	1.51405700
H	-1.84449400	3.46801900	1.43277800
H	-0.43601600	2.79317400	2.30632800
H	-0.43272600	4.49107300	1.74503500
O	-0.41861600	3.81000500	-1.24255400
C	3.67042000	-2.27161700	-0.24678900
C	2.41075600	-2.57836100	-0.81630700
C	2.07722200	-3.86027400	-1.24958300
C	3.02392200	-4.85733300	-1.05754700
C	4.26795900	-4.58524000	-0.45669100
C	4.60302800	-3.30578200	-0.05313000
C	3.66811200	-0.88299900	0.01804200
C	2.43786700	-0.35931500	-0.35882700
H	1.11965300	-4.07397400	-1.71817400
H	2.80008400	-5.86952800	-1.37956800
H	4.97605800	-5.39591800	-0.31952500
H	5.56816000	-3.09789400	0.39861700
H	4.45330400	-0.30728500	0.48803500
C	0.55189400	-1.36906000	-1.73686300
N	0.85331800	-1.25201600	-3.02238600
C	-0.15727600	-1.36963900	-3.88841800
C	-1.45660100	-1.65017800	-3.47797400
C	-1.67739800	-1.70990800	-2.11193000

N	-0.67756000	-1.55024700	-1.22528500
H	0.09213800	-1.23999400	-4.93901800
H	-2.26826500	-1.77772200	-4.18381900
H	-2.66754200	-1.85285000	-1.68645900
N	1.63856200	-1.42107900	-0.82763600
C	-0.11573300	-2.02867900	2.14486000
C	-0.75119000	-0.86104900	2.66095900
C	-2.17265400	-0.95348700	2.41982900
C	-2.41923800	-2.18282600	1.73190600
C	-1.14122700	-2.81703900	1.53623700
C	-0.94967900	-4.12309200	0.85020700
H	0.07972900	-4.25817200	0.50789000
H	-1.17969100	-4.94995900	1.53220200
H	-1.61363900	-4.23223800	-0.01342000
C	1.31836000	-2.38499100	2.31651000
H	1.98120600	-1.53404700	2.12917700
H	1.51093600	-2.72251200	3.34225100
H	1.62495400	-3.19520300	1.65021700
C	-0.04937600	0.24033200	3.37498800
H	-0.71579400	1.08258100	3.57728900
H	0.32890800	-0.10808300	4.34290300
H	0.81813500	0.60487800	2.81043700
C	-3.18409700	0.03094500	2.89327000
H	-4.14016700	-0.08163900	2.37711500
H	-3.36980800	-0.08843400	3.96674000
H	-2.85321800	1.06257700	2.73418400
C	-3.73386200	-2.80855000	1.41310200

H	-3.91710000	-3.67463000	2.06046300
H	-4.56606400	-2.11699500	1.56528400
H	-3.78793500	-3.17629100	0.38224800
Co	-1.14377300	-0.94647200	0.65598500
C	6.04650600	5.13798800	0.29653000
H	5.97379700	5.68299300	1.23996500
H	7.06230800	4.74276000	0.20911300
H	5.92317400	5.86650500	-0.51217300
C	-7.14589500	2.58988800	-1.42078000
H	-7.48441200	3.30848900	-0.66622300
H	-7.15965200	3.11716600	-2.37894700
H	-7.88527800	1.78746800	-1.46271800

Zero-point correction= 0.703361 (Hartree/Particle)

Thermal correction to Energy= 0.749112

Thermal correction to Enthalpy= 0.750056

Thermal correction to Gibbs Free Energy= 0.623658

Sum of electronic and zero-point Energies= -2312.102456

Sum of electronic and thermal Energies= -2312.056706

Sum of electronic and thermal Enthalpies= -2312.055761

Sum of electronic and thermal Free Energies= -2312.182159

E(RM06L) = -2312.805817 A.U.

(T)C-TS4

1 3

Number of imaginary frequencies: 1

C	2.26249400	0.66665400	-0.05400700
C	3.55841400	1.33452400	0.09713600
C	4.57003200	1.17472200	-0.86239700

C	3.82101500	2.15584000	1.20738300
C	5.78406200	1.83258100	-0.72589100
H	4.38232500	0.55083700	-1.73222000
C	5.04015100	2.80311300	1.33900400
H	3.07847800	2.23452500	1.99983000
C	6.04261000	2.66376600	0.37031900
H	6.54851300	1.70670000	-1.48862800
H	5.23117800	3.41437600	2.21765500
C	1.09537100	1.34392300	0.27288400
P	0.77641100	3.06943400	0.39153100
C	-1.55078200	0.92934100	0.21589900
C	-2.72587500	1.66323200	-0.17946300
C	-2.63404200	2.97946400	-0.68171300
C	-3.99516900	1.06292900	-0.13785600
C	-3.77221800	3.66023700	-1.07943300
H	-1.66072600	3.45306300	-0.79430800
C	-5.12822500	1.75170600	-0.54434700
H	-4.06671300	0.03841900	0.21556300
C	-5.04333100	3.06824300	-1.01204200
H	-3.67836500	4.67260000	-1.46546800
H	-6.09958600	1.26421200	-0.50111900
C	-0.26758200	1.13523900	0.25730700
C	-0.09888000	3.57397200	1.88950800
H	-1.15985200	3.73453600	1.67326400
H	0.00928900	2.81259600	2.66403600
H	0.32658300	4.51626100	2.24107000
O	0.76123300	4.02187300	-0.76203100

C	2.75737300	-2.91551900	-0.67378200
C	1.42352300	-2.73055300	-1.10568400
C	0.64844800	-3.76989300	-1.60552400
C	1.22195800	-5.03738200	-1.61638600
C	2.53002700	-5.25495200	-1.15157400
C	3.30616600	-4.20751500	-0.68368000
C	3.24937500	-1.64206700	-0.28511800
C	2.24941600	-0.70515700	-0.47007500
H	-0.36789300	-3.60865400	-1.95209000
H	0.64274100	-5.87614100	-1.99017500
H	2.93845300	-6.26009100	-1.17141700
H	4.32184600	-4.37586500	-0.33919700
H	4.21144700	-1.42348900	0.15816000
C	0.14508500	-0.82135800	-1.84072100
N	0.56834300	-0.13744200	-2.88675400
C	-0.38347300	0.28019000	-3.73245000
C	-1.72633800	-0.04489500	-3.56676500
C	-2.06793700	-0.73468500	-2.41289600
N	-1.13538800	-1.09742600	-1.51762500
H	-0.04599100	0.88175400	-4.57285800
H	-2.48112600	0.26529500	-4.27882100
H	-3.09866400	-0.96286300	-2.15311900
N	1.09333800	-1.37076700	-0.94272100
C	-0.60437200	-2.44105800	2.02112600
C	-0.88844000	-1.19964800	2.63607100
C	-2.29031700	-0.90480700	2.40989400
C	-2.85944600	-1.98734900	1.66602500

C	-1.80963900	-2.91261300	1.38676000
C	-1.99155700	-4.20176200	0.66330700
H	-1.04021900	-4.63379600	0.34429000
H	-2.48946400	-4.94229000	1.30089700
H	-2.61905900	-4.08167900	-0.22724400
C	0.70781300	-3.14337100	2.05606000
H	1.54766200	-2.45671500	1.90386500
H	0.85902000	-3.61915300	3.03190700
H	0.77927400	-3.92810600	1.29896500
C	0.05944300	-0.34684700	3.40411500
H	-0.17258000	0.71591600	3.27549200
H	0.01469900	-0.55475200	4.48002300
H	1.09535100	-0.50077100	3.08493100
C	-3.00585700	0.25518000	3.00700900
H	-3.99635200	0.40375300	2.57125900
H	-3.13645700	0.10971500	4.08573100
H	-2.44803500	1.18906000	2.87464900
C	-4.29447500	-2.20386800	1.32147700
H	-4.69172200	-3.07900500	1.84864800
H	-4.92005000	-1.35353300	1.60464200
H	-4.44864700	-2.39095100	0.25195100
Co	-1.28022400	-0.99575400	0.55495700
C	7.34209700	3.39202500	0.49754600
H	8.15676400	2.85862400	0.00228400
H	7.28074800	4.38298200	0.03375900
H	7.61973800	3.54737500	1.54289200
C	-6.26277700	3.82641300	-1.42659200

H	-6.09915700	4.37700500	-2.35719200
H	-7.12380100	3.16925400	-1.56535600
H	-6.53856300	4.56934100	-0.67000600

Zero-point correction= 0.701893 (Hartree/Particle)

Thermal correction to Energy= 0.748326

Thermal correction to Enthalpy= 0.749270

Thermal correction to Gibbs Free Energy= 0.620233

Sum of electronic and zero-point Energies= -2312.091181

Sum of electronic and thermal Energies= -2312.044749

Sum of electronic and thermal Enthalpies= -2312.043804

Sum of electronic and thermal Free Energies= -2312.172842

E(RM06L) = -2312.793074 A.U.

(S)C-TS5

1 1

Number of imaginary frequencies: 1

C	-2.09711000	0.73606800	0.17069500
C	-3.42642200	1.35624800	0.06745100
C	-3.70735100	2.25630500	-0.96975600
C	-4.44251100	1.07403400	0.99244700
C	-4.95493900	2.84895600	-1.08029200
H	-2.93453400	2.46847300	-1.70657700
C	-5.68453800	1.68237200	0.88615400
H	-4.23907700	0.39242600	1.81494800
C	-5.96526400	2.58160700	-0.14945200
H	-5.15361200	3.53595900	-1.89924100
H	-6.45335800	1.46512100	1.62391600
C	-0.95084300	1.49307400	-0.02426500

P	-0.79246800	3.29865600	0.19109800
C	1.58877600	1.31008900	0.11189600
C	2.91171200	1.75486200	0.30697400
C	3.17702800	3.14079500	0.22560700
C	3.98573200	0.88949900	0.57775300
C	4.46014900	3.61949600	0.42495700
H	2.35464400	3.82187400	0.02314600
C	5.26996800	1.38376000	0.75039700
H	3.79694300	-0.17732300	0.61434400
C	5.53504500	2.75672700	0.68519200
H	4.63988200	4.69021300	0.36788000
H	6.08821900	0.69285700	0.94157400
C	0.38398100	0.99430000	-0.06280200
C	-0.17729300	3.84186700	-1.45907300
H	0.17541800	4.87262900	-1.39293500
H	0.64620800	3.20506100	-1.79464500
H	-0.99416800	3.80798800	-2.18773700
O	-2.02827300	4.05539700	0.61821700
C	-2.57274200	-2.90927500	0.42469300
C	-1.21297800	-2.79185600	0.76187700
C	-0.42547100	-3.87270100	1.11716600
C	-1.02070900	-5.13385300	1.08195500
C	-2.36235900	-5.28475700	0.70619300
C	-3.14742700	-4.18696700	0.37951300
C	-3.07047200	-1.59827800	0.17284100
C	-2.06795900	-0.67930300	0.37225900
H	0.61671500	-3.75256800	1.39730300

H	-0.43459000	-6.00660800	1.35171000
H	-2.79715600	-6.27904900	0.68276600
H	-4.19026000	-4.31065400	0.10464400
H	-4.06588900	-1.34087000	-0.16104100
C	-0.02849900	-1.02822000	1.80825300
N	-0.54807000	-0.59289100	2.93023600
C	0.33968500	-0.38796000	3.91687800
C	1.69409000	-0.67236900	3.77461800
C	2.13390200	-1.09582500	2.52602300
N	1.26854400	-1.24260100	1.51335700
H	-0.06205700	0.00038700	4.84909800
H	2.38950100	-0.54276300	4.59466300
H	3.18013700	-1.29852600	2.31925700
N	-0.83857700	-1.39527000	0.68295100
C	0.40706800	-2.26001800	-2.15110100
C	0.56868100	-0.86740700	-2.49015500
C	1.96286200	-0.52597500	-2.32622600
C	2.59077100	-1.62829500	-1.69371500
C	1.62194000	-2.70704700	-1.58227100
C	1.96160100	-4.07656200	-1.11276000
H	1.07529700	-4.69806200	-0.97439300
H	2.60935800	-4.57709900	-1.84253600
H	2.51279800	-4.05872300	-0.16626100
C	-0.83370000	-3.04670400	-2.34971500
H	-1.73177600	-2.45316700	-2.15768800
H	-0.88906200	-3.37534300	-3.39469800
H	-0.87257900	-3.93988900	-1.72153600

C	-0.48008500	0.00136300	-3.08987700
H	-0.27394800	1.06094800	-2.91326100
H	-0.54202800	-0.14987000	-4.17412900
H	-1.46884400	-0.21355800	-2.67190600
C	2.60361900	0.73241200	-2.78285200
H	3.53996500	0.94015700	-2.25973100
H	2.82994300	0.66115200	-3.85360100
H	1.94648000	1.59634000	-2.65051200
C	4.03659800	-1.79615000	-1.38771500
H	4.48887600	-2.48187400	-2.11446300
H	4.58756100	-0.85535900	-1.43503900
H	4.20136600	-2.24268500	-0.40077400
Co	0.96748400	-1.00769400	-0.50609800
C	-7.29515200	3.25982600	-0.24209500
H	-7.57628800	3.46348600	-1.27850400
H	-8.08851600	2.66485300	0.21694900
H	-7.27705000	4.22456600	0.27737800
C	6.91425000	3.29410400	0.89254300
H	7.66060900	2.49799600	0.92910200
H	7.19848600	3.98836900	0.09639600
H	6.98242400	3.85374300	1.83150400

Zero-point correction= 0.702771 (Hartree/Particle)

Thermal correction to Energy= 0.748224

Thermal correction to Enthalpy= 0.749169

Thermal correction to Gibbs Free Energy= 0.624565

Sum of electronic and zero-point Energies= -2312.071049

Sum of electronic and thermal Energies= -2312.025595

Sum of electronic and thermal Enthalpies= -2312.024651

Sum of electronic and thermal Free Energies= -2312.149255

E(RM06L) = -2312.773820 A.U.

(S)C-TS6

1 1

Number of imaginary frequencies: 1

C	1.67542600	-0.58448500	-0.72874100
C	3.01159200	-1.10758300	-1.02246300
C	3.31638700	-2.47820100	-0.96132400
C	4.04644300	-0.21791600	-1.35602500
C	4.59889700	-2.92649000	-1.23703400
H	2.56859900	-3.19245700	-0.62551000
C	5.32731000	-0.67787400	-1.62920800
H	3.84414500	0.85058900	-1.40647100
C	5.62969600	-2.04205200	-1.58255300
H	4.81492400	-3.99024900	-1.16612200
H	6.10828200	0.03347500	-1.88721500
C	0.49919900	-1.27376900	-0.72163000
P	-0.04340100	-3.00945800	-0.55036900
C	-1.43923800	-2.00654700	0.05642400
C	-2.63289500	-2.32623200	0.76904200
C	-3.46208900	-1.31130500	1.29217000
C	-3.01238100	-3.66760700	0.97178700
C	-4.62224800	-1.62973400	1.97277900
H	-3.17641200	-0.27091300	1.14538200
C	-4.17726300	-3.97581500	1.65512300
H	-2.37214800	-4.46478800	0.60030700

C	-5.00450100	-2.96812200	2.16896000
H	-5.25318200	-0.83518100	2.36641300
H	-4.45615800	-5.01603600	1.80197300
C	-0.79341100	-0.79736600	-0.21893900
C	-0.41391200	-3.74287800	-2.16882800
H	-0.99165000	-4.65815000	-2.01977400
H	-0.96190500	-3.07817600	-2.83957900
H	0.53352000	-4.01649600	-2.64064400
O	0.66453900	-3.96467300	0.35735100
C	0.91444300	2.97057200	0.06297300
C	1.84956300	2.61435200	1.05236400
C	2.26184400	3.48959800	2.05149500
C	1.71566000	4.76974100	2.03386100
C	0.78765500	5.15223300	1.05766300
C	0.37834900	4.25823600	0.07511100
C	0.67114100	1.79087000	-0.76110700
C	1.53431100	0.78465400	-0.24680500
H	2.99542000	3.19366500	2.79069100
H	2.02270100	5.48493300	2.79034600
H	0.38211400	6.15905300	1.07109900
H	-0.36454100	4.55245600	-0.66082800
H	0.62391400	1.84915600	-1.84332200
C	3.00114900	0.47385600	1.71238500
N	4.06436900	1.07932900	2.23068200
C	4.82492000	0.30157600	3.01026600
C	4.53478900	-1.03746400	3.24231100
C	3.37397000	-1.53301700	2.65644200

N	2.58489100	-0.77373700	1.89434600
H	5.69889500	0.77701500	3.45053200
H	5.17307100	-1.65898000	3.85897000
H	3.05026100	-2.56300300	2.79490500
N	2.20719500	1.26537200	0.83251500
C	-2.83092800	0.22342700	-2.15719400
C	-3.40508700	1.31078600	-1.44291300
C	-2.66240100	2.50750600	-1.77592800
C	-1.64008800	2.14564900	-2.68485900
C	-1.67088900	0.71498100	-2.85456200
C	-0.78379600	-0.06976700	-3.75449300
H	0.23939600	0.31831500	-3.76127300
H	-0.72416300	-1.11479100	-3.44257400
H	-1.14596500	-0.05349800	-4.78921900
C	-3.40438400	-1.14074100	-2.26570200
H	-3.96030200	-1.43478400	-1.37292400
H	-4.10391500	-1.16318100	-3.10982500
H	-2.64319200	-1.89957600	-2.45490400
C	-4.61286700	1.30157600	-0.57882300
H	-4.40942600	1.78942900	0.38050600
H	-5.42571700	1.85928100	-1.05817200
H	-4.97481400	0.29062200	-0.38221100
C	-2.99122800	3.86424200	-1.26922800
H	-2.35818800	4.63375400	-1.71655600
H	-4.03061700	4.11813700	-1.50341100
H	-2.88089400	3.91139700	-0.18066200
C	-0.71748100	3.08110000	-3.38212600

H	-1.22977700	3.51241400	-4.24949000
H	-0.39752300	3.91375900	-2.75075800
H	0.17666100	2.58177700	-3.76366500
Co	-1.42681400	1.09466100	-0.84117900
O	-0.53407300	0.58628300	2.00104700
O	-1.85262400	1.98102600	0.85952900
C	-1.24273100	1.62956700	1.92450500
C	-1.35374000	2.52836300	3.11443600
H	-2.31655800	3.03957300	3.12810000
H	-1.19472300	1.97521700	4.03923400
H	-0.57319200	3.29323600	3.03252300
H	-0.73924300	-0.02296200	0.79479400
C	7.00119000	-2.54500600	-1.90358200
H	7.05699100	-2.90412600	-2.93743600
H	7.75693100	-1.76373400	-1.79406400
H	7.28386600	-3.38589300	-1.26452300
C	-6.24362900	-3.30404600	2.93244500
H	-7.03418500	-2.56720300	2.76873700
H	-6.63081400	-4.29011100	2.66680900
H	-6.04391600	-3.31797200	4.01010900

Zero-point correction= 0.764527 (Hartree/Particle)

Thermal correction to Energy= 0.814955

Thermal correction to Enthalpy= 0.815899

Thermal correction to Gibbs Free Energy= 0.680975

Sum of electronic and zero-point Energies= -2541.169303

Sum of electronic and thermal Energies= -2541.118875

Sum of electronic and thermal Enthalpies= -2541.117930

Sum of electronic and thermal Free Energies= -2541.252854

E(RM06L) = -2541.933830 A.U.

(T)C-TS6

1 3

Number of imaginary frequencies: 1

C	1.73765500	-0.69457000	-0.65776100
C	2.98499400	-1.35870100	-1.04055200
C	3.19423400	-2.74068900	-0.88101900
C	4.02633200	-0.59332600	-1.59229500
C	4.38706400	-3.32114200	-1.27926300
H	2.44981700	-3.35403200	-0.37930200
C	5.21437300	-1.18716200	-1.99470100
H	3.89224900	0.47832300	-1.72154700
C	5.41845800	-2.56286900	-1.85274700
H	4.53457900	-4.38822600	-1.12836200
H	6.00087800	-0.57365900	-2.42749100
C	0.51141800	-1.28638500	-0.55768700
P	-0.13353300	-2.97894100	-0.32614500
C	-1.45392800	-1.87740400	0.29547500
C	-2.67273300	-2.08175100	0.99715100
C	-3.41446700	-0.99824500	1.52088400
C	-3.18712600	-3.38544700	1.16669900
C	-4.62252900	-1.21392500	2.15678100
H	-3.02497900	0.01601300	1.42781200
C	-4.39704800	-3.58978000	1.80439300
H	-2.61604900	-4.23290900	0.79426500
C	-5.13970600	-2.51206300	2.31176000

H	-5.18164100	-0.37035300	2.55573000
H	-4.78088100	-4.59960400	1.92270700
C	-0.74082500	-0.71561300	-0.03743600
C	-0.62643700	-3.69296200	-1.91921300
H	-1.28723000	-4.54594900	-1.74762600
H	-1.12050300	-2.97000600	-2.57074000
H	0.27497700	-4.05854800	-2.41822700
O	0.50990800	-3.96926500	0.59121500
C	1.51328600	2.98843100	-0.30255700
C	2.39207800	2.63855400	0.75296700
C	2.90705200	3.59818300	1.62484100
C	2.53153000	4.92043600	1.41677700
C	1.67039900	5.28846700	0.37164500
C	1.15907900	4.33083900	-0.49046300
C	1.14881500	1.77352100	-0.96216400
C	1.78896000	0.73469000	-0.32779800
H	3.58901700	3.32179900	2.41716300
H	2.92752900	5.68722800	2.07545600
H	1.40979200	6.33340900	0.23490000
H	0.49461000	4.61865300	-1.30144700
H	0.60715400	1.66155600	-1.88990100
C	3.15875700	0.46256700	1.72811500
N	4.11840300	1.04688700	2.44563600
C	4.67299100	0.27648400	3.38593700
C	4.30272400	-1.04654600	3.59401800
C	3.28723400	-1.53412400	2.77858800
N	2.69624600	-0.78104400	1.85194400

H	5.45214700	0.74510900	3.98445600
H	4.77539500	-1.66017000	4.35136300
H	2.91754600	-2.55515700	2.86426300
N	2.56002800	1.24557400	0.71944500
C	-3.20775700	0.09035000	-1.94403000
C	-3.76285900	1.25316300	-1.36756900
C	-2.93654100	2.36545000	-1.76790300
C	-1.92699000	1.90227000	-2.67020500
C	-2.03947900	0.49425100	-2.73896600
C	-1.20445800	-0.41363900	-3.57201100
H	-0.83101800	0.09831000	-4.46230100
H	-0.32865200	-0.79031100	-3.02553600
H	-1.77874800	-1.28105600	-3.91017000
C	-3.79768600	-1.27342000	-1.94220200
H	-4.44907900	-1.44260300	-1.08097600
H	-4.40397600	-1.41467700	-2.84518900
H	-3.03594700	-2.05774600	-1.93904400
C	-4.96352800	1.35571100	-0.49379800
H	-4.75365900	1.92942800	0.41589300
H	-5.78286000	1.86727400	-1.01069900
H	-5.32595600	0.37154000	-0.18901300
C	-3.12575500	3.77667900	-1.35415700
H	-2.16839000	4.27140600	-1.16742200
H	-3.63596900	4.33776200	-2.14638000
H	-3.72570200	3.85897900	-0.44656300
C	-0.98976100	2.77543200	-3.42793900
H	-1.51255800	3.26190500	-4.25940400

H	-0.57687000	3.57511200	-2.80628800
H	-0.15119700	2.21980000	-3.85390200
Co	-1.72811700	0.96766900	-0.67383100
O	-0.24260800	0.95089100	1.95207400
O	-1.58745400	2.28167000	0.74310500
C	-0.80829900	2.05792400	1.73975900
C	-0.57487700	3.19463700	2.68101400
H	-1.52641400	3.64284700	2.97248200
H	-0.02119000	2.86843800	3.55966400
H	0.00001600	3.96591400	2.15686300
H	-0.57041200	0.15174900	0.89698700
C	6.68925400	-3.21110000	-2.30030300
H	6.53991600	-3.77139400	-3.23006300
H	7.47676500	-2.47744800	-2.48571100
H	7.05826200	-3.92786200	-1.56113500
C	-6.42482000	-2.74127400	3.03522600
H	-7.09444500	-1.88134100	2.96090300
H	-6.94924200	-3.62411000	2.66247200
H	-6.24090300	-2.91004400	4.10260000

Zero-point correction= 0.762905 (Hartree/Particle)

Thermal correction to Energy= 0.813945

Thermal correction to Enthalpy= 0.814889

Thermal correction to Gibbs Free Energy= 0.676738

Sum of electronic and zero-point Energies= -2541.162216

Sum of electronic and thermal Energies= -2541.111175

Sum of electronic and thermal Enthalpies= -2541.110231

Sum of electronic and thermal Free Energies= -2541.248383

E(RM06L) = -2541.925120 A.U.