Electronic Supplementary Information (ESI)

DFT rationalization of mechanism and chemoselectivity in versatile Au-catalyzed reactions of diazoesters with allyl-functionalized sulfides, selenides, amines, or ethers

Caicai Gao [a], Teng Cao [a], Alexander M. Kirillov [b,c], Ran Fang[a], and Lizi Yang[d]*

[a]Key Laboratory of Chemical Additives for China National Light Industry, College of Chemistry and Chemical Engineering, Shaanxi University of Science and Technology, Xi'an 710021, P. R. China.

[b]Centro de Química Estrutural and Departamento de Engenharia Química, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001, Lisbon, Portugal.

[c]Research Institute of Chemistry, Peoples' Friendship University of Russia (RUDN University), 6 Miklukho-Maklaya st., Moscow, 117198, Russian Federation.

[d]College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou 730000, P. R. China

*Corresponding author.
E-mail address:
fangr@lzu.edu.cn (R. Fang).

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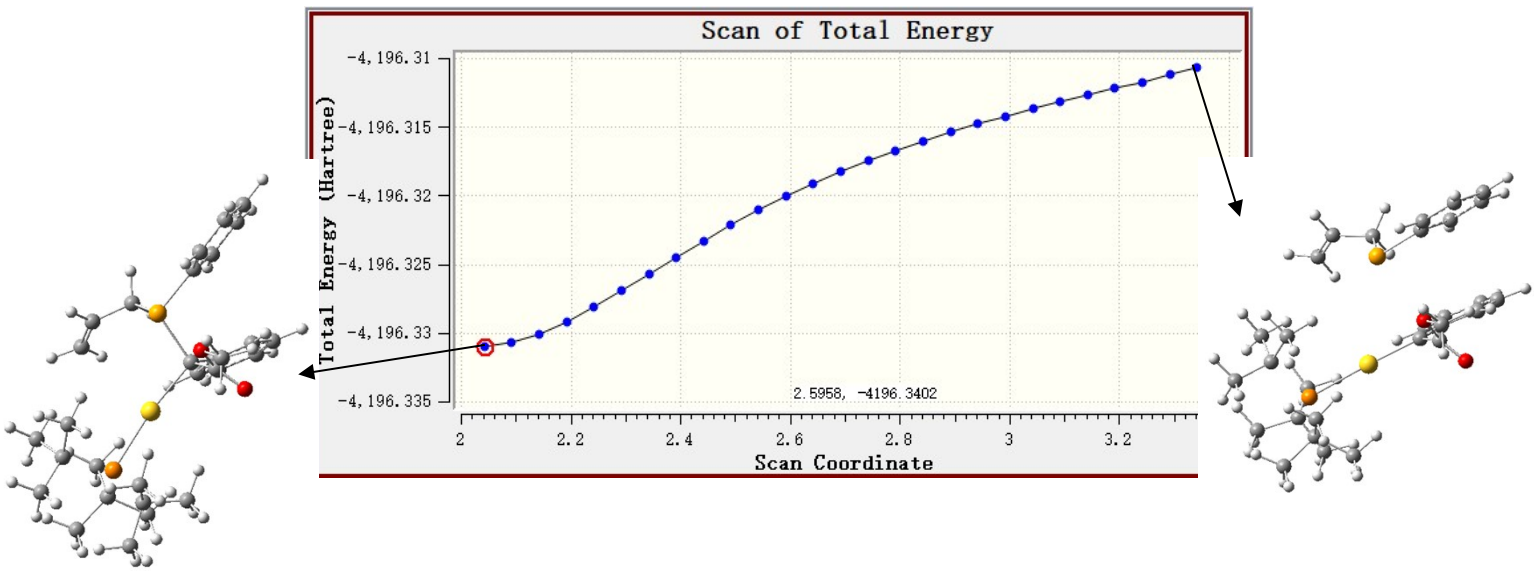

Figure S1. Scan results for **A-1a**.

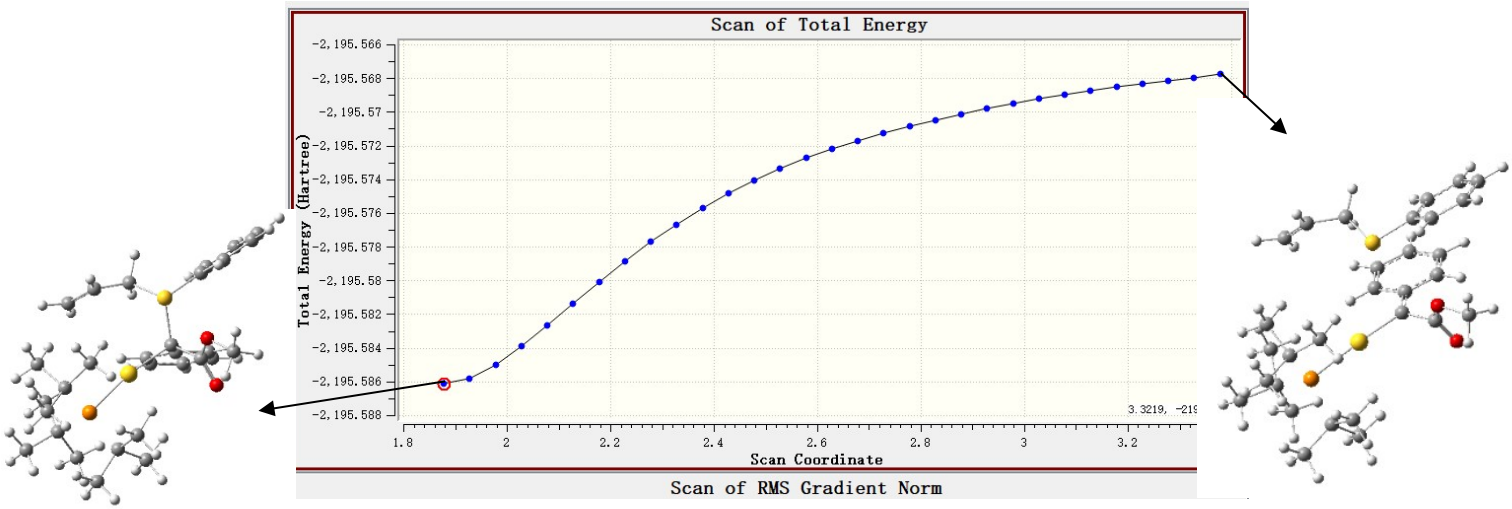

Figure S2. Scan results for **B-1a**.

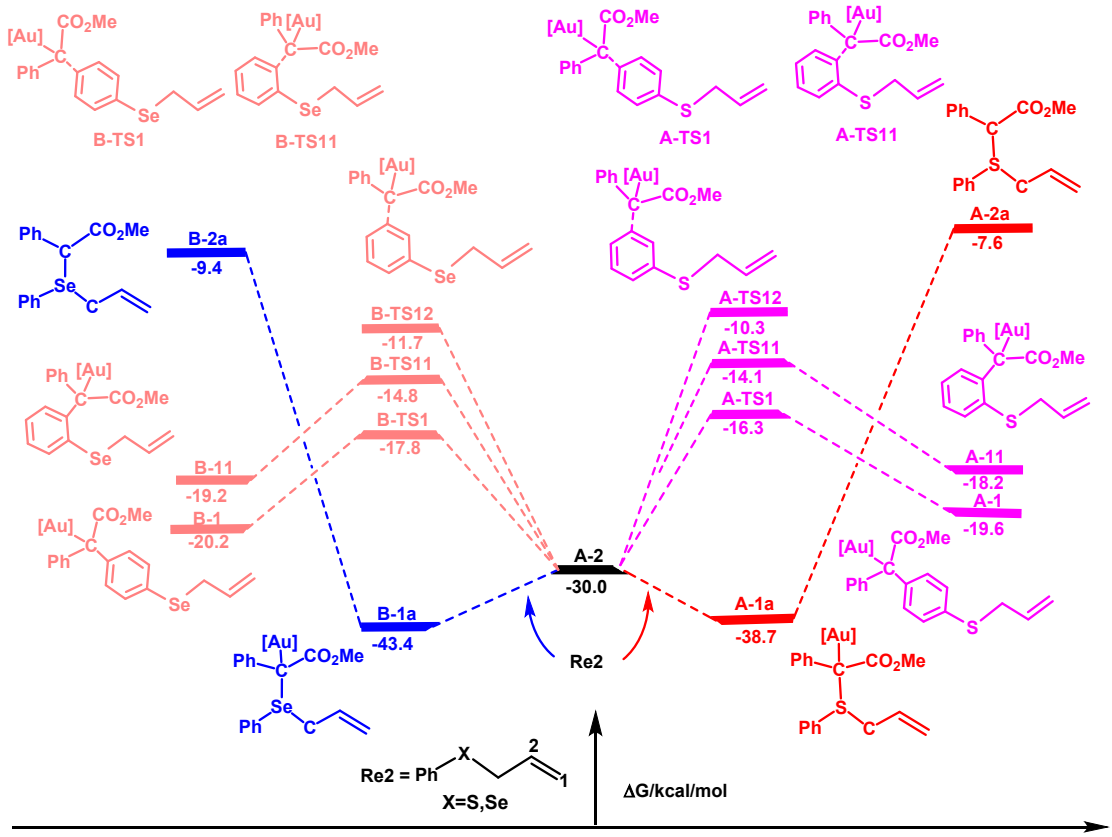

Figure S3. Additional calculation results for the series **A** and **B**. Relative energies are in kcal/mol.

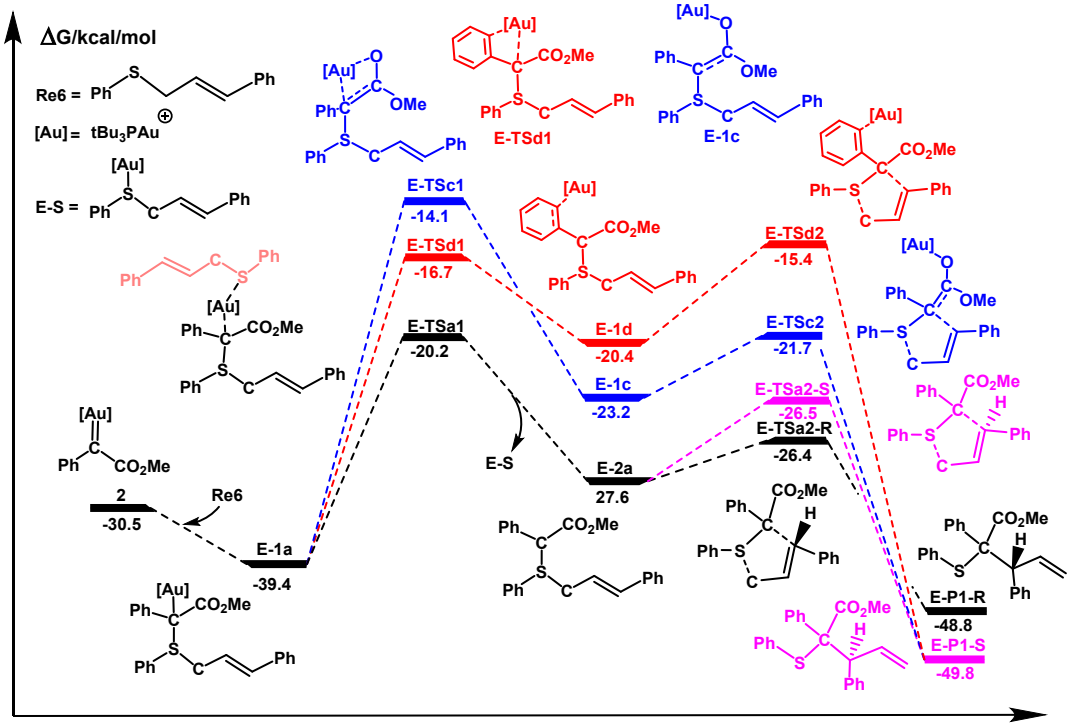

Figure S4 Computational energy profiles for the series **E**. Relative energies are in kcal/mol.

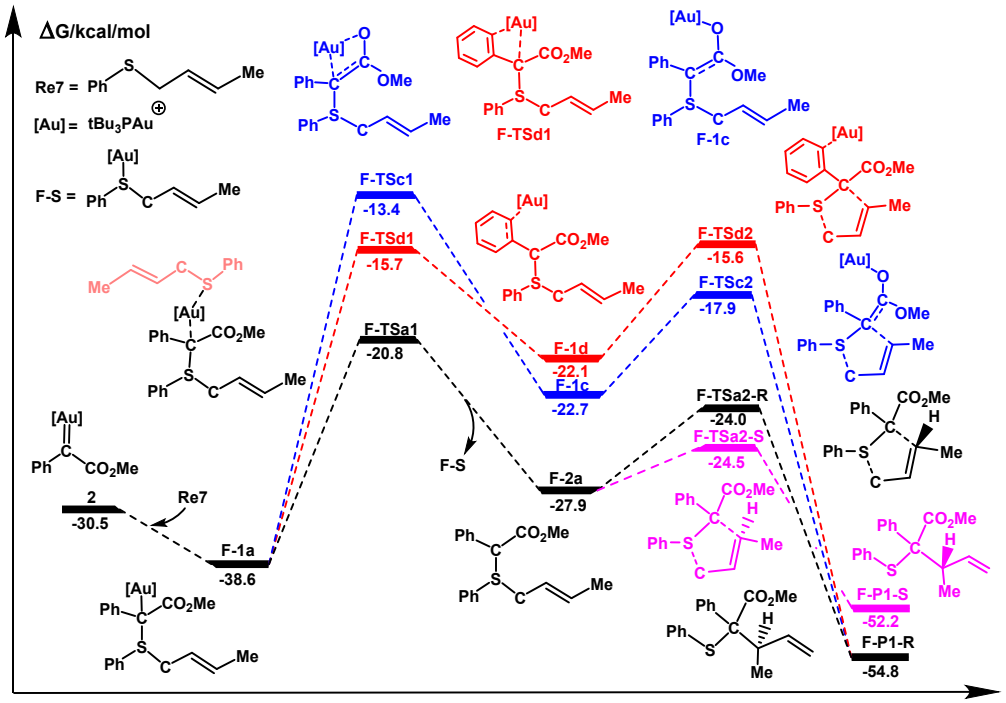

Figure S5 Computational energy profiles for the series **F**. Relative energies are in kcal/mol.

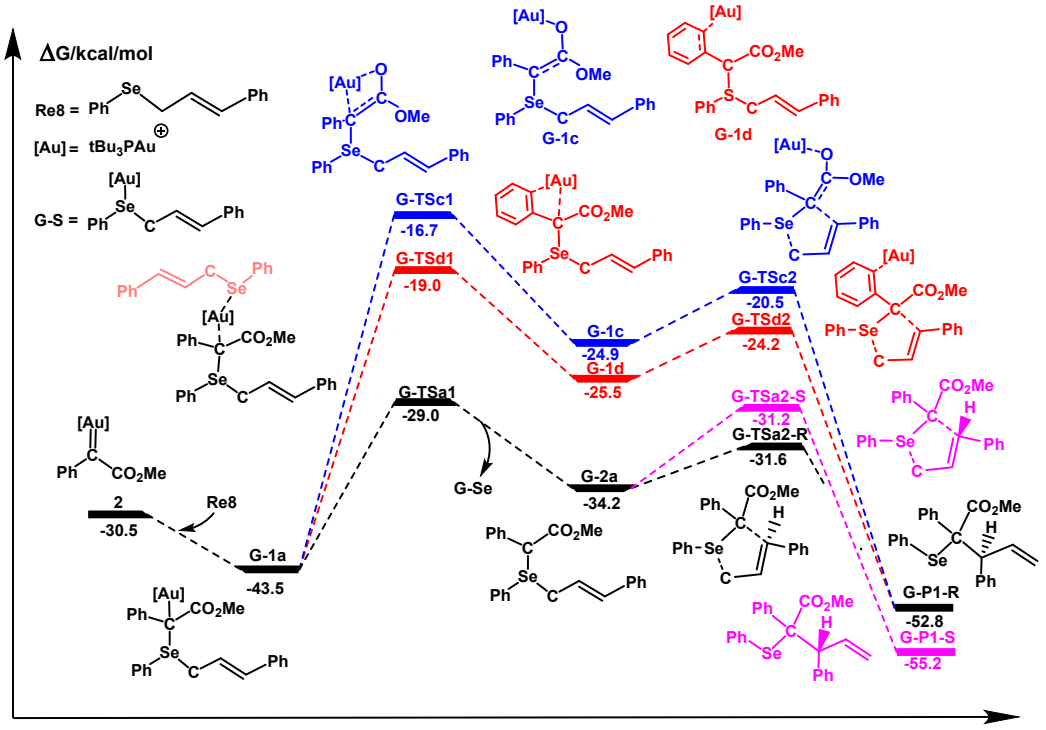

Figure S6 Computational energy profiles for the series **G**. Relative energies are in kcal/mol.

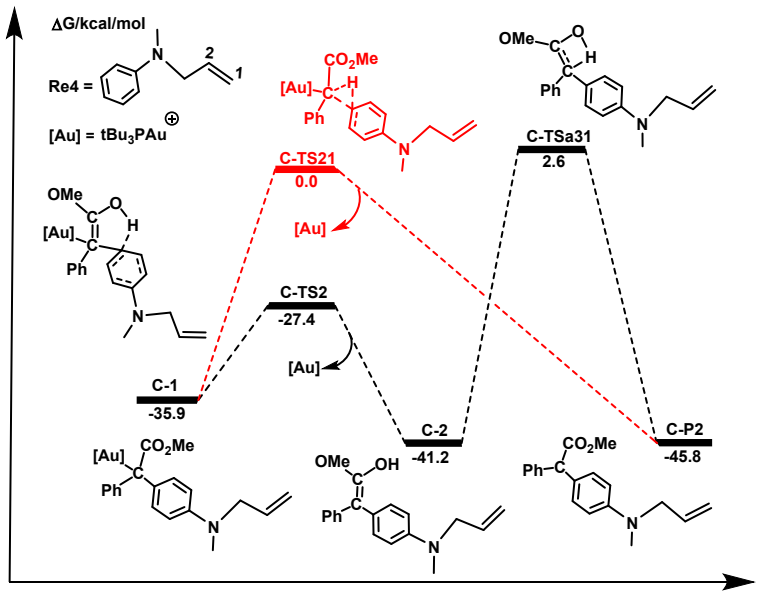

Figure S7. Additional calculation results for the series **C**. Relative energies are in kcal/mol.

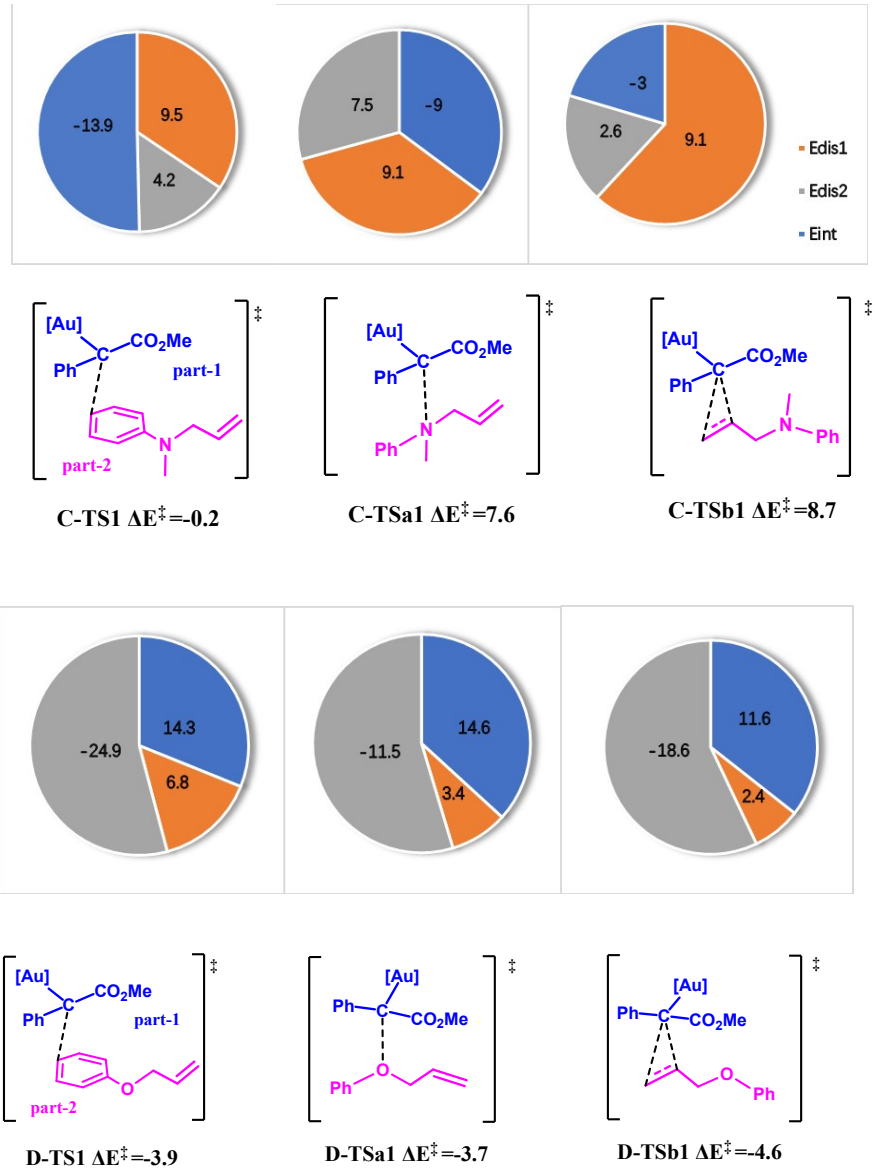

Figure S8 Distortion/interaction analysis for the reaction in series **C** and **D**. The values are in kcal/mol. $\Delta E^{\ddagger}$, the activation energy. $\Delta E_{dist\text{-}1}$, the distortion energy of Part-1. $\Delta E_{dist\text{-}2}$, the distortion energy of Part-2. $\Delta E_{int} = \Delta E^{\ddagger} - \Delta E_{dist}$, the interaction energy.

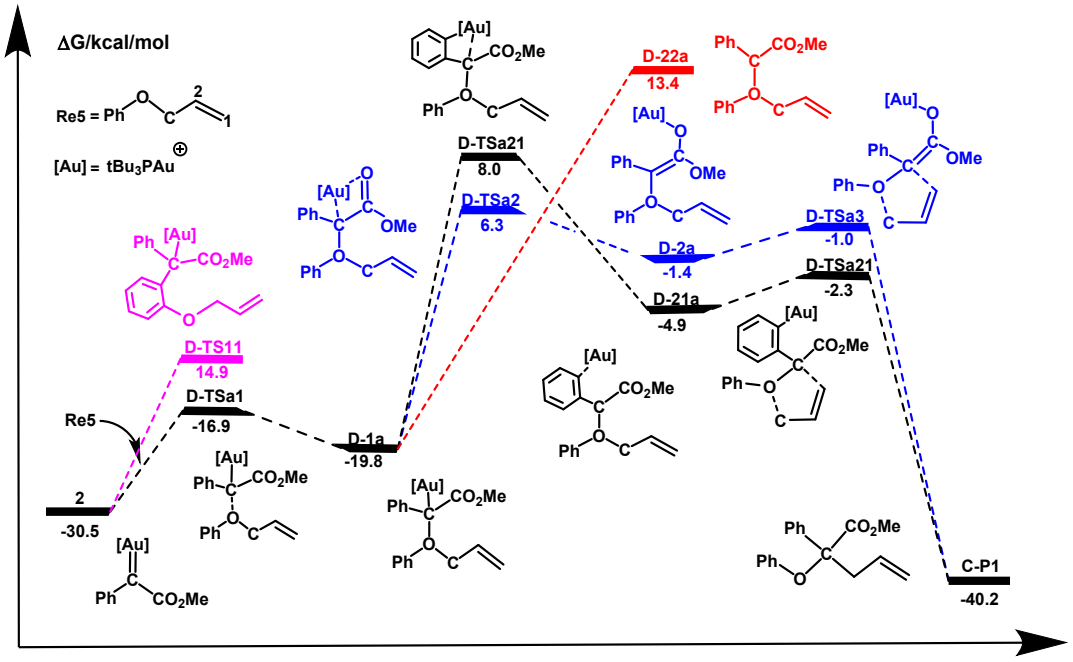

Figure S9 Additional calculation results for the series **D**. Relative energies are in kcal/mol.

Figure S10 Selected key intermediates and transition states for different pathways. Representative bond lengths are in Å.

The Cartesian coordinates of the stationary points

Re1

C	-1.63861	0.32449	0.00018
C	-2.75918	-0.62707	0.00027
O	-2.61396	-1.83352	0.00004

O	-3.95938	-0.00044	0.00003
C	-5.10285	-0.87215	-0.00022
H	-5.10246	-1.50677	0.88901
H	-5.97045	-0.21317	-0.00039
H	-5.1021	-1.50674	-0.88947
N	-1.92649	1.60846	0.00015
N	-2.13331	2.72834	0.00018
C	-0.17546	-0.15591	0.0001
C	0.11034	-1.52148	0.00013
C	0.86405	0.77414	-0.0001
C	1.43537	-1.95682	0.00064
H	-0.70941	-2.25446	0.00107
C	2.18953	0.33883	-0.00059
H	0.63897	1.85046	-0.00031
C	2.47534	-1.0264	-0.00008
H	1.66072	-3.03316	0.00129
H	3.00893	1.07236	-0.00117
H	3.52	-1.36988	0.00025

Zero-point correction= 0.158236 (Hartree/Particle)
Thermal correction to Energy= 0.170018
Thermal correction to Enthalpy= 0.170962
Thermal correction to Gibbs Free Energy= 0.118793
Sum of electronic and zero-point Energies= -607.536620
Sum of electronic and thermal Energies= -607.524838
Sum of electronic and thermal Enthalpies= -607.523894
Sum of electronic and thermal Free Energies= -607.576063
E(RB3LYP) = -607.901197369 A.U

A-re2

C	-4.34130400	-0.28104300	0.58034000
H	-4.21952200	-1.21685300	1.12027400
C	-3.29638500	0.48294500	0.26028000
H	-3.45180000	1.40831100	-0.29256200
S	-0.92846400	-0.18481300	-0.97296400
C	0.76247600	-0.07354300	-0.37231800
C	1.38116300	1.17416600	-0.21215800
C	1.48562100	-1.24128300	-0.09713800
C	2.70084700	1.25108600	0.23303800
H	0.82706200	2.07825700	-0.44522400
C	2.80938800	-1.16052300	0.33853000
H	1.00740400	-2.20665000	-0.22843200
C	3.41722900	0.08422200	0.50776300
H	3.17267000	2.22179700	0.35547600
H	3.36392400	-2.07075700	0.54785900

H	4.44679600	0.14539700	0.84806600
C	-1.87560200	0.15153000	0.59595100
H	-1.38152000	0.99348200	1.09104900
H	-1.81443800	-0.72472700	1.24661000
H	-5.35574700	0.00341900	0.31858100

Zero-point correction= 0.162752 (Hartree/Particle)
Thermal correction to Energy= 0.172709
Thermal correction to Enthalpy= 0.173653
Thermal correction to Gibbs Free Energy= 0.124868
Sum of electronic and zero-point Energies= -746.992678
Sum of electronic and thermal Energies= -746.982721
Sum of electronic and thermal Enthalpies= -746.981777
Sum of electronic and thermal Free Energies= -747.030562
E(RB3LYP) = -747.314476070 A.U

CAT

P	0.62653600	-0.00024100	-0.00014600
Au	-1.70049900	0.00036300	0.00037000
C	1.15131300	1.50436600	-1.09820200
C	0.26692800	1.56693100	-2.36511900
C	0.91926000	2.82196900	-0.32910500
C	2.63932100	1.40312900	-1.50489000
H	0.34555600	0.69038600	-3.00426900
H	-0.78727700	1.72093800	-2.11511900
H	0.59217100	2.43130000	-2.95390000
H	1.59168800	2.95164100	0.51942000
H	1.11443500	3.64742500	-1.02159000
H	-0.11460800	2.92476000	0.01277600
H	2.89702700	2.31204800	-2.05905700
H	3.31290900	1.34537600	-0.64810000
H	2.84033500	0.55825400	-2.16547900
C	1.15177800	0.19826400	1.85107300
C	0.27203700	1.26864600	2.53794500
C	0.91514000	-1.12486100	2.60912300
C	2.64092400	0.59673500	1.96581100
H	0.35888500	2.26025700	2.10001300
H	-0.78409500	0.98230600	2.54306500
H	0.59500200	1.34250800	3.58187000
H	1.58456300	-1.92742100	2.29773700
H	1.11135400	-0.93721300	3.66986800
H	-0.12020900	-1.46806300	2.52759100
H	2.89908600	0.62394500	3.02989200
H	3.31191100	-0.11926800	1.48829700
H	2.84465200	1.58958500	1.56204100

C	1.15042300	-1.70345100	-0.75397100
C	0.26763000	-2.83191300	-0.17169300
C	0.91487100	-1.69770400	-2.27907000
C	2.63877500	-2.00529300	-0.46532800
H	0.35275200	-2.95001500	0.90629400
H	-0.78788400	-2.68980100	-0.42322900
H	0.58856400	-3.77324200	-0.63048300
H	1.58355000	-1.02547800	-2.81750600
H	1.11273500	-2.70965800	-2.64730000
H	-0.12076600	-1.45698900	-2.53605700
H	2.89464400	-2.94172500	-0.97240700
H	3.31218500	-1.23623600	-0.84755900
H	2.84183600	-2.15158200	0.59669400

Zero-point correction= 0.372082 (Hartree/Particle)
Thermal correction to Energy= 0.392010
Thermal correction to Enthalpy= 0.392954
Thermal correction to Gibbs Free Energy= 0.326369
Sum of electronic and zero-point Energies= -949.818631
Sum of electronic and thermal Energies= -949.798703
Sum of electronic and thermal Enthalpies= -949.797759
Sum of electronic and thermal Free Energies= -949.864344
E(RB3LYP) = -950.516544585 A.U.

TS1

C	-2.30969800	-0.40876300	0.18781900
C	-2.61044300	-1.68505600	-0.56080600
O	-2.71812000	-1.67001600	-1.76680200
O	-2.65395400	-2.77767300	0.21215200
C	-2.84108500	-4.03406900	-0.48736400
H	-2.00116400	-4.21535500	-1.16051200
H	-2.88498600	-4.79183800	0.29253900
H	-3.76944600	-4.00982600	-1.06027000
N	-2.61227800	-0.85236500	1.83100300
N	-2.67385500	-0.88239700	2.93755500
C	-3.20124600	0.75550900	-0.03477000
C	-4.48142400	0.59890000	-0.60422000
C	-2.77501100	2.04535600	0.33967800
C	-5.29745400	1.70637200	-0.81077800
H	-4.82522800	-0.38250900	-0.91113100
C	-3.60129700	3.14774900	0.14788700
H	-1.79236700	2.17351200	0.78441700
C	-4.86221800	2.97957400	-0.43156600
H	-6.27492200	1.57758300	-1.26407700
H	-3.26289500	4.13632200	0.44094100

H	-5.50453600	3.84039300	-0.58993500
P	2.17408200	0.17565600	-0.07914100
Au	-0.18305400	-0.13183900	0.16059300
C	2.79287800	-1.09037500	-1.40539500
C	2.11123900	-2.45835100	-1.15906900
C	2.34251100	-0.63408100	-2.81093400
C	4.32547000	-1.27286900	-1.40475600
H	2.35533000	-2.90509900	-0.19724000
H	1.02246400	-2.38327700	-1.23858400
H	2.45081000	-3.15110100	-1.93729300
H	2.86624900	0.25577500	-3.16237900
H	2.57363500	-1.44008600	-3.51578200
H	1.26403800	-0.45798300	-2.86316000
H	4.59598400	-1.93581900	-2.23425700
H	4.86204600	-0.33370600	-1.55062100
H	4.69394300	-1.74100700	-0.48987700
C	2.47043600	1.99727800	-0.66349800
C	1.41541300	2.36423600	-1.73553900
C	2.23679800	2.96226800	0.51979000
C	3.88343400	2.24136200	-1.23431200
H	1.48417000	1.76786000	-2.64311900
H	0.39552400	2.27876300	-1.34840600
H	1.57251900	3.41060100	-2.02072100
H	3.01333100	2.90230400	1.28345200
H	2.24980100	3.98581200	0.12964400
H	1.26261900	2.80602500	0.99313000
H	3.97646400	3.30464700	-1.48252300
H	4.67659000	2.00460300	-0.52250300
H	4.06763000	1.68257100	-2.15343900
C	3.00860900	-0.14796900	1.63714800
C	2.15968000	0.51167100	2.75072600
C	3.00529400	-1.66222000	1.94015600
C	4.45717800	0.37669800	1.71767500
H	2.09821700	1.59550200	2.67598400
H	1.14187600	0.10991800	2.77065900
H	2.62413200	0.27759600	3.71518600
H	3.67282900	-2.23225000	1.29333200
H	3.35795000	-1.80164800	2.96789300
H	2.00026900	-2.09085800	1.88020900
H	4.87258000	0.10080000	2.69336900
H	5.10554100	-0.05608800	0.95390900
H	4.51419500	1.46385700	1.64154100

Zero-point correction= 0.528872 (Hartree/Particle)

Thermal correction to Energy= 0.562575

Thermal correction to Enthalpy= 0.563520

Thermal correction to Gibbs Free Energy= 0.463328

Sum of electronic and zero-point Energies= -1557.373767

Sum of electronic and thermal Energies= -1557.340063

Sum of electronic and thermal Enthalpies= -1557.339119

Sum of electronic and thermal Free Energies= -1557.439311

E(RB3LYP) = -1558.43876655 A.U.

1

C	2.45129500	-0.54382400	-0.33093100
C	2.67544200	-1.68316600	0.66258700
O	2.72179300	-1.51076200	1.85618600
O	2.76776300	-2.86206000	0.03664000
C	2.94397400	-4.02093900	0.89209900
H	2.08551000	-4.12656000	1.55788700
H	3.01662500	-4.86764000	0.21238700
H	3.85596800	-3.91369700	1.48109300
N	2.64981800	-0.98231200	-1.61960300
N	2.79578100	-1.32469400	-2.67758000
C	3.06962100	0.81853200	-0.06074300
C	2.94073200	1.38013200	1.22008200
C	3.74471400	1.53111600	-1.06130800
C	3.49553100	2.63129600	1.48727200
H	2.43781100	0.82901000	2.00415500
C	4.28658500	2.78614200	-0.78441600
H	3.87026200	1.12058700	-2.05886200
C	4.16515800	3.34106300	0.48972500
H	3.40143500	3.04939500	2.48473200
H	4.81219400	3.32278100	-1.56788300
H	4.59235900	4.31538400	0.70400900
P	-2.09662200	0.17624200	0.03679900
Au	0.21610400	-0.22674400	-0.21692900
C	-3.04371500	-1.32957100	-0.72661700
C	-2.37931400	-1.72706400	-2.06651400
C	-2.90619000	-2.55249400	0.20594500
C	-4.54239600	-1.04253300	-0.96188900
H	-2.42939600	-0.95279600	-2.82946300
H	-1.33044900	-2.00679000	-1.92835100
H	-2.90598600	-2.60493900	-2.45707600
H	-3.46020900	-2.44378600	1.13900000
H	-3.32135400	-3.42201800	-0.31489900
H	-1.86093500	-2.77910800	0.43720200
H	-5.01337100	-1.95851800	-1.33560300
H	-5.06818400	-0.75801100	-0.04845700

H	-4.71118300	-0.26835400	-1.71273700
C	-2.43025400	0.33592000	1.93670100
C	-1.64071900	-0.75873200	2.69464100
C	-1.88838300	1.69037400	2.44337400
C	-3.92798500	0.22550200	2.29246400
H	-1.94435800	-1.77292200	2.44281900
H	-0.56221300	-0.67229600	2.53200300
H	-1.82141300	-0.62153100	3.76660000
H	-2.46058100	2.54497600	2.08089400
H	-1.96328200	1.69421500	3.53608000
H	-0.83412600	1.83473800	2.18891500
H	-4.04081500	0.40102200	3.36803900
H	-4.54127900	0.96580500	1.77607000
H	-4.33584200	-0.76571900	2.08595000
C	-2.50909000	1.82179900	-0.89727800
C	-1.39517800	2.86123100	-0.62508700
C	-2.50133300	1.56652100	-2.42002700
C	-3.87579500	2.41444600	-0.49352800
H	-1.31369000	3.15603300	0.41922000
H	-0.41614600	2.50285500	-0.95735200
H	-1.62830000	3.76332900	-1.20168100
H	-3.33196200	0.94441800	-2.75507600
H	-2.60019700	2.53376400	-2.92420300
H	-1.56189700	1.11860700	-2.75778000
H	-4.06672000	3.29518200	-1.11678900
H	-4.70285100	1.72006200	-0.65224000
H	-3.90011800	2.74882100	0.54518400

Zero-point correction= 0.530941 (Hartree/Particle)
Thermal correction to Energy= 0.564631
Thermal correction to Enthalpy= 0.565575
Thermal correction to Gibbs Free Energy= 0.464884
Sum of electronic and zero-point Energies= -1557.380504
Sum of electronic and thermal Energies= -1557.346814
Sum of electronic and thermal Enthalpies= -1557.345870
Sum of electronic and thermal Free Energies= -1557.446561
E(RB3LYP) = -1558.44909250 A.U.

TS11

C	-3.18752100	-0.25391500	0.56895300
C	-2.96239800	-1.43791600	-0.18234900
O	-1.81853600	-1.67243500	-0.67472300
O	-3.91686200	-2.35659100	-0.26073700
C	-3.54606100	-3.65902000	-0.77611200
H	-2.75540000	-4.09777700	-0.16445800

H	-4.45663900	-4.25202500	-0.71226900
H	-3.21259500	-3.57638500	-1.81160000
N	-4.97656700	-0.55824500	1.28283300
N	-5.68271700	-0.56339900	2.13849400
C	-3.18729800	1.09469600	0.06984400
C	-3.34432700	1.40007300	-1.30634300
C	-3.00959900	2.15918600	0.98711000
C	-3.30196200	2.71720800	-1.74522100
H	-3.49708500	0.59266800	-2.01634300
C	-2.98838200	3.47684200	0.54672700
H	-2.89313300	1.92143200	2.03980700
C	-3.13114500	3.75371200	-0.81853100
H	-3.41973600	2.94504800	-2.79983400
H	-2.86164600	4.28876900	1.25561400
H	-3.11463200	4.78375300	-1.16266000
P	2.19165000	0.12234100	0.12773900
Au	0.06801500	-0.71244400	-0.27897300
C	2.44999800	0.11861700	2.04421800
C	1.16561500	0.63618300	2.73489000
C	2.64914600	-1.33254500	2.53385000
C	3.65402100	0.97236200	2.49503000
H	0.92730900	1.67069900	2.49528400
H	0.29760400	0.01789300	2.48791000
H	1.31781700	0.57755200	3.81845800
H	3.60163700	-1.76458200	2.22417200
H	2.64284000	-1.32289500	3.62916600
H	1.83709700	-1.98965300	2.20914400
H	3.76997600	0.86019300	3.57871300
H	4.59264100	0.65860200	2.03491500
H	3.51254600	2.03673500	2.29823400
C	3.45345400	-1.05066400	-0.75387500
C	3.02308000	-2.52282400	-0.54425700
C	3.41165400	-0.80611300	-2.27816100
C	4.90155500	-0.86314200	-0.25296000
H	3.01176300	-2.83681400	0.49746500
H	2.03564700	-2.71795400	-0.97274300
H	3.74244400	-3.16074300	-1.06981200
H	3.82544900	0.15950100	-2.57108600
H	4.02390800	-1.57652000	-2.75916800
H	2.39853400	-0.89799700	-2.68019500
H	5.55843700	-1.50425700	-0.85126700
H	5.26046500	0.16176500	-0.36429000
H	5.02833400	-1.16202400	0.78932400
C	2.28128600	1.91514100	-0.59286200

C	1.58426100	1.94572100	-1.97473100
C	1.48471800	2.88179700	0.31104700
C	3.72566800	2.44113100	-0.73391700
H	2.06163400	1.31704700	-2.72358500
H	0.53271300	1.65305500	-1.90154900
H	1.61698100	2.97649300	-2.34571100
H	1.95646200	3.05150100	1.27963100
H	1.43744000	3.85174300	-0.19611200
H	0.45566200	2.54601700	0.46861800
H	3.68169500	3.47537200	-1.09332100
H	4.26805700	2.45026100	0.21338100
H	4.31142100	1.87601000	-1.46078100

Zero-point correction= 0.527844 (Hartree/Particle)
Thermal correction to Energy= 0.561977
Thermal correction to Enthalpy= 0.562922
Thermal correction to Gibbs Free Energy= 0.459556
Sum of electronic and zero-point Energies= -1557.351724
Sum of electronic and thermal Energies= -1557.317591
Sum of electronic and thermal Enthalpies= -1557.316646
Sum of electronic and thermal Free Energies= -1557.420012
E(RB3LYP) = -1558.40702209 A.U.

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C	-3.73710100	-0.22891100	0.23461300
C	-3.09032700	-1.44064400	-0.20139700
O	-1.95482300	-1.49929000	-0.72211200
O	-3.82565000	-2.53596100	-0.03299400
C	-3.24478700	-3.80528800	-0.41525500
H	-2.33564900	-3.99420700	0.15868400
H	-4.00850500	-4.54418700	-0.18059700
H	-3.01909400	-3.80855300	-1.48284600
N	-4.89739900	-0.39262100	0.86324700
N	-5.87810600	-0.50379000	1.41667800
C	-3.28544300	1.16059800	-0.02382100
C	-2.82804100	1.52632500	-1.30150900
C	-3.37525400	2.13716700	0.98097600
C	-2.46536600	2.84781800	-1.56121000
H	-2.77838900	0.78382400	-2.09113400
C	-3.02523100	3.45933000	0.70947800
H	-3.72760100	1.86529000	1.97226100
C	-2.56887400	3.81768200	-0.56085700
H	-2.12490500	3.12366500	-2.55460500
H	-3.11095100	4.20829800	1.49059600
H	-2.30440000	4.84893900	-0.77312500

P	2.16315500	0.06708500	0.14332500
Au	-0.01798700	-0.58781000	-0.28781100
C	2.81347100	-1.05010900	1.58657100
C	1.72032300	-1.18338400	2.67408700
C	3.07264100	-2.47851000	1.06023300
C	4.10885800	-0.50775900	2.22798200
H	1.44847100	-0.24083000	3.14478700
H	0.81111200	-1.64361500	2.27614200
H	2.10718000	-1.84219200	3.45945500
H	3.92523600	-2.53863200	0.38337900
H	3.29898500	-3.11807500	1.92009400
H	2.19364200	-2.89961800	0.56343300
H	4.45011800	-1.23079500	2.97718300
H	4.91952100	-0.38069200	1.50808300
H	3.95689900	0.44033600	2.74730800
C	3.17626200	-0.22404800	-1.48112500
C	2.75275200	-1.56910800	-2.11864300
C	2.83000900	0.87161000	-2.51333400
C	4.70174900	-0.22587700	-1.24430700
H	2.95521800	-2.43651200	-1.49357400
H	1.69057700	-1.57479100	-2.38065200
H	3.32158900	-1.69540300	-3.04655400
H	3.21669900	1.85466900	-2.24161000
H	3.29661700	0.59566200	-3.46505800
H	1.75286100	0.94751300	-2.68887100
H	5.19959300	-0.32365100	-2.21535400
H	5.06193400	0.69805100	-0.78796300
H	5.03179200	-1.06592900	-0.63067000
C	2.16075500	1.93219500	0.64808100
C	1.20658600	2.71285900	-0.28502800
C	1.58942900	2.08045200	2.07486000
C	3.56480800	2.57208300	0.59822100
H	1.52193000	2.71953700	-1.32660800
H	0.18542000	2.32683400	-0.23712400
H	1.18216100	3.75435400	0.05499800
H	2.24655100	1.67615600	2.84549100
H	1.47392200	3.15003000	2.28034000
H	0.60108500	1.62152900	2.17070600
H	3.48644300	3.60118100	0.96607100
H	4.29049400	2.05680300	1.22966100
H	3.96611600	2.62573000	-0.41543600

Zero-point correction= 0.531757 (Hartree/Particle)

Thermal correction to Energy= 0.565308

Thermal correction to Enthalpy= 0.566252

Thermal correction to Gibbs Free Energy= 0.465177

Sum of electronic and zero-point Energies= -1557.392604

Sum of electronic and thermal Energies= -1557.359053

Sum of electronic and thermal Enthalpies= -1557.358109

Sum of electronic and thermal Free Energies= -1557.459184

E(RB3LYP) = -1558.45250544 A.U.

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C	-2.33772500	0.34707800	0.09390900
C	-2.74937400	1.75800700	0.31637300
O	-2.88432100	2.15761500	1.45611900
O	-2.88237300	2.47265600	-0.79777400
C	-3.19132100	3.88142200	-0.61870500
H	-2.40723000	4.36428400	-0.03275300
H	-3.23567300	4.29284200	-1.62492700
H	-4.15010700	3.99520100	-0.10989600
C	-3.34528800	-0.64256200	0.03393600
C	-4.73441800	-0.30442800	0.07153100
C	-2.98808400	-2.01980000	-0.08740800
C	-5.70123600	-1.28880800	-0.01560200
H	-5.02998400	0.73389400	0.17742100
C	-3.96132000	-2.99876500	-0.17712500
H	-1.93502700	-2.28020500	-0.10810300
C	-5.31521700	-2.63276700	-0.14137300
H	-6.75359100	-1.02755000	0.01409800
H	-3.68384500	-4.04313200	-0.27155600
H	-6.07865300	-3.40241300	-0.20998500
P	2.10073500	-0.14748100	-0.01631000
Au	-0.30251700	0.08576400	0.04476600
C	2.84819500	1.57991700	-0.47023400
C	1.99788600	2.22050300	-1.59456700
C	2.73529400	2.52840800	0.74432200
C	4.32345100	1.51693900	-0.91854300
H	2.01916900	1.66880300	-2.53253200
H	0.95304500	2.34132700	-1.29228900
H	2.39998700	3.21987800	-1.79605900
H	3.39924400	2.25647700	1.56574600
H	3.02717700	3.53209800	0.41634500
H	1.71126800	2.59508000	1.12393600
H	4.67991900	2.53992000	-1.08441600
H	4.97499300	1.06449700	-0.16858800
H	4.45496200	0.97773200	-1.85854900
C	2.68696700	-0.71530700	1.74042700
C	1.89872400	0.07660700	2.81196500

C	2.32324100	-2.20108800	1.95093400
C	4.20079200	-0.53363600	1.97496700
H	2.08923500	1.14776900	2.79577500
H	0.81949100	-0.07972200	2.71835800
H	2.19992400	-0.29317200	3.79861900
H	2.91703600	-2.87986100	1.33741200
H	2.52608600	-2.45420200	2.99730800
H	1.26129700	-2.39416200	1.77079900
H	4.44654700	-0.92271600	2.96958000
H	4.81017400	-1.08143000	1.25325500
H	4.50597400	0.51402400	1.95780900
C	2.54686400	-1.46701600	-1.35945400
C	1.56536900	-2.65868300	-1.24535200
C	2.32519200	-0.86651100	-2.76502400
C	3.99509300	-1.98780800	-1.25721400
H	1.62897900	-3.19345400	-0.29952600
H	0.52966000	-2.33760400	-1.39386300
H	1.80480400	-3.37322100	-2.04107100
H	3.05522700	-0.09869500	-3.02305800
H	2.43425000	-1.67215000	-3.49933300
H	1.31863100	-0.45322300	-2.88172200
H	4.17800000	-2.67528500	-2.09086100
H	4.73718100	-1.19030200	-1.32557800
H	4.17470200	-2.54685100	-0.33701800

Zero-point correction= 0.521047 (Hartree/Particle)
Thermal correction to Energy= 0.552915
Thermal correction to Enthalpy= 0.553859
Thermal correction to Gibbs Free Energy= 0.456271
Sum of electronic and zero-point Energies= -1447.893282
Sum of electronic and thermal Energies= -1447.861414
Sum of electronic and thermal Enthalpies= -1447.860470
Sum of electronic and thermal Free Energies= -1447.958058
E(RB3LYP) = -1448.91237568 A.U.

A-1a

C	1.53504500	0.01703700	0.40242100
C	1.59590200	1.16125000	1.39130700
O	1.41833000	1.02921500	2.58364800
O	1.81051200	2.36649300	0.80643600
C	1.77694500	3.50137500	1.69775800
H	2.52590900	3.39128300	2.48425900
H	1.99358200	4.36789100	1.07422200
H	0.78963200	3.59517300	2.15488300
C	2.07597300	-1.28843600	0.93410800

C	3.14041100	-1.31940200	1.85450700
C	1.53826400	-2.51741300	0.51011700
C	3.63885200	-2.53032900	2.33282900
H	3.56392900	-0.39215700	2.22252400
C	2.04647000	-3.73064300	0.97683800
H	0.69758400	-2.51701500	-0.17744500
C	3.09932100	-3.74059100	1.89230900
H	4.44958300	-2.52686100	3.05509200
H	1.60846700	-4.66481900	0.63798400
H	3.48861100	-4.68188000	2.26798200
P	-3.00102900	0.12457800	-0.01226100
Au	-0.61443600	0.00616500	0.02358700
C	-3.74070100	-1.66389500	-0.06313000
C	-2.94679500	-2.50706900	-1.08938900
C	-3.53372000	-2.35184300	1.30475900
C	-5.24036000	-1.70474000	-0.42142500
H	-3.05402300	-2.16116600	-2.11604900
H	-1.88079000	-2.53127300	-0.84615500
H	-3.32259200	-3.53596200	-1.05018600
H	-4.15085400	-1.92680400	2.09704100
H	-3.82472100	-3.40308400	1.20165300
H	-2.48718300	-2.33260300	1.62302500
H	-5.58519400	-2.74342000	-0.36166800
H	-5.85398400	-1.11864200	0.26488700
H	-5.43846800	-1.36131300	-1.43867900
C	-3.51798300	1.02567200	1.62509700
C	-2.66238900	0.48261100	2.79609800
C	-3.18308800	2.52920700	1.51377100
C	-5.01401100	0.87392000	1.97166500
H	-2.80494900	-0.57892400	2.98845100
H	-1.59453000	0.66012000	2.63992900
H	-2.95603800	1.01986300	3.70527400
H	-3.82958600	3.06461100	0.81695300
H	-3.33025200	2.98258200	2.50031000
H	-2.13950100	2.69625700	1.23078600
H	-5.22576200	1.47506000	2.86325100
H	-5.67298000	1.22855800	1.17677800
H	-5.28730200	-0.15546100	2.21077400
C	-3.56325300	1.14316300	-1.56129200
C	-2.60753800	2.34734400	-1.74299500
C	-3.40316000	0.27789800	-2.83007300
C	-5.01720800	1.65335700	-1.48552200
H	-2.65093100	3.06802000	-0.92863300
H	-1.56868600	2.02278800	-1.85495300

H	-2.89344200	2.87483900	-2.66040000
H	-4.12621100	-0.53677100	-2.88752000
H	-3.57226000	0.91844700	-3.70283700
H	-2.39399200	-0.13542600	-2.91636200
H	-5.25540400	2.16559500	-2.42490400
H	-5.74329300	0.84751000	-1.36296100
H	-5.16774800	2.37631700	-0.68186000
C	0.29831600	-1.99445100	-3.26943400
H	0.55177900	-2.92407300	-2.76706400
C	1.03772500	-0.89216800	-3.13195200
H	0.76850300	0.01702500	-3.66603600
S	2.37164400	0.58937100	-1.17909000
C	4.14795100	0.74456400	-0.90064300
C	4.99451800	-0.35880400	-0.73297300
C	4.64702400	2.05268600	-0.86241900
C	6.35772100	-0.13879900	-0.53340800
H	4.61061200	-1.37163400	-0.75326400
C	6.01156700	2.25520300	-0.65713100
H	3.97789200	2.89571200	-0.99594800
C	6.86489000	1.16211400	-0.49367300
H	7.02230500	-0.98753000	-0.40704300
H	6.40649100	3.26577700	-0.63246200
H	7.92708700	1.32320600	-0.33866900
C	2.31077200	-0.85210900	-2.34311800
H	2.48494300	-1.77160600	-1.78085700
H	3.17081200	-0.65904100	-2.99276700
H	-0.57293700	-2.01072000	-3.91609900

Zero-point correction= 0.687237 (Hartree/Particle)
Thermal correction to Energy= 0.729429
Thermal correction to Enthalpy= 0.730373
Thermal correction to Gibbs Free Energy= 0.611492
Sum of electronic and zero-point Energies= -2194.898904
Sum of electronic and thermal Energies= -2194.856712
Sum of electronic and thermal Enthalpies= -2194.855768
Sum of electronic and thermal Free Energies= -2194.974649
E(RB3LYP) = -2196.27022791 A.U.

A-TSa1
1 1

C	-1.88013400	0.62349500	0.88090200
C	-1.39821500	0.59757400	2.25746900
O	-0.71534100	1.46566600	2.79058200
O	-1.76077800	-0.53962200	2.94333800
C	-1.20713100	-0.67073100	4.26347300

H	-1.46965200	0.19041800	4.88125900
H	-1.63889600	-1.58365800	4.67375900
H	-0.11790800	-0.75378600	4.21848300
C	-2.13986600	1.95314600	0.24635400
C	-2.73513400	3.00387200	0.96853100
C	-1.81766700	2.18249100	-1.10199400
C	-3.00061600	4.23302700	0.36345400
H	-2.96628000	2.86526500	2.02009300
C	-2.09290700	3.40599400	-1.71382400
H	-1.34599800	1.38690200	-1.67142400
C	-2.68679800	4.43695900	-0.98222100
H	-3.45295800	5.03174700	0.94403600
H	-1.84112300	3.55412400	-2.76021300
H	-2.89744200	5.39234800	-1.45354400
P	1.76248300	-2.32262300	-0.20212600
Au	0.70742700	-0.22843800	0.21377400
C	2.32538200	-2.31493100	-2.05918000
C	1.19772500	-1.69931800	-2.92238400
C	3.54491000	-1.38264800	-2.22644400
C	2.68772400	-3.70923300	-2.61309800
H	0.27302200	-2.27368700	-2.91079700
H	0.97023400	-0.67602300	-2.60923600
H	1.54622600	-1.65919700	-3.96082100
H	4.45496300	-1.78341000	-1.77757900
H	3.74040400	-1.27139400	-3.29887100
H	3.35755900	-0.38260500	-1.82602500
H	3.06511100	-3.58803000	-3.63500400
H	3.47016900	-4.20490700	-2.03575100
H	1.82745000	-4.37886600	-2.67058300
C	3.30157600	-2.49699900	0.96814600
C	4.03526100	-1.13964700	1.05319600
C	2.82741000	-2.81326900	2.40409100
C	4.30363400	-3.58382500	0.52361100
H	4.44904800	-0.80766300	0.10264800
H	3.37015200	-0.35933900	1.43158800
H	4.86883500	-1.24485100	1.75702800
H	2.43397100	-3.82472600	2.51268200
H	3.69159000	-2.73295100	3.07285800
H	2.07543400	-2.09975400	2.75454100
H	5.09535100	-3.65419400	1.27858000
H	3.85104700	-4.57284100	0.43781800
H	4.78911000	-3.34524400	-0.42442800
C	0.53524900	-3.78657000	0.12417500
C	-0.23514500	-3.51875700	1.43865700

C	-0.51734100	-3.80524900	-1.00292900
C	1.20204900	-5.17565700	0.20525600
H	0.39135600	-3.58977800	2.32611100
H	-0.71980000	-2.53985300	1.44115700
H	-1.01791700	-4.28038800	1.53553400
H	-0.11446800	-4.13804800	-1.96025400
H	-1.30692000	-4.51236500	-0.72311600
H	-0.97780600	-2.82330000	-1.13691600
H	0.41512100	-5.93131700	0.31256500
H	1.77397700	-5.42756200	-0.68924300
H	1.85735700	-5.27535200	1.07227200
C	-6.91075200	-0.94462500	0.90699700
H	-7.13644900	0.01367000	0.44675500
C	-5.74632600	-1.17640000	1.51766000
H	-5.55568500	-2.14717400	1.97176800
S	-3.13176200	-0.65798300	0.62923100
C	-3.78758000	-0.53839400	-1.04378100
C	-3.66420700	-1.69055400	-1.82766500
C	-4.47398400	0.58315100	-1.52534800
C	-4.20378700	-1.71093800	-3.11497600
H	-3.16882700	-2.56885400	-1.42978400
C	-5.01347800	0.54835900	-2.81077600
H	-4.58151300	1.47558900	-0.92151500
C	-4.87508800	-0.59148100	-3.60697400
H	-4.10952000	-2.60488100	-3.72329800
H	-5.54392500	1.41639800	-3.18928100
H	-5.30012200	-0.60895900	-4.60576600
C	-4.65750300	-0.16525700	1.64040300
H	-4.95423500	0.83443800	1.31800100
H	-4.24000500	-0.11937300	2.64885800
H	-7.68561900	-1.70305300	0.86039200
C	3.81589200	4.40694700	2.44541400
H	4.67260900	3.76297500	2.26239600
C	2.56531000	3.94451800	2.40085000
H	1.72727300	4.61383400	2.58617600
S	1.22052600	2.36638000	0.54085300
C	2.39098500	2.84844600	-0.73969000
C	1.92903900	3.74560200	-1.71039500
C	3.70481600	2.36785200	-0.80202500
C	2.77503800	4.14571400	-2.74698100
H	0.91702000	4.13246700	-1.64508500
C	4.54985700	2.78830800	-1.82981200
H	4.07300300	1.67599600	-0.05235500
C	4.08604900	3.67209900	-2.80733700

H	2.41191200	4.84216400	-3.49683100
H	5.57224200	2.42352400	-1.86706300
H	4.74642800	3.99473300	-3.60632500
C	2.21214700	2.52133800	2.11072200
H	3.09673900	1.88365600	2.05168200
H	1.51577100	2.10860600	2.84522400
H	4.02899700	5.44531200	2.67870200

Zero-point correction= 0.851055 (Hartree/Particle)
Thermal correction to Energy= 0.904301
Thermal correction to Enthalpy= 0.905245
Thermal correction to Gibbs Free Energy= 0.760073
Sum of electronic and zero-point Energies= -2941.860278
Sum of electronic and thermal Energies= -2941.807031
Sum of electronic and thermal Enthalpies= -2941.806087
Sum of electronic and thermal Free Energies= -2941.951259
E(RB3LYP) = -2943.57739136 A.U.

A-2a

C	1.01063200	-0.13563400	0.31791200
C	1.98848900	-0.71517200	1.21364000
O	2.72603500	-0.07315000	1.94882300
O	2.04565000	-2.09253900	1.17178700
C	3.01495300	-2.67207400	2.04613300
H	2.81012300	-2.41768500	3.09008500
H	2.93788400	-3.75090100	1.89905900
H	4.02411700	-2.32857800	1.80174600
C	0.80786000	1.33411700	0.29034600
C	0.51242900	2.03519800	1.47454200
C	0.90197900	2.07713000	-0.90049000
C	0.29949700	3.41173900	1.46291800
H	0.46453200	1.48475200	2.40762900
C	0.66652900	3.45357700	-0.91817000
H	1.20382100	1.57409700	-1.81320300
C	0.36084400	4.12707500	0.26432000
H	0.07709500	3.92822400	2.39270000
H	0.74680200	4.00208900	-1.85302400
H	0.18697500	5.19929300	0.25565200
C	1.89581900	-0.57085500	-3.74689000
H	1.62376700	0.46382300	-3.93834600
C	1.14237900	-1.36886200	-2.98926400
H	1.44960700	-2.40010900	-2.82258000
S	-0.03549900	-1.22527200	-0.46798300
C	-1.77710300	-0.86477000	-0.07049700
C	-2.38654300	0.36725500	-0.33298900

C	-2.48229800	-1.88558200	0.57479000
C	-3.71360800	0.56562900	0.04923600
H	-1.83525600	1.16786700	-0.81249200
C	-3.81025100	-1.67716000	0.94938100
H	-1.99386200	-2.83258300	0.78325800
C	-4.42585300	-0.45277600	0.68641400
H	-4.18959300	1.52115900	-0.14929900
H	-4.36031300	-2.47026300	1.44676500
H	-5.45846800	-0.29016900	0.98020900
C	-0.13009600	-0.94713000	-2.33394100
H	-0.37926000	0.09704300	-2.53038900
H	-0.97570300	-1.57998700	-2.62608700
H	2.80829100	-0.92844600	-4.21319600

Zero-point correction= 0.312898 (Hartree/Particle)
Thermal correction to Energy= 0.333694
Thermal correction to Enthalpy= 0.334638
Thermal correction to Gibbs Free Energy= 0.260195
Sum of electronic and zero-point Energies= -1245.014262
Sum of electronic and thermal Energies= -1244.993466
Sum of electronic and thermal Enthalpies= -1244.992522
Sum of electronic and thermal Free Energies= -1245.066965
E(RB3LYP) = -1245.67925844 A.U.

A-TSc1
1 1

C	-1.91971200	0.07651400	-0.33901600
C	-1.80033400	-0.61062500	-1.61086800
O	-1.04905000	-0.28279800	-2.52542100
O	-2.56817400	-1.74385800	-1.71078900
C	-2.39483200	-2.49407900	-2.92978600
H	-1.36853500	-2.85767800	-3.01588000
H	-3.08965000	-3.33086500	-2.85790800
H	-2.62496900	-1.87604000	-3.79958400
C	-1.45270300	1.49857100	-0.17138800
C	-1.25032300	2.35571200	-1.28836100
C	-1.25845600	2.07110500	1.12011600
C	-0.89000200	3.68885200	-1.11296900
H	-1.37691200	1.95587100	-2.28526300
C	-0.91330900	3.41506000	1.27722300
H	-1.42083800	1.46558900	2.00595900
C	-0.72876400	4.23404200	0.16462200
H	-0.75248900	4.31429400	-1.99021500
H	-0.79357800	3.81578300	2.27943500
H	-0.46604100	5.27979100	0.28794400

P	2.97557000	-0.21479300	0.04681900
Au	0.71862600	0.34547500	0.06280300
C	3.29797400	-1.59069600	1.37256200
C	2.51282500	-1.24922700	2.66120200
C	2.73858100	-2.93834300	0.86950900
C	4.79298900	-1.76712700	1.71317000
H	2.83273300	-0.32421900	3.13684900
H	1.43820400	-1.18272100	2.46856000
H	2.67581800	-2.05914400	3.38182600
H	3.30287000	-3.35400200	0.03408600
H	2.80518400	-3.65950600	1.69183500
H	1.68615600	-2.86094300	0.58191100
H	4.89210100	-2.60467300	2.41295300
H	5.40283800	-2.00191500	0.83879800
H	5.21738100	-0.88985200	2.20401500
C	3.38289000	-0.84915100	-1.73741900
C	2.25223300	-1.78864600	-2.22256700
C	3.39929000	0.34402600	-2.71781400
C	4.73585200	-1.58812400	-1.81990000
H	2.13456200	-2.68057400	-1.60932100
H	1.28933900	-1.27343900	-2.28445400
H	2.51085500	-2.12271900	-3.23412800
H	4.24900000	1.01093300	-2.56738200
H	3.48209300	-0.05817000	-3.73330300
H	2.47339600	0.92430100	-2.67394600
H	4.92649700	-1.83948100	-2.86928700
H	5.57506900	-0.98138800	-1.47520800
H	4.73887400	-2.52745600	-1.26298700
C	3.97689300	1.39338200	0.46231000
C	3.34504600	2.59646600	-0.27801100
C	3.85604900	1.70576600	1.96976100
C	5.47089200	1.28873500	0.08862900
H	3.37926500	2.51219400	-1.36229800
H	2.30498000	2.75485500	0.02117700
H	3.91045800	3.49395500	-0.00193800
H	4.39196300	0.99575600	2.60081200
H	4.30189500	2.69074400	2.14616600
H	2.81329800	1.75736500	2.29613600
H	5.97278700	2.20616800	0.41597500
H	5.97400300	0.45215300	0.57708500
H	5.62903800	1.20554800	-0.98792600
C	-1.26028000	-3.21411300	2.64690900
H	-1.94828100	-3.23037200	3.48849900
C	-1.62369500	-2.76234500	1.44456100

H	-0.91914100	-2.76398900	0.61723500
S	-3.04750000	-0.42115800	0.91037700
C	-4.78910900	-0.13895200	0.47081700
C	-5.36431700	-0.55429700	-0.73543200
C	-5.53522100	0.55195100	1.43265400
C	-6.71111900	-0.27708300	-0.96677200
H	-4.77002300	-1.07782700	-1.47357500
C	-6.88344800	0.81810700	1.18722500
H	-5.07085300	0.87855100	2.35816400
C	-7.46917800	0.40415200	-0.00962800
H	-7.17001700	-0.59446100	-1.89800200
H	-7.46971500	1.35183900	1.92842000
H	-8.51688700	0.61475700	-0.20023900
C	-3.00007500	-2.27128400	1.13471900
H	-3.40337300	-2.70411700	0.22046800
H	-3.69252100	-2.42895400	1.96554400
H	-0.26390200	-3.60495900	2.82656200

Zero-point correction= 0.686677 (Hartree/Particle)
Thermal correction to Energy= 0.728273
Thermal correction to Enthalpy= 0.729217
Thermal correction to Gibbs Free Energy= 0.610770
Sum of electronic and zero-point Energies= -2194.868391
Sum of electronic and thermal Energies= -2194.826795
Sum of electronic and thermal Enthalpies= -2194.825851
Sum of electronic and thermal Free Energies= -2194.944298
E(RB3LYP) = -2196.23459110 A.U.

A-1c

C	-2.48680000	0.05322000	0.22222600
C	-1.98201100	-1.02793500	-0.51036900
O	-0.82644200	-1.12237900	-1.02927700
O	-2.81771400	-2.09164000	-0.68037300
C	-2.27541900	-3.25187200	-1.34028600
H	-1.41598800	-3.64527700	-0.79295600
H	-3.08557600	-3.98102800	-1.34580700
H	-1.97305200	-3.01250900	-2.36155100
C	-1.76928000	1.35032200	0.35359500
C	-1.30202200	2.02550000	-0.79039700
C	-1.58437700	1.96369500	1.60646600
C	-0.67332200	3.26646300	-0.68210100
H	-1.45440900	1.57927100	-1.76818900
C	-0.97083900	3.21176900	1.71219000
H	-1.93433900	1.45959000	2.50314400
C	-0.51166000	3.86882400	0.56826100

H	-0.33564100	3.77634700	-1.57992600
H	-0.85238900	3.67128400	2.68923500
H	-0.04433300	4.84571600	0.64906200
P	3.36688500	-0.01606300	-0.01335600
Au	1.13819700	-0.46550900	-0.45940600
C	3.57236500	0.20498900	1.89682000
C	2.40058800	1.06041700	2.43398500
C	3.45889100	-1.16810500	2.59496500
C	4.91241200	0.85786600	2.29736700
H	2.37581000	2.07236400	2.03519500
H	1.43313100	0.59450800	2.22739400
H	2.51009800	1.13798500	3.52189100
H	4.30956000	-1.82275300	2.39983500
H	3.42984800	-0.99471800	3.67633900
H	2.53707500	-1.69084400	2.32337000
H	4.96700300	0.89091400	3.39140400
H	5.77936800	0.29481200	1.94693800
H	5.00396600	1.88614700	1.94286700
C	4.39466600	-1.52697200	-0.65160500
C	3.67682100	-2.84221600	-0.26355700
C	4.43980600	-1.50730900	-2.19541000
C	5.83849300	-1.55505000	-0.10633200
H	3.58269700	-2.99341500	0.80998600
H	2.67875200	-2.89871000	-0.70723800
H	4.26515600	-3.67692700	-0.66129800
H	5.04405700	-0.69393800	-2.59856000
H	4.89802800	-2.44399900	-2.53129300
H	3.43875800	-1.45793300	-2.63373800
H	6.36791700	-2.39355300	-0.57269800
H	6.39921700	-0.64809800	-0.33903900
H	5.87652400	-1.71524600	0.97288500
C	3.86246200	1.59959700	-0.95891200
C	3.22076600	1.57804000	-2.36716500
C	3.26979100	2.82846800	-0.23597700
C	5.38859200	1.78652000	-1.09130600
H	3.57942400	0.77108900	-3.00339300
H	2.13103500	1.50939800	-2.30793300
H	3.46885100	2.52156500	-2.86656000
H	3.74497500	3.03264600	0.72452100
H	3.44454900	3.70465700	-0.87040800
H	2.18993400	2.74228800	-0.08981200
H	5.57686500	2.75366900	-1.57094000
H	5.90037900	1.79945500	-0.12688100
H	5.85445000	1.02438200	-1.71829500

C	-3.53754400	-1.96377900	4.01030400
H	-4.44881200	-1.59861600	4.47752200
C	-3.39463000	-2.01490900	2.68435900
H	-2.47362900	-2.39020300	2.24608100
S	-4.06690700	0.07093500	0.96785200
C	-5.41017600	0.26306700	-0.23832800
C	-5.44983500	-0.41471800	-1.46106600
C	-6.41414300	1.16689800	0.12599800
C	-6.52254500	-0.18397700	-2.32167100
H	-4.65955200	-1.10442800	-1.72990000
C	-7.48517500	1.38145100	-0.74342000
H	-6.35742600	1.70164100	1.06939300
C	-7.53822400	0.70789600	-1.96429400
H	-6.56560800	-0.70294900	-3.27424100
H	-8.26859300	2.08062700	-0.46882600
H	-8.36869900	0.88078100	-2.64166000
C	-4.45951300	-1.59496200	1.72386700
H	-4.58528900	-2.29150900	0.89607200
H	-5.41884700	-1.41764700	2.21653000
H	-2.75116300	-2.30267100	4.67719700

Zero-point correction= 0.687225 (Hartree/Particle)
Thermal correction to Energy= 0.729533
Thermal correction to Enthalpy= 0.730477
Thermal correction to Gibbs Free Energy= 0.608929
Sum of electronic and zero-point Energies= -2194.893666
Sum of electronic and thermal Energies= -2194.851358
Sum of electronic and thermal Enthalpies= -2194.850413
Sum of electronic and thermal Free Energies= -2194.971962
E(RB3LYP) = -2196.24777510 A.U.

A-TSc2

C	2.56839300	0.86581700	-0.26920600
C	1.72245700	1.89532100	-0.79624600
O	0.49706800	1.80757000	-1.08211900
O	2.33214600	3.07979300	-0.97752600
C	1.55258400	4.16546700	-1.51711900
H	0.71413400	4.40384100	-0.85914300
H	2.24241600	5.00609500	-1.57667100
H	1.17628000	3.91016500	-2.50961600
C	2.12594700	-0.55464700	-0.27433200
C	1.61289800	-1.11814500	-1.45907700
C	2.27050400	-1.38887300	0.84612800
C	1.25738200	-2.46622800	-1.51657900
H	1.51353100	-0.49800400	-2.34474900

C	1.91902800	-2.73741400	0.78741200
H	2.67213300	-0.97950600	1.76550100
C	1.41227800	-3.28270800	-0.39392500
H	0.88020300	-2.88203900	-2.44650200
H	2.05005900	-3.36455700	1.66435700
H	1.15331400	-4.33616200	-0.44327300
P	-3.19375300	-0.35398800	0.19750200
Au	-1.18340000	0.62124300	-0.42398900
C	-4.56078600	1.00718200	-0.00317700
C	-4.03391200	2.35279900	0.55013600
C	-4.83837400	1.23846100	-1.50490300
C	-5.88397300	0.64909700	0.70607800
H	-3.83407400	2.33848300	1.61968700
H	-3.12329900	2.67095500	0.03435700
H	-4.80147200	3.11414200	0.37133400
H	-5.34264400	0.39876200	-1.98406100
H	-5.50247800	2.10490700	-1.59559200
H	-3.92512200	1.46926800	-2.06137300
H	-6.61785300	1.43128300	0.48177400
H	-6.30737500	-0.29839300	0.36771700
H	-5.78020800	0.61244700	1.79214300
C	-3.53058200	-1.85017900	-0.98149000
C	-3.12334000	-1.46231800	-2.42361600
C	-2.63102600	-3.04185500	-0.58662200
C	-5.00270300	-2.31397600	-0.97105300
H	-3.70138600	-0.63920600	-2.83904000
H	-2.06312900	-1.20097800	-2.48342900
H	-3.28821800	-2.33408800	-3.06698100
H	-2.91597400	-3.49632800	0.36319000
H	-2.74302900	-3.81383100	-1.35610600
H	-1.57317200	-2.76834300	-0.55034700
H	-5.08882200	-3.19768100	-1.61322000
H	-5.35099500	-2.60192500	0.02280800
H	-5.68461900	-1.56211100	-1.37139700
C	-3.05335000	-0.93336300	2.03672500
C	-1.68162100	-1.61620900	2.25006500
C	-3.07921800	0.29530600	2.97171600
C	-4.17927700	-1.90296800	2.45530100
H	-1.54760100	-2.52311300	1.66446500
H	-0.85335600	-0.94165500	2.01684700
H	-1.60237500	-1.89267700	3.30772300
H	-4.05752400	0.77471200	3.02061300
H	-2.83900200	-0.04610700	3.98453300
H	-2.33171500	1.04341900	2.69199500

H	-4.06570100	-2.12330000	3.52271300
H	-5.17635800	-1.48159500	2.31568000
H	-4.13100400	-2.85605100	1.92584300
C	1.90464400	1.87999100	2.07426600
H	1.68874300	2.80430800	1.55091300
C	3.15970100	1.65478300	2.59798500
H	3.31651700	0.78614800	3.23472300
S	4.26743400	1.30219800	-0.21037100
C	5.17154100	-0.25106000	-0.12438300
C	5.38941300	-0.95166500	-1.31804200
C	5.74860200	-0.69296900	1.07051300
C	6.16762200	-2.10841600	-1.30497800
H	4.95860000	-0.59236100	-2.24660200
C	6.53466200	-1.84661300	1.07058900
H	5.58934400	-0.14624700	1.99224600
C	6.74155700	-2.55612700	-0.11302900
H	6.33394600	-2.65260300	-2.22945500
H	6.98460400	-2.18818800	1.99769600
H	7.35469500	-3.45196000	-0.10878400
C	4.27589500	2.33858000	2.12116300
H	4.15532800	3.29017200	1.61401800
H	5.27351600	2.12850200	2.49206900
H	1.05167900	1.27653600	2.36529400

Zero-point correction= 0.685839 (Hartree/Particle)
Thermal correction to Energy= 0.727533
Thermal correction to Enthalpy= 0.728478
Thermal correction to Gibbs Free Energy= 0.610054
Sum of electronic and zero-point Energies= -2194.873508
Sum of electronic and thermal Energies= -2194.831814
Sum of electronic and thermal Enthalpies= -2194.830870
Sum of electronic and thermal Free Energies= -2194.949294
E(RB3LYP) = -2196.23701365 A.U.

A-TSd1

1 1

C	-1.91971200	0.07651400	-0.33901600
C	-1.80033400	-0.61062500	-1.61086800
O	-1.04905000	-0.28279800	-2.52542100
O	-2.56817400	-1.74385800	-1.71078900
C	-2.39483200	-2.49407900	-2.92978600
H	-1.36853500	-2.85767800	-3.01588000
H	-3.08965000	-3.33086500	-2.85790800
H	-2.62496900	-1.87604000	-3.79958400
C	-1.45270300	1.49857100	-0.17138800

C	-1.25032300	2.35571200	-1.28836100
C	-1.25845600	2.07110500	1.12011600
C	-0.89000200	3.68885200	-1.11296900
H	-1.37691200	1.95587100	-2.28526300
C	-0.91330900	3.41506000	1.27722300
H	-1.42083800	1.46558900	2.00595900
C	-0.72876400	4.23404200	0.16462200
H	-0.75248900	4.31429400	-1.99021500
H	-0.79357800	3.81578300	2.27943500
H	-0.46604100	5.27979100	0.28794400
P	2.97557000	-0.21479300	0.04681900
Au	0.71862600	0.34547500	0.06280300
C	3.29797400	-1.59069600	1.37256200
C	2.51282500	-1.24922700	2.66120200
C	2.73858100	-2.93834300	0.86950900
C	4.79298900	-1.76712700	1.71317000
H	2.83273300	-0.32421900	3.13684900
H	1.43820400	-1.18272100	2.46856000
H	2.67581800	-2.05914400	3.38182600
H	3.30287000	-3.35400200	0.03408600
H	2.80518400	-3.65950600	1.69183500
H	1.68615600	-2.86094300	0.58191100
H	4.89210100	-2.60467300	2.41295300
H	5.40283800	-2.00191500	0.83879800
H	5.21738100	-0.88985200	2.20401500
C	3.38289000	-0.84915100	-1.73741900
C	2.25223300	-1.78864600	-2.22256700
C	3.39929000	0.34402600	-2.71781400
C	4.73585200	-1.58812400	-1.81990000
H	2.13456200	-2.68057400	-1.60932100
H	1.28933900	-1.27343900	-2.28445400
H	2.51085500	-2.12271900	-3.23412800
H	4.24900000	1.01093300	-2.56738200
H	3.48209300	-0.05817000	-3.73330300
H	2.47339600	0.92430100	-2.67394600
H	4.92649700	-1.83948100	-2.86928700
H	5.57506900	-0.98138800	-1.47520800
H	4.73887400	-2.52745600	-1.26298700
C	3.97689300	1.39338200	0.46231000
C	3.34504600	2.59646600	-0.27801100
C	3.85604900	1.70576600	1.96976100
C	5.47089200	1.28873500	0.08862900
H	3.37926500	2.51219400	-1.36229800
H	2.30498000	2.75485500	0.02117700

H	3.91045800	3.49395500	-0.00193800
H	4.39196300	0.99575600	2.60081200
H	4.30189500	2.69074400	2.14616600
H	2.81329800	1.75736500	2.29613600
H	5.97278700	2.20616800	0.41597500
H	5.97400300	0.45215300	0.57708500
H	5.62903800	1.20554800	-0.98792600
C	-1.26028000	-3.21411300	2.64690900
H	-1.94828100	-3.23037200	3.48849900
C	-1.62369500	-2.76234500	1.44456100
H	-0.91914100	-2.76398900	0.61723500
S	-3.04750000	-0.42115800	0.91037700
C	-4.78910900	-0.13895200	0.47081700
C	-5.36431700	-0.55429700	-0.73543200
C	-5.53522100	0.55195100	1.43265400
C	-6.71111900	-0.27708300	-0.96677200
H	-4.77002300	-1.07782700	-1.47357500
C	-6.88344800	0.81810700	1.18722500
H	-5.07085300	0.87855100	2.35816400
C	-7.46917800	0.40415200	-0.00962800
H	-7.17001700	-0.59446100	-1.89800200
H	-7.46971500	1.35183900	1.92842000
H	-8.51688700	0.61475700	-0.20023900
C	-3.00007500	-2.27128400	1.13471900
H	-3.40337300	-2.70411700	0.22046800
H	-3.69252100	-2.42895400	1.96554400
H	-0.26390200	-3.60495900	2.82656200

Zero-point correction= 0.686851 (Hartree/Particle)
Thermal correction to Energy= 0.728381
Thermal correction to Enthalpy= 0.729325
Thermal correction to Gibbs Free Energy= 0.611564
Sum of electronic and zero-point Energies= -2194.872383
Sum of electronic and thermal Energies= -2194.830853
Sum of electronic and thermal Enthalpies= -2194.829909
Sum of electronic and thermal Free Energies= -2194.947670
E(RB3LYP) = -2196.23459110 A.U.

A-1d

C	-2.46535900	0.67677300	-0.50896200
C	-1.72502700	1.59648600	-1.35202500
O	-0.65066000	1.34179700	-1.90004600
O	-2.30612200	2.82107500	-1.47981400
C	-1.62820100	3.74711700	-2.34266800
H	-1.53849600	3.34221600	-3.35346400

H	-2.24583100	4.64505200	-2.34657000
H	-0.62923400	3.97335100	-1.96177000
C	-1.99137900	-0.66641400	-0.22174400
C	-1.08991900	-1.34196300	-1.12256600
C	-2.42896900	-1.41746700	0.89476800
C	-0.73891900	-2.70350400	-0.90783200
H	-0.91575700	-0.90192500	-2.09880200
C	-2.04531600	-2.73958300	1.09723900
H	-3.11146200	-0.97339400	1.60714600
C	-1.19204600	-3.40058400	0.20754700
H	-0.13466000	-3.20330600	-1.65959300
H	-2.42610700	-3.26697300	1.96748400
H	-0.91285600	-4.43608500	0.36836200
P	3.19291600	0.02046800	0.18401500
Au	1.01772100	-0.67524200	-0.38346700
C	3.29720400	0.20134100	2.10806200
C	2.00163100	0.87513100	2.62077000
C	3.33984600	-1.19542100	2.76519700
C	4.52072600	1.01372700	2.58201300
H	1.85714400	1.88761900	2.24814000
H	1.11707200	0.28626500	2.36017800
H	2.05751300	0.93058000	3.71421400
H	4.27790300	-1.72432400	2.59169100
H	3.24471600	-1.06120100	3.84846600
H	2.50930700	-1.82853000	2.44007200
H	4.53877300	1.00790200	3.67784800
H	5.46670000	0.59014600	2.23988400
H	4.47876300	2.05831000	2.26849900
C	4.43417700	-1.32597600	-0.44950900
C	3.87190800	-2.73175900	-0.12940100
C	4.53964200	-1.24644300	-1.98852200
C	5.84620800	-1.19192600	0.15859300
H	3.78042900	-2.93685500	0.93550900
H	2.89315900	-2.88722600	-0.59177800
H	4.56042300	-3.47480700	-0.54757100
H	5.05272200	-0.35030600	-2.33948200
H	5.12505200	-2.10658400	-2.33160000
H	3.55999900	-1.30555800	-2.47203900
H	6.49351400	-1.94785700	-0.30017900
H	6.30047900	-0.21778700	-0.03102800
H	5.85713000	-1.37357300	1.23473800
C	3.50881500	1.71894500	-0.69091000
C	2.93734200	1.66524400	-2.12905600
C	2.71871900	2.82861500	0.03646000

C	5.00032400	2.11078300	-0.73858400
H	3.40257500	0.90898200	-2.75844900
H	1.85570800	1.50631600	-2.12996600
H	3.12854600	2.63739500	-2.59879700
H	3.11289900	3.06038000	1.02701700
H	2.79848900	3.74292100	-0.56208400
H	1.65566000	2.58418400	0.11723300
H	5.08088000	3.11071300	-1.17973300
H	5.46215600	2.15381000	0.24981800
H	5.59029900	1.43887700	-1.36459000
C	-1.63350000	2.47288200	2.90443400
H	-1.46872800	1.50693900	3.37498600
C	-2.72844200	2.72889900	2.18648300
H	-2.86903300	3.70699800	1.73163400
S	-3.94031800	1.32913300	0.12903100
C	-5.19990500	0.02153900	0.05896500
C	-6.06817400	-0.24045000	1.12138300
C	-5.34014200	-0.64039600	-1.16533100
C	-7.07957500	-1.19028400	0.95333900
H	-5.97856100	0.27131900	2.07168900
C	-6.35154600	-1.58740600	-1.31566400
H	-4.66254000	-0.42398500	-1.98441900
C	-7.22195800	-1.86431300	-0.25876400
H	-7.75403400	-1.39875300	1.77784000
H	-6.45974700	-2.10575800	-2.26313800
H	-8.00993000	-2.60042300	-0.38161200
C	-3.81980400	1.73229100	1.97493400
H	-3.66669100	0.81814300	2.55000100
H	-4.80266200	2.15640800	2.20329600
H	-0.87617200	3.23305200	3.06710000

Zero-point correction= 0.686887 (Hartree/Particle)
Thermal correction to Energy= 0.729236
Thermal correction to Enthalpy= 0.730180
Thermal correction to Gibbs Free Energy= 0.608598
Sum of electronic and zero-point Energies= -2194.880567
Sum of electronic and thermal Energies= -2194.838218
Sum of electronic and thermal Enthalpies= -2194.837274
Sum of electronic and thermal Free Energies= -2194.958856
E(RB3LYP) = -2196.24175070 A.U

A-TSd2

C	-2.53338500	0.89383500	-0.31075900
C	-1.69849900	1.86696600	-1.01941900
O	-0.53560000	1.68121000	-1.38370800

O	-2.32545200	3.04800100	-1.21727700
C	-1.57260000	4.06317600	-1.90139400
H	-1.25854300	3.71210000	-2.88683400
H	-2.25038600	4.91067300	-1.99683900
H	-0.68833600	4.34476100	-1.32400600
C	-2.06927900	-0.49004100	-0.13484700
C	-1.20432400	-1.10549900	-1.09773600
C	-2.49614700	-1.29214500	0.94018000
C	-0.83738900	-2.46861300	-0.96894300
H	-1.01612700	-0.59048100	-2.03441100
C	-2.10985300	-2.62829800	1.06225800
H	-3.16503500	-0.87488600	1.68352500
C	-1.27433200	-3.22815900	0.12068300
H	-0.25874600	-2.93203900	-1.76273900
H	-2.47538500	-3.20718400	1.90534700
H	-0.99102700	-4.27113200	0.21305300
P	3.22076700	-0.04598900	0.17111300
Au	0.99631200	-0.61255600	-0.33560000
C	3.38375400	0.17680500	2.08660900
C	2.13761100	0.92647600	2.61291000
C	3.37718200	-1.20279600	2.78082200
C	4.65853700	0.94043400	2.50352500
H	2.02051800	1.92645200	2.19887400
H	1.22200200	0.36181300	2.41403800
H	2.23476900	1.02995700	3.69965900
H	4.28229000	-1.78341300	2.59738200
H	3.31966000	-1.03460000	3.86192900
H	2.50666800	-1.80141100	2.49748300
H	4.70813200	0.95959500	3.59805600
H	5.57255500	0.46347800	2.14565200
H	4.65727100	1.97813600	2.16552900
C	4.36195500	-1.48046000	-0.45637400
C	3.72792500	-2.84166200	-0.08383000
C	4.43213200	-1.44801000	-1.99839900
C	5.79485600	-1.41120500	0.11285400
H	3.64614000	-3.01159500	0.98797500
H	2.73333900	-2.95245800	-0.52473800
H	4.36467200	-3.63412900	-0.49308700
H	4.97823300	-0.58746000	-2.38599100
H	4.96658600	-2.34461000	-2.33095600
H	3.43812000	-1.47283800	-2.45484300
H	6.38234700	-2.22156600	-0.33323800
H	6.30230100	-0.47492900	-0.12555700
H	5.82521100	-1.55393300	1.19441200

C	3.60729100	1.60809200	-0.76107600
C	3.00230100	1.54805600	-2.18523000
C	2.89628400	2.78128500	-0.05088300
C	5.11738700	1.91205900	-0.85101100
H	3.41901500	0.75947300	-2.80890200
H	1.91519800	1.43894300	-2.15558600
H	3.22327000	2.50105200	-2.68001600
H	3.31243300	3.01027600	0.93110300
H	3.03027300	3.67475300	-0.67076600
H	1.82024000	2.60785200	0.03731000
H	5.24355500	2.89492900	-1.31881600
H	5.60228600	1.95323400	0.12616200
H	5.65497900	1.19316900	-1.47233300
C	-1.65544900	1.95737300	1.90694200
H	-1.66626000	0.92411000	2.23335800
C	-2.75092700	2.77165600	2.08758600
H	-2.67319000	3.82461800	1.82764400
S	-4.19908300	1.36952900	-0.09427500
C	-5.19910800	-0.12663100	-0.11022200
C	-6.11816500	-0.33731100	0.92357700
C	-5.16867400	-0.98678300	-1.21619000
C	-6.99509200	-1.42244600	0.85729200
H	-6.15965600	0.33956900	1.77023700
C	-6.03916300	-2.07432500	-1.26470400
H	-4.47863800	-0.80156700	-2.03233700
C	-6.95251800	-2.29485600	-0.23032800
H	-7.70876900	-1.58317700	1.65941700
H	-6.01307600	-2.74204700	-2.12043700
H	-7.63383200	-3.13853400	-0.27775500
C	-4.01955000	2.23691400	2.30903400
H	-4.12453200	1.23895600	2.72285700
H	-4.89503100	2.87439600	2.37207000
H	-0.68846300	2.36396300	1.63151400

Zero-point correction= 0.685471 (Hartree/Particle)
Thermal correction to Energy= 0.727277
Thermal correction to Enthalpy= 0.728221
Thermal correction to Gibbs Free Energy= 0.610515
Sum of electronic and zero-point Energies= -2194.865358
Sum of electronic and thermal Energies= -2194.823552
Sum of electronic and thermal Enthalpies= -2194.822607
Sum of electronic and thermal Free Energies= -2194.940313
E(RB3LYP) = -2196.22897407 A.U.

A-TSb11

C	0.89175300	0.20892300	-0.35697000
C	1.23465600	-0.81046700	-1.40051900
O	1.18322200	-0.51609900	-2.57977000
O	1.43619300	-2.06378600	-0.95389600
C	1.59931600	-3.06045500	-1.99225800
H	2.47203000	-2.82846500	-2.60511800
H	1.73790200	-4.00401900	-1.46641000
H	0.71013500	-3.09556700	-2.62431300
C	1.49178400	1.53989000	-0.47254200
C	2.60503000	1.79940800	-1.30823700
C	0.94526000	2.61939800	0.25995200
C	3.12365500	3.08475100	-1.41810800
H	3.03895600	0.99401600	-1.88702600
C	1.47919000	3.89903000	0.16397700
H	0.08965300	2.43792800	0.90431800
C	2.56852600	4.13618900	-0.68019400
H	3.96099300	3.27147800	-2.08341000
H	1.04395800	4.71343900	0.73443500
H	2.98033300	5.13717200	-0.76675700
P	-3.57880700	-0.11184200	0.21063000
Au	-1.19420100	0.03784700	0.01531800
C	-4.05788800	-1.97648700	0.41811200
C	-3.19435500	-2.82812600	-0.54351600
C	-3.69933900	-2.44668400	1.84490400
C	-5.55084600	-2.26466700	0.15821700
H	-3.36675300	-2.61152900	-1.59600700
H	-2.12650600	-2.70498300	-0.33902500
H	-3.44416500	-3.88287200	-0.38104900
H	-4.34839100	-2.02294700	2.61242500
H	-3.82385800	-3.53439000	1.88543400
H	-2.65800200	-2.22820100	2.10044000
H	-5.74262600	-3.32346800	0.36650100
H	-6.21273100	-1.68225200	0.80182900
H	-5.83863500	-2.08737300	-0.87961700
C	-4.13280700	0.91575100	1.75718900
C	-3.15883500	0.63347200	2.92655000
C	-4.00078700	2.42247900	1.44456500
C	-5.57661700	0.62416300	2.21580300
H	-3.19173300	-0.39302400	3.28682900
H	-2.12532600	0.86714600	2.65318100
H	-3.43493500	1.28243300	3.76541000
H	-4.73580300	2.77729700	0.72140700
H	-4.17004700	2.97841700	2.37334700
H	-2.99984800	2.68139200	1.08634500

H	-5.81639400	1.28839300	3.05404000
H	-6.31524200	0.80966600	1.43372700
H	-5.70374300	-0.39907900	2.57376300
C	-4.34270500	0.61926800	-1.41233500
C	-3.56252900	1.89689100	-1.80782000
C	-4.14257800	-0.37875700	-2.57442700
C	-5.84408000	0.95269700	-1.29161600
H	-3.64260000	2.70348600	-1.08130600
H	-2.50162100	1.68723100	-1.97370700
H	-3.97622800	2.26779400	-2.75251400
H	-4.74873200	-1.28018900	-2.47624700
H	-4.45251700	0.11642900	-3.50112200
H	-3.09369400	-0.66474200	-2.69592300
H	-6.20360800	1.29419300	-2.26896500
H	-6.44862600	0.08946700	-1.00688600
H	-6.03950300	1.75839500	-0.58131800
C	1.50790000	-0.58749800	1.55311000
H	0.95241100	-1.51837700	1.54426900
C	2.87363600	-0.60344100	1.41327500
H	3.41726000	0.33292200	1.53071700
S	4.66958700	-1.47221300	-0.48301600
C	6.17211900	-0.73105300	0.16193000
C	6.34831100	0.65851500	0.11470800
C	7.19307800	-1.55058700	0.66578800
C	7.53674400	1.22392600	0.58066900
H	5.56085300	1.28836500	-0.28695000
C	8.37455100	-0.97742800	1.13511300
H	7.06417400	-2.62853100	0.67726300
C	8.54727100	0.40856200	1.09300800
H	7.67252300	2.30056800	0.54242600
H	9.16429400	-1.61356000	1.52294400
H	9.47091400	0.85079900	1.45359600
C	3.70290800	-1.78397600	1.08284400
H	4.43320200	-1.97220400	1.87611700
H	3.10291500	-2.68036900	0.92633000
H	1.05069600	0.24782000	2.06754400

Zero-point correction=	0.686174 (Hartree/Particle)
Thermal correction to Energy=	0.728004
Thermal correction to Enthalpy=	0.728949
Thermal correction to Gibbs Free Energy=	0.609568
Sum of electronic and zero-point Energies=	-2194.868539
Sum of electronic and thermal Energies=	-2194.826709
Sum of electronic and thermal Enthalpies=	-2194.825764
Sum of electronic and thermal Free Energies=	-2194.945145

E(RB3LYP) = -2196.23042419 A.U.

A-P1

C	-0.48644700	0.02174200	0.06363700
C	-0.30262300	1.52950100	-0.15183600
O	0.49081800	2.21103100	0.46590600
O	-1.04941400	2.00832700	-1.16588200
C	-0.81326200	3.38268800	-1.51062400
H	0.20827000	3.51484100	-1.87666100
H	-1.53102100	3.61369400	-2.29715100
H	-0.96472000	4.03157000	-0.64501900
C	-1.90756000	-0.50333300	-0.16876500
C	-3.02642100	0.30769200	0.07986000
C	-2.13040700	-1.84767100	-0.50132500
C	-4.31969300	-0.20340200	-0.02060300
H	-2.89249100	1.34721600	0.35327400
C	-3.42468100	-2.35829100	-0.60523000
H	-1.28450600	-2.49957700	-0.68775800
C	-4.52664600	-1.53818100	-0.36884800
H	-5.16695500	0.44779100	0.17412000
H	-3.56700500	-3.40130700	-0.87292300
H	-5.53460200	-1.93371300	-0.45285900
C	-0.59309900	1.06641000	3.43748400
H	0.32295200	1.64301500	3.34603500
C	-0.87735800	0.07267700	2.59533700
H	-1.81442000	-0.46991100	2.70597500
S	0.63057300	-0.72650500	-1.29349100
C	2.29540900	-0.64332300	-0.62703500
C	2.89393600	-1.81477300	-0.14068600
C	3.03979000	0.54440100	-0.67309700
C	4.21790900	-1.79683200	0.29874700
H	2.31958800	-2.73508300	-0.11443300
C	4.35875700	0.55917700	-0.22022400
H	2.58242500	1.45150200	-1.04972200
C	4.95050800	-0.60949600	0.26312800
H	4.67441900	-2.70936000	0.67089100
H	4.92642100	1.48447000	-0.25184100
H	5.98041500	-0.59524900	0.60758800
C	0.02708800	-0.37585100	1.47409400
H	0.11790000	-1.46787600	1.48995400
H	1.02319800	0.04712700	1.61183800
H	-1.27146200	1.34125500	4.24027800

Zero-point correction= 0.314870 (Hartree/Particle)

Thermal correction to Energy= 0.335118

Thermal correction to Enthalpy= 0.336062

Thermal correction to Gibbs Free Energy= 0.263785

Sum of electronic and zero-point Energies= -1245.076279

Sum of electronic and thermal Energies= -1245.056031

Sum of electronic and thermal Enthalpies= -1245.055087

Sum of electronic and thermal Free Energies= -1245.127364

E(RB3LYP) = -1245.73478237 A.U.

A-P3

C	1.81461400	0.26450600	0.44343900
C	1.71898400	1.67866800	-0.07019300
O	2.28564700	2.08726200	-1.06083600
O	0.91810300	2.46857500	0.69061000
C	0.78773800	3.82555900	0.23102300
H	0.37262200	3.85419800	-0.77918900
H	0.11499800	4.31044700	0.93793300
H	1.76142100	4.32047100	0.22419500
C	3.05751000	-0.45712800	-0.01553700
C	3.17609300	-0.89650100	-1.34085500
C	4.11908300	-0.68495300	0.86693000
C	4.32506200	-1.55813500	-1.76939200
H	2.36438200	-0.71151800	-2.03744200
C	5.27141700	-1.34790900	0.44019000
H	4.04536000	-0.33911300	1.89408500
C	5.37628000	-1.78789100	-0.87882100
H	4.40078900	-1.89442000	-2.79940400
H	6.08532500	-1.51841600	1.13900200
H	6.27067200	-2.30602600	-1.21233600
C	1.20712100	-0.08551100	1.79026400
H	0.73726000	0.72191800	2.33987100
C	0.52236200	-0.57535700	0.55060600
H	0.69291700	-1.62048300	0.30437100
S	-2.11823700	-0.96982900	1.09424400
C	-3.62807400	-0.61381500	0.20825500
C	-3.78225900	0.45693500	-0.68239300
C	-4.72353200	-1.45528200	0.46150700
C	-5.00921600	0.67090000	-1.31427400
H	-2.95767800	1.13085200	-0.88505400
C	-5.94697400	-1.22426100	-0.16172500
H	-4.61042000	-2.29466000	1.14156600
C	-6.09649700	-0.16264100	-1.05737000
H	-5.11148100	1.50217700	-2.00627700
H	-6.78394400	-1.88501800	0.04535500
H	-7.04878400	0.01048500	-1.54898400

C	-0.83557000	-0.06905700	0.12120400
H	-0.92828600	1.00284400	0.30000600
H	-1.00674900	-0.27300100	-0.94023600
H	1.73855300	-0.80894600	2.39928800

Zero-point correction= 0.314669 (Hartree/Particle)
Thermal correction to Energy= 0.334895
Thermal correction to Enthalpy= 0.335840
Thermal correction to Gibbs Free Energy= 0.263952
Sum of electronic and zero-point Energies= -1245.072245
Sum of electronic and thermal Energies= -1245.052018
Sum of electronic and thermal Enthalpies= -1245.051074
Sum of electronic and thermal Free Energies= -1245.122962
E(RB3LYP) = -1245.73456793 A.U.

Re3

C	-4.25321200	-0.26757100	0.85067100
H	-4.30504500	0.61466600	1.48403100
C	-3.08469500	-0.79713700	0.48314500
H	-3.06419100	-1.66928400	-0.16863800
C	1.00112100	0.11920100	-0.20601000
C	1.72995300	1.10897900	0.46229600
C	1.60634500	-1.10836800	-0.49830600
C	3.05148900	0.86909400	0.84192600
H	1.25926000	2.06251900	0.67881700
C	2.92697800	-1.34721500	-0.11556800
H	1.03963200	-1.86730700	-1.02819000
C	3.65029900	-0.35900400	0.55501700
H	3.61242600	1.64126600	1.36063900
H	3.39112300	-2.30210000	-0.34515100
H	4.67911500	-0.54407300	0.84986300
C	-1.75198300	-0.25332800	0.87250100
H	-1.83613300	0.56284100	1.59135100
H	-1.08946100	-1.02916100	1.26258400
H	-5.19811300	-0.69904000	0.53550500
Se	-0.81607000	0.45417000	-0.75573100

Zero-point correction= 0.161791 (Hartree/Particle)
Thermal correction to Energy= 0.172081
Thermal correction to Enthalpy= 0.173026
Thermal correction to Gibbs Free Energy= 0.123231
Sum of electronic and zero-point Energies= -2748.189351
Sum of electronic and thermal Energies= -2748.179061
Sum of electronic and thermal Enthalpies= -2748.178116
Sum of electronic and thermal Free Energies= -2748.227911
E(RB3LYP) = -2750.64618048 A.U.

B-1a

C	1.36173700	0.04829700	-0.56206200
C	1.47929400	-1.08665900	-1.55002400
O	1.32850200	-0.95950800	-2.74619500
O	1.70578500	-2.29022100	-0.95938600
C	1.71357600	-3.42613400	-1.85008400
H	2.47606200	-3.30075600	-2.62111000
H	1.93491300	-4.28805100	-1.22179900
H	0.73771200	-3.53953300	-2.32695000
C	1.90838800	1.36222800	-1.04723000
C	3.00205500	1.42049000	-1.93264500
C	1.34257500	2.57926600	-0.62306000
C	3.50020300	2.64440800	-2.37640900
H	3.44878300	0.50405100	-2.30059100
C	1.84993200	3.80517000	-1.05524200
H	0.48174000	2.55681900	0.03901500
C	2.93135600	3.84146900	-1.93626300
H	4.33362300	2.66178600	-3.07217400
H	1.38988200	4.72884800	-0.71688000
H	3.32075000	4.79288500	-2.28531200
P	-3.14679800	-0.14057900	0.02077200
Au	-0.76305800	0.01323400	-0.13423400
C	-3.90547800	1.64033500	-0.01675000
C	-3.08237900	2.55853800	0.91819600
C	-3.75665900	2.23194600	-1.43585700
C	-5.38991600	1.69265900	0.39848100
H	-3.13454800	2.27351700	1.96732400
H	-2.02961400	2.58910300	0.62318300
H	-3.48115900	3.57608300	0.83488300
H	-4.40775700	1.75513800	-2.16920900
H	-4.04125800	3.28913500	-1.39451300
H	-2.72441100	2.18477600	-1.79590200
H	-5.74749000	2.72272300	0.28706200
H	-6.02496200	1.05918200	-0.22316100
H	-5.54287300	1.41283800	1.44272700
C	-3.72720000	-1.15870700	-1.52500000
C	-2.93008800	-0.69390300	-2.76878200
C	-3.37127000	-2.64792900	-1.32344300
C	-5.23779500	-1.04167700	-1.81612800
H	-3.10818700	0.34433700	-3.04171400
H	-1.85273000	-0.83164800	-2.63952900
H	-3.24169900	-1.31118400	-3.61926800
H	-3.97046300	-3.13324400	-0.55199200

H	-3.57086100	-3.17380600	-2.26362400
H	-2.31125200	-2.78731800	-1.09042200
H	-5.48156100	-1.70280500	-2.65555300
H	-5.85981700	-1.34665300	-0.97228600
H	-5.52981800	-0.03239700	-2.11204200
C	-3.62440300	-1.05445900	1.66056800
C	-2.63917300	-2.22768100	1.88264000
C	-3.42877400	-0.10120400	2.85946300
C	-5.07114900	-1.59087300	1.67999200
H	-2.67897000	-2.98639100	1.10350700
H	-1.60670800	-1.87431200	1.96172500
H	-2.89755400	-2.71634500	2.82930000
H	-4.17217900	0.69631700	2.89743300
H	-3.53930900	-0.68596800	3.77962500
H	-2.42863600	0.34254000	2.86978800
H	-5.26512400	-2.03476700	2.66330900
H	-5.81502000	-0.80685700	1.52584300
H	-5.23967100	-2.37398100	0.93832600
C	0.24298500	2.11246500	3.26110000
H	0.33579800	2.97160400	2.60247900
C	1.10122900	1.09075200	3.21361700
H	0.99040600	0.25664700	3.90421800
C	4.15826500	-0.73219300	0.77587100
C	4.98004200	0.38538000	0.59631300
C	4.67361000	-2.03061300	0.69791200
C	6.33867600	0.19068100	0.34127800
H	4.58177600	1.39192000	0.64571700
C	6.03238700	-2.20956400	0.43768900
H	4.02596700	-2.88910400	0.84175100
C	6.86326200	-1.10108300	0.26128700
H	6.98489800	1.05186900	0.20362100
H	6.44050000	-3.21369900	0.38072500
H	7.92106700	-1.24373000	0.06400600
C	2.28422400	1.04879800	2.30209700
H	2.34844700	1.91438500	1.64068200
H	3.22126700	0.92704800	2.85258400
H	-0.56528100	2.13514400	3.98498400
Se	2.26198600	-0.59136300	1.15654800

Zero-point correction= 0.685362 (Hartree/Particle)
Thermal correction to Energy= 0.728301
Thermal correction to Enthalpy= 0.729245
Thermal correction to Gibbs Free Energy= 0.607526
Sum of electronic and zero-point Energies= -4195.645619
Sum of electronic and thermal Energies= -4195.602679

Sum of electronic and thermal Enthalpies= -4195.601735

Sum of electronic and thermal Free Energies= -4195.723455

E(RB3LYP) = -4199.60711577 A.U.

B-TSa1

1 1

C	-1.82422200	-0.57143900	-0.08091100
C	-1.78120000	-0.67791000	-1.53261500
O	-1.28710000	-1.60855800	-2.16287100
O	-2.30666500	0.41618300	-2.17597600
C	-2.20907500	0.40562500	-3.60933200
H	-2.66571000	-0.49721200	-4.01951700
H	-2.74493400	1.29279200	-3.94701400
H	-1.16417100	0.45152700	-3.92759800
C	-1.89999700	-1.82065400	0.73046100
C	-2.58734400	-2.96223100	0.27406600
C	-1.26527600	-1.89692400	1.98492900
C	-2.63725300	-4.12533700	1.04241100
H	-3.05913400	-2.94509700	-0.70231900
C	-1.32943400	-3.05410900	2.76305200
H	-0.70275900	-1.03648700	2.33679100
C	-2.01634200	-4.17536000	2.29265100
H	-3.16415600	-4.99604000	0.66293600
H	-0.83149700	-3.08487400	3.72829400
H	-2.06090500	-5.08099100	2.88998800
P	1.81684400	2.47596700	-0.01495400
Au	0.77663600	0.33267000	-0.15805600
C	2.75811600	2.53181200	1.68023400
C	1.85816900	1.89594200	2.76595600
C	4.02099900	1.64531300	1.60538500
C	3.17120900	3.95052400	2.12573700
H	0.91928400	2.42364400	2.92265400
H	1.62669600	0.85373100	2.52718400
H	2.40680900	1.90657500	3.71505100
H	4.80406700	2.06553600	0.97265100
H	4.43675500	1.56532200	2.61607900
H	3.79332100	0.63092700	1.26626900
H	3.74683200	3.86844800	3.05497300
H	3.80615800	4.45565600	1.39542800
H	2.31378000	4.59228700	2.33763300
C	3.06837900	2.69128000	-1.48361000
C	3.81120900	1.35567900	-1.71044300
C	2.29906100	2.97309100	-2.79272700
C	4.10295200	3.81559600	-1.26191500

H	4.39504100	1.03030100	-0.85177100
H	3.10727700	0.56022000	-1.96863500
H	4.50156400	1.48448600	-2.55226100
H	1.85121900	3.96694300	-2.82205800
H	3.01156600	2.91830200	-3.62343700
H	1.52077300	2.22716200	-2.97931600
H	4.71031500	3.91149100	-2.16934500
H	3.64221400	4.78708700	-1.07611800
H	4.78875500	3.59805600	-0.44114800
C	0.48488200	3.88334000	-0.09728600
C	-0.52710400	3.55079200	-1.21947100
C	-0.31967400	3.89281100	1.21958400
C	1.05904000	5.29520800	-0.33791700
H	-0.09574300	3.59339500	-2.21769100
H	-0.97913300	2.56547500	-1.08527300
H	-1.33080100	4.29584000	-1.18259500
H	0.25502100	4.26083500	2.07085700
H	-1.17390400	4.56774200	1.09257200
H	-0.71236300	2.90152300	1.46141500
H	0.23453000	6.01668400	-0.29640000
H	1.78779800	5.59355400	0.41760800
H	1.52076600	5.39978600	-1.32137200
C	-1.77931600	1.11953200	4.20454500
H	-1.63163800	0.06595400	4.42409500
C	-2.58920000	1.52899800	3.22506400
H	-2.73095800	2.59432400	3.05219800
C	-4.85356900	0.30690800	-0.18791300
C	-5.47325300	-0.85493400	0.28159500
C	-5.47244400	1.12559600	-1.13538600
C	-6.73908500	-1.18893100	-0.20298900
H	-4.98264700	-1.49791300	1.00365500
C	-6.73803400	0.77984700	-1.61265200
H	-4.97668200	2.02127900	-1.49602100
C	-7.37023300	-0.37417200	-1.14629600
H	-7.23052200	-2.08736700	0.15747400
H	-7.22816300	1.41349400	-2.34533700
H	-8.35510800	-0.63963200	-1.51768800
C	-3.40680600	0.60619900	2.38260400
H	-3.23869500	-0.44672100	2.61075500
H	-4.47310400	0.83719600	2.44889700
H	-1.25773200	1.83006200	4.83790700
C	3.34406100	-4.33469700	-3.12716600
H	4.19280200	-3.65665200	-3.16954100
C	2.12100300	-3.91308600	-2.79736600

H	1.29297900	-4.61879700	-2.76231400
C	2.88649700	-2.72256000	0.35624100
C	2.82531800	-3.59738800	1.44619100
C	4.11392600	-2.17853600	-0.03549100
C	3.98852300	-3.91212800	2.15244600
H	1.87550500	-4.03644800	1.73581100
C	5.27542700	-2.51148900	0.66352600
H	4.17163500	-1.50333900	-0.88198100
C	5.21483800	-3.37383300	1.76087300
H	3.93553900	-4.59119700	2.99820200
H	6.22876200	-2.09613500	0.34966900
H	6.12024000	-3.62908000	2.30285800
C	1.78624700	-2.50046600	-2.46531500
H	2.61578700	-1.81424100	-2.63984100
H	0.88850300	-2.14220100	-2.97300200
H	3.53776400	-5.37302500	-3.37663700
Se	-3.07666800	0.85767300	0.41664200
Se	1.21395100	-2.33717500	-0.54448600

Zero-point correction= 0.848196 (Hartree/Particle)
Thermal correction to Energy= 0.902552
Thermal correction to Enthalpy= 0.903496
Thermal correction to Gibbs Free Energy= 0.754713
Sum of electronic and zero-point Energies= -6943.353730
Sum of electronic and thermal Energies= -6943.299374
Sum of electronic and thermal Enthalpies= -6943.298430
Sum of electronic and thermal Free Energies= -6943.447213
E(RB3LYP) = -6950.25130102 A.U.

B-2a

C	-0.96136000	-0.29626600	-0.39904100
C	-1.66788800	-1.29511100	-1.16714100
O	-2.69432100	-1.13329000	-1.81610800
O	-1.05105300	-2.53221400	-1.13423700
C	-1.73557600	-3.56490400	-1.84568000
H	-1.83057000	-3.31600300	-2.90605400
H	-1.12698200	-4.46191000	-1.72070500
H	-2.73768300	-3.72834600	-1.43891100
C	-1.34523000	1.11885800	-0.32546100
C	-2.63412800	1.55221800	-0.72295300
C	-0.46651200	2.11472200	0.15992900
C	-3.00255000	2.89165500	-0.63612200
H	-3.32857400	0.82259600	-1.11554600
C	-0.84431800	3.45406800	0.24096200
H	0.54906200	1.85555400	0.43260900

C	-2.11884800	3.85816000	-0.15085800
H	-4.00115200	3.18115200	-0.95345400
H	-0.12825700	4.18419600	0.60956200
H	-2.41482700	4.90091600	-0.08707500
C	-2.04220500	-0.89824100	2.96101100
H	-2.47146700	-0.13446900	2.31919500
C	-0.72110900	-1.01324500	3.12890600
H	-0.31869200	-1.80180200	3.76193900
C	2.10978200	-0.12486100	-0.06690500
C	2.13219700	0.39116000	-1.36090200
C	3.26912500	-0.18004800	0.70768400
C	3.32748700	0.89972800	-1.87024900
H	1.21879700	0.40536900	-1.94809300
C	4.46094300	0.33025700	0.18982500
H	3.25789100	-0.61772300	1.70201200
C	4.48937900	0.87346300	-1.09605600
H	3.34966600	1.31569600	-2.87301100
H	5.36551400	0.29839500	0.78984500
H	5.41779400	1.26921700	-1.49634100
C	0.26377600	-0.16292900	2.40313000
H	-0.07184700	0.86049900	2.24615100
H	1.26142000	-0.17581300	2.84342700
H	-2.73560400	-1.55701800	3.47423000
Se	0.45972700	-0.99025200	0.56066100

Zero-point correction= 0.311909 (Hartree/Particle)
Thermal correction to Energy= 0.332984
Thermal correction to Enthalpy= 0.333928
Thermal correction to Gibbs Free Energy= 0.259131
Sum of electronic and zero-point Energies= -3246.231608
Sum of electronic and thermal Energies= -3246.210533
Sum of electronic and thermal Enthalpies= -3246.209589
Sum of electronic and thermal Free Energies= -3246.284386
E(RB3LYP) = -3249.01436305 A.U.

B-TSa2

C	1.05744800	0.19730200	-0.21444300
C	2.36775200	0.05153000	-0.84892500
O	3.08201100	0.94614600	-1.27511700
O	2.77668600	-1.26087500	-0.89869400
C	4.03167900	-1.48143600	-1.55239700
H	4.83863300	-0.95028300	-1.04116900
H	4.19841300	-2.55832600	-1.51139300
H	3.99567800	-1.14228900	-2.59107500
C	0.41050500	1.50080700	0.00649400

C	0.84738300	2.67859600	-0.63975300
C	-0.67952900	1.61701100	0.89474100
C	0.22276300	3.89986900	-0.39667300
H	1.68787800	2.62524000	-1.31742100
C	-1.29360000	2.84148700	1.13778100
H	-1.03961400	0.73750000	1.41083800
C	-0.85021700	3.99529500	0.49063000
H	0.58257000	4.78705700	-0.91089400
H	-2.12567200	2.89094500	1.83495700
H	-1.33167500	4.95111400	0.67539000
C	2.26905900	-0.13176500	2.10792800
H	2.71347700	0.84956700	2.22970500
C	1.10114900	-0.47600600	2.74199400
H	0.53846500	0.30294000	3.25114700
C	-1.73106700	-1.01719200	-0.35843800
C	-2.10302600	-0.36844700	-1.53900100
C	-2.70115600	-1.51353200	0.51389400
C	-3.45501400	-0.18846700	-1.82632800
H	-1.34098000	0.00202200	-2.21574500
C	-4.05339500	-1.34323300	0.21091800
H	-2.40680000	-2.02327800	1.42551200
C	-4.43159000	-0.67616100	-0.95466900
H	-3.74490500	0.32819000	-2.73636700
H	-4.80862500	-1.72707200	0.89044200
H	-5.48361800	-0.53887000	-1.18551800
C	0.46510700	-1.70204300	2.49870600
H	1.05458500	-2.57103400	2.22567200
H	-0.50025100	-1.91948500	2.94665500
H	2.87724700	-0.88409200	1.61726000
Se	0.13470900	-1.41010900	-0.03653700

Zero-point correction= 0.311076 (Hartree/Particle)
Thermal correction to Energy= 0.331433
Thermal correction to Enthalpy= 0.332377
Thermal correction to Gibbs Free Energy= 0.260683
Sum of electronic and zero-point Energies= -3246.220550
Sum of electronic and thermal Energies= -3246.200193
Sum of electronic and thermal Enthalpies= -3246.199249
Sum of electronic and thermal Free Energies= -3246.270943
E(RB3LYP) = -3249.00499663 A.U.

B-1c

C	-2.25550600	0.33803000	0.05822500
C	-1.80628600	-0.93118700	-0.32274000
O	-0.67763200	-1.21610700	-0.83764600

O	-2.68118600	-1.95521700	-0.13910300
C	-2.24496700	-3.27063100	-0.52603000
H	-1.36089500	-3.57202700	0.04049200
H	-3.08358200	-3.92801600	-0.29700300
H	-2.01800000	-3.30678500	-1.59350200
C	-1.49468800	1.59256100	-0.15469400
C	-0.91836400	1.87882600	-1.40848500
C	-1.36225200	2.55442400	0.86494100
C	-0.23922700	3.07751100	-1.62830300
H	-1.02483200	1.16321600	-2.21737600
C	-0.69992000	3.76081600	0.63792400
H	-1.78639100	2.35487500	1.84550600
C	-0.13316400	4.02819100	-0.60981000
H	0.18115200	3.28153000	-2.60909400
H	-0.62578400	4.49103700	1.43849400
H	0.37476100	4.97074300	-0.79030600
P	3.55847500	-0.13719200	0.02653700
Au	1.32143700	-0.57273800	-0.39524500
C	3.67963600	0.80749500	1.70916000
C	2.57303400	1.88783200	1.76639500
C	3.38709500	-0.16953900	2.86865600
C	5.05387300	1.46923100	1.94660200
H	2.68268700	2.67221600	1.02044800
H	1.57571300	1.45471500	1.65204900
H	2.61967700	2.36490100	2.75218800
H	4.17760400	-0.90542900	3.02130700
H	3.31073800	0.41519600	3.79191600
H	2.43575100	-0.69261400	2.73282300
H	5.04620800	1.93140100	2.94031500
H	5.87943200	0.75505300	1.92921900
H	5.26933600	2.26285900	1.22855500
C	4.46936500	-1.84241000	0.11795100
C	3.60596500	-2.84701900	0.91907700
C	4.60398500	-2.43357100	-1.30289800
C	5.87109500	-1.75335000	0.75817700
H	3.45007200	-2.56309200	1.95808200
H	2.62752300	-2.99508600	0.45342600
H	4.12456600	-3.81246900	0.91883300
H	5.31046600	-1.88885600	-1.93029700
H	4.98315700	-3.45691900	-1.20754600
H	3.64061200	-2.48906800	-1.81808100
H	6.34039200	-2.74204400	0.70175400
H	6.52924100	-1.05226700	0.24188700
H	5.83370300	-1.47792400	1.81381400

C	4.24987100	0.93802700	-1.42623500
C	3.69358400	0.40187900	-2.76756400
C	3.72885800	2.38487500	-1.29124600
C	5.79180400	0.96464900	-1.48441600
H	4.00504100	-0.61528900	-2.99753800
H	2.60077000	0.44020400	-2.79278200
H	4.06730300	1.04750500	-3.57047900
H	4.16987600	2.92100700	-0.44985600
H	4.01027400	2.92853400	-2.20002300
H	2.63932200	2.42583100	-1.20820100
H	6.09537700	1.65730800	-2.27740600
H	6.24461200	1.31667100	-0.55576300
H	6.22190400	-0.00820700	-1.72965000
C	-3.17038100	-0.39745800	4.42057000
H	-4.08604300	0.04325300	4.80730800
C	-3.08738300	-0.87894100	3.17731700
H	-2.15785500	-1.31832400	2.82348000
C	-5.29710100	0.02517200	-0.47015500
C	-4.93641600	-0.31891600	-1.76990300
C	-6.63436300	0.06277500	-0.06833300
C	-5.93916700	-0.65700400	-2.68079200
H	-3.89395300	-0.31677300	-2.06782000
C	-7.62702100	-0.28486300	-0.98596700
H	-6.91192800	0.36299900	0.93825600
C	-7.27949800	-0.64552100	-2.28958700
H	-5.67004900	-0.92800300	-3.69703200
H	-8.66909300	-0.26374000	-0.68283000
H	-8.05436800	-0.90924300	-3.00247500
C	-4.21812500	-0.87016300	2.20961400
H	-4.30549000	-1.78193500	1.62269400
H	-5.17086500	-0.60638600	2.67250100
H	-2.32728100	-0.44329700	5.10237000
Se	-3.95255800	0.59580000	0.83185100

Zero-point correction= 0.685599 (Hartree/Particle)
Thermal correction to Energy= 0.728528
Thermal correction to Enthalpy= 0.729472
Thermal correction to Gibbs Free Energy= 0.606294
Sum of electronic and zero-point Energies= -4195.636066
Sum of electronic and thermal Energies= -4195.593137
Sum of electronic and thermal Enthalpies= -4195.592193
Sum of electronic and thermal Free Energies= -4195.715371
E(RB3LYP) = -4199.58426729 A.U.

B-TSc2

C	-2.34720400	-0.78907300	-0.24036000
C	-1.52530200	-1.84997700	-0.73539800
O	-0.29179000	-1.81231700	-0.99422200
O	-2.16716700	-3.02283200	-0.89769700
C	-1.41259500	-4.14443800	-1.39806800
H	-0.59574600	-4.39472800	-0.71787300
H	-2.12765500	-4.96402800	-1.45404200
H	-1.00865400	-3.92267400	-2.38776800
C	-1.88712900	0.62254300	-0.29944400
C	-1.33324300	1.13097700	-1.49135200
C	-2.05448300	1.50657400	0.77954600
C	-0.95977700	2.47144800	-1.59494700
H	-1.21827900	0.47395700	-2.34816400
C	-1.68576700	2.84765600	0.67436800
H	-2.49038700	1.14201200	1.70212100
C	-1.13708200	3.33668700	-0.51273400
H	-0.55207600	2.84360900	-2.53055100
H	-1.83639200	3.51304800	1.51938400
H	-0.86372000	4.38414300	-0.59858800
P	3.43183000	0.34240900	0.19667400
Au	1.40513000	-0.62603900	-0.37963200
C	4.74198000	-1.08218100	0.25617400
C	4.13005200	-2.31405600	0.96552700
C	5.08104700	-1.54186200	-1.17925900
C	6.04803700	-0.67725000	0.97348600
H	3.84872100	-2.13210200	2.00079700
H	3.25161400	-2.68682200	0.43113100
H	4.88199100	-3.11113700	0.96606400
H	5.64662200	-0.80244300	-1.74762200
H	5.70846800	-2.43682000	-1.10527200
H	4.18619800	-1.81805100	-1.74455700
H	6.75610100	-1.50976400	0.89472000
H	6.52585800	0.19742100	0.52822700
H	5.90111100	-0.48438700	2.03788400
C	3.88256900	1.63775000	-1.16838600
C	3.52911100	1.05477200	-2.55800000
C	3.00985100	2.89991800	-0.99849500
C	5.36955800	2.05069000	-1.14783200
H	4.08806600	0.15708700	-2.81520100
H	2.46207500	0.82789600	-2.63705200
H	3.76440100	1.81383600	-3.31264100
H	3.26946900	3.48663300	-0.11621900
H	3.17923700	3.54255500	-1.86964800
H	1.94293500	2.66292700	-0.96868200

H	5.52054400	2.83004400	-1.90314500
H	5.68072300	2.46607500	-0.18747000
H	6.04010700	1.22755200	-1.40077400
C	3.24686200	1.18903800	1.92579600
C	1.90262300	1.95186500	1.97551900
C	3.17238400	0.10929500	3.02779900
C	4.40091000	2.15951200	2.25501800
H	1.83856400	2.77557200	1.26804400
H	1.05272600	1.28875200	1.79387600
H	1.79050300	2.37313500	2.98112800
H	4.11587500	-0.41581000	3.18140200
H	2.92541100	0.60735900	3.97171900
H	2.38571400	-0.62491800	2.83053900
H	4.24977100	2.54258900	3.27055200
H	5.38034100	1.67807000	2.23315800
H	4.42722800	3.02446800	1.58975500
C	-1.79284700	-1.68956700	2.09829900
H	-1.56127700	-2.64180500	1.63500700
C	-3.05069500	-1.46504300	2.62390900
H	-3.22015500	-0.56852400	3.21714200
C	-5.04140400	0.52996500	-0.10767600
C	-5.16537800	1.32109400	-1.25530200
C	-5.61660900	0.93732400	1.09924700
C	-5.84373200	2.53783000	-1.18236900
H	-4.73646200	0.99128000	-2.19548700
C	-6.30223800	2.15205100	1.16064200
H	-5.53441400	0.31722100	1.98414100
C	-6.41264800	2.95345700	0.02331500
H	-5.93610800	3.15416200	-2.07131000
H	-6.75066100	2.46817000	2.09756200
H	-6.94807500	3.89651800	0.07394900
C	-4.15558100	-2.19008800	2.18919600
H	-4.02150200	-3.15970300	1.72059000
H	-5.15396600	-1.98408800	2.56070900
H	-0.94788100	-1.06356700	2.36383500
Se	-4.20222600	-1.20306100	-0.27984000

Zero-point correction=	0.685093 (Hartree/Particle)
Thermal correction to Energy=	0.727152
Thermal correction to Enthalpy=	0.728096
Thermal correction to Gibbs Free Energy=	0.609294
Sum of electronic and zero-point Energies=	-4195.618175
Sum of electronic and thermal Energies=	-4195.576115
Sum of electronic and thermal Enthalpies=	-4195.575171
Sum of electronic and thermal Free Energies=	-4195.693974

E(RB3LYP) = -4199.57279116 A.U.

B-1d

C	-2.25801400	0.59118000	-0.58071800
C	-1.50484400	1.51663700	-1.39603500
O	-0.41670600	1.27765600	-1.92491600
O	-2.09277800	2.74186800	-1.52214800
C	-1.41184000	3.68078700	-2.36807900
H	-1.30410200	3.28447500	-3.38056500
H	-2.03731500	4.57332500	-2.37410200
H	-0.42078400	3.91316800	-1.97072900
C	-1.77526500	-0.73553300	-0.25829700
C	-0.83759300	-1.41059800	-1.12393600
C	-2.22101900	-1.47286700	0.86508600
C	-0.46869600	-2.76214100	-0.87534400
H	-0.65597000	-0.98993900	-2.10758200
C	-1.81588900	-2.78184300	1.10295400
H	-2.92435600	-1.02461500	1.55450600
C	-0.93236700	-3.44505900	0.24381900
H	0.16013300	-3.26553900	-1.60423100
H	-2.20331900	-3.29838900	1.97682000
H	-0.63793500	-4.47177300	0.43155000
P	3.41482500	0.02989300	0.19518800
Au	1.24935100	-0.69231500	-0.38007800
C	3.50677000	0.22084400	2.11880800
C	2.20253100	0.88654100	2.62014200
C	3.55668700	-1.17283300	2.78185100
C	4.72009300	1.04564900	2.59746500
H	2.05640400	1.89872700	2.24720900
H	1.32364900	0.29336400	2.35024400
H	2.24765100	0.94117300	3.71409500
H	4.50081600	-1.69384400	2.61746700
H	3.45205300	-1.03557000	3.86386000
H	2.73447100	-1.81461200	2.45262500
H	4.72859200	1.04766600	3.69344300
H	5.67240300	0.62710100	2.26676500
H	4.67273300	2.08765700	2.27624800
C	4.67313400	-1.30680700	-0.42496400
C	4.12424400	-2.71717400	-0.10167500
C	4.78612800	-1.23334900	-1.96380300
C	6.08001900	-1.15496200	0.19050900
H	4.02885500	-2.91866200	0.96359200
H	3.14995900	-2.88547900	-0.56891700
H	4.82326600	-3.45451000	-0.51251500

H	5.29294900	-0.33423600	-2.31621400
H	5.38108100	-2.08970100	-2.29991400
H	3.80959900	-1.30343900	-2.45211800
H	6.73891600	-1.90421700	-0.26266900
H	6.52351400	-0.17580500	0.00134700
H	6.08623600	-1.33400000	1.26711300
C	3.72059600	1.72708800	-0.68611600
C	3.15821700	1.66172400	-2.12745400
C	2.91614400	2.83308800	0.03107400
C	5.20861600	2.13289900	-0.72716700
H	3.63532700	0.90810700	-2.75110400
H	2.07835400	1.49132900	-2.13453600
H	3.34218300	2.63401300	-2.59985000
H	3.30226700	3.07366500	1.02274600
H	2.99101600	3.74510700	-0.57158700
H	1.85491900	2.57926800	0.10685000
H	5.28223700	3.13136400	-1.17284300
H	5.66432000	2.18516400	0.26363700
H	5.80853700	1.46361500	-1.34648900
C	-1.53768700	2.19301700	2.94575100
H	-1.37386500	1.17203400	3.28088400
C	-2.66654400	2.56030800	2.33317800
H	-2.79973700	3.59269000	2.01576600
C	-5.11873600	-0.23024200	-0.00829300
C	-6.09299800	-0.38671300	0.97930600
C	-5.07865300	-1.07008100	-1.12344800
C	-7.02695700	-1.41837800	0.85430300
H	-6.14336300	0.27297200	1.83818300
C	-6.01666800	-2.09657900	-1.23474300
H	-4.32383900	-0.92936800	-1.88980400
C	-6.98892400	-2.27300900	-0.24779300
H	-7.78435300	-1.54751200	1.62112300
H	-5.98649400	-2.75586400	-2.09657900
H	-7.71791700	-3.07178000	-0.34017200
C	-3.78883400	1.62847600	2.05228900
H	-3.69388400	0.66596500	2.55378700
H	-4.76502000	2.07276600	2.26138000
H	-0.75035600	2.91024500	3.15380700
Se	-3.89220500	1.28711200	0.02412800

Zero-point correction= 0.685201 (Hartree/Particle)
Thermal correction to Energy= 0.728186
Thermal correction to Enthalpy= 0.729131
Thermal correction to Gibbs Free Energy= 0.605938
Sum of electronic and zero-point Energies= -4195.623321

Sum of electronic and thermal Energies= -4195.580335

Sum of electronic and thermal Enthalpies= -4195.579391

Sum of electronic and thermal Free Energies= -4195.702583

E(RB3LYP) = -4199.57647645 A.U.

B-TSd2

C	-2.30452700	0.80948300	-0.31102400
C	-1.48685800	1.81968900	-0.97524100
O	-0.31533000	1.68182800	-1.33330300
O	-2.14244800	2.99645400	-1.12989400
C	-1.41468500	4.05572500	-1.77294900
H	-1.08271600	3.74716300	-2.76667500
H	-2.11582400	4.88636200	-1.84614400
H	-0.54408300	4.34309700	-1.17809900
C	-1.82785400	-0.57308000	-0.18780000
C	-0.94245000	-1.14030300	-1.16238800
C	-2.24875200	-1.41902900	0.85577700
C	-0.55458800	-2.50124500	-1.07805700
H	-0.75450600	-0.59034600	-2.07926700
C	-1.84357000	-2.75267000	0.93348200
H	-2.92829700	-1.03637200	1.60776300
C	-0.99077800	-3.30588800	-0.02126200
H	0.04148800	-2.92640300	-1.88036600
H	-2.20632400	-3.36653500	1.75270900
H	-0.69144100	-4.34686200	0.03726900
P	3.44300400	-0.03742000	0.19105800
Au	1.23262600	-0.62314700	-0.35298900
C	3.57769100	0.17789900	2.10936300
C	2.31886500	0.91607000	2.62194800
C	3.57229100	-1.20494900	2.79724500
C	4.84112100	0.94877100	2.54697200
H	2.20337000	1.91929200	2.21532600
H	1.40936400	0.34902500	2.40287500
H	2.39764200	1.00995500	3.71105800
H	4.48450700	-1.77746100	2.62364900
H	3.49884300	-1.04198200	3.87819600
H	2.71063300	-1.80941400	2.49957400
H	4.87661700	0.96251800	3.64214400
H	5.76307000	0.48037400	2.19818800
H	4.83640400	1.98818500	2.21430000
C	4.60669200	-1.45819700	-0.42733700
C	3.98055700	-2.82708600	-0.06975300
C	4.69678900	-1.41766600	-1.96818500
C	6.03093900	-1.37912300	0.16181700

H	3.88865800	-3.00397300	1.00013800
H	2.99180000	-2.94393600	-0.52193400
H	4.62873100	-3.61157300	-0.47647400
H	5.23915600	-0.54997400	-2.34508200
H	5.24428800	-2.30738000	-2.29806900
H	3.70898800	-1.45025300	-2.43754400
H	6.63169700	-2.18212900	-0.27987000
H	6.53370000	-0.43726100	-0.06433900
H	6.04669800	-1.52719400	1.24292600
C	3.82686400	1.62479600	-0.72772700
C	3.23963300	1.56662800	-2.15929200
C	3.09686500	2.78799700	-0.02048300
C	5.33517000	1.94220800	-0.79799400
H	3.66902600	0.78351300	-2.78131300
H	2.15308800	1.44945400	-2.14212100
H	3.45917600	2.52333700	-2.64746400
H	3.50003800	3.01549100	0.96724400
H	3.23029700	3.68571900	-0.63435600
H	2.02146100	2.60464100	0.05435100
H	5.45848700	2.92754100	-1.26137500
H	5.80769000	1.98491600	0.18520100
H	5.88672100	1.22982600	-1.41449500
C	-1.55628600	1.81492000	1.93660800
H	-1.60927900	0.78322300	2.26422400
C	-2.62929800	2.66480400	2.09264500
H	-2.50890700	3.71558400	1.84032600
C	-5.07728600	-0.41803400	-0.08485000
C	-5.90977800	-0.67587200	1.00850300
C	-5.03812200	-1.30188500	-1.16966800
C	-6.68800600	-1.83594600	1.02499100
H	-5.96317700	0.01939700	1.83951900
C	-5.80967000	-2.46325200	-1.13866500
H	-4.41689300	-1.08269800	-2.03159400
C	-6.63400800	-2.73209300	-0.04306000
H	-7.33560200	-2.03463700	1.87344700
H	-5.77659000	-3.15072600	-1.97839300
H	-7.23984600	-3.63273100	-0.02754500
C	-3.92172700	2.17270200	2.27835700
H	-4.06807800	1.17998100	2.69276100
H	-4.77427300	2.84106900	2.33650600
H	-0.56635500	2.19253100	1.70479200
Se	-4.13444400	1.26997400	-0.19052800

Zero-point correction= 0.684470 (Hartree/Particle)

Thermal correction to Energy= 0.726692

Thermal correction to Enthalpy=	0.727636
Thermal correction to Gibbs Free Energy=	0.608647
Sum of electronic and zero-point Energies=	-4195.610073
Sum of electronic and thermal Energies=	-4195.567850
Sum of electronic and thermal Enthalpies=	-4195.566906
Sum of electronic and thermal Free Energies=	-4195.685895

E(RB3LYP) = -4199.56384297 A.U.

B-P1

C	-0.60878900	0.16120800	0.18602500
C	-0.49421300	1.63845800	-0.18276100
O	0.25440900	2.42478100	0.36292000
O	-1.25644800	1.96529300	-1.24759900
C	-1.07067600	3.29701300	-1.75113300
H	-0.05726800	3.41629100	-2.14370700
H	-1.80258900	3.41243200	-2.55014100
H	-1.23536900	4.03685500	-0.96472000
C	-1.99011600	-0.46871300	0.02135900
C	-3.15925800	0.29115400	0.17706100
C	-2.12084700	-1.85609000	-0.14484500
C	-4.41557500	-0.31367500	0.14870300
H	-3.09259000	1.36298200	0.31971400
C	-3.37679700	-2.46062100	-0.17655200
H	-1.22569100	-2.45431700	-0.27767100
C	-4.53146400	-1.69184800	-0.03163100
H	-5.30526600	0.29797500	0.26768200
H	-3.44979600	-3.53539300	-0.31552500
H	-5.51058400	-2.16092800	-0.05969300
C	-0.66729300	1.43329100	3.47489800
H	0.21216800	2.05103300	3.31695500
C	-0.91650000	0.36926900	2.71146900
H	-1.81919500	-0.21376300	2.88565700
C	2.34306700	-0.55843400	-0.43230900
C	2.91684700	-1.71538000	0.10792300
C	3.06731000	0.63967500	-0.44467700
C	4.20812900	-1.67412600	0.63505600
H	2.34997800	-2.64055500	0.10976000
C	4.35232400	0.67945800	0.09689000
H	2.61780600	1.53453600	-0.85938400
C	4.92477500	-0.47619500	0.63314400
H	4.65070500	-2.57474400	1.05069900
H	4.90833800	1.61240000	0.09450100
H	5.92841300	-0.44318400	1.04695400
C	-0.02076500	-0.10211800	1.59272500

H	0.14675500	-1.18104700	1.68372900
H	0.94824300	0.39336600	1.66347200
H	-1.33812300	1.72597500	4.27772100
Se	0.60145400	-0.67395500	-1.24107800

Zero-point correction= 0.314248 (Hartree/Particle)
Thermal correction to Energy= 0.334878
Thermal correction to Enthalpy= 0.335822
Thermal correction to Gibbs Free Energy= 0.262503
Sum of electronic and zero-point Energies= -3246.282646
Sum of electronic and thermal Energies= -3246.262016
Sum of electronic and thermal Enthalpies= -3246.261072
Sum of electronic and thermal Free Energies= -3246.334390
E(RB3LYP) = -3249.06785047 A.U.

B-P3

C	-2.04341700	0.37119600	-0.32353000
C	-1.91877400	1.75292300	0.26408900
O	-2.49882700	2.12837800	1.26032200
O	-1.07236300	2.55341900	-0.43327500
C	-0.90273500	3.87541200	0.10731700
H	-0.50638900	3.82948700	1.12440800
H	-0.19901700	4.37558300	-0.55765300
H	-1.85771600	4.40527500	0.12622700
C	-3.31678500	-0.33581400	0.06825200
C	-3.47879400	-0.84447400	1.36381900
C	-4.36464800	-0.48069700	-0.84768300
C	-4.65673000	-1.49249400	1.73021700
H	-2.67761300	-0.72415900	2.08627900
C	-5.54604700	-1.12938500	-0.48323800
H	-4.25659900	-0.08063700	-1.85187400
C	-5.69404200	-1.63889200	0.80636000
H	-4.76607900	-1.88306100	2.73785400
H	-6.34888600	-1.23459200	-1.20733700
H	-6.61117400	-2.14622200	1.09128700
C	-1.41149000	0.06627200	-1.67043300
H	-0.90228100	0.88207200	-2.17075900
C	-0.76908500	-0.49710300	-0.43916800
H	-0.96436700	-1.55039100	-0.25181700
C	3.50951400	-0.52293400	-0.08332900
C	4.25326000	0.62541400	-0.37531200
C	3.91683100	-1.36617500	0.95638900
C	5.39106100	0.93202900	0.37275100
H	3.93856400	1.27124300	-1.18882100
C	5.05322200	-1.05656400	1.70501800

H	3.34340800	-2.26248000	1.17066500
C	5.79093900	0.09258700	1.41408400
H	5.96480400	1.82487300	0.14113700
H	5.36413900	-1.71484200	2.51120300
H	6.67727500	0.33096900	1.99480200
C	0.59538300	-0.04950300	0.01322400
H	0.73600300	1.02249900	-0.11047000
H	0.79764300	-0.33952000	1.04628200
H	-1.94993400	-0.61124300	-2.32464800
Se	1.95122800	-0.96058900	-1.13106200

Zero-point correction= 0.315255 (Hartree/Particle)
Thermal correction to Energy= 0.335383
Thermal correction to Enthalpy= 0.336327
Thermal correction to Gibbs Free Energy= 0.261846
Sum of electronic and zero-point Energies= -3246.277426
Sum of electronic and thermal Energies= -3246.257297
Sum of electronic and thermal Enthalpies= -3246.256353
Sum of electronic and thermal Free Energies= -3246.330834
E(RB3LYP) = -3249.06505566 A.U.

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Re4

C	4.16549000	-0.52623800	0.04401200
H	4.48147400	-0.01941000	-0.86524200
C	2.87843300	-0.76096400	0.29851900
H	2.58616200	-1.26058000	1.22158400
C	-0.60767200	0.15414700	0.02004600
C	-1.03612800	-1.19049300	0.07773000
C	-1.60148900	1.15302200	-0.03118800
C	-2.38916100	-1.51225500	0.06280800
H	-0.30699300	-1.98871300	0.16818500
C	-2.95509000	0.81639000	-0.03110800
H	-1.32204000	2.19814900	-0.08848500
C	-3.36533900	-0.51462100	0.00880300
H	-2.68198300	-2.55766200	0.11104800
H	-3.69370400	1.61237600	-0.07505200
H	-4.41991800	-0.77098600	0.00430100
C	1.74311100	-0.36959000	-0.61227900
H	2.14388500	0.14743600	-1.49936500
H	1.23823600	-1.26526700	-0.98338400
H	4.95139800	-0.83830300	0.72507500
N	0.75476000	0.47723500	0.06091900
C	1.15430700	1.86688300	0.18810100
H	0.61906700	2.34550600	1.01263000
H	2.22205100	1.90205800	0.41763300

H	0.98028100	2.45705800	-0.72802700

Zero-point correction= 0.207028 (Hartree/Particle)
Thermal correction to Energy= 0.217684
Thermal correction to Enthalpy= 0.218628
Thermal correction to Gibbs Free Energy= 0.169742
Sum of electronic and zero-point Energies= -443.419106
Sum of electronic and thermal Energies= -443.408451
Sum of electronic and thermal Enthalpies= -443.407507
Sum of electronic and thermal Free Energies= -443.456392
E(RB3LYP) = -443.785504195 A.U.

C-TS1

C	0.88680200	-1.03813500	0.44119100
C	0.78333300	-2.53547200	0.40104800
O	0.84370400	-3.21625800	1.40847400
O	0.48145500	-3.05099100	-0.81133700
C	0.21805700	-4.47014300	-0.82513200
H	-0.65910700	-4.70011500	-0.21631900
H	0.03833600	-4.72116700	-1.86975600
H	1.07436800	-5.02510300	-0.43624900
C	1.85110600	-0.45122100	1.35425800
C	2.93772900	-1.18356300	1.90067200
C	1.72237300	0.90667600	1.73973800
C	3.80388700	-0.60168300	2.81947000
H	3.06324400	-2.22608500	1.63785000
C	2.59559200	1.48969000	2.65026800
H	0.90618100	1.48743900	1.32198800
C	3.63706000	0.73408100	3.19838200
H	4.60590700	-1.19283500	3.25107300
H	2.45893100	2.52557000	2.94557700
H	4.30989100	1.18144200	3.92428000
P	-3.29955000	0.51232400	-0.14105300
Au	-1.02701200	-0.22759000	0.12891800
C	-3.80584000	0.25093600	-1.99258500
C	-2.64906400	0.72588100	-2.90550500
C	-3.97186600	-1.25933000	-2.27408700
C	-5.10484000	0.97821400	-2.39567800
H	-2.43586500	1.79038800	-2.82753200
H	-1.72659200	0.17376700	-2.70140800
H	-2.93088800	0.52559500	-3.94560400
H	-4.84876700	-1.69167700	-1.79127500
H	-4.10358100	-1.39035900	-3.35398600
H	-3.08662900	-1.83155700	-1.98049300
H	-5.34609900	0.71456500	-3.43200500

H	-5.95763300	0.68857600	-1.77935900
H	-5.00787700	2.06501600	-2.35816400
C	-4.40239100	-0.57737900	1.02322200
C	-3.90843400	-2.04289200	0.95174300
C	-4.20561600	-0.13355800	2.48991000
C	-5.90787700	-0.52927500	0.68747800
H	-4.01561900	-2.49317400	-0.03338800
H	-2.86102800	-2.12838200	1.25560500
H	-4.50626100	-2.63860900	1.65096300
H	-4.64245400	0.84240800	2.70583800
H	-4.71374900	-0.86050700	3.13311200
H	-3.15136200	-0.12529700	2.78158600
H	-6.45014800	-1.11466800	1.43891300
H	-6.31590400	0.48317700	0.70867000
H	-6.13705500	-0.97083900	-0.28435400
C	-3.44438700	2.38177600	0.34276400
C	-2.60196000	2.63716800	1.61597000
C	-2.81360200	3.25131000	-0.76659900
C	-4.89124800	2.85833600	0.58604500
H	-2.95053100	2.09120700	2.49043700
H	-1.54910300	2.38692600	1.45648900
H	-2.65768200	3.70591100	1.85332800
H	-3.40373800	3.27055900	-1.68359700
H	-2.75527700	4.28238300	-0.40032800
H	-1.79514900	2.93134600	-1.00724500
H	-4.87424800	3.93548000	0.78874900
H	-5.53970900	2.70065200	-0.27770400
H	-5.35079900	2.37859800	1.45186600
C	8.87364800	0.78093500	-1.13854900
H	9.24727400	1.29638900	-0.25650600
C	7.61921100	0.33719500	-1.21385900
H	7.27299500	-0.17551000	-2.11035000
C	4.27247400	0.62949600	-0.95739400
C	4.19538800	-0.79109900	-1.12577300
C	3.10228700	1.39808000	-1.27463400
C	3.01468200	-1.38893600	-1.49378600
H	5.08035600	-1.40232400	-1.00703800
C	1.93276100	0.77826300	-1.63363200
H	3.13842100	2.47844100	-1.22761300
C	1.81968700	-0.63803000	-1.65091300
H	2.98335400	-2.46375700	-1.63767400
H	1.06047500	1.38199700	-1.86540200
H	0.95709400	-1.10629100	-2.10359600
C	6.60565100	0.50093100	-0.10995700

H	6.28675400	-0.46472100	0.29006400
H	7.04789300	1.05002200	0.72690400
H	9.57949900	0.63351600	-1.94974600
N	5.40649100	1.24341000	-0.54249900
C	5.52433300	2.70284800	-0.55313800
H	6.56468200	2.96774600	-0.36789500
H	5.24454200	3.11725900	-1.52586800
H	4.89954900	3.15887700	0.22324300

Zero-point correction= 0.730821 (Hartree/Particle)
Thermal correction to Energy= 0.773784
Thermal correction to Enthalpy= 0.774728
Thermal correction to Gibbs Free Energy= 0.653311
Sum of electronic and zero-point Energies= -1891.310012
Sum of electronic and thermal Energies= -1891.267049
Sum of electronic and thermal Enthalpies= -1891.266105
Sum of electronic and thermal Free Energies= -1891.387522
E(RB3LYP) = -1892.71817792 A.U.

C-TS11

C	-1.32692800	0.50734600	0.34149200
C	-1.61022400	1.95118400	0.00926400
O	-2.00830200	2.42308300	-1.04224300
O	-1.25291700	2.71821400	1.06036700
C	-1.30880300	4.14590800	0.84373500
H	-2.32035700	4.45275400	0.57066900
H	-1.01226000	4.59094700	1.79227600
H	-0.61966300	4.43683700	0.04778300
C	-1.99624200	-0.06581600	1.49918200
C	-3.16399700	0.51557400	2.05403800
C	-1.49139500	-1.24123300	2.10955700
C	-3.77923300	-0.03951400	3.17245600
H	-3.56399700	1.42819700	1.62565700
C	-2.11425200	-1.79993700	3.21653900
H	-0.59800900	-1.69909500	1.69782000
C	-3.26180300	-1.20102500	3.75215000
H	-4.65857600	0.43474500	3.59753600
H	-1.70637700	-2.69602700	3.67392800
H	-3.74187900	-1.63219700	4.62553000
P	3.11897800	-0.05987400	-0.15599200
Au	0.73434000	0.16537200	0.02372100
C	3.74745800	1.09704100	-1.57724300
C	2.77421100	0.98543100	-2.77598000
C	3.68427300	2.56884200	-1.11283500
C	5.18318200	0.78679900	-2.04890700

H	2.73967100	-0.00711000	-3.22181300
H	1.75693100	1.27106400	-2.49139200
H	3.10823600	1.68072500	-3.55452600
H	4.43020100	2.81119400	-0.35485400
H	3.88880000	3.20702300	-1.97962800
H	2.69379200	2.83941600	-0.73506100
H	5.46927500	1.52781100	-2.80423300
H	5.91573700	0.84712200	-1.24161600
H	5.27027000	-0.19506000	-2.51771400
C	3.88245200	0.46841200	1.54515000
C	3.15751900	1.74005500	2.04934900
C	3.60245700	-0.62740300	2.59735200
C	5.40142900	0.73492300	1.49486400
H	3.31603700	2.61173200	1.41731900
H	2.08001700	1.57926500	2.14706700
H	3.54995600	1.98262100	3.04357000
H	4.17012000	-1.54304700	2.42659800
H	3.90496100	-0.24150200	3.57713100
H	2.53842700	-0.87435500	2.65982600
H	5.74612300	0.97124200	2.50816900
H	5.97458500	-0.12851800	1.15153200
H	5.65729900	1.58889900	0.86502100
C	3.54597200	-1.90890200	-0.54538400
C	2.62925000	-2.82275300	0.30394200
C	3.20748600	-2.22163700	-2.01922000
C	5.02086700	-2.27885300	-0.28548900
H	2.77693400	-2.71653500	1.37719000
H	1.57270800	-2.64311800	0.08295700
H	2.85121700	-3.86475300	0.04559200
H	3.87510100	-1.73129400	-2.72836600
H	3.31616000	-3.30143500	-2.17069600
H	2.17476300	-1.95854900	-2.26603600
H	5.18047100	-3.31867200	-0.59347700
H	5.71635600	-1.66012000	-0.85549700
H	5.29006300	-2.21343900	0.77026900
C	-7.10031300	1.37028500	-2.30929200
H	-7.55754300	1.87782300	-1.46275000
C	-5.87781500	0.84498200	-2.23617500
H	-5.44374200	0.34515400	-3.10135400
C	-3.54665800	-1.12162500	-0.87625600
C	-2.39563600	-0.44850400	-1.43151200
C	-3.44525500	-2.52663900	-0.66661400
C	-1.33534500	-1.23826300	-1.97846500
H	-2.49367200	0.55779500	-1.81462300

C	-2.34777300	-3.23005300	-1.11827200
H	-4.25110000	-3.06885900	-0.19137500
C	-1.28578000	-2.59910300	-1.81099200
H	-0.55499900	-0.71850800	-2.52498200
H	-2.32249500	-4.30615800	-0.96979200
H	-0.46944800	-3.18826900	-2.21417200
C	-5.00899900	0.89975900	-1.00431700
H	-4.09198500	1.45452900	-1.19938700
H	-5.53298200	1.42611700	-0.20013100
H	-7.68486000	1.32798500	-3.22288500
N	-4.67212500	-0.45270800	-0.50608000
C	-5.78867700	-1.17992100	0.10387700
H	-6.57449900	-0.46645600	0.34859900
H	-6.21136500	-1.92885000	-0.57521900
H	-5.46587400	-1.66889900	1.02708400

Zero-point correction= 0.730521 (Hartree/Particle)
Thermal correction to Energy= 0.772572
Thermal correction to Enthalpy= 0.773516
Thermal correction to Gibbs Free Energy= 0.656159
Sum of electronic and zero-point Energies= -1891.302741
Sum of electronic and thermal Energies= -1891.260691
Sum of electronic and thermal Enthalpies= -1891.259746
Sum of electronic and thermal Free Energies= -1891.377104
E(RB3LYP) = -1892.71088992 A.U.

C-TS12

C	1.19460100	-0.14275600	0.36352900
C	1.31469400	-1.38533000	1.20676500
O	1.10043100	-1.38521800	2.40451800
O	1.57290100	-2.52502300	0.51643500
C	1.51511300	-3.74013400	1.29322800
H	0.50727700	-3.89178500	1.68559000
H	1.78269500	-4.53906300	0.60273700
H	2.21821100	-3.69578100	2.12724400
C	1.73477100	1.10819100	0.98671300
C	2.70836600	1.08250300	2.00530900
C	1.26301700	2.36718800	0.56908600
C	3.16005100	2.25893500	2.59805400
H	3.08328300	0.13283200	2.36975400
C	1.72102800	3.54709800	1.15262400
H	0.52160600	2.41579300	-0.22317300
C	2.67055300	3.49703300	2.17425500
H	3.89296600	2.20885100	3.39773200
H	1.33085600	4.50266600	0.81521100

H	3.02433700	4.41286000	2.63800000
P	-3.32409500	-0.06526200	-0.16979000
Au	-0.93450200	-0.08505200	-0.00533300
C	-3.91571000	1.76814900	-0.35952000
C	-3.09729900	2.66495600	0.60043600
C	-3.59450500	2.26254500	-1.78717000
C	-5.42075400	1.97430400	-0.08915300
H	-3.27291400	2.45398900	1.65323700
H	-2.02281700	2.58263300	0.41417400
H	-3.38791600	3.70688200	0.42343700
H	-4.21959000	1.79976700	-2.55195400
H	-3.78635100	3.34060900	-1.82640400
H	-2.54299000	2.10839800	-2.04782700
H	-5.67031600	3.02264700	-0.28992000
H	-6.05549000	1.36135500	-0.73149700
H	-5.69230500	1.77697300	0.94947800
C	-3.85102600	-1.11840800	-1.70933500
C	-2.91142900	-0.78766900	-2.89397000
C	-3.63462000	-2.61657700	-1.40190600
C	-5.31532900	-0.90205100	-2.14367300
H	-2.99584200	0.23822800	-3.24843200
H	-1.86513900	-0.97853300	-2.63686400
H	-3.17305000	-1.44445300	-3.73153200
H	-4.33465900	-3.00972700	-0.66400800
H	-3.79425700	-3.18008000	-2.32792600
H	-2.61361300	-2.82187700	-1.06651200
H	-5.53714300	-1.58226800	-2.97407000
H	-6.02960400	-1.11849400	-1.34708600
H	-5.49980500	0.11173800	-2.50384300
C	-4.02155500	-0.84213300	1.46176800
C	-3.16225300	-2.07129300	1.84831600
C	-3.86606100	0.16517700	2.62287100
C	-5.50262300	-1.26290100	1.36230000
H	-3.19512700	-2.87742200	1.11716300
H	-2.11647300	-1.79601300	2.01403100
H	-3.55063900	-2.47127800	2.79200900
H	-4.53286900	1.02406000	2.53734700
H	-4.12622500	-0.35050200	3.55377600
H	-2.83640500	0.51944400	2.72642000
H	-5.82876700	-1.62166000	2.34525400
H	-6.15889100	-0.43617600	1.08399200
H	-5.66201900	-2.08031800	0.65636900
C	8.01359700	-2.33908600	-0.04885100
H	8.62728500	-1.79591200	0.66645700

C	6.77683500	-1.94489100	-0.35152000
H	6.18828300	-2.50722700	-1.07605200
C	4.37299900	0.32705400	-1.19101100
C	3.40620900	-0.65136300	-0.90393100
C	3.93138900	1.41190100	-2.00081700
C	2.01865500	-0.48385500	-1.24834100
H	3.66540200	-1.55029600	-0.36070100
C	2.62216200	1.51017800	-2.50196400
H	4.63293600	2.19615200	-2.26045100
C	1.66916500	0.58375200	-2.15446600
H	1.49244400	-1.42243900	-1.40997700
H	2.37648500	2.34380000	-3.15214000
H	0.64458900	0.66804900	-2.49977700
C	6.11366400	-0.72800400	0.24350400
H	5.24778900	-1.00770100	0.85268200
H	6.80858400	-0.22202700	0.92308500
H	8.45635600	-3.22434000	-0.49432400
N	5.67484200	0.24360400	-0.76625800
C	6.69384900	1.13621200	-1.30489000
H	7.67583300	0.73097800	-1.05849200
H	6.63290400	1.19779500	-2.39696200
H	6.62228200	2.15125200	-0.89035300

Zero-point correction= 0.729807 (Hartree/Particle)
Thermal correction to Energy= 0.772749
Thermal correction to Enthalpy= 0.773693
Thermal correction to Gibbs Free Energy= 0.652556
Sum of electronic and zero-point Energies= -1891.288422
Sum of electronic and thermal Energies= -1891.245480
Sum of electronic and thermal Enthalpies= -1891.244536
Sum of electronic and thermal Free Energies= -1891.365673
E(RB3LYP) = -1892.69261562 A.U.

C-2

C	-1.03462300	1.34250100	-0.51940100
C	-0.81840800	1.56626600	-1.91298900
O	-1.44602400	0.87156200	-2.84716300
O	0.00854500	2.48142500	-2.37229100
C	0.25947400	2.55988600	-3.79876600
H	-0.66909700	2.74869200	-4.33875100
H	0.94802400	3.39495800	-3.91187100
H	0.71624400	1.63257300	-4.15066500
C	-0.77536300	2.43716400	0.49874600
C	-0.55454300	3.78631600	0.17680100
C	-0.81865300	2.08470500	1.86322500

C	-0.36768200	4.73859100	1.18138100
H	-0.53376700	4.10722300	-0.85643800
C	-0.63290500	3.03668500	2.86252300
H	-1.02059800	1.05324200	2.13697500
C	-0.40056800	4.37229000	2.52629400
H	-0.20481500	5.77597800	0.90420700
H	-0.67523900	2.73477000	3.90492800
H	-0.25691300	5.11749400	3.30246300
P	2.93522200	-0.96733300	0.22840900
Au	0.89746600	0.14646600	-0.26174200
C	2.79721400	-2.81192200	-0.34503100
C	1.40235800	-3.36041800	0.03867500
C	2.87474000	-2.88360800	-1.88610800
C	3.88740400	-3.72585600	0.25350500
H	1.21499600	-3.37991200	1.11047900
H	0.60360300	-2.78494900	-0.43716300
H	1.33024600	-4.39186500	-0.32510200
H	3.86528000	-2.65020700	-2.27866100
H	2.64570500	-3.91132800	-2.18891200
H	2.13864100	-2.23110300	-2.36556100
H	3.77893600	-4.72572600	-0.18179700
H	4.89860200	-3.38199700	0.02877700
H	3.79421400	-3.83748300	1.33537200
C	4.34661100	-0.05182200	-0.73122900
C	3.86300600	0.27214200	-2.16534300
C	4.62920000	1.30806200	-0.05610900
C	5.66187200	-0.85555700	-0.80405400
H	3.66227900	-0.61003200	-2.77077100
H	2.96244500	0.89344800	-2.15151100
H	4.65283000	0.84154500	-2.66852100
H	5.10551300	1.20924100	0.91983400
H	5.32254700	1.86520400	-0.69586400
H	3.72386400	1.91324400	0.04979400
H	6.41749900	-0.23919600	-1.30421800
H	6.05407000	-1.11253200	0.18155500
H	5.56333000	-1.77387500	-1.38571900
C	3.21583800	-0.85699500	2.14202900
C	2.85207700	0.56451800	2.63330800
C	2.24347100	-1.82168800	2.85553100
C	4.66006900	-1.18814700	2.57430700
H	3.50008200	1.34372100	2.23711700
H	1.81811000	0.82922200	2.39634600
H	2.95513300	0.57939000	3.72434400
H	2.48777800	-2.87272500	2.69648400

H	2.31265700	-1.63583400	3.93289100
H	1.20365900	-1.64908300	2.56138400
H	4.70532700	-1.17086500	3.66911200
H	4.98460100	-2.17913900	2.25212400
H	5.38454000	-0.45437900	2.21514700
C	-9.32607300	-1.27783500	0.11511000
H	-9.63504000	-2.03368400	0.83401900
C	-8.08306500	-0.79688500	0.09750400
H	-7.80056600	-0.04202200	-0.63572600
C	-4.67035300	-1.03843300	0.15107300
C	-4.62204500	0.36326900	0.37722600
C	-3.47326500	-1.64777700	-0.29738700
C	-3.45909800	1.08898300	0.17977800
H	-5.51255900	0.89868000	0.68318800
C	-2.31109900	-0.90280300	-0.48489900
H	-3.43466100	-2.71684100	-0.46500400
C	-2.26221400	0.48391500	-0.25444200
H	-3.47835600	2.15947800	0.36059300
H	-1.40815400	-1.42620500	-0.79290400
H	-2.10326400	0.29479000	-2.40036100
C	-6.99289400	-1.24263000	1.04000800
H	-6.67500400	-0.42071400	1.68860700
H	-7.37815500	-2.02161600	1.70836500
H	-10.08538700	-0.92736500	-0.57705900
N	-5.81437900	-1.77464200	0.34636200
C	-5.89332300	-3.15904900	-0.09597800
H	-6.94172200	-3.46049200	-0.11511300
H	-5.50200600	-3.27245900	-1.11235500
H	-5.34604500	-3.84467700	0.56681800

Zero-point correction= 0.732531 (Hartree/Particle)
Thermal correction to Energy= 0.775661
Thermal correction to Enthalpy= 0.776605
Thermal correction to Gibbs Free Energy= 0.654318
Sum of electronic and zero-point Energies= -1891.341585
Sum of electronic and thermal Energies= -1891.298455
Sum of electronic and thermal Enthalpies= -1891.297511
Sum of electronic and thermal Free Energies= -1891.419798
E(RB3LYP) = -1892.74319919 A.U.

C-3

C	1.84491300	-0.43256900	-0.03806900
C	2.42788000	-1.64728100	-0.24104100
O	1.74928200	-2.81578800	-0.37957900
O	3.76213800	-1.80942400	-0.34635300

C	4.29362500	-3.13754200	-0.30750900
H	3.94082700	-3.73508600	-1.15190000
H	5.37533600	-3.01252700	-0.36587000
H	4.02974300	-3.64515600	0.62540900
C	2.60670600	0.83612900	0.05373800
C	3.80854600	1.06737700	-0.64506800
C	2.11043700	1.88647600	0.85233100
C	4.48329400	2.28158200	-0.53508700
H	4.21234000	0.28934000	-1.28060900
C	2.78513200	3.10057000	0.95786600
H	1.18476300	1.74120900	1.40004600
C	3.97955500	3.30741200	0.26619200
H	5.40644100	2.42897900	-1.08960800
H	2.37645000	3.88658800	1.58744900
H	4.50707600	4.25344200	0.34710300
C	-6.99136100	0.95237000	-0.95119200
H	-7.39921200	1.33286600	-0.01720700
C	-5.68787600	0.71484300	-1.09565800
H	-5.30464800	0.32411600	-2.03773100
C	-2.50852400	-0.29877700	0.24482600
C	-1.79751700	0.46730100	-0.70890200
C	-1.74762000	-1.10828800	1.10950900
C	-0.41363300	0.42307900	-0.78360900
H	-2.33728900	1.07414400	-1.42817000
C	-0.35423200	-1.14026800	1.02456700
H	-2.23328600	-1.69249100	1.88199400
C	0.35593500	-0.38709500	0.07452100
H	0.09343200	1.02016300	-1.53578300
H	0.19653300	-1.74225100	1.74364000
H	0.80096600	-2.60770600	-0.33926000
C	-4.65701900	0.93678600	-0.01864100
H	-3.95219300	1.71288600	-0.32816400
H	-5.15006600	1.31513300	0.89077500
H	-7.69780100	0.78708800	-1.75891900
N	-3.90423700	-0.28126100	0.29307400
C	-4.60475000	-1.21460600	1.15619900
H	-5.66357000	-1.20994800	0.88658500
H	-4.22764200	-2.23038200	1.00891500
H	-4.52084500	-0.96488700	2.22741100

Zero-point correction= 0.358580 (Hartree/Particle)
Thermal correction to Energy= 0.380052
Thermal correction to Enthalpy= 0.380996
Thermal correction to Gibbs Free Energy= 0.304988
Sum of electronic and zero-point Energies= -941.480906

Sum of electronic and thermal Energies= -941.459433

Sum of electronic and thermal Enthalpies= -941.458489

Sum of electronic and thermal Free Energies= -941.534497

E(RB3LYP) = -942.178178204 A.U.

C-TS3

C	1.26531200	0.17298400	-0.29102500
C	1.85109200	1.29689700	-0.93712400
O	3.06704400	1.48665400	-1.23883300
O	0.98179500	2.31453400	-1.20907900
C	1.54925000	3.50939500	-1.74125700
H	2.04986400	3.32398800	-2.69553000
H	0.70934400	4.19119700	-1.88405000
H	2.27595700	3.95299000	-1.05240300
H	4.26961400	0.99178700	-0.56969400
O	2.21365900	0.51904600	2.28080700
H	2.16556400	-0.41470900	2.53658300
H	1.84880400	0.51337900	1.28749200
O	4.51036500	1.27230400	2.26023100
H	4.52674900	2.21901600	2.45406200
H	3.41282700	0.90472500	2.29771600
O	5.14876600	0.81449800	-0.04163700
H	5.83073200	1.36234300	-0.44991900
H	4.87736200	1.09976300	1.23210300
C	1.94470700	-1.15456200	-0.31978800
C	1.52249300	-2.16575500	0.57709100
C	3.01052300	-1.48378600	-1.18307800
C	2.13349600	-3.41723900	0.61678000
H	0.67494800	-1.96901800	1.22936000
C	3.62068900	-2.73672800	-1.14015400
H	3.35602800	-0.74839300	-1.89873700
C	3.19534600	-3.71416800	-0.23961900
H	1.77319000	-4.16524600	1.31874900
H	4.43548700	-2.95115800	-1.82720700
H	3.67514000	-4.68794200	-0.21049500
C	-0.22525800	0.17325900	-0.07873500
C	-0.85654700	1.04421000	0.81904800
C	-1.06293500	-0.71901200	-0.77273600
C	-2.23954200	1.05476700	1.00061300
H	-0.25507800	1.75179300	1.38295400
C	-2.43889900	-0.74022200	-0.58290200
H	-0.61870600	-1.42697400	-1.46644700
C	-3.06833100	0.16016100	0.30099900
H	-2.66792800	1.77216300	1.69074600

H	-3.03002900	-1.48166600	-1.11155400
N	-4.46294000	0.11181600	0.50524800
C	-5.03225300	0.91990200	1.56863300
H	-6.07771200	0.63221400	1.70456500
H	-4.50572600	0.73602300	2.50898500
H	-5.00144500	2.00426200	1.36023300
C	-5.34779200	-0.02461200	-0.65650400
H	-4.75149800	-0.37393400	-1.50335500
H	-5.76021300	0.95616100	-0.95150200
C	-6.47516800	-0.99138500	-0.40321100
H	-6.17044200	-1.98750900	-0.08364800
C	-7.76833400	-0.70018400	-0.54240800
H	-8.54516000	-1.43827600	-0.36670800
H	-8.09720900	0.29048900	-0.84868900

Zero-point correction= 0.433914 (Hartree/Particle)
Thermal correction to Energy= 0.463278
Thermal correction to Enthalpy= 0.464222
Thermal correction to Gibbs Free Energy= 0.371399
Sum of electronic and zero-point Energies= -1170.724076
Sum of electronic and thermal Energies= -1170.694711
Sum of electronic and thermal Enthalpies= -1170.693767
Sum of electronic and thermal Free Energies= -1170.786591
E(RB3LYP) = -1171.58789833 A.U.

C-TS31

C	1.88512800	-0.41578500	0.42239000
C	2.51864000	-1.66118200	0.03246200
O	3.44996300	-1.99038400	0.86477000
O	2.16586200	-2.44710300	-0.95697400
C	2.76811100	-3.76133400	-1.01399300
H	2.76955800	-4.21775000	-0.02252700
H	2.15704400	-4.33329300	-1.71115200
H	3.79348100	-3.68252700	-1.38026500
C	2.69393500	0.82336300	0.18778400
C	3.73213900	0.88671000	-0.75898700
C	2.42954100	1.98347200	0.94339500
C	4.49172600	2.04564200	-0.92367700
H	3.94291800	0.02221800	-1.38310600
C	3.17080100	3.14679100	0.75970600
H	1.63452700	1.95951200	1.68285400
C	4.21424100	3.18521000	-0.17003600
H	5.29063200	2.06044800	-1.66026400
H	2.94223800	4.02572400	1.35662200
H	4.79731400	4.09113400	-0.30589300

C	-6.91152200	1.35923800	-0.73722800
H	-7.32973200	1.44666700	0.26323900
C	-5.61199200	1.13592700	-0.93152200
H	-5.21892000	1.04124700	-1.94327000
C	-2.46672600	-0.29542600	0.19785500
C	-1.67769800	0.70432400	-0.40959300
C	-1.78472700	-1.32691400	0.87256700
C	-0.29118200	0.67681500	-0.33398100
H	-2.15162500	1.49268600	-0.98565800
C	-0.39420700	-1.33912800	0.94238700
H	-2.33825400	-2.11028700	1.37671800
C	0.39613000	-0.34627300	0.34314500
H	0.27467600	1.45921300	-0.82946400
H	0.09041500	-2.13696000	1.50136300
H	2.88428500	-1.04557100	1.43534000
C	-4.59585600	0.98922000	0.17142300
H	-3.87365100	1.80793200	0.11929600
H	-5.09660800	1.08114800	1.14982400
H	-7.60412600	1.47360400	-1.56558200
N	-3.86566900	-0.27933200	0.08954900
C	-4.62141000	-1.42295100	0.56733100
H	-5.65389800	-1.32708100	0.22272400
H	-4.21348300	-2.34917400	0.15368600
H	-4.63413100	-1.50998500	1.66773800

Zero-point correction= 0.352736 (Hartree/Particle)
Thermal correction to Energy= 0.373993
Thermal correction to Enthalpy= 0.374937
Thermal correction to Gibbs Free Energy= 0.299326
Sum of electronic and zero-point Energies= -941.410747
Sum of electronic and thermal Energies= -941.389490
Sum of electronic and thermal Enthalpies= -941.388546
Sum of electronic and thermal Free Energies= -941.464157
E(RB3LYP) = -942.102675179 A.U.

C-TS21

C	-0.86143000	1.77974900	-0.66100900
C	-0.19689400	2.05663600	-1.99940600
O	0.78094800	2.76239300	-2.14247200
O	-0.84001500	1.45706100	-3.02899100
C	-0.27840400	1.69797900	-4.33760500
H	0.72649500	1.27525300	-4.40495100
H	-0.95142500	1.20158900	-5.03533100
H	-0.23102000	2.76917100	-4.54043500
C	-0.69699400	2.84141800	0.41178800

C	-0.66326200	4.20286900	0.07480900
C	-0.59637600	2.48932900	1.76904800
C	-0.51114400	5.17816000	1.06064500
H	-0.73070600	4.50558000	-0.96450700
C	-0.45588500	3.46458600	2.75587900
H	-0.65187600	1.44212400	2.05651900
C	-0.40755800	4.81491300	2.40385200
H	-0.47956900	6.22518300	0.77522000
H	-0.38431700	3.16862500	3.79825500
H	-0.29454700	5.57610600	3.16950900
P	2.66571000	-1.15113200	0.30248800
Au	0.85397900	0.26992100	-0.12555700
C	2.10073400	-2.95904700	-0.08570700
C	0.68661200	-3.19493900	0.49796100
C	1.97068200	-3.14168000	-1.61369500
C	3.06688300	-4.02674700	0.46957600
H	0.64168000	-3.12291100	1.58297700
H	-0.04637700	-2.49980100	0.07839600
H	0.37504900	-4.21013600	0.22632400
H	2.92949600	-3.13233400	-2.13359200
H	1.51539200	-4.12066100	-1.79957900
H	1.31751700	-2.38630700	-2.06064900
H	2.71485900	-5.01331200	0.14788200
H	4.08659200	-3.90869700	0.09911100
H	3.09484400	-4.03769400	1.56060300
C	4.09943000	-0.59377500	-0.87587000
C	3.51906000	-0.25640800	-2.27039000
C	4.72844700	0.71404100	-0.34821300
C	5.20488100	-1.66125400	-1.02096600
H	3.02510500	-1.09626100	-2.75578700
H	2.81792300	0.58159500	-2.22127600
H	4.35134700	0.05000500	-2.91418800
H	5.29377900	0.57749500	0.57446100
H	5.43321200	1.07498300	-1.10522700
H	3.98289800	1.50033200	-0.20027600
H	6.01101600	-1.24141700	-1.63267600
H	5.64186900	-1.95144100	-0.06378200
H	4.85570700	-2.56270500	-1.52813500
C	3.17540000	-0.95958200	2.16050900
C	3.14733600	0.53862400	2.54858700
C	2.13297900	-1.66006500	3.05930700
C	4.57325600	-1.53822800	2.46885600
H	3.87293000	1.14478400	2.01024300
H	2.15843600	0.98106400	2.40118300

H	3.38799900	0.61288800	3.61520600
H	2.16028600	-2.74781200	2.98153700
H	2.36216700	-1.40744600	4.10034000
H	1.11465600	-1.31496400	2.85662800
H	4.75698800	-1.43697300	3.54446900
H	4.66094900	-2.59849800	2.22423600
H	5.37240600	-0.99919800	1.95718000
C	-8.80151900	-1.60732600	0.89441100
H	-8.95955700	-2.60642800	1.29475800
C	-7.58196100	-1.08016400	0.78868900
H	-7.45378600	-0.07782000	0.38163300
C	-4.32757800	-1.04310400	-0.09721100
C	-4.18611700	0.14194500	0.67091600
C	-3.34266800	-1.27136000	-1.10121300
C	-3.13513800	1.01908300	0.46340600
H	-4.92424900	0.40696500	1.41682600
C	-2.29453700	-0.39616000	-1.30814400
H	-3.39438200	-2.15918100	-1.71860500
C	-2.15097200	0.76227900	-0.51346400
H	-3.08397300	1.92147800	1.06085000
H	-1.57378500	-0.61002700	-2.08638000
H	-1.97944400	1.94014800	-1.13169700
C	-6.31807100	-1.79713700	1.19352700
H	-5.82515500	-1.28947000	2.02805300
H	-6.55975400	-2.80361800	1.55157400
H	-9.68920600	-1.05760100	0.59758500
N	-5.35293700	-1.92879700	0.09313800
C	-5.59048800	-3.01143700	-0.85553200
H	-6.57976900	-3.42919800	-0.66738300
H	-5.57854300	-2.64778300	-1.88827100
H	-4.84928900	-3.81568100	-0.75742600

Zero-point correction= 0.727083 (Hartree/Particle)
Thermal correction to Energy= 0.770350
Thermal correction to Enthalpy= 0.771295
Thermal correction to Gibbs Free Energy= 0.648954
Sum of electronic and zero-point Energies= -1891.272671
Sum of electronic and thermal Energies= -1891.229404
Sum of electronic and thermal Enthalpies= -1891.228459
Sum of electronic and thermal Free Energies= -1891.350800
E(RB3LYP) = -1892.67270763 A.U.

C-TSb1
1 1

C	0.85288000	0.44587400	-0.57076200

C	1.21508100	-0.36615400	-1.77965500
O	1.15831300	0.13177000	-2.88890400
O	1.45749600	-1.66959800	-1.55908800
C	1.64887100	-2.47023000	-2.74970800
H	2.48144200	-2.08297800	-3.33984600
H	1.86584000	-3.47421400	-2.38854900
H	0.74271600	-2.46402200	-3.35880700
C	1.42219200	1.78085100	-0.43754400
C	2.50086500	2.23413400	-1.23987300
C	0.87808000	2.68263900	0.50850900
C	2.98647800	3.53063000	-1.11303700
H	2.92242800	1.57799400	-1.99226200
C	1.38063400	3.97023000	0.64811800
H	0.05063600	2.35280100	1.12970800
C	2.43390600	4.39991000	-0.16650100
H	3.79742900	3.86671600	-1.75128000
H	0.94822600	4.64529400	1.37982000
H	2.82010100	5.40973100	-0.06694000
C	1.57342800	-0.80743900	1.21107200
H	1.01501900	-1.67898000	0.89406100
C	2.88565900	-0.66186700	0.86784700
H	3.31754100	-1.34204600	0.13821300
C	6.04988400	-0.59375900	0.87326600
C	7.14251500	-1.42754100	1.19937800
C	5.99314700	-0.06938300	-0.43773200
C	8.13812100	-1.69565900	0.26397000
H	7.22507800	-1.86444200	2.18644400
C	6.99820800	-0.34943700	-1.36177100
H	5.17307800	0.56647600	-0.74852600
C	8.07990600	-1.16168600	-1.02418500
H	8.96835800	-2.33438100	0.55095100
H	6.92740800	0.07495700	-2.35934200
H	8.85824300	-1.37694700	-1.74861300
C	3.82744000	0.35182600	1.44593800
H	4.02147100	1.15959700	0.72898200
H	3.39001200	0.83221500	2.32589600
H	1.14097700	-0.20951700	2.00737700
Au	-1.17752000	0.08830100	-0.10360100
P	-3.52455900	-0.29565500	0.20367700
C	-4.46608300	0.63587600	-1.20913200
C	-3.82269100	-2.20576900	0.08849700
C	-4.04944200	0.37745200	1.94006100
C	-3.83044300	2.03455700	-1.40046600
H	-4.33920000	2.52711900	-2.23679100

H	-3.93019600	2.68411900	-0.53290200
H	-2.76921800	1.96339100	-1.65653100
C	-4.26558800	-0.10975400	-2.54738400
H	-4.78649300	-1.06716100	-2.58913000
H	-4.68054000	0.51486100	-3.34605900
H	-3.20770500	-0.26780700	-2.77714300
C	-5.97852000	0.79046100	-0.94632900
H	-6.19290100	1.42836200	-0.08692600
H	-6.43552100	1.26813100	-1.82037300
H	-6.48251300	-0.16657000	-0.79904300
C	-2.97108200	-2.78014000	-1.07000400
H	-3.10987200	-3.86724500	-1.08666700
H	-3.25414300	-2.40154500	-2.05014300
H	-1.90448900	-2.58425400	-0.92255600
C	-3.30995300	-2.89017100	1.37493600
H	-3.92241400	-2.67515300	2.25158700
H	-3.34483000	-3.97401900	1.21910500
C	-5.30104200	-2.59241600	-0.12677300
H	-5.68797700	-2.25108000	-1.08861700
H	-5.37932200	-3.68562400	-0.12049600
H	-5.95712100	-2.21618200	0.66058700
C	-4.09108500	1.92126700	1.90940600
H	-4.91006400	2.31744700	1.30811400
H	-4.24508700	2.27602400	2.93454200
H	-3.15058300	2.35200200	1.55278100
C	-2.96274800	0.00002400	2.97595200
H	-2.84346200	-1.07243600	3.11732100
H	-1.98883200	0.41944900	2.70487100
H	-3.24941700	0.42765100	3.94352700
C	-5.41809500	-0.14809700	2.42073700
H	-5.41804300	-1.22674000	2.58683100
H	-5.65584400	0.32501600	3.38024200
H	-6.22825600	0.09249300	1.72993500
H	-2.27085700	-2.62684200	1.59489200
N	5.07512500	-0.29264500	1.83353200
C	5.09631800	-0.97920800	3.12042800
H	4.26398300	-0.62067800	3.72830700
H	5.01201100	-2.07096800	3.02912100
H	6.02196700	-0.75191300	3.65932200

Zero-point correction=	0.730046 (Hartree/Particle)
Thermal correction to Energy=	0.773004
Thermal correction to Enthalpy=	0.773948
Thermal correction to Gibbs Free Energy=	0.650959
Sum of electronic and zero-point Energies=	-1891.296518

Sum of electronic and thermal Energies= -1891.253560

Sum of electronic and thermal Enthalpies= -1891.252616

Sum of electronic and thermal Free Energies= -1891.375605

E(RB3LYP) = -1892.70236777 A.U.

C-TSa1

1 1

C	1.13987800	-0.21634700	1.04968900
C	1.52313200	-1.61440900	1.41693700
O	1.78575000	-1.92396500	2.56432800
O	1.42325100	-2.49700200	0.41041900
C	1.70861700	-3.86993000	0.76864600
H	1.01785900	-4.20930100	1.54258600
H	1.57338300	-4.44151700	-0.14842400
H	2.73346700	-3.96118800	1.13343100
C	1.95679300	0.84715000	1.51455300
C	3.24025300	0.63194300	2.10815300
C	1.48633100	2.19427700	1.42558900
C	3.96801500	1.69469200	2.62521200
H	3.62515700	-0.37505000	2.19542500
C	2.22462300	3.24714200	1.93410600
H	0.51882700	2.37219700	0.96834900
C	3.46411800	2.99655500	2.54593200
H	4.93004200	1.51203300	3.09228200
H	1.84393200	4.26157800	1.87422600
H	4.03531500	3.82205500	2.96056900
P	-3.16163700	0.04470100	-0.19443500
Au	-0.81231600	-0.05673100	0.39022400
C	-4.13875500	-0.90963700	1.17985200
C	-3.36478800	-2.20083000	1.54167300
C	-4.17757700	-0.06081600	2.46987400
C	-5.58306700	-1.27517000	0.77896200
H	-3.27946100	-2.90673000	0.71759300
H	-2.35868300	-1.97632000	1.90849300
H	-3.90483700	-2.70656400	2.35023300
H	-4.81252800	0.82179900	2.38401300
H	-4.59711600	-0.68007500	3.27026900
H	-3.17791600	0.24830000	2.78936400
H	-6.07423200	-1.74355300	1.63954000
H	-6.17915100	-0.40439400	0.50022400
H	-5.62367800	-1.99532500	-0.04051200
C	-3.71096900	1.90014400	-0.25880200
C	-3.07108900	2.65551000	0.93102500
C	-3.14577000	2.55997000	-1.53582100

C	-5.24016500	2.10360400	-0.22638300
H	-3.41942200	2.31856700	1.90535400
H	-1.98023100	2.57579300	0.91434400
H	-3.32886900	3.71684900	0.84077200
H	-3.62093100	2.20285600	-2.45022700
H	-3.33646800	3.63722500	-1.47611500
H	-2.06316600	2.42513900	-1.62321000
H	-5.45173400	3.17463300	-0.32430700
H	-5.75340600	1.59604600	-1.04528100
H	-5.68721900	1.77578300	0.71409900
C	-3.41520300	-0.79946600	-1.91892300
C	-2.27621900	-0.35013100	-2.86479000
C	-3.26276500	-2.32960400	-1.77165200
C	-4.77760000	-0.49234800	-2.57348400
H	-2.28107300	0.71568500	-3.08547500
H	-1.29715100	-0.61229700	-2.45289400
H	-2.39032700	-0.88167500	-3.81651000
H	-4.08759000	-2.79391900	-1.23013000
H	-3.25199200	-2.76829600	-2.77566000
H	-2.32116300	-2.60299900	-1.28588300
H	-4.85238000	-1.06210400	-3.50676400
H	-5.62277100	-0.78280500	-1.94680200
H	-4.88976000	0.56182200	-2.83307600
C	3.78226100	2.94355200	-3.15893200
H	3.89359400	3.58172400	-2.28469600
C	3.10970400	1.79459100	-3.10922300
H	3.01918800	1.18340600	-4.00640600
C	3.95859000	-0.51271400	-1.13369500
C	4.36249200	-1.86825400	-1.15285000
C	4.87760400	0.43953700	-0.63681800
C	5.61893200	-2.24404500	-0.69006800
H	3.70133800	-2.63127700	-1.54149800
C	6.13729200	0.04628800	-0.18451300
H	4.63489000	1.49274600	-0.64129300
C	6.51942200	-1.29311100	-0.20041700
H	5.90213100	-3.29194400	-0.72537500
H	6.82683700	0.80526500	0.17329900
H	7.50234100	-1.59237900	0.14811000
C	2.40661100	1.27474300	-1.87708900
H	2.65274600	1.89404700	-1.01042800
H	1.32085600	1.35304000	-2.00510700
H	4.24194700	3.29634500	-4.07673900
N	2.67271700	-0.14084200	-1.56343000
C	1.95135600	-1.08942400	-2.41985300

H	1.69439800	-1.98784400	-1.85997500
H	1.02265000	-0.62369600	-2.75015200
H	2.53652300	-1.36958500	-3.30611700

Zero-point correction= 0.731287 (Hartree/Particle)
Thermal correction to Energy= 0.773639
Thermal correction to Enthalpy= 0.774583
Thermal correction to Gibbs Free Energy= 0.655696
Sum of electronic and zero-point Energies= -1891.297113
Sum of electronic and thermal Energies= -1891.254762
Sum of electronic and thermal Enthalpies= -1891.253818
Sum of electronic and thermal Free Energies= -1891.372705
E(RB3LYP) = -1892.71557907 A.U

C-1a
1 1

C	-1.51548700	-0.17430900	-0.31193800
C	-1.63832700	-1.21676600	-1.42231900
O	-0.85415900	-1.24061700	-2.35083900
O	-2.68308800	-2.06540600	-1.34309100
C	-2.79986900	-3.02132500	-2.42403700
H	-1.91793700	-3.66398000	-2.46141200
H	-3.69429100	-3.60039300	-2.19881100
H	-2.90380700	-2.50074000	-3.37734200
C	-1.97253700	1.15849100	-0.89426400
C	-2.93429600	1.20780600	-1.92313000
C	-1.40187500	2.37470300	-0.48403200
C	-3.30822900	2.41549400	-2.50953000
H	-3.40733800	0.29363600	-2.26632200
C	-1.78502500	3.58787700	-1.05509000
H	-0.63714000	2.36852600	0.28392600
C	-2.73902100	3.61293500	-2.07338000
H	-4.04573000	2.41953500	-3.30630200
H	-1.32487800	4.51109800	-0.71590200
H	-3.02811500	4.55486200	-2.52937500
P	3.04689200	-0.08304900	0.09752300
Au	0.65162000	-0.11390600	0.02189200
C	3.67299400	-1.58433600	1.15004400
C	2.80874700	-1.70251600	2.42784700
C	3.45096000	-2.89483800	0.36272500
C	5.15985800	-1.49217100	1.55122400
H	2.90023200	-0.85250700	3.10149600
H	1.75098400	-1.82929700	2.18035600
H	3.13118500	-2.59292500	2.97977200
H	4.11428200	-2.99509200	-0.49689900

H	3.66475800	-3.73477700	1.03324100
H	2.41640500	-3.00055300	0.02259400
H	5.43681000	-2.41225200	2.07872400
H	5.82552500	-1.39885200	0.69135700
H	5.35986800	-0.66250200	2.23163600
C	3.65305200	-0.24060800	-1.73786300
C	2.79300000	-1.30221700	-2.46654600
C	3.40126700	1.09242100	-2.47732800
C	5.14439900	-0.61272600	-1.87335500
H	2.91369400	-2.30767300	-2.06746100
H	1.72866500	-1.05295200	-2.45484600
H	3.11382900	-1.33047900	-3.51434500
H	4.05647100	1.89958500	-2.14592000
H	3.60614000	0.93103700	-3.54133300
H	2.36021700	1.41849100	-2.39468900
H	5.40402800	-0.61889700	-2.93820200
H	5.80920700	0.10075100	-1.38242800
H	5.36526200	-1.61005500	-1.48750900
C	3.65533900	1.58275900	0.87495700
C	2.77751700	2.73647600	0.33479200
C	3.42973500	1.55867700	2.40292700
C	5.13925400	1.90258700	0.59647800
H	2.85362800	2.88079800	-0.74087100
H	1.72387900	2.58122000	0.58188800
H	3.10080900	3.66707800	0.81546600
H	4.09789600	0.87374200	2.92646300
H	3.63268300	2.56276900	2.79191300
H	2.39538700	1.31067300	2.66039800
H	5.39952700	2.83034100	1.11920100
H	5.81614800	1.12613900	0.95761700
H	5.34000700	2.06693400	-0.46367800
C	-2.18102700	2.70423300	2.79962500
H	-1.12667100	2.88193900	2.60670300
C	-2.75015800	1.51463900	2.60033600
H	-3.79819800	1.37461900	2.84464100
C	-3.84325300	-0.70980100	0.89834500
C	-4.52097900	-1.92023100	1.08299300
C	-4.57339800	0.44424400	0.59222500
C	-5.91015000	-1.97015500	0.96354300
H	-3.99894000	-2.83929500	1.30558200
C	-5.96272700	0.38157800	0.47155300
H	-4.07949500	1.39305500	0.45438000
C	-6.63876400	-0.82252000	0.65624100
H	-6.41722500	-2.91813700	1.11262700

H	-6.51067000	1.28802300	0.23470600
H	-7.71928700	-0.86618600	0.56521200
C	-1.95935300	0.28786800	2.26012200
H	-0.90579800	0.52300200	2.09839600
H	-2.03483500	-0.38820500	3.11636500
H	-2.75271200	3.54409700	3.18122900
N	-2.34477000	-0.62451700	1.04414200
C	-1.75903300	-1.95994800	1.44709000
H	-1.91110200	-2.68604900	0.65626200
H	-0.69451500	-1.80885300	1.61311400
H	-2.23455100	-2.29709500	2.36695500

Zero-point correction= 0.733807 (Hartree/Particle)
Thermal correction to Energy= 0.775891
Thermal correction to Enthalpy= 0.776836
Thermal correction to Gibbs Free Energy= 0.659316
Sum of electronic and zero-point Energies= -1891.300429
Sum of electronic and thermal Energies= -1891.258345
Sum of electronic and thermal Enthalpies= -1891.257401
Sum of electronic and thermal Free Energies= -1891.374921
E(RB3LYP) = -1892.71827238 A.U.

C-P1

C	1.94846800	0.55706300	-0.76643000
C	2.44271400	1.84616600	-0.10095700
O	3.12281800	2.68099300	-0.65614800
O	2.02575700	1.96609900	1.18056100
C	2.44582100	3.16707800	1.85060400
H	2.06872500	4.04811200	1.32634200
H	2.02252300	3.10745700	2.85297000
H	3.53620100	3.22346100	1.89492800
C	2.75269200	-0.67292700	-0.34275800
C	3.18938600	-0.89127800	0.97079100
C	3.05019500	-1.63962100	-1.31391400
C	3.90097300	-2.04702500	1.30097100
H	2.97604900	-0.15397200	1.73663600
C	3.75843500	-2.79389600	-0.98516400
H	2.72053400	-1.48408100	-2.33790700
C	4.18776400	-3.00225600	0.32686000
H	4.23357300	-2.19638000	2.32436300
H	3.97934500	-3.52788700	-1.75488200
H	4.74353400	-3.89886700	0.58518200
C	-6.69514200	-1.14906000	1.30126500
H	-7.13174000	-1.69682900	0.46894100
C	-5.40930200	-0.79844500	1.30551000

H	-4.99778200	-0.24021700	2.14579600
C	-2.40749900	0.17809100	-0.45505500
C	-1.55780200	-0.39907400	0.51416400
C	-1.79246700	0.87499100	-1.51391900
C	-0.17587700	-0.29754800	0.41626800
H	-1.98128200	-0.90943300	1.37264000
C	-0.40492900	0.97745700	-1.59180300
H	-2.39170800	1.32339200	-2.29706200
C	0.43327100	0.39385000	-0.63790500
H	0.43758400	-0.76192100	1.18137600
H	0.03148200	1.51859600	-2.42852400
H	2.16993600	0.72957200	-1.82330100
C	-4.43625600	-1.11039600	0.19766100
H	-3.65586900	-1.78140600	0.56551700
H	-4.95566700	-1.65520300	-0.60731400
H	-7.35706300	-0.91291200	2.12888600
N	-3.79953700	0.09497100	-0.34038000
C	-4.63550800	0.84969200	-1.25648100
H	-5.66344500	0.82870100	-0.88688800
H	-4.31543800	1.89446200	-1.29497000
H	-4.63096300	0.44666400	-2.28361300

Zero-point correction= 0.359338 (Hartree/Particle)
Thermal correction to Energy= 0.380691
Thermal correction to Enthalpy= 0.381635
Thermal correction to Gibbs Free Energy= 0.305262
Sum of electronic and zero-point Energies= -941.511981
Sum of electronic and thermal Energies= -941.490628
Sum of electronic and thermal Enthalpies= -941.489684
Sum of electronic and thermal Free Energies= -941.566057
E(RB3LYP) = -942.211366208 A.U.

Re5

C	4.22879100	0.10688800	0.42131600
H	4.17002800	0.86759200	1.19603600
C	3.17135600	-0.22302800	-0.31728200
H	3.24905500	-0.99436000	-1.08150100
C	-0.47162600	-0.23678300	-0.02486900
C	-1.38532500	-1.29826300	0.05810400
C	-0.93844400	1.08257600	-0.05514500
C	-2.74980000	-1.03901400	0.10769200
H	-0.99868900	-2.31180700	0.08139900
C	-2.31500600	1.32600700	-0.00523500
H	-0.25105200	1.91778400	-0.11433600
C	-3.22601800	0.27631400	0.07570400

H	-3.44744300	-1.86930100	0.17107000
H	-2.66882000	2.35291200	-0.02939000
H	-4.29224800	0.47566500	0.11415700
C	1.82870200	0.43232200	-0.20082400
H	1.80058900	1.11243200	0.66179400
H	1.61398200	1.02496700	-1.10418500
H	5.19455900	-0.36736800	0.27745400
O	0.84678200	-0.59633000	-0.06615700

Zero-point correction= 0.166319 (Hartree/Particle)
Thermal correction to Energy= 0.175425
Thermal correction to Enthalpy= 0.176369
Thermal correction to Gibbs Free Energy= 0.131300
Sum of electronic and zero-point Energies= -424.013496
Sum of electronic and thermal Energies= -424.004390
Sum of electronic and thermal Enthalpies= -424.003446
Sum of electronic and thermal Free Energies= -424.048514
E(RB3LYP) = -424.329669321 A.U.

D-TSa1

C	-1.46446600	0.35002300	0.63036500
C	-1.61972900	0.03112000	2.09022900
O	-1.27544900	0.84172700	2.92757300
O	-2.04004600	-1.21331500	2.38714900
C	-2.02704800	-1.54065200	3.79795000
H	-2.67239700	-0.85810100	4.35362300
H	-2.39805500	-2.56260600	3.86035700
H	-1.01102900	-1.47298000	4.19141700
C	-2.10125200	1.59615800	0.15654800
C	-3.09511300	2.25981600	0.90429000
C	-1.72990100	2.13913900	-1.09119100
C	-3.67632200	3.43280500	0.43010900
H	-3.39302600	1.87384600	1.87214200
C	-2.32332100	3.30159700	-1.57203400
H	-0.97196100	1.63258100	-1.68159900
C	-3.29537400	3.95444200	-0.80798800
H	-4.42883700	3.93927500	1.02612900
H	-2.02389500	3.70567500	-2.53411200
H	-3.75148600	4.86871500	-1.17557500
P	2.97115200	-0.02095600	-0.19169100
Au	0.59825800	0.09734200	0.16080900
C	3.32921000	-1.26609000	-1.63095400
C	2.40850200	-2.49903000	-1.46754400
C	2.93766500	-0.62019800	-2.97811300
C	4.79775800	-1.73267200	-1.70671900

H	2.59808700	-3.07385400	-0.56293000
H	1.35326100	-2.21040800	-1.47508500
H	2.57635400	-3.16713100	-2.32000200
H	3.60128900	0.19265300	-3.27472400
H	3.00402300	-1.38853000	-3.75644100
H	1.90754100	-0.25082600	-2.97100100
H	4.91131200	-2.38616000	-2.57936700
H	5.50018700	-0.90585500	-1.82827000
H	5.09896500	-2.31309900	-0.83277800
C	3.60645100	1.75149400	-0.64409600
C	2.61148500	2.40392600	-1.63431500
C	3.59932700	2.64628600	0.61570800
C	5.02312600	1.76526600	-1.25557100
H	2.53439100	1.88441600	-2.58807600
H	1.60998600	2.48171100	-1.20108100
H	2.95963200	3.42151300	-1.84522100
H	4.36259000	2.36928700	1.34394800
H	3.81603800	3.67288900	0.30042200
H	2.62343900	2.65744500	1.10968500
H	5.32171900	2.80745700	-1.41677300
H	5.76984100	1.31191800	-0.60074300
H	5.06888200	1.26750400	-2.22615100
C	3.77192400	-0.63244200	1.46180300
C	3.08781500	0.08758700	2.64965300
C	3.48371300	-2.13788400	1.64772600
C	5.29587400	-0.40378600	1.53605300
H	3.25233500	1.16312100	2.66378300
H	2.00836800	-0.08943900	2.66657600
H	3.50556500	-0.31778100	3.57827700
H	4.02678200	-2.76988300	0.94379600
H	3.81054300	-2.42488000	2.65328100
H	2.41523900	-2.36240100	1.57584500
H	5.66711900	-0.83195200	2.47417200
H	5.83718500	-0.88800500	0.72115400
H	5.56179900	0.65484000	1.54228600
C	-2.58138600	-3.95297500	-2.02816300
H	-3.18194800	-4.50278900	-1.30774700
C	-1.91344700	-2.84979100	-1.68817800
H	-1.31981900	-2.31180800	-2.42517400
C	-3.79337400	-0.76642500	-0.46817300
C	-4.22770300	-0.29654600	-1.70383000
C	-4.68173100	-1.09036400	0.55493900
C	-5.59867800	-0.14814200	-1.92045400
H	-3.50465200	-0.05556200	-2.47392900

C	-6.04981800	-0.93938900	0.32211200
H	-4.30837500	-1.44816900	1.50647000
C	-6.50813700	-0.46921100	-0.91087400
H	-5.95308800	0.21574200	-2.87955600
H	-6.75651700	-1.18928900	1.10720500
H	-7.57336000	-0.35444500	-1.08446700
C	-1.88635500	-2.31014900	-0.29778000
H	-2.48600600	-2.89791400	0.39798300
H	-0.87097700	-2.21473900	0.09130300
H	-2.54482000	-4.35274400	-3.03655000
O	-2.39200500	-0.91321100	-0.27473500

Zero-point correction= 0.689635 (Hartree/Particle)
Thermal correction to Energy= 0.730756
Thermal correction to Enthalpy= 0.731701
Thermal correction to Gibbs Free Energy= 0.615179
Sum of electronic and zero-point Energies= -1871.893600
Sum of electronic and thermal Energies= -1871.852478
Sum of electronic and thermal Enthalpies= -1871.851534
Sum of electronic and thermal Free Energies= -1871.968055
E(RB3LYP) = -1873.24791788 A.U.

D-1a

C	-1.80786900	0.69539700	0.38399200
C	-2.00077300	0.85907000	1.86740900
O	-1.56871200	1.82520400	2.46438200
O	-2.62156500	-0.17364900	2.48117900
C	-2.71038600	-0.05678600	3.92072100
H	-3.24990600	0.85069900	4.19749300
H	-3.25014500	-0.94343700	4.25067500
H	-1.71161800	-0.02616700	4.36069100
C	-2.22395800	1.86289400	-0.47151000
C	-2.95689000	2.95086900	0.03483200
C	-1.89902200	1.85928500	-1.84168300
C	-3.34857200	3.99650700	-0.80283800
H	-3.19431200	3.00191100	1.09116900
C	-2.30865500	2.89265800	-2.68023500
H	-1.31031400	1.03967600	-2.24369400
C	-3.03475400	3.96854000	-2.16158300
H	-3.90287400	4.83318900	-0.38888300
H	-2.04794100	2.86840500	-3.73409000
H	-3.34388900	4.78191900	-2.81074000
P	2.65881100	0.00552400	-0.00194400
Au	0.28322800	0.23624500	0.15188800
C	3.12978900	-0.49992400	-1.80944100

C	2.14978400	-1.59479300	-2.29451400
C	2.92140400	0.70718600	-2.75037600
C	4.57927300	-1.00531300	-1.96332100
H	2.22252500	-2.52615700	-1.73639200
H	1.11176500	-1.25346700	-2.24885000
H	2.38221000	-1.82118100	-3.34166200
H	3.65430600	1.50025900	-2.59820500
H	3.03686400	0.35752600	-3.78241100
H	1.91708900	1.13133000	-2.65835000
H	4.76797600	-1.20374500	-3.02468100
H	5.31972300	-0.27433700	-1.63331200
H	4.75784400	-1.93956800	-1.42803600
C	3.41872400	1.73017700	0.44836400
C	2.59159800	2.84561500	-0.23718700
C	3.27865200	1.97354400	1.96803300
C	4.90211600	1.88226600	0.05105200
H	2.61887500	2.80832000	-1.32451800
H	1.54546800	2.82800800	0.08130500
H	3.01220500	3.81128900	0.06568200
H	3.92959000	1.33654700	2.56854800
H	3.57033500	3.00985800	2.17123200
H	2.24635400	1.85510000	2.31040500
H	5.25864300	2.85429000	0.41063000
H	5.54256900	1.11774100	0.49480500
H	5.05104900	1.87022000	-1.03068200
C	3.23958800	-1.34407200	1.25738000
C	2.44320000	-1.18108400	2.57481500
C	2.88577900	-2.74777500	0.71759200
C	4.75086600	-1.29900700	1.56542600
H	2.62120500	-0.23461400	3.08139700
H	1.36657700	-1.27951000	2.40679100
H	2.74904400	-1.98113700	3.25887600
H	3.48998100	-3.04173700	-0.14182300
H	3.08595200	-3.47518300	1.51239800
H	1.82749900	-2.83320400	0.45364900
H	4.99622400	-2.13554400	2.22985400
H	5.36658000	-1.40344000	0.67019200
H	5.04849200	-0.38446000	2.08152800
C	-5.81187900	-2.26536900	-0.10237800
H	-5.99260800	-2.18375700	-1.17133400
C	-4.95583700	-1.46153900	0.53105400
H	-4.78579700	-1.54873900	1.60019900
C	-2.19748700	-1.75519700	-0.55767500
C	-1.77233900	-2.70418400	0.36352200

C	-2.15258700	-1.96311500	-1.93125800
C	-1.26764100	-3.91302300	-0.12084000
H	-1.84271200	-2.49185200	1.42338700
C	-1.65121200	-3.18044800	-2.39858400
H	-2.50010000	-1.19815200	-2.61719900
C	-1.20890200	-4.15130800	-1.49662900
H	-0.93511000	-4.67287700	0.57926400
H	-1.61086500	-3.36803200	-3.46678200
H	-0.82590500	-5.09725100	-1.86611800
C	-4.24007000	-0.35707300	-0.16116800
H	-4.47744800	-0.29441900	-1.22425300
H	-4.39990100	0.61501100	0.30385200
H	-6.37588200	-3.02496700	0.42930000
O	-2.74078000	-0.53212500	-0.06420400

Zero-point correction= 0.689809 (Hartree/Particle)
Thermal correction to Energy= 0.731676
Thermal correction to Enthalpy= 0.732620
Thermal correction to Gibbs Free Energy= 0.613382
Sum of electronic and zero-point Energies= -1871.894162
Sum of electronic and thermal Energies= -1871.852295
Sum of electronic and thermal Enthalpies= -1871.851350
Sum of electronic and thermal Free Energies= -1871.970589
E(RB3LYP) = -1873.25075934 A.U.

D-TSa2
1 1

C	-1.97349100	0.19827600	-0.23422100
C	-1.84699600	1.11230600	-1.33113900
O	-0.87854600	1.03991000	-2.12253800
O	-2.75548500	2.10002200	-1.43951500
C	-2.45891000	3.13070300	-2.40783200
H	-2.44583600	2.71603400	-3.41683200
H	-3.26066300	3.86121100	-2.30471600
H	-1.49109100	3.58808800	-2.19228100
C	-1.86482300	-1.27372900	-0.37989600
C	-1.91331100	-1.89909900	-1.64145300
C	-1.70851900	-2.09539400	0.75584200
C	-1.79333100	-3.28365500	-1.75818700
H	-2.02559300	-1.29453600	-2.53499800
C	-1.62432900	-3.48082100	0.63840000
H	-1.64553100	-1.63874700	1.74024200
C	-1.65852200	-4.08364900	-0.62195800
H	-1.82910500	-3.73953600	-2.74332500
H	-1.51847600	-4.09065700	1.53114200

H	-1.58341600	-5.16247500	-0.71582400
P	2.91657100	-0.08229700	0.22266800
Au	0.72709800	0.31394900	-0.41770900
C	2.94886100	-0.58262000	2.09249600
C	1.99847200	0.34488800	2.88530900
C	2.38529500	-2.01152100	2.25126100
C	4.35740100	-0.52496800	2.72118700
H	2.30684800	1.38896900	2.88642600
H	0.97843800	0.28699200	2.49454300
H	1.98208300	0.00624600	3.92760500
H	3.04676900	-2.77877300	1.84778400
H	2.27564500	-2.21429500	3.32245600
H	1.39817600	-2.11712300	1.79189700
H	4.29291900	-0.89341200	3.75132500
H	5.08061100	-1.15232300	2.19759600
H	4.75489700	0.49055900	2.76982700
C	3.56912400	-1.53155500	-0.88859900
C	2.47809800	-2.62311900	-1.00693400
C	3.80962600	-1.00819200	-2.32153800
C	4.87261500	-2.16670200	-0.35943000
H	2.23112300	-3.10357300	-0.06252200
H	1.55413200	-2.23033400	-1.44031300
H	2.85583400	-3.40065000	-1.68064200
H	4.66082700	-0.33032100	-2.39327700
H	4.02995200	-1.86933100	-2.96164600
H	2.92408600	-0.51451400	-2.73197700
H	5.20656100	-2.91948300	-1.08247000
H	5.68365100	-1.44475200	-0.24628700
H	4.73403700	-2.68153400	0.59336900
C	3.93848600	1.53696200	-0.07592900
C	3.50668000	2.17197800	-1.41926500
C	3.60137300	2.57290500	1.01875900
C	5.46412900	1.30188000	-0.08815500
H	3.71662000	1.54907500	-2.28641400
H	2.44030200	2.41435500	-1.42588400
H	4.06422800	3.10711800	-1.54549300
H	3.99093500	2.30244500	2.00128500
H	4.06859900	3.52365200	0.73974200
H	2.52441600	2.74916300	1.09746800
H	5.96191100	2.27220600	-0.19581900
H	5.83245500	0.84992100	0.83477200
H	5.78638200	0.68339900	-0.92762900
C	-1.48134500	3.58383500	1.75272700
H	-0.56950200	3.12218000	2.12295400

C	-2.59677700	2.87601900	1.56748200
H	-3.50637300	3.34699600	1.20411600
C	-4.41057400	0.07754700	0.64809300
C	-4.80707800	-0.90529400	1.54765300
C	-5.25022500	0.60035300	-0.32600100
C	-6.11787300	-1.37948900	1.46604400
H	-4.11536600	-1.29836300	2.28296500
C	-6.55478400	0.10542100	-0.39533100
H	-4.88807300	1.36106200	-1.00447100
C	-6.98866600	-0.87701500	0.49705600
H	-6.45077400	-2.14775200	2.15626600
H	-7.23225500	0.49731900	-1.14715400
H	-8.00506600	-1.25242700	0.43680600
C	-2.68599700	1.43427300	1.92509000
H	-1.73526300	1.02810500	2.26853300
H	-3.48119400	1.22691300	2.64369500
H	-1.44603000	4.65090400	1.55785800
O	-3.05469200	0.58023600	0.74069000

Zero-point correction= 0.689251 (Hartree/Particle)
Thermal correction to Energy= 0.730425
Thermal correction to Enthalpy= 0.731369
Thermal correction to Gibbs Free Energy= 0.613125
Sum of electronic and zero-point Energies= -1871.856526
Sum of electronic and thermal Energies= -1871.815352
Sum of electronic and thermal Enthalpies= -1871.814408
Sum of electronic and thermal Free Energies= -1871.932651
E(RB3LYP) = -1873.20612372 A.U.

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1 1

C	1.94988200	-0.17557400	0.54054100
C	1.78356200	-1.04603000	1.65831700
O	1.00175600	-0.84438800	2.59061200
O	2.52487500	-2.20442000	1.58301500
C	2.28991200	-3.14230400	2.65009000
H	1.25861300	-3.50272200	2.62858900
H	2.98220400	-3.96547200	2.47226000
H	2.48163800	-2.68216300	3.62128500
C	1.54119200	1.23196500	0.45961600
C	1.09722400	1.95692800	1.61204500
C	1.61976000	1.96328000	-0.76647600
C	0.80223700	3.31794900	1.52869400
H	1.02212900	1.43002200	2.55461200
C	1.33697200	3.32603400	-0.81820600

H	1.93055100	1.44903000	-1.66898500
C	0.93544700	4.01742600	0.32737000
H	0.48680400	3.83815100	2.42842100
H	1.43183800	3.84959200	-1.76512800
H	0.72346600	5.08056100	0.28201900
P	-2.91709800	-0.23872200	-0.20156400
Au	-0.69469900	0.39127600	0.08316200
C	-3.04341300	-1.41198100	-1.73792100
C	-2.16543300	-0.85424400	-2.88291600
C	-2.45650800	-2.79400500	-1.37936100
C	-4.48814200	-1.59658400	-2.24855300
H	-2.49726900	0.11087900	-3.26016200
H	-1.12047800	-0.75872600	-2.57378000
H	-2.20534800	-1.56344600	-3.71763300
H	-3.07045900	-3.35056000	-0.67057500
H	-2.40419000	-3.38969300	-2.29744800
H	-1.44117300	-2.71387800	-0.97940600
H	-4.47359400	-2.31680200	-3.07442800
H	-5.16119000	-1.99285300	-1.48613800
H	-4.91601400	-0.67180000	-2.63939400
C	-3.45730500	-1.15166500	1.42049400
C	-2.33148900	-2.11514300	1.86939800
C	-3.62415100	-0.12553600	2.56289100
C	-4.77456500	-1.93925500	1.25580000
H	-2.13213300	-2.91372700	1.15664800
H	-1.39458200	-1.59033200	2.07801400
H	-2.65569600	-2.58947300	2.80297300
H	-4.48186000	0.53482900	2.42777900
H	-3.79205800	-0.68355300	3.49040400
H	-2.72381300	0.47800700	2.70754200
H	-5.04366600	-2.36553900	2.22873200
H	-5.60895900	-1.31253700	0.93505700
H	-4.68123900	-2.77365600	0.55782700
C	-3.95111700	1.37595700	-0.47798900
C	-3.44954500	2.47353200	0.49094700
C	-3.70211100	1.91324400	-1.90386200
C	-5.46678300	1.16868500	-0.27267100
H	-3.58465500	2.22464100	1.54192900
H	-2.39337800	2.70486600	0.32651600
H	-4.02550100	3.38498100	0.29403500
H	-4.14749100	1.29202400	-2.68221600
H	-4.16820900	2.90184100	-1.97797800
H	-2.63572600	2.03919100	-2.11313800
H	-5.97902900	2.10692300	-0.51339100

H	-5.88253400	0.39623500	-0.92213700
H	-5.71921700	0.92300300	0.76050900
C	4.13979700	-2.28615300	-3.27925900
H	4.73340100	-3.01248300	-2.72992100
C	3.15824900	-1.59536700	-2.69503300
H	2.56915500	-0.87995400	-3.26555800
C	4.34344800	-0.10355300	-0.26440400
C	5.07894000	-0.61724300	0.79612300
C	4.85025800	0.82310500	-1.16548700
C	6.38980500	-0.16483800	0.95694900
H	4.63716600	-1.34038300	1.46866000
C	6.16477100	1.26171500	-0.98555300
H	4.24457800	1.19381300	-1.98204500
C	6.93141900	0.77073900	0.07177800
H	6.98637800	-0.54821900	1.77842700
H	6.58277200	1.98840800	-1.67452900
H	7.95119100	1.11646000	0.20685600
C	2.76338400	-1.81437000	-1.28071700
H	1.69522200	-1.98098900	-1.14222100
H	3.33821400	-2.58761000	-0.77461800
H	4.37581700	-2.15978200	-4.33110800
O	2.96734900	-0.54211200	-0.46229600

Zero-point correction= 0.689862 (Hartree/Particle)
Thermal correction to Energy= 0.730785
Thermal correction to Enthalpy= 0.731729
Thermal correction to Gibbs Free Energy= 0.615322
Sum of electronic and zero-point Energies= -1871.859643
Sum of electronic and thermal Energies= -1871.818720
Sum of electronic and thermal Enthalpies= -1871.817776
Sum of electronic and thermal Free Energies= -1871.934183
E(RB3LYP) = -1873.21115687 A.U.

D-2a

C	2.68053500	-0.50991900	0.39729400
C	2.42422700	-0.05929400	1.72580400
O	1.46527600	-0.41068000	2.41434800
O	3.36488000	0.82409300	2.19839900
C	3.12119000	1.31146100	3.52959800
H	3.09110400	0.48700100	4.24532100
H	3.95206400	1.98084100	3.75355100
H	2.17388900	1.85342700	3.57714300
C	1.99493400	-1.51645000	-0.32448500
C	0.93357600	-2.29346500	0.29459800
C	2.32314800	-1.85892200	-1.67070500

C	0.37586500	-3.41111800	-0.40211100
H	0.86817300	-2.26532300	1.37954900
C	1.71071400	-2.91383200	-2.32494900
H	3.10885300	-1.31550600	-2.18223200
C	0.72813100	-3.70920900	-1.70581000
H	-0.33369500	-4.03706900	0.13208200
H	2.01540700	-3.14109400	-3.34324800
H	0.28062600	-4.54574100	-2.23066000
P	-2.79771600	0.44666900	0.04164200
Au	-0.91332000	-0.97388500	0.07686300
C	-2.88475000	1.30761900	-1.69071700
C	-1.45840100	1.72808200	-2.11982400
C	-3.36660900	0.29254400	-2.75042300
C	-3.81272100	2.54035900	-1.72148300
H	-1.00016500	2.46503500	-1.46254300
H	-0.79090400	0.86346700	-2.18330700
H	-1.52363700	2.17352400	-3.11953300
H	-4.41595400	0.01805800	-2.63620300
H	-3.26327200	0.75813200	-3.73691700
H	-2.75976900	-0.61747500	-2.75357700
H	-3.85494300	2.91911400	-2.74910100
H	-4.83521100	2.30671400	-1.41941500
H	-3.44782700	3.35587600	-1.09443000
C	-4.37486200	-0.63341700	0.35248900
C	-4.26256700	-1.94328600	-0.46449500
C	-4.42866800	-1.05771800	1.83703700
C	-5.69312500	0.08384000	-0.00759000
H	-4.25580200	-1.79066700	-1.54227100
H	-3.36576000	-2.50825300	-0.19413600
H	-5.13283000	-2.56606400	-0.22822900
H	-4.63687200	-0.22868800	2.51454800
H	-5.24633300	-1.77788200	1.95156400
H	-3.50943900	-1.55586100	2.15851800
H	-6.52857700	-0.57356400	0.25854600
H	-5.82866700	1.01859300	0.53962800
H	-5.78091000	0.29378800	-1.07520000
C	-2.56319800	1.75256200	1.45216800
C	-2.00878500	1.04571000	2.71382400
C	-1.48548100	2.77426900	1.03035300
C	-3.85990300	2.50867900	1.80757400
H	-2.67536000	0.28834000	3.12209400
H	-1.03400000	0.58457800	2.53023900
H	-1.87260200	1.80798200	3.49018800
H	-1.81067200	3.43770500	0.22757400

H	-1.26336800	3.40570600	1.89789000
H	-0.55199600	2.28598300	0.73550900
H	-3.62208200	3.27072200	2.55851900
H	-4.29986800	3.02202600	0.95039500
H	-4.61861100	1.85691500	2.24412600
C	5.60066500	-2.55648300	0.90914200
H	5.58274800	-2.19792400	1.93499200
C	5.42119600	-1.73140100	-0.12591800
H	5.44702400	-2.10463400	-1.14588800
C	3.59320200	1.48494700	-0.79469800
C	2.79583100	1.63888800	-1.92205600
C	4.21872100	2.54840600	-0.15759200
C	2.62074300	2.92724000	-2.43066500
H	2.32488900	0.78173300	-2.38665600
C	4.03786100	3.82789200	-0.69006600
H	4.81040800	2.39489700	0.73464400
C	3.24300900	4.01907200	-1.82078000
H	2.00731000	3.07057100	-3.31439600
H	4.51923000	4.67402800	-0.21046200
H	3.11045600	5.01629800	-2.22768200
C	5.23841200	-0.27456300	0.06210100
H	5.35790300	0.04876800	1.09414800
H	5.82601500	0.33466600	-0.62489200
H	5.78552500	-3.61613300	0.76461200
O	3.78712000	0.13275200	-0.30736000

Zero-point correction= 0.690784 (Hartree/Particle)
Thermal correction to Energy= 0.732153
Thermal correction to Enthalpy= 0.733098
Thermal correction to Gibbs Free Energy= 0.615897
Sum of electronic and zero-point Energies= -1871.873193
Sum of electronic and thermal Energies= -1871.831823
Sum of electronic and thermal Enthalpies= -1871.830879
Sum of electronic and thermal Free Energies= -1871.948080
E(RB3LYP) = -1873.22400528 A.U.

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C	-2.71483300	-0.60253400	-0.22585000
C	-2.12126200	0.07529500	-1.29714500
O	-0.95766800	-0.15981700	-1.77635600
O	-2.86469700	1.06192000	-1.85019600
C	-2.25126100	1.83192700	-2.89665900
H	-1.99103400	1.19877100	-3.74786700
H	-3.00173000	2.56693100	-3.18715400
H	-1.35199200	2.33799800	-2.53681700

C	-2.26659700	-1.82642900	0.43077900
C	-2.83992300	-2.23168900	1.65767100
C	-1.29222800	-2.67683000	-0.14498100
C	-2.44458600	-3.41102400	2.28711100
H	-3.60305700	-1.61713300	2.12325800
C	-0.89911600	-3.84946600	0.49654500
H	-0.86887200	-2.42385400	-1.10869800
C	-1.46613600	-4.22612600	1.71700900
H	-2.90667400	-3.69160000	3.22923000
H	-0.15676500	-4.48707800	0.02418500
H	-1.16088900	-5.14534300	2.20681600
P	3.01421000	0.25900800	0.20029400
Au	0.92012900	0.03981700	-0.77025600
C	3.08181900	-0.91185100	1.74173800
C	1.74997300	-0.80275000	2.52197200
C	3.18272000	-2.37899600	1.27087600
C	4.26056700	-0.60546500	2.68917100
H	1.56432100	0.18734100	2.93335400
H	0.89594500	-1.08601500	1.90099700
H	1.79388500	-1.50393500	3.36307000
H	4.14277200	-2.61776500	0.81208200
H	3.07735400	-3.02265200	2.15104300
H	2.37814900	-2.64194700	0.57812500
H	4.26360300	-1.35479000	3.48886000
H	5.23097400	-0.65917000	2.19220500
H	4.17282500	0.37096300	3.16941000
C	4.32626100	-0.25812400	-1.12601500
C	3.82771800	-1.52005700	-1.87141100
C	4.45250600	0.85020700	-2.19500900
C	5.72117300	-0.53662400	-0.52663100
H	3.70845400	-2.39142500	-1.23021100
H	2.87723200	-1.33752000	-2.38096400
H	4.56986000	-1.77541100	-2.63621000
H	4.93531200	1.75460800	-1.82219500
H	5.07842300	0.46452300	-3.00697100
H	3.48410400	1.11567200	-2.62885200
H	6.41538900	-0.74265200	-1.34903300
H	6.12160500	0.31234200	0.03059700
H	5.73126400	-1.41215600	0.12522000
C	3.24563200	2.10766100	0.72430300
C	2.70310000	3.02802400	-0.39532100
C	2.38912700	2.40322200	1.97495100
C	4.71372100	2.47801600	1.02180400
H	3.23144700	2.92659300	-1.34113100

H	1.63889900	2.85282700	-0.57692800
H	2.81852400	4.06667200	-0.06512000
H	2.76563400	1.91975900	2.87720700
H	2.41596700	3.48363500	2.15428300
H	1.34197400	2.12104200	1.83073300
H	4.74325000	3.51258400	1.38181700
H	5.16104800	1.85212900	1.79582200
H	5.34545200	2.43105900	0.13317800
C	-4.58849400	-2.04407500	-2.33262600
H	-4.15927500	-2.82825800	-1.71616200
C	-5.33780600	-1.05647700	-1.79798700
H	-5.75030600	-0.27412400	-2.42853800
C	-4.08292400	1.15855300	0.83402400
C	-4.84787300	2.14262400	0.21969000
C	-3.47278900	1.35099600	2.06988500
C	-5.01794300	3.36206000	0.88010000
H	-5.27978400	1.97023200	-0.75858400
C	-3.64097000	2.58113800	2.70792500
H	-2.88261200	0.55976200	2.51770600
C	-4.41674200	3.58319200	2.11997700
H	-5.61440100	4.14068600	0.41532800
H	-3.17431900	2.74788400	3.67370300
H	-4.55135700	4.53329700	2.62676800
C	-5.48020300	-0.93764300	-0.37545100
H	-5.32902900	-1.83389900	0.21817200
H	-6.19940000	-0.23751500	0.03556400
H	-4.40940600	-2.10644200	-3.40143800
O	-3.95911900	-0.11808300	0.21371400

Zero-point correction= 0.689387 (Hartree/Particle)
Thermal correction to Energy= 0.730418
Thermal correction to Enthalpy= 0.731362
Thermal correction to Gibbs Free Energy= 0.614458
Sum of electronic and zero-point Energies= -1871.878290
Sum of electronic and thermal Energies= -1871.837259
Sum of electronic and thermal Enthalpies= -1871.836315
Sum of electronic and thermal Free Energies= -1871.953219
E(RB3LYP) = -1873.22161092 A.U.

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1 1

C	-1.10948200	0.94360200	0.36792900
C	-0.99827500	2.44209400	0.43978300
O	-0.88870900	3.02266200	1.50295600
O	-0.89908700	3.07219500	-0.75271000

C	-0.62075700	4.48748400	-0.67771600
H	0.34890100	4.65930400	-0.20558200
H	-0.61360300	4.83570700	-1.70975000
H	-1.39252800	5.00090500	-0.10079200
C	-1.96069600	0.29433300	1.37274400
C	-2.99419900	0.98282000	2.05256400
C	-1.74855800	-1.06192200	1.71020200
C	-3.73703200	0.35858900	3.04899700
H	-3.18095300	2.02592500	1.82671700
C	-2.49971800	-1.69031300	2.69829600
H	-0.96792400	-1.61219000	1.19390400
C	-3.49330100	-0.97896600	3.37585100
H	-4.50299700	0.91704800	3.57844400
H	-2.30620200	-2.72908400	2.94721500
H	-4.07283400	-1.46257200	4.15658800
P	3.15081200	-0.46798000	-0.16893000
Au	0.85991800	0.21667200	0.04241400
C	3.24109000	-2.07264200	-1.25243000
C	2.09933500	-3.02732700	-0.82813400
C	2.96914400	-1.71088500	-2.72866900
C	4.58858700	-2.81779400	-1.16062200
H	2.19497700	-3.39919100	0.19021500
H	1.12079700	-2.54717800	-0.92495900
H	2.11176700	-3.89653900	-1.49589600
H	3.77951600	-1.14327900	-3.18730500
H	2.86973100	-2.64290000	-3.29618900
H	2.03509400	-1.15345900	-2.84921600
H	4.56462000	-3.66907900	-1.85082500
H	5.43731400	-2.19350700	-1.44603200
H	4.77828100	-3.22148700	-0.16431600
C	4.12279300	0.97955000	-1.01243000
C	3.27533000	1.54660500	-2.17760300
C	4.29049800	2.13848000	-0.00575100
C	5.51254300	0.57179500	-1.54349300
H	3.09938500	0.83358200	-2.98071400
H	2.30607000	1.91536400	-1.82860900
H	3.81736000	2.39576700	-2.60961300
H	4.98420400	1.90680500	0.80306800
H	4.70153000	2.99932500	-0.54469600
H	3.33437400	2.44844100	0.42651900
H	6.00931400	1.46411500	-1.94138100
H	6.15878600	0.16111000	-0.76544100
H	5.45563000	-0.15159100	-2.35953000
C	3.83570700	-0.80552200	1.61048000

C	3.30927200	0.29083800	2.56913500
C	3.26809600	-2.14145500	2.14007200
C	5.37605300	-0.85467500	1.68673000
H	3.65967900	1.29225300	2.32677600
H	2.21603500	0.31087400	2.59967100
H	3.66429600	0.05732300	3.57939900
H	3.67704900	-3.01562500	1.63114300
H	3.54206900	-2.22936300	3.19708900
H	2.17591900	-2.17441900	2.08434200
H	5.66540200	-1.12259500	2.70933100
H	5.81001100	-1.60220900	1.02009600
H	5.83875000	0.10972000	1.46838500
C	-8.71379200	-1.28003100	-1.59274400
H	-9.09961200	-2.06458000	-0.94647100
C	-7.53726600	-0.69717700	-1.36432100
H	-7.17708600	0.08318500	-2.03238200
C	-4.36694500	-0.82617200	-0.95440900
C	-4.40172000	0.58955700	-0.99182200
C	-3.18015600	-1.52113700	-1.32810200
C	-3.25451700	1.27972100	-1.32013000
H	-5.31861900	1.12761800	-0.78814200
C	-2.04809100	-0.81872400	-1.63779700
H	-3.21866400	-2.60433900	-1.36065200
C	-2.01349300	0.60890000	-1.52671500
H	-3.27403100	2.36256300	-1.37282800
H	-1.14418200	-1.34624600	-1.92535400
H	-1.21998400	1.15040000	-2.02453700
C	-6.66764200	-1.05043100	-0.19550200
H	-6.47534100	-0.19775500	0.46517400
H	-7.11624200	-1.84946100	0.39644600
H	-9.33955000	-0.98797600	-2.43003900
O	-5.38584100	-1.60651500	-0.61554600

Zero-point correction= 0.689592 (Hartree/Particle)
Thermal correction to Energy= 0.730882
Thermal correction to Enthalpy= 0.731826
Thermal correction to Gibbs Free Energy= 0.614161
Sum of electronic and zero-point Energies= -1871.892450
Sum of electronic and thermal Energies= -1871.851160
Sum of electronic and thermal Enthalpies= -1871.850216
Sum of electronic and thermal Free Energies= -1871.967881
E(RB3LYP) = -1892.70836148 A.U.

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1 1

C	-1.17939700	1.00558000	-0.18864200
C	-0.83751000	2.30771200	-0.86005300
O	-0.31285700	3.25935000	-0.31216800
O	-1.12358900	2.31900400	-2.19702100
C	-0.68252000	3.49170600	-2.90884500
H	0.40648200	3.57088200	-2.87527700
H	-1.02421700	3.35790000	-3.93495800
H	-1.11554500	4.39269700	-2.46979000
C	-1.70489300	1.15736800	1.23485300
C	-2.30729600	2.34295200	1.69091800
C	-1.64943100	0.07366900	2.12838600
C	-2.82112900	2.43890500	2.98464700
H	-2.34707700	3.21234000	1.04492800
C	-2.17295600	0.16220600	3.41892100
H	-1.17454500	-0.85141900	1.81207900
C	-2.76109800	1.34979300	3.85507700
H	-3.26621300	3.37380700	3.31296200
H	-2.10600800	-0.69234800	4.08632200
H	-3.15785200	1.42879900	4.86271600
P	3.10806000	-0.57997600	-0.01358400
Au	0.82495700	0.14207900	-0.14112200
C	3.58818800	-1.46262900	-1.66941400
C	2.43045800	-2.40043500	-2.08987100
C	3.71167600	-0.41242500	-2.79515100
C	4.89941900	-2.27198200	-1.59471700
H	2.25581800	-3.22020500	-1.39512300
H	1.49560400	-1.84445000	-2.20913500
H	2.68268500	-2.84283300	-3.06060700
H	4.58146300	0.23591900	-2.68324700
H	3.82816800	-0.94489900	-3.74580500
H	2.81417400	0.20818300	-2.87455000
H	5.11462100	-2.68162700	-2.58849400
H	5.75618600	-1.66175700	-1.30240800
H	4.83065800	-3.11826300	-0.90860400
C	4.18302700	1.01018200	0.25170900
C	3.65542900	2.13933800	-0.66805300
C	3.99727000	1.51950900	1.69824400
C	5.68740200	0.79710800	-0.01593900
H	3.74572300	1.91609000	-1.72991000
H	2.61174900	2.38622600	-0.45363500
H	4.25176800	3.03821100	-0.47318500
H	4.47135700	0.87905100	2.44347700
H	4.47274400	2.50366800	1.77311100
H	2.94220700	1.64858300	1.95667500

H	6.21859400	1.72452000	0.22710700
H	6.11943600	0.00517000	0.59875200
H	5.90062900	0.57372200	-1.06344200
C	3.30627000	-1.79041500	1.48494100
C	2.48869800	-1.24874700	2.68267900
C	2.68083400	-3.15565200	1.12427600
C	4.76696900	-2.01269400	1.92855400
H	2.86589200	-0.30908400	3.08078800
H	1.43524000	-1.10693300	2.42537900
H	2.53857100	-1.98792600	3.49070200
H	3.25179300	-3.70565700	0.37494300
H	2.66082400	-3.77279700	2.02945700
H	1.64848300	-3.05117800	0.77634200
H	4.77620700	-2.74638500	2.74299400
H	5.39803300	-2.40691800	1.12986800
H	5.22999400	-1.10263000	2.31404300
C	-8.83136600	-2.11069900	-1.21300600
H	-9.21562200	-2.75143300	-0.42339000
C	-7.74408600	-1.35859000	-1.04172800
H	-7.38361600	-0.72486300	-1.84985300
C	-4.61360800	-1.20057200	-0.32303000
C	-4.66982300	0.16655300	-0.73799500
C	-3.37994000	-1.92893700	-0.37081500
C	-3.52127700	0.77858100	-1.13683800
H	-5.61169900	0.70043800	-0.74958700
C	-2.23590400	-1.29365400	-0.72614500
H	-3.40630700	-2.97648600	-0.09181000
C	-2.19100300	0.13614400	-1.09397800
H	-3.55269500	1.80771800	-1.48075400
H	-1.29356900	-1.83397300	-0.73788400
H	-1.73915200	0.22110800	-2.09412700
C	-6.98969600	-1.31508700	0.24944700
H	-6.88517700	-0.30648200	0.65949400
H	-7.44943200	-1.95443200	1.00309000
H	-9.38400200	-2.10337300	-2.14695700
O	-5.63869400	-1.89085700	0.10407700

Zero-point correction=	0.690589 (Hartree/Particle)
Thermal correction to Energy=	0.732008
Thermal correction to Enthalpy=	0.732953
Thermal correction to Gibbs Free Energy=	0.614920
Sum of electronic and zero-point Energies=	-1871.898833
Sum of electronic and thermal Energies=	-1871.857414
Sum of electronic and thermal Enthalpies=	-1871.856470
Sum of electronic and thermal Free Energies=	-1871.974502

E(RB3LYP) = -1873.25570566 A.U.

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1 1

C	-1.19028700	1.13009800	-0.50560800
C	-1.06250300	1.61404500	-1.90582000
O	-1.71233800	1.04606500	-2.81280900
O	-0.22529900	2.60701000	-2.17930300
C	-0.08450200	2.97293900	-3.57324400
H	-1.05303100	3.24864900	-3.99334900
H	0.59603200	3.82266600	-3.57665500
H	0.33489100	2.13864700	-4.13882100
C	-1.21456800	2.09856500	0.66492800
C	-0.92619900	3.47031500	0.56265400
C	-1.55406800	1.59692300	1.93800500
C	-0.97487100	4.29785300	1.68748100
H	-0.66000200	3.90023900	-0.39378500
C	-1.60563500	2.42507500	3.05653600
H	-1.77855000	0.53955400	2.05229700
C	-1.31373300	3.78583600	2.93886700
H	-0.75144200	5.35500700	1.57536000
H	-1.87289200	2.00502900	4.02205800
H	-1.35213900	4.43461000	3.80830500
P	2.90602700	-0.82260400	0.15840700
Au	0.74569500	0.11511800	-0.25023900
C	3.30801000	-2.13125200	-1.21175400
C	2.04020800	-2.97571700	-1.48573500
C	3.63011800	-1.40969500	-2.53894400
C	4.48184200	-3.06783100	-0.85724700
H	1.69848900	-3.54621200	-0.62396200
H	1.21432800	-2.34886400	-1.83481500
H	2.27274600	-3.69257000	-2.28162000
H	4.58506600	-0.88280800	-2.52098700
H	3.69509000	-2.16573400	-3.32932400
H	2.84157900	-0.70675500	-2.82346300
H	4.66908800	-3.72921700	-1.71117700
H	5.40948200	-2.52746300	-0.65773900
H	4.26654900	-3.70886800	-0.00008000
C	4.18201900	0.63388300	0.11244800
C	3.84913800	1.55746400	-1.08493100
C	4.01609700	1.50017600	1.38049100
C	5.65147500	0.17567300	0.00701200
H	3.96512900	1.07501900	-2.05384300
H	2.83240400	1.95559700	-1.01870000

H	4.54066700	2.40757700	-1.05932400
H	4.36447700	1.00296900	2.28689600
H	4.62513200	2.40238100	1.25638000
H	2.98090300	1.82285300	1.52647900
H	6.29588100	1.06136900	0.04796400
H	5.95051400	-0.48048000	0.82630200
H	5.86670300	-0.33196300	-0.93517600
C	2.88303000	-1.65480400	1.90846600
C	2.10889800	-0.74412800	2.89228600
C	2.09044700	-2.97841200	1.83925600
C	4.28669700	-1.94034300	2.48107700
H	2.58577100	0.21863200	3.06359900
H	1.08522100	-0.55838700	2.55474800
H	2.05321700	-1.25816000	3.85891200
H	2.59936400	-3.75692600	1.26978300
H	1.96792800	-3.35509300	2.86074800
H	1.08898100	-2.83228600	1.42293400
H	4.17392400	-2.46992100	3.43410500
H	4.89102400	-2.57200700	1.82794800
H	4.84694900	-1.02680000	2.68930400
C	-8.88630700	-2.32107400	-0.59867400
H	-9.25080800	-3.05396700	0.11685600
C	-7.80425200	-1.58135700	-0.35720600
H	-7.46375600	-0.85606500	-1.09393500
C	-4.68533900	-1.35073500	0.30446200
C	-4.82724400	0.04198900	0.06641200
C	-3.41875200	-1.97297800	0.13682400
C	-3.72793700	0.77355800	-0.30768600
H	-5.78494800	0.53205700	0.18762000
C	-2.33283900	-1.23182800	-0.24589500
H	-3.34711500	-3.03723500	0.33227000
C	-2.42909800	0.17932600	-0.56031900
H	-3.83671400	1.84186000	-0.47241200
H	-1.36650700	-1.71256900	-0.36687100
H	-2.42155100	0.21693400	-1.79979900
C	-7.02317700	-1.67813400	0.91761100
H	-6.96990400	-0.72761200	1.45910400
H	-7.44977100	-2.42910600	1.58356300
H	-9.45397800	-2.21356700	-1.51741100
O	-5.66046300	-2.15917900	0.68736100

Zero-point correction= 0.687308 (Hartree/Particle)

Thermal correction to Energy= 0.728079

Thermal correction to Enthalpy= 0.729023

Thermal correction to Gibbs Free Energy= 0.612877

Sum of electronic and zero-point Energies= -1871.902023

Sum of electronic and thermal Energies= -1871.861253

Sum of electronic and thermal Enthalpies= -1871.860309

Sum of electronic and thermal Free Energies= -1871.976454

E(RB3LYP) = -1873.24776488 A.U.

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1 1

C	1.28993100	1.16639400	0.49131500
C	1.11893700	1.36464700	1.89465000
O	1.70297500	0.59885200	2.80182600
O	0.37675600	2.33017900	2.39186300
C	0.15900500	2.39477400	3.82524100
H	1.10953300	2.49861200	4.34976600
H	-0.46011100	3.27789700	3.96962300
H	-0.36179400	1.49771200	4.16607100
C	1.09329800	2.30818800	-0.48806400
C	1.01351700	3.66140500	-0.12187300
C	1.04919700	1.99397500	-1.86176400
C	0.87669300	4.65663600	-1.09221600
H	1.06325900	3.95175900	0.91946000
C	0.91558000	2.98882100	-2.82722900
H	1.13983100	0.95684800	-2.17203600
C	0.82284400	4.32937800	-2.44645700
H	0.82250200	5.69575700	-0.78122000
H	0.88849400	2.71570100	-3.87799200
H	0.71943600	5.10770100	-3.19600000
P	-2.85325800	-0.85176500	-0.20720600
Au	-0.73263000	0.11996100	0.24358600
C	-2.78699800	-2.72546400	0.27892300
C	-1.44413400	-3.32668000	-0.19932100
C	-2.79447900	-2.86322700	1.81722700
C	-3.95115700	-3.55645600	-0.30175600
H	-1.31636300	-3.31733100	-1.27997100
H	-0.59295800	-2.80760600	0.24933900
H	-1.40426500	-4.37239200	0.12614400
H	-3.74964000	-2.59176300	2.26887600
H	-2.61229700	-3.91527700	2.06279500
H	-1.99894900	-2.27671500	2.28697100
H	-3.86717100	-4.58096800	0.07815700
H	-4.93204100	-3.18102300	-0.00444600
H	-3.92105100	-3.61752000	-1.39114700
C	-4.16402700	0.09432300	0.85904500
C	-3.59494500	0.32388300	2.27964900

C	-4.39888000	1.49823600	0.25969600
C	-5.51755900	-0.63937300	0.96355300
H	-3.40386100	-0.59532000	2.83027100
H	-2.66885500	0.90552300	2.24768100
H	-4.33156600	0.90050300	2.85053700
H	-4.93581400	1.47475800	-0.68918400
H	-5.01753400	2.06663500	0.96287400
H	-3.46442000	2.05106100	0.12504400
H	-6.21080800	-0.00801500	1.53094500
H	-5.97371200	-0.82777100	-0.01007400
H	-5.44093400	-1.58862000	1.49666900
C	-3.21655100	-0.64109400	-2.09728300
C	-2.79872200	0.77998900	-2.54589300
C	-2.33628400	-1.62374800	-2.90080000
C	-4.69620700	-0.87700200	-2.46627600
H	-3.38700700	1.57451500	-2.09088300
H	-1.74299300	0.97967400	-2.34306900
H	-2.94586800	0.84763600	-3.62976200
H	-2.63025900	-2.66634600	-2.77384200
H	-2.44975600	-1.38649100	-3.96418800
H	-1.27491000	-1.52192100	-2.65544200
H	-4.79491600	-0.81279500	-3.55574700
H	-5.05900800	-1.86144100	-2.16530300
H	-5.35930400	-0.12106600	-2.04183600
C	9.06324300	-1.84319200	0.26803200
H	9.44775300	-2.71731100	-0.25209500
C	7.86160900	-1.33749500	-0.00744500
H	7.50272700	-0.46390300	0.53409000
C	4.68923100	-1.44827900	-0.31248900
C	4.76478000	-0.06411700	-0.54429700
C	3.48565200	-1.98779000	0.16982400
C	3.65965000	0.74768100	-0.29958100
H	5.67899900	0.39260200	-0.90352600
C	2.38769700	-1.16551700	0.40010400
H	3.42930500	-3.05814300	0.33667700
C	2.44419000	0.22544900	0.17353700
H	3.74500000	1.81396600	-0.48384000
H	1.45762600	-1.61606500	0.73877700
H	2.30522900	-0.02290400	2.34163800
C	6.95263800	-1.90336800	-1.06054200
H	6.77424000	-1.19052300	-1.87633900
H	7.38795600	-2.80550600	-1.49575400
H	9.71150700	-1.39904400	1.01692400
O	5.68463400	-2.33795000	-0.52317800

Zero-point correction= 0.692107 (Hartree/Particle)
Thermal correction to Energy= 0.733355
Thermal correction to Enthalpy= 0.734300
Thermal correction to Gibbs Free Energy= 0.616786
Sum of electronic and zero-point Energies= -1871.930823
Sum of electronic and thermal Energies= -1871.889575
Sum of electronic and thermal Enthalpies= -1871.888631
Sum of electronic and thermal Free Energies= -1872.006144
E(RB3LYP) = -1873.28405525 A.U.

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0 1

C	-1.03388600	-0.20940200	-0.26187800
C	-1.63377400	-1.35852500	-0.84936400
O	-2.85176900	-1.54872400	-1.13987500
O	-0.77597700	-2.39729000	-1.06970600
C	-1.35584100	-3.61249700	-1.53997700
H	-1.85780000	-3.46963300	-2.50074700
H	-0.52243700	-4.30788900	-1.65087300
H	-2.08403800	-4.01402000	-0.82740900
H	-4.04919200	-1.00006100	-0.49967100
O	-1.98836200	-0.40834700	2.32283800
H	-1.93181100	0.53514600	2.53728000
H	-1.62282900	-0.45324800	1.33066700
O	-4.29182900	-1.14211200	2.33860600
H	-4.31785100	-2.07831200	2.57737600
H	-3.19278800	-0.78402400	2.35888300
O	-4.92471500	-0.78312800	0.01802200
H	-5.61650000	-1.33676700	-0.36518100
H	-4.65753700	-1.01361500	1.30365000
C	-1.69451700	1.12422000	-0.36567300
C	-1.26476200	2.17609700	0.47914500
C	-2.75103200	1.42007500	-1.25188200
C	-1.86019700	3.43523500	0.44888900
H	-0.42368000	2.00396300	1.14657800
C	-3.34596100	2.68087600	-1.27896400
H	-3.10158000	0.65229200	-1.93016400
C	-2.91357900	3.69920000	-0.42863900
H	-1.49493600	4.21477200	1.11294000
H	-4.15419100	2.86861100	-1.98137500
H	-3.38151900	4.67881700	-0.45375400
C	0.45784200	-0.21969500	-0.05424900
C	1.07477600	-1.06308600	0.88914300
C	1.30041700	0.62070600	-0.79489700

C	2.45113500	-1.07502100	1.07406000
H	0.45927400	-1.72825100	1.48769200
C	2.68658900	0.63256800	-0.61741400
H	0.86325300	1.28688700	-1.53275200
C	3.27033300	-0.22250300	0.32259000
H	2.91599700	-1.73084100	1.80344400
H	3.29124800	1.29902100	-1.22140400
C	5.49112900	0.56977800	-0.12548000
H	5.18251900	1.61457000	0.04099700
H	5.44629100	0.37742600	-1.20679500
C	6.87980200	0.35275200	0.39553600
H	6.98366900	0.40388800	1.47811700
C	7.94378000	0.14002200	-0.37607700
H	8.93863100	0.02634400	0.04333400
H	7.86077000	0.07535000	-1.45833100
O	4.61434200	-0.30355200	0.58240200

Zero-point correction= 0.386279 (Hartree/Particle)
Thermal correction to Energy= 0.412232
Thermal correction to Enthalpy= 0.413176
Thermal correction to Gibbs Free Energy= 0.327100
Sum of electronic and zero-point Energies= -1151.297977
Sum of electronic and thermal Energies= -1151.272024
Sum of electronic and thermal Enthalpies= -1151.271080
Sum of electronic and thermal Free Energies= -1151.357155
E(RB3LYP) = -1152.13264045 A.U.

C-P3

C	-0.33568500	0.12368900	0.26897700
C	-0.12153900	1.10488900	-0.90945100
O	-0.16601100	2.31375100	-0.82444600
O	0.09995700	0.43907500	-2.05253100
C	0.31293700	1.25904000	-3.21499700
H	1.19210000	1.89324600	-3.07850900
H	0.46713500	0.56271600	-4.03817800
H	-0.55730500	1.89237800	-3.40226600
C	-1.69036400	-0.57357200	0.07331600
C	-2.80277200	0.15736900	-0.36631800
C	-1.84639200	-1.93038400	0.37493300
C	-4.04541600	-0.45971000	-0.50629700
H	-2.70078600	1.21424600	-0.59321400
C	-3.09185600	-2.54478700	0.23518200
H	-0.98990200	-2.50384900	0.70632100
C	-4.19489800	-1.81426700	-0.20612500

H	-4.89590400	0.12070600	-0.85186100
H	-3.19631200	-3.60020900	0.47006100
H	-5.16200400	-2.29577800	-0.31722400
C	-1.45173800	2.98830100	2.19800300
H	-0.57416500	3.58250500	1.95945700
C	-1.45602000	1.66249400	2.06563700
H	-2.36193500	1.10781200	2.30107200
C	1.99954100	-0.71065400	0.25524200
C	2.76015300	-1.88280600	0.37658500
C	2.64710000	0.52672600	0.15644000
C	4.14867100	-1.81864200	0.40045300
H	2.23833900	-2.83147400	0.44656800
C	4.04465500	0.57387100	0.18340300
H	2.09316100	1.45119600	0.05924400
C	4.80345200	-0.58709200	0.30546100
H	4.72212100	-2.73629700	0.49509000
H	4.53577700	1.53988200	0.10807600
H	5.88737700	-0.53639000	0.32697500
C	-0.26207400	0.84207300	1.65183000
H	-0.12261800	0.02846800	2.37440700
H	0.63469800	1.46330300	1.68653900
H	-2.33129200	3.52720400	2.53791200
O	0.64292700	-0.92518900	0.22146400

Zero-point correction= 0.317962 (Hartree/Particle)
Thermal correction to Energy= 0.337512
Thermal correction to Enthalpy= 0.338456
Thermal correction to Gibbs Free Energy= 0.268265
Sum of electronic and zero-point Energies= -922.098983
Sum of electronic and thermal Energies= -922.079433
Sum of electronic and thermal Enthalpies= -922.078488
Sum of electronic and thermal Free Energies= -922.148680
E(RB3LYP) = -922.747665195 A.U.

D-P2

C	-1.54847200	0.23088800	-0.42708400
C	-1.49328200	1.66268600	0.04510900
O	-2.15880300	2.10858400	0.95469100
O	-0.60994000	2.42125300	-0.65357500
C	-0.51427300	3.79192300	-0.22748700
H	-0.20707500	3.85164500	0.81930200
H	0.23411300	4.24807600	-0.87498200
H	-1.47793300	4.29387100	-0.33922000
C	-2.83781700	-0.46446600	-0.06519100
C	-3.06131900	-0.91592600	1.24180300

C	-3.83976400	-0.65176500	-1.02362700
C	-4.25542000	-1.54996800	1.57978000
H	-2.29489700	-0.76402700	1.99575300
C	-5.03704800	-1.28653200	-0.68808000
H	-3.68205200	-0.29749400	-2.03848100
C	-5.24689100	-1.73874200	0.61438700
H	-4.41290400	-1.89652800	2.59704400
H	-5.80383000	-1.42633300	-1.44464000
H	-6.17656700	-2.23518400	0.87685500
C	-0.82535200	-0.16762200	-1.70327600
H	-0.29838300	0.61604200	-2.23509900
C	-0.26491400	-0.61856000	-0.39148000
H	-0.45524200	-1.65519200	-0.12471400
C	3.36978600	-0.70171100	-0.09247400
C	3.79305400	0.30652000	0.78183900
C	4.31361800	-1.56083200	-0.67524200
C	5.15600200	0.44375300	1.06445000
H	3.08156500	0.98173800	1.24169400
C	5.66428100	-1.41027300	-0.38452800
H	3.96079500	-2.33437500	-1.34941500
C	6.09668800	-0.40617500	0.48872900
H	5.47592700	1.22833900	1.74447000
H	6.38538100	-2.08172400	-0.84198200
H	7.15207800	-0.29139700	0.71464000
C	1.05284500	-0.10940400	0.13555400
H	1.21034700	0.93969100	-0.13559000
H	1.08693700	-0.19344700	1.23155200
H	-1.30992000	-0.90677100	-2.33218600
O	2.06891000	-0.92979800	-0.44412800

Zero-point correction= 0.319784 (Hartree/Particle)
Thermal correction to Energy= 0.338786
Thermal correction to Enthalpy= 0.339730
Thermal correction to Gibbs Free Energy= 0.268988
Sum of electronic and zero-point Energies= -922.102463
Sum of electronic and thermal Energies= -922.083462
Sum of electronic and thermal Enthalpies= -922.082517
Sum of electronic and thermal Free Energies= -922.153260
E(RB3LYP) = -922.749578281 A.U.
E-re2
0 1

C	-1.91299500	-0.52768800	0.39560000
H	-1.68600000	-1.58072400	0.56429500
C	-0.88735700	0.33853000	0.39597900
H	-1.05760200	1.39991500	0.22715100

S	1.49021600	0.17906100	-0.98675300
C	3.17910900	0.06567600	-0.38080900
C	3.80017900	1.17383600	0.21218400
C	3.89808800	-1.12710300	-0.53249300
C	5.11796900	1.08314700	0.66061500
H	3.24973300	2.10436900	0.31134100
C	5.21984100	-1.21089600	-0.09157900
H	3.41809800	-1.98177500	-0.99835600
C	5.83006200	-0.10845400	0.50836700
H	5.59163400	1.94609900	1.11982200
H	5.77111500	-2.13862000	-0.21525100
H	6.85810700	-0.17547800	0.85214300
C	0.53534500	-0.06674600	0.59989200
H	1.02218600	0.55575100	1.35721000
H	0.61374300	-1.11435900	0.90178800
C	-3.33946900	-0.23023900	0.20567000
C	-3.82793100	1.05313100	-0.10446900
C	-4.27067500	-1.27540900	0.33602300
C	-5.19084200	1.27678300	-0.27086100
H	-3.13647700	1.88141300	-0.22340100
C	-5.63632200	-1.05242500	0.16973300
H	-3.91303700	-2.27448600	0.57207300
C	-6.10319000	0.22628400	-0.13384200
H	-5.54507700	2.27501400	-0.51179200
H	-6.33456600	-1.87754000	0.27661200
H	-7.16618900	0.40488000	-0.26566100

Zero-point correction= 0.244241 (Hartree/Particle)
Thermal correction to Energy= 0.258733
Thermal correction to Enthalpy= 0.259677
Thermal correction to Gibbs Free Energy= 0.197915
Sum of electronic and zero-point Energies= -977.978378
Sum of electronic and thermal Energies= -977.963885
Sum of electronic and thermal Enthalpies= -977.962941
Sum of electronic and thermal Free Energies= -978.024703
E(RB3LYP) = -978.463153830 A.U.

E-tsa1-s
1 1

C	-1.12779800	-1.10636000	-0.48918500
C	-0.59494600	-1.17851900	-1.84527400
O	0.47287800	-1.68875400	-2.16784200
O	-1.40396100	-0.57630900	-2.78225300
C	-0.87173500	-0.51806800	-4.11563900
H	-0.62977700	-1.51828300	-4.48099000

H	-1.65479000	-0.06627100	-4.72472800
H	0.03222900	0.09616600	-4.14477500
C	-0.73958400	-2.16940600	0.48870700
C	-0.61421600	-3.51615400	0.10143000
C	-0.50695900	-1.84902200	1.83751200
C	-0.27193300	-4.50178600	1.02821700
H	-0.75642400	-3.78800800	-0.93970300
C	-0.17694200	-2.83380300	2.76914900
H	-0.58873000	-0.81218400	2.15172500
C	-0.05813400	-4.16618700	2.36713000
H	-0.17225200	-5.53341600	0.70329200
H	-0.00955600	-2.55966500	3.80702400
H	0.20432100	-4.93482900	3.08801400
P	0.46003500	3.40993900	-0.19798700
Au	0.62129800	1.03730600	-0.13448900
C	0.84227300	4.06158600	1.59000600
C	0.13250900	3.14923600	2.61937500
C	2.35323700	3.92985200	1.88041000
C	0.41908600	5.52673200	1.82787500
H	-0.95335500	3.15967900	2.54172300
H	0.47340900	2.11315800	2.53366900
H	0.39265300	3.50189700	3.62411900
H	2.96378600	4.62723500	1.30486300
H	2.51403000	4.16385500	2.93883800
H	2.71701700	2.91232900	1.71537700
H	0.74224600	5.82169300	2.83289300
H	0.88053000	6.22078600	1.12315300
H	-0.66263900	5.66730000	1.78871300
C	1.76722000	4.09811300	-1.45856100
C	3.08825600	3.31000900	-1.30560300
C	1.28382100	3.83667700	-2.90216500
C	2.05671100	5.60579700	-1.29621800
H	3.55421000	3.42620600	-0.32893800
H	2.93292500	2.24323900	-1.48714600
H	3.79653500	3.68094600	-2.05548500
H	0.43986800	4.46331600	-3.19248900
H	2.10766400	4.07412000	-3.58439300
H	1.01906900	2.78733800	-3.06260000
H	2.75220700	5.91177300	-2.08637000
H	1.16281200	6.22382600	-1.39476600
H	2.53349200	5.84216800	-0.34331600
C	-1.31692000	3.95467500	-0.74726100
C	-1.77149800	3.06708800	-1.92980200
C	-2.29847000	3.67587500	0.40940200

C	-1.43595400	5.43814400	-1.15314200
H	-1.20193800	3.23925500	-2.84127100
H	-1.71483800	2.00267800	-1.69020400
H	-2.81813700	3.30621000	-2.15264600
H	-2.17598600	4.35863200	1.25125600
H	-3.31880000	3.81203200	0.03205000
H	-2.20920500	2.64930000	0.77319600
H	-2.48885100	5.65526100	-1.36791800
H	-1.11737900	6.12170800	-0.36469500
H	-0.87339800	5.67119900	-2.05858500
C	-6.22597600	-2.38880300	-0.70234000
H	-5.89050800	-3.13164400	0.02163400
C	-5.28668600	-1.77929700	-1.45078100
H	-5.56465200	-1.03037200	-2.18871800
S	-2.87653800	-0.63453500	-0.53268900
C	-3.55567900	-0.67260800	1.13387800
C	-4.11926800	0.52509200	1.58664200
C	-3.62853000	-1.83434600	1.91265900
C	-4.73230600	0.57052000	2.84000600
H	-4.09544300	1.40799100	0.95817600
C	-4.24828200	-1.77786600	3.16052700
H	-3.20255500	-2.76735500	1.56541400
C	-4.79410600	-0.57926400	3.62725600
H	-5.17105800	1.49928000	3.19067800
H	-4.30371000	-2.67511300	3.76891900
H	-5.27617100	-0.54626000	4.59943100
C	-3.83869500	-2.07855900	-1.33841700
H	-3.61581300	-2.96965400	-0.74900600
H	-3.33707100	-2.13915600	-2.30649800
C	5.80556700	-1.84979200	-1.24204200
H	6.15069000	-0.81532300	-1.23087300
C	4.48127800	-2.06647500	-1.32218700
H	4.07980700	-3.07688200	-1.33664800
S	2.38987100	-0.93798000	0.13402500
C	3.53061800	-0.45137200	1.43811800
C	3.47704000	-1.18197200	2.63157200
C	4.44091800	0.60526800	1.30846300
C	4.31814000	-0.84398500	3.69379200
H	2.78669700	-2.01497200	2.71935600
C	5.29239000	0.92329800	2.36729800
H	4.49335300	1.17499500	0.38690500
C	5.22924700	0.20478900	3.56368400
H	4.27231100	-1.41495300	4.61636500
H	6.00531100	1.73538600	2.25724500

H	5.89237600	0.45681800	4.38547500
C	3.47453800	-0.97136500	-1.39272600
H	3.93712000	0.00857800	-1.53062300
H	2.72778800	-1.13523700	-2.17335600
C	6.87668600	-2.85203600	-1.18220300
C	8.21190800	-2.41184900	-1.15607100
C	6.63446700	-4.23876500	-1.14762700
C	9.26928600	-3.31831400	-1.09932300
H	8.41841200	-1.34466500	-1.18185000
C	7.68920200	-5.14397500	-1.09079400
H	5.61541400	-4.61273700	-1.16322600
C	9.01162000	-4.68905800	-1.06674500
H	10.29240800	-2.95460600	-1.08102800
H	7.48188700	-6.20982200	-1.06482400
H	9.83200400	-5.39904500	-1.02276200
C	-7.67743900	-2.19113500	-0.74391300
C	-8.31129900	-1.29133800	-1.62288000
C	-8.48086600	-2.93805600	0.13679900
C	-9.69446600	-1.14642400	-1.61441300
H	-7.72178400	-0.70465000	-2.32078000
C	-9.86668200	-2.79251500	0.14588200
H	-8.00861100	-3.64038600	0.81914500
C	-10.47842200	-1.89533800	-0.73013600
H	-10.16663700	-0.44974500	-2.30069300
H	-10.46754100	-3.37997400	0.83348900
H	-11.55804700	-1.78024600	-0.72848100

Zero-point correction= 1.013851 (Hartree/Particle)
Thermal correction to Energy= 1.076301
Thermal correction to Enthalpy= 1.077245
Thermal correction to Gibbs Free Energy= 0.906936
Sum of electronic and zero-point Energies= -3403.824495
Sum of electronic and thermal Energies= -3403.762044
Sum of electronic and thermal Enthalpies= -3403.761100
Sum of electronic and thermal Free Energies= -3403.931409
E(RB3LYP) = -3405.87706768 A.U.

E-1a

1 1

C	-1.88060900	-0.52596900	0.22985100
C	-2.27633800	-1.90179200	-0.25983100
O	-2.34359200	-2.87795000	0.45708100
O	-2.48925300	-1.95464900	-1.59882900
C	-2.77087400	-3.26680200	-2.12878400

H	-3.66327900	-3.68484500	-1.65895700
H	-2.92729900	-3.12212800	-3.19710700
H	-1.92676100	-3.93667800	-1.95206000
C	-2.35771000	-0.20690500	1.62603900
C	-3.58116000	-0.70297200	2.11445900
C	-1.59530800	0.61340000	2.47748500
C	-4.01839300	-0.39128600	3.40109600
H	-4.18342000	-1.35844700	1.49624500
C	-2.03831800	0.93707200	3.76083800
H	-0.63474200	0.98420000	2.13154600
C	-3.25330700	0.43439900	4.22741100
H	-4.95873800	-0.79896000	3.75966400
H	-1.42704800	1.56803600	4.39929800
H	-3.59583200	0.67388400	5.22943200
P	2.59922100	-1.31442800	-0.05777900
Au	0.28515200	-0.71941300	0.04519500
C	3.49188000	-0.63190800	1.51855400
C	3.00950200	0.81421900	1.77816200
C	3.05944800	-1.45350200	2.75344200
C	5.03163900	-0.64805400	1.42214300
H	3.27386800	1.51877700	0.99239300
H	1.92509300	0.84854200	1.91680700
H	3.47568000	1.16771800	2.70529000
H	3.45851600	-2.46835400	2.75498800
H	3.45099300	-0.95415500	3.64676100
H	1.97124900	-1.50113000	2.85565700
H	5.44343200	-0.29864800	2.37601600
H	5.43474600	-1.64659600	1.24268300
H	5.41162300	0.01990900	0.64679300
C	2.66681700	-3.25204100	-0.08850000
C	1.63241600	-3.81507600	0.91695400
C	2.23272900	-3.76367800	-1.47962600
C	4.06155800	-3.82585600	0.23811900
H	1.83608100	-3.54725500	1.95187700
H	0.61329100	-3.49790300	0.67833200
H	1.66096900	-4.90898100	0.85349600
H	2.96113900	-3.55089500	-2.26304600
H	2.13253600	-4.85319500	-1.42235200
H	1.26077000	-3.36175600	-1.78056000
H	4.02523200	-4.91522100	0.12252600
H	4.83917800	-3.45341200	-0.43103300
H	4.36891300	-3.62585600	1.26636600
C	3.38461500	-0.57812700	-1.66634100
C	2.37665900	-0.73797100	-2.83002200

C	3.59243200	0.94051700	-1.48542200
C	4.72953800	-1.22297500	-2.05996700
H	2.17145200	-1.77429300	-3.09228700
H	1.42467000	-0.24870700	-2.60336500
H	2.79959600	-0.25334700	-3.71766900
H	4.38752200	1.18376500	-0.77947900
H	3.88568100	1.36139800	-2.45368600
H	2.67667500	1.44997700	-1.17411600
H	5.12191100	-0.69918000	-2.93939900
H	5.48232700	-1.14415000	-1.27321700
H	4.62933100	-2.27465200	-2.33447800
C	0.15704300	3.43182300	0.12647900
H	-0.11083400	3.37879300	1.18201400
C	-0.70754600	2.91340900	-0.76437800
H	-0.49788100	2.94380700	-1.83096900
S	-2.44259700	0.72225000	-1.06129700
C	-4.24765300	0.77013600	-1.09589000
C	-5.01376700	1.33043000	-0.06549600
C	-4.85514400	0.22347200	-2.23305700
C	-6.40364000	1.34322700	-0.18724600
H	-4.54684000	1.74825800	0.81830400
C	-6.24589500	0.24085900	-2.33778000
H	-4.24758000	-0.20301600	-3.02370900
C	-7.01835500	0.79984100	-1.31767700
H	-7.00483000	1.77884000	0.60451900
H	-6.72305600	-0.17562200	-3.21913000
H	-8.10022200	0.81591500	-1.40472700
C	-2.05544200	2.41040900	-0.36846300
H	-2.19437800	2.38026900	0.71414000
H	-2.85304600	3.01381300	-0.81460400
C	1.42823900	4.11157600	-0.14867000
C	2.22481500	4.51301900	0.93946000
C	1.88133000	4.40342300	-1.45006600
C	3.43735400	5.17109500	0.73922200
H	1.88277600	4.31096200	1.95144400
C	3.09129000	5.06090200	-1.64975000
H	1.27853700	4.13169800	-2.31126100
C	3.87529000	5.44607600	-0.55690300
H	4.03425100	5.47598300	1.59340000
H	3.42103100	5.28542900	-2.65970200
H	4.81486600	5.96589300	-0.71715400

Zero-point correction=	0.768655 (Hartree/Particle)
Thermal correction to Energy=	0.815407
Thermal correction to Enthalpy=	0.816351

Thermal correction to Gibbs Free Energy= 0.686249

Sum of electronic and zero-point Energies= -2425.881729

Sum of electronic and thermal Energies= -2425.834977

Sum of electronic and thermal Enthalpies= -2425.834033

Sum of electronic and thermal Free Energies= -2425.964135

E(RB3LYP) = -2427.42167729 A.U

E-tsa2

0 1

C	0.32852400	0.59292000	-0.71144100
C	-0.56389500	1.49689800	-1.43707000
O	-1.39583100	1.18534100	-2.27743100
O	-0.39739400	2.81409500	-1.07557200
C	-1.19724000	3.74499300	-1.81064800
H	-2.26268800	3.53733800	-1.68039300
H	-0.94799700	4.72766700	-1.40805400
H	-0.96618300	3.70364500	-2.87864600
C	0.20952800	-0.87159500	-0.79566500
C	-0.49366900	-1.49972200	-1.85212100
C	0.78724900	-1.72073600	0.17708400
C	-0.60563400	-2.88583400	-1.91827900
H	-0.95989700	-0.88365400	-2.60715700
C	0.66957000	-3.10658900	0.10278400
H	1.34244700	-1.29706700	1.00413100
C	-0.02742000	-3.70463600	-0.94713400
H	-1.15349700	-3.32880800	-2.74574300
H	1.13153500	-3.71972600	0.87214400
H	-0.11503800	-4.78540200	-1.00847000
C	-1.66653400	0.91220400	1.59263100
C	-0.59118300	0.41673500	2.28805600
H	-0.55803400	-0.64058000	2.53515800
S	1.47233000	1.39506100	0.29264300
C	3.03327400	0.49770800	0.25043000
C	3.46396600	-0.16001400	-0.90744400
C	3.87892300	0.59645600	1.36063600
C	4.73372200	-0.73381600	-0.93771800
H	2.80834000	-0.22517500	-1.76776000
C	5.15105900	0.02471300	1.31554800
H	3.55401200	1.12109900	2.25336200
C	5.57991300	-0.64556700	0.16982000
H	5.06229300	-1.24984600	-1.83485900
H	5.80379500	0.10390800	2.17978800
H	6.56849800	-1.09312300	0.13788000
C	0.57590400	1.17761400	2.51247100

H	0.49563800	2.25876100	2.57046500
H	1.38838100	0.74798000	3.09062900
H	-1.65814600	1.97359600	1.34928400
C	-2.86410100	0.19242500	1.19163700
C	-3.95141600	0.92038200	0.66584000
C	-2.99067500	-1.20998500	1.28696000
C	-5.12416200	0.28251500	0.27498400
H	-3.86685100	1.99989900	0.57319500
C	-4.16280000	-1.84516300	0.89332000
H	-2.15849500	-1.80582900	1.64561000
C	-5.23686700	-1.10430200	0.39097900
H	-5.94892100	0.86541400	-0.12430200
H	-4.23748400	-2.92604900	0.96841300
H	-6.14940500	-1.60613900	0.08312600

Zero-point correction= 0.393354 (Hartree/Particle)
Thermal correction to Energy= 0.417978
Thermal correction to Enthalpy= 0.418922
Thermal correction to Gibbs Free Energy= 0.336599
Sum of electronic and zero-point Energies= -1475.998746
Sum of electronic and thermal Energies= -1475.974122
Sum of electronic and thermal Enthalpies= -1475.973178
Sum of electronic and thermal Free Energies= -1476.055501
E(RB3LYP) = -1476.82905428 A.U.

E-2a
0 1

C	-0.82934400	0.24724700	1.03741300
C	-0.52809900	0.08108700	2.44346900
O	-0.58666500	0.97285500	3.27904200
O	-0.14294100	-1.19685900	2.79023000
C	0.15792000	-1.36898800	4.17573100
H	-0.71117700	-1.14579600	4.80141400
H	0.44368300	-2.41646700	4.28809700
H	0.97965200	-0.71746500	4.48609500
C	-1.27361800	1.56648900	0.52512300
C	-2.37464700	2.22094700	1.10903900
C	-0.62733900	2.21113400	-0.54527500
C	-2.82005400	3.45046300	0.62953100
H	-2.86916900	1.75518100	1.95413100
C	-1.08606900	3.43281000	-1.04258700
H	0.26841600	1.76650200	-0.96631700
C	-2.18770900	4.05758500	-0.45834700
H	-3.67067600	3.93401500	1.10216200
H	-0.56601000	3.90655400	-1.87107800

H	-2.54129300	5.01262900	-0.83621200
C	2.55319800	-0.19385500	-1.29598000
H	2.20308700	0.69630800	-1.81853500
C	1.66672700	-1.17730500	-1.06647200
H	1.97887700	-2.09204800	-0.56697000
S	-0.87299800	-1.17390400	0.09985100
C	-2.47929800	-1.34522600	-0.73902300
C	-2.98784600	-0.39446100	-1.63090800
C	-3.22166600	-2.48470700	-0.41261600
C	-4.24568400	-0.59827800	-2.19933000
H	-2.42437600	0.50086200	-1.86679800
C	-4.47697100	-2.67983500	-0.98994200
H	-2.81990300	-3.20907900	0.28923100
C	-4.98851400	-1.73784000	-1.88335000
H	-4.64602300	0.13889600	-2.88876200
H	-5.05276100	-3.56581800	-0.73996100
H	-5.96617300	-1.88917400	-2.33097100
C	0.23396700	-1.10229300	-1.45053400
H	-0.01179100	-0.20144400	-2.01487000
H	-0.10123200	-1.98267200	-2.00964400
C	3.98097600	-0.18163000	-0.95325200
C	4.58422600	-1.15288900	-0.13234300
C	4.78982000	0.84896000	-1.46296000
C	5.94461200	-1.09847400	0.15255700
H	3.98278200	-1.94665900	0.29930300
C	6.15282900	0.90359800	-1.17842000
H	4.33961700	1.61310700	-2.09144400
C	6.73672200	-0.07207600	-0.37054300
H	6.38972600	-1.85545300	0.79171200
H	6.75702600	1.70913800	-1.58519300
H	7.79771700	-0.03139400	-0.14307500

Zero-point correction= 0.394346 (Hartree/Particle)
Thermal correction to Energy= 0.419674
Thermal correction to Enthalpy= 0.420618
Thermal correction to Gibbs Free Energy= 0.334272
Sum of electronic and zero-point Energies= -1476.000243
Sum of electronic and thermal Energies= -1475.974915
Sum of electronic and thermal Enthalpies= -1475.973971
Sum of electronic and thermal Free Energies= -1476.060317
E(RB3LYP) = -1476.82863254 A.U.

E-tsc1
1 1

C	-2.10709300	-0.49277100	-0.23827900

C	-1.97037700	-1.63513500	-1.12257200
O	-1.19624700	-2.58283500	-0.88581000
O	-2.70694200	-1.60757900	-2.25195800
C	-2.43429000	-2.64067200	-3.22140100
H	-2.68210200	-3.62136800	-2.81170300
H	-3.07043700	-2.41022300	-4.07519400
H	-1.38139900	-2.62566600	-3.51160300
C	-2.17801100	-0.73185100	1.23947600
C	-2.90713400	-1.81880100	1.76073200
C	-1.54223400	0.13106000	2.15385300
C	-2.98901900	-2.03704100	3.13497000
H	-3.40603400	-2.50215800	1.08058500
C	-1.64834900	-0.07105300	3.53207800
H	-0.94285800	0.95214700	1.77267000
C	-2.36960800	-1.15812900	4.02758900
H	-3.54871500	-2.88863300	3.51040100
H	-1.15286700	0.61157500	4.21662600
H	-2.44450900	-1.32312600	5.09808200
P	2.93262700	-0.96284100	-0.01547600
Au	0.62254200	-1.05302700	-0.19178900
C	3.40245800	-1.35712100	1.82121100
C	2.46356900	-0.57502200	2.76963000
C	3.15391100	-2.85423100	2.10555000
C	4.86925200	-1.01533900	2.15637600
H	2.57563800	0.50542700	2.69917300
H	1.41355300	-0.82426600	2.59451700
H	2.70748500	-0.86378700	3.79845200
H	3.86014100	-3.51043100	1.59570400
H	3.28183400	-3.01866400	3.18100400
H	2.13528700	-3.15790200	1.84737700
H	5.06870300	-1.32496300	3.18842200
H	5.58309700	-1.53763800	1.51718100
H	5.07360100	0.05538500	2.09849000
C	3.62596900	-2.32083200	-1.21493400
C	2.76480000	-3.60231000	-1.10381200
C	3.48637400	-1.83471500	-2.67419800
C	5.10328100	-2.67423900	-0.94127000
H	2.80371600	-4.07294900	-0.12353000
H	1.71607900	-3.41137700	-1.34726800
H	3.14993700	-4.32810000	-1.82920800
H	4.16233600	-1.01540700	-2.92226700
H	3.74044400	-2.67130000	-3.33413700
H	2.46100100	-1.53384100	-2.90864300
H	5.43682700	-3.38070000	-1.70975800

H	5.76463700	-1.80730100	-0.98842000
H	5.24439500	-3.16462100	0.02373900
C	3.54657000	0.79873800	-0.53222000
C	2.74771900	1.26982400	-1.77009900
C	3.22811400	1.80256600	0.59579000
C	5.05735000	0.85722700	-0.84343100
H	2.91846500	0.66171700	-2.65649100
H	1.67325300	1.29026600	-1.56699800
H	3.05916000	2.29367500	-2.00459700
H	3.84765500	1.65972300	1.48249300
H	3.42642000	2.81213400	0.22140700
H	2.17462200	1.76790400	0.88569000
H	5.32328000	1.89858400	-1.05749700
H	5.67628400	0.53020700	-0.00568400
H	5.33066700	0.27138400	-1.72284100
C	-0.74991000	3.61108700	0.37972200
H	-0.92312200	3.45351600	1.44482500
C	-1.62923500	3.07338800	-0.48296900
H	-1.52497000	3.22591300	-1.55473700
S	-3.14269000	0.76631500	-0.95159600
C	-4.88521700	0.46617500	-0.54760200
C	-5.37968600	0.49410500	0.76229000
C	-5.71783600	0.15725100	-1.62889500
C	-6.73088300	0.22303400	0.97951400
H	-4.73142300	0.71847600	1.60150700
C	-7.06704600	-0.11195800	-1.39577500
H	-5.31566800	0.13007600	-2.63638300
C	-7.57210700	-0.07838700	-0.09476300
H	-7.12540000	0.24668700	1.99051900
H	-7.72074900	-0.34531700	-2.23025400
H	-8.62236700	-0.28702400	0.08364800
C	-2.86016000	2.35821500	-0.03370900
H	-2.86681600	2.15896200	1.03956200
H	-3.76825300	2.91460800	-0.29382900
C	0.41994700	4.44267800	0.06869900
C	0.83503300	4.73308500	-1.24526500
C	1.16048400	4.98301300	1.13513700
C	1.95103000	5.53153700	-1.47752200
H	0.28301400	4.33696000	-2.09211600
C	2.27767900	5.78457600	0.90318800
H	0.84915800	4.77669700	2.15616500
C	2.67788400	6.06062900	-0.40498700
H	2.25238200	5.75069800	-2.49762200
H	2.83001100	6.19751200	1.74186000

H	3.54356200	6.68904300	-0.59080900

Zero-point correction= 0.768229 (Hartree/Particle)
Thermal correction to Energy= 0.814360
Thermal correction to Enthalpy= 0.815304
Thermal correction to Gibbs Free Energy= 0.686135
Sum of electronic and zero-point Energies= -2425.850911
Sum of electronic and thermal Energies= -2425.804780
Sum of electronic and thermal Enthalpies= -2425.803836
Sum of electronic and thermal Free Energies= -2425.933005
E(RB3LYP) = -2427.38135200 A.U.

E-tsc2

1 1

C	2.67887400	0.35795200	-0.77780400
C	1.73219700	0.89998200	-1.72510400
O	0.47992900	0.90623900	-1.64283100
O	2.30476900	1.52656900	-2.76675300
C	1.44548100	2.07887200	-3.78171700
H	0.81444000	2.86925000	-3.36924400
H	2.12043700	2.48508100	-4.53362100
H	0.81545900	1.29981600	-4.21608700
C	2.22046000	-0.63770200	0.23044200
C	1.45184400	-1.74450200	-0.17954100
C	2.64680400	-0.58931300	1.56566500
C	1.12131300	-2.76015300	0.71841600
H	1.15285300	-1.83075000	-1.22010600
C	2.30580500	-1.59814600	2.46697500
H	3.27541000	0.22964400	1.89164400
C	1.54256500	-2.68840700	2.04775900
H	0.55908000	-3.62198400	0.37055900
H	2.65356900	-1.53996500	3.49407300
H	1.29564900	-3.48371300	2.74457900
P	-3.37069700	-0.59962600	0.04993800
Au	-1.27665300	0.11346100	-0.63834300
C	-4.65114400	0.70254600	-0.59862400
C	-4.10026900	2.12729800	-0.35207100
C	-4.80782300	0.56208700	-2.12909400
C	-6.03931200	0.57363900	0.06366500
H	-3.96236700	2.36664500	0.70036700
H	-3.14729500	2.28365200	-0.86525800
H	-4.82210300	2.84354300	-0.76082900
H	-5.32466300	-0.35043900	-2.42853300
H	-5.41325800	1.40317800	-2.48424700
H	-3.84595800	0.61178000	-2.64821000

H	-6.71415800	1.29721600	-0.40719500
H	-6.48348500	-0.41487800	-0.06467300
H	-6.01733100	0.80516500	1.12994300
C	-3.69610300	-2.33472100	-0.74914000
C	-3.17499600	-2.33135100	-2.20576300
C	-2.88091500	-3.41068300	-0.00050600
C	-5.18536200	-2.73943500	-0.73832600
H	-3.67758000	-1.61237300	-2.84953900
H	-2.10027800	-2.13213600	-2.24552100
H	-3.34552900	-3.32724800	-2.62995400
H	-3.25418600	-3.60803900	1.00497800
H	-2.96163200	-4.34734900	-0.56309500
H	-1.82051900	-3.15249700	0.05958500
H	-5.26842800	-3.75782200	-1.13419800
H	-5.61667000	-2.74619200	0.26444100
H	-5.80053600	-2.10014800	-1.37377000
C	-3.40413400	-0.70826200	1.98126200
C	-2.08529900	-1.34944400	2.47311300
C	-3.44319100	0.71313800	2.58309500
C	-4.60400500	-1.51209800	2.52544500
H	-1.95626100	-2.38299700	2.15865400
H	-1.21124000	-0.78303500	2.14188000
H	-2.09424300	-1.34007200	3.56905500
H	-4.39039800	1.22613100	2.41080800
H	-3.32446300	0.61801500	3.66809300
H	-2.62361300	1.33969400	2.22082000
H	-4.57919800	-1.46785500	3.62013500
H	-5.56624000	-1.10681400	2.20706700
H	-4.56615800	-2.56722900	2.24913700
C	2.73125900	2.63643600	0.19252100
H	2.67212200	2.99340700	-0.83094000
C	4.04985000	2.60988700	0.73385900
H	4.17944100	2.43085000	1.79846000
S	4.33022500	0.19269400	-1.44335700
C	5.11434000	-1.11924600	-0.49893000
C	4.91400900	-2.45252700	-0.88184000
C	6.02202200	-0.81270800	0.52192400
C	5.60142000	-3.47297900	-0.22511700
H	4.23249000	-2.68542000	-1.69303400
C	6.71217800	-1.83883800	1.16881500
H	6.18675400	0.22157400	0.80107600
C	6.49983000	-3.16810800	0.79979900
H	5.44395200	-4.50512500	-0.52314600
H	7.41780600	-1.59786000	1.95817800

H	7.04008800	-3.96438100	1.30275800
C	5.15494200	2.75377200	-0.04164900
H	5.08292000	3.00707300	-1.09303900
C	1.53180800	2.86717000	0.98975100
C	1.46855500	2.62687000	2.38035300
C	0.40312700	3.44517900	0.36834400
C	0.33821400	2.96996300	3.11369900
H	2.31477300	2.18653700	2.89562400
C	-0.72504900	3.79579400	1.10627800
H	0.43672100	3.65831200	-0.69555700
C	-0.76088000	3.56375800	2.48339300
H	0.31901600	2.79239900	4.18479900
H	-1.56560600	4.27279100	0.61118600
H	-1.62918700	3.85800100	3.06540700
H	6.15393100	2.71764200	0.38080300

Zero-point correction= 0.767603 (Hartree/Particle)
Thermal correction to Energy= 0.813851
Thermal correction to Enthalpy= 0.814795
Thermal correction to Gibbs Free Energy= 0.687090
Sum of electronic and zero-point Energies= -2425.855076
Sum of electronic and thermal Energies= -2425.808827
Sum of electronic and thermal Enthalpies= -2425.807883
Sum of electronic and thermal Free Energies= -2425.935589
E(RB3LYP) = -2427.38135200 A.U.

E-tsd1
1 1

C	-2.08180900	-0.45530700	0.34951900
C	-1.94558400	-0.38452400	1.79042400
O	-1.21183300	-1.10284000	2.46547300
O	-2.67822100	0.61518000	2.37995100
C	-2.48198000	0.76272600	3.79994600
H	-1.44162000	1.01012100	4.02275700
H	-3.14021300	1.57740800	4.10191600
H	-2.74536400	-0.15818300	4.32351000
C	-1.77856800	-1.72805000	-0.39387800
C	-1.75879600	-2.98831100	0.26584000
C	-1.58437200	-1.74173600	-1.80627000
C	-1.56557900	-4.16863700	-0.44560900
H	-1.88974900	-3.02031400	1.33949700
C	-1.40629600	-2.93732800	-2.50643500
H	-1.61269600	-0.80913100	-2.36079600
C	-1.39860700	-4.15794100	-1.83435000
H	-1.56500800	-5.11178700	0.09314100

H	-1.27910300	-2.90383700	-3.58443000
H	-1.26651800	-5.08664000	-2.38013100
P	2.84965000	-0.82666800	0.08304300
Au	0.53708300	-0.91989300	-0.13808600
C	3.55178800	0.48433500	-1.15602600
C	2.81201900	0.35491500	-2.50848600
C	3.24779800	1.90475300	-0.63596400
C	5.07250100	0.35000400	-1.38527400
H	2.97013100	-0.59931300	-3.00740100
H	1.73521700	0.50426400	-2.38861400
H	3.18631600	1.14001000	-3.17522300
H	3.80797200	2.16572600	0.26253700
H	3.53844300	2.62083800	-1.41217200
H	2.18265700	2.05579800	-0.44471900
H	5.39540000	1.16798300	-2.03911400
H	5.64787400	0.42728000	-0.46068300
H	5.34461000	-0.58230300	-1.88315300
C	3.23981300	-0.34192900	1.91517800
C	2.27414900	0.78422800	2.35658400
C	2.94793800	-1.53687400	2.84979900
C	4.70068100	0.11136800	2.12187000
H	2.34056400	1.68680200	1.75123900
H	1.23825700	0.43334800	2.35241400
H	2.52803800	1.05853600	3.38722300
H	3.65568300	-2.35870400	2.73312200
H	3.03837000	-1.18190400	3.88244600
H	1.92927800	-1.91465900	2.72682600
H	4.85653100	0.29567300	3.19080300
H	5.42577900	-0.64477800	1.81501200
H	4.93279400	1.04158800	1.60021000
C	3.52478200	-2.59557000	-0.32589100
C	2.60920400	-3.66162100	0.32272400
C	3.45163600	-2.84056100	-1.84907300
C	4.97773700	-2.81338800	0.14922900
H	2.56596900	-3.60422500	1.40835100
H	1.58762200	-3.60589700	-0.06338500
H	3.00886200	-4.64865600	0.06300700
H	4.16239400	-2.24019600	-2.41841900
H	3.70171900	-3.89137700	-2.03228100
H	2.44476200	-2.67181200	-2.24153400
H	5.30436300	-3.80486700	-0.18438800
H	5.67601300	-2.08521400	-0.26722400
H	5.07176500	-2.79698300	1.23658800
C	-1.16561000	3.84670000	-0.63762200

H	-1.78869300	4.13352800	-1.48577700
C	-1.64797000	2.92628800	0.21711900
H	-1.05757500	2.57656100	1.05877200
S	-3.10607300	0.63222400	-0.57417100
C	-4.87481400	0.25472800	-0.37866700
C	-5.46700300	-0.01821400	0.85905700
C	-5.62003600	0.23054000	-1.56261400
C	-6.83045200	-0.30750600	0.90202300
H	-4.87321300	-0.00321400	1.76487100
C	-6.98525100	-0.05531400	-1.50255000
H	-5.14197100	0.42784500	-2.51753000
C	-7.58803900	-0.32396600	-0.27299000
H	-7.30267700	-0.52030900	1.85611600
H	-7.57143500	-0.07518800	-2.41582600
H	-8.64861400	-0.55121900	-0.22881900
C	-3.02720200	2.38094100	0.11087000
H	-3.53614600	2.33772300	1.07238800
H	-3.63781600	2.92623800	-0.61333700
C	0.12398600	4.54265600	-0.55601400
C	0.88130200	4.60481200	0.62971700
C	0.61395000	5.20251200	-1.69730000
C	2.09497400	5.28653600	0.66160400
H	0.50034400	4.14813600	1.53824500
C	1.83251000	5.87847000	-1.66707100
H	0.03223200	5.18050000	-2.61528400
C	2.57799400	5.92162100	-0.48735800
H	2.65789200	5.34128400	1.58884500
H	2.19352400	6.38123500	-2.55916300
H	3.51955700	6.46146100	-0.45627700

Zero-point correction= 0.768476 (Hartree/Particle)
Thermal correction to Energy= 0.814528
Thermal correction to Enthalpy= 0.815472
Thermal correction to Gibbs Free Energy= 0.686070
Sum of electronic and zero-point Energies= -2425.854283
Sum of electronic and thermal Energies= -2425.808231
Sum of electronic and thermal Enthalpies= -2425.807287
Sum of electronic and thermal Free Energies= -2425.936689
E(RB3LYP) = -2427.38543024 A.U.

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1 1

C	2.73927500	0.38369700	0.53195600
C	1.79250200	1.09621000	1.35361100
O	0.53839100	1.08601300	1.28019300

O	2.36739800	1.89280600	2.27082300
C	1.50935300	2.59402400	3.18922000
H	0.93285600	1.88608000	3.78937500
H	2.18314300	3.16626300	3.82559000
H	0.82662600	3.25756200	2.65577000
C	2.29612100	-0.76793100	-0.30000200
C	1.45794400	-1.75271900	0.25776500
C	2.78376900	-0.98407500	-1.59996400
C	1.11102400	-2.89649900	-0.46299400
H	1.11518000	-1.64213800	1.28182600
C	2.42945900	-2.12177400	-2.32487900
H	3.47543200	-0.27625200	-2.04234400
C	1.58923500	-3.08300300	-1.76120600
H	0.48789600	-3.65405700	0.00356100
H	2.82528100	-2.26360200	-3.32602200
H	1.32751000	-3.97664400	-2.31960000
P	-3.36096900	-0.68415900	0.03279900
Au	-1.24951900	0.15053800	0.49748100
C	-3.36828400	-1.47523500	-1.73264200
C	-2.56933800	-0.56518600	-2.69465600
C	-2.62309900	-2.82665800	-1.70249600
C	-4.78779700	-1.69949300	-2.29442800
H	-3.01166800	0.41973200	-2.82977600
H	-1.53781600	-0.43363900	-2.35713700
H	-2.54160200	-1.05165000	-3.67643500
H	-3.15666000	-3.59906200	-1.14737600
H	-2.52974800	-3.18104200	-2.73504900
H	-1.61148000	-2.72632000	-1.30084300
H	-4.69918500	-2.21425600	-3.25768600
H	-5.40607800	-2.32551800	-1.64868100
H	-5.32069700	-0.76560500	-2.48166400
C	-3.76650600	-2.01050400	1.38496500
C	-2.52623000	-2.90691900	1.61265300
C	-4.04060900	-1.31057100	2.73419200
C	-4.97760000	-2.89733100	1.02491900
H	-2.21678700	-3.45945200	0.72790300
H	-1.67267500	-2.32457800	1.97071900
H	-2.77682500	-3.63952400	2.38816900
H	-4.97753500	-0.75247400	2.74766800
H	-4.11658800	-2.08405500	3.50622600
H	-3.22340800	-0.64229600	3.02133000
H	-5.17212300	-3.57231700	1.86600700
H	-5.88980800	-2.32271000	0.85502400
H	-4.79664400	-3.52388900	0.14948600

C	-4.59879700	0.80224000	0.13124100
C	-4.23032500	1.69914800	1.33798000
C	-4.44106900	1.68669200	-1.12465000
C	-6.07329700	0.36327000	0.25535800
H	-4.31210100	1.19756500	2.30049600
H	-3.21762300	2.10144300	1.24492200
H	-4.92490800	2.54688800	1.35209800
H	-4.80900400	1.21037900	-2.03447000
H	-5.03822400	2.59285800	-0.97400100
H	-3.40415700	1.99888300	-1.27726300
H	-6.70251400	1.25993000	0.22692600
H	-6.39474800	-0.28375000	-0.56249200
H	-6.28376100	-0.14313200	1.19905400
C	2.74686800	2.40301300	-0.96699300
H	3.13302900	1.69592300	-1.69176500
C	3.72100900	3.15792500	-0.26299300
H	3.39687200	3.95119600	0.40443000
C	5.21721600	-1.04422900	0.50286800
C	6.24102300	-0.86882400	-0.43595900
C	4.93667000	-2.32400600	1.00145000
C	6.96605500	-1.97238500	-0.88961500
H	6.47998300	0.12378500	-0.80169900
C	5.65691100	-3.42253500	0.53475600
H	4.16405600	-2.45522500	1.75122200
C	6.67093400	-3.24918700	-0.41065900
H	7.76146700	-1.83141200	-1.61510600
H	5.43510800	-4.41297500	0.92047500
H	7.23606400	-4.10613900	-0.76424600
C	5.04523300	2.85732400	-0.31858300
H	5.42617100	2.13527800	-1.03203400
H	5.78001000	3.40046400	0.26570200
S	4.39469800	0.39365600	1.20052500
C	1.38644400	2.85461800	-1.22352200
C	0.76411100	3.88042600	-0.47888100
C	0.67925100	2.30690200	-2.31581700
C	-0.49184900	4.36061700	-0.83572100
H	1.27845000	4.32459200	0.36672800
C	-0.57406700	2.79421500	-2.67594100
H	1.14200500	1.51823300	-2.90215900
C	-1.16262100	3.82822900	-1.94147200
H	-0.94161000	5.16711700	-0.26420600
H	-1.08170500	2.38511700	-3.54432700
H	-2.12788700	4.22833800	-2.23701000

Zero-point correction= 0.767110 (Hartree/Particle)

Thermal correction to Energy= 0.813543
Thermal correction to Enthalpy= 0.814487
Thermal correction to Gibbs Free Energy= 0.685832
Sum of electronic and zero-point Energies= -2425.855697
Sum of electronic and thermal Energies= -2425.809263
Sum of electronic and thermal Enthalpies= -2425.808319
Sum of electronic and thermal Free Energies= -2425.936974
E(RB3LYP) = -2427.39459869 A.U.

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0 1

C	0.73186600	-0.18255800	-0.48347300
C	1.96639300	-0.60459900	-1.13581200
O	2.85966900	0.13116100	-1.54300000
O	2.08343100	-1.96935700	-1.24211700
C	3.27475400	-2.42444100	-1.89112400
H	4.16827000	-2.09989500	-1.35080600
H	3.20758700	-3.51305600	-1.89535500
H	3.33305500	-2.04396500	-2.91438500
C	0.40328700	1.24072000	-0.28220700
C	0.99151200	2.25280400	-1.07652300
C	-0.51854300	1.65671400	0.70422900
C	0.67630200	3.59506900	-0.88092200
H	1.70800200	1.97435800	-1.83599800
C	-0.82732900	3.00109800	0.89460100
H	-1.00529400	0.92120700	1.33212900
C	-0.23251800	3.98443800	0.10394800
H	1.14871800	4.34391300	-1.51103900
H	-1.53962100	3.27797600	1.66717800
H	-0.47510400	5.03282700	0.25046000
C	2.35384200	-0.55672500	1.88750900
C	1.14890000	-0.55713700	2.53883800
H	0.80944200	0.37236600	2.99153600
S	-0.29200600	-1.47272200	0.02617200
C	-2.01052300	-0.97546000	-0.16408400
C	-2.42977900	-0.20434100	-1.25439700
C	-2.94994000	-1.50021400	0.73000500
C	-3.78814300	0.05335100	-1.43045400
H	-1.69886000	0.19275600	-1.94898400
C	-4.30815300	-1.24455600	0.53739400
H	-2.62656900	-2.10677900	1.56991000
C	-4.73038000	-0.46389500	-0.53880800
H	-4.10963700	0.65895700	-2.27248900
H	-5.03366800	-1.65388200	1.23407500

H	-5.78705200	-0.26140100	-0.68411400
C	0.23025400	-1.61975500	2.42981800
H	0.59466100	-2.62580300	2.24948600
H	-0.72837200	-1.56002000	2.93602600
H	2.67680900	-1.48234200	1.41243400
C	3.31243600	0.58452800	1.84148800
H	3.53333900	0.84622000	0.79734500
H	2.91635500	1.46957600	2.34640200
H	4.26981500	0.31586100	2.30823000

Zero-point correction= 0.340146 (Hartree/Particle)
Thermal correction to Energy= 0.361580
Thermal correction to Enthalpy= 0.362524
Thermal correction to Gibbs Free Energy= 0.289306
Sum of electronic and zero-point Energies= -1284.306745
Sum of electronic and thermal Energies= -1284.285311
Sum of electronic and thermal Enthalpies= -1284.284367
Sum of electronic and thermal Free Energies= -1284.357585
E(RB3LYP) = -1285.01213914 A.U.

F-tsd2

1 1

C	-2.66065800	0.89964700	-0.28501600
C	-1.89226200	1.82249800	-1.12093500
O	-0.70674300	1.67627700	-1.42977500
O	-2.59562500	2.91402700	-1.49142700
C	-1.90786500	3.86456800	-2.32131400
H	-1.59092000	3.39956100	-3.25789800
H	-2.63175100	4.65504200	-2.51611300
H	-1.03080100	4.26638300	-1.80842800
C	-2.10129800	-0.42712200	0.02740000
C	-1.21628200	-1.09407300	-0.88013200
C	-2.48933600	-1.13976400	1.17619300
C	-0.80524000	-2.42845600	-0.63403800
H	-1.05295300	-0.65938200	-1.86110200
C	-2.04877000	-2.44238400	1.42171800
H	-3.17900500	-0.68266700	1.87594100
C	-1.20326200	-3.09793900	0.52844100
H	-0.23003700	-2.94909700	-1.39422500
H	-2.38647500	-2.95327100	2.31860900
H	-0.88550300	-4.11899500	0.71060300
P	3.31880900	-0.10634500	0.09541700
Au	1.03067500	-0.55685000	-0.24540000
C	3.67099500	-0.11462600	1.99758300
C	2.54298000	0.65891200	2.71979200

C	3.61557200	-1.56124900	2.53483800
C	5.03754600	0.50153800	2.36687300
H	2.49537400	1.71274900	2.45235900
H	1.56434900	0.20954400	2.52560500
H	2.72797700	0.60214100	3.79839400
H	4.45463300	-2.17335100	2.20247300
H	3.66547900	-1.51668200	3.62824500
H	2.68080300	-2.06397800	2.27041500
H	5.17629800	0.40950900	3.45011300
H	5.87441700	-0.01062400	1.88875300
H	5.10198900	1.56394800	2.12589500
C	4.30104600	-1.51988100	-0.79958800
C	3.62596800	-2.88144300	-0.50924200
C	4.22199700	-1.32020500	-2.32925900
C	5.78362600	-1.59191600	-0.37515700
H	3.64044400	-3.16387100	0.54134400
H	2.58779700	-2.89432300	-0.85213800
H	4.17051800	-3.65381700	-1.06394800
H	4.77679500	-0.45037700	-2.68167200
H	4.66762700	-2.19975300	-2.80673100
H	3.18914000	-1.24735200	-2.68277200
H	6.27714300	-2.36221400	-0.97834800
H	6.32307800	-0.65766900	-0.53935300
H	5.90536800	-1.88066000	0.67046000
C	3.72745000	1.61716800	-0.68902500
C	2.94919800	1.75827900	-2.01932300
C	3.21992300	2.74981800	0.22881000
C	5.23646700	1.82506100	-0.93817300
H	3.20465100	1.00001500	-2.75742600
H	1.86747000	1.73958700	-1.86020400
H	3.20311500	2.73202500	-2.45401300
H	3.78699900	2.84110100	1.15624100
H	3.33582900	3.69531000	-0.31231200
H	2.15925300	2.64083100	0.46539200
H	5.38490200	2.84392500	-1.31314300
H	5.83406300	1.72504300	-0.02943800
H	5.63899200	1.14736500	-1.69272500
C	-1.99910200	2.23586000	1.78888200
H	-1.97106300	1.24338800	2.22851100
C	-3.18745400	2.96440700	1.89529700
H	-3.18700000	3.99719600	1.55160700
C	-5.18746200	-0.44344400	-0.25204300
C	-6.06021700	-0.77333600	0.79099000
C	-5.04115100	-1.30782100	-1.34607100

C	-6.77206700	-1.97413100	0.74703800
H	-6.19033800	-0.09511000	1.62807100
C	-5.74328700	-2.51184800	-1.37330000
H	-4.39328800	-1.03347600	-2.17215800
C	-6.60924600	-2.84722300	-0.32876200
H	-7.45117400	-2.22506500	1.55618400
H	-5.62701300	-3.18086400	-2.22064900
H	-7.16195100	-3.78104900	-0.35991700
C	-4.38714100	2.37884000	2.22222400
H	-4.42424900	1.38901100	2.66471800
H	-5.31288300	2.94380300	2.22431600
S	-4.40327800	1.17497400	-0.25405900
C	-0.67814800	2.88449200	1.53035100
H	-0.08702100	2.32110000	0.79971300
H	-0.79606900	3.90706300	1.16023300
H	-0.09417300	2.92693300	2.46011400

Zero-point correction= 0.713496 (Hartree/Particle)
Thermal correction to Energy= 0.756944
Thermal correction to Enthalpy= 0.757888
Thermal correction to Gibbs Free Energy= 0.635742
Sum of electronic and zero-point Energies= -2234.158302
Sum of electronic and thermal Energies= -2234.114854
Sum of electronic and thermal Enthalpies= -2234.113910
Sum of electronic and thermal Free Energies= -2234.236056
E(RB3LYP) = -2235.56746079 A.U.

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0 1

C	-0.06270900	-0.49583900	-0.62181400
C	0.84748500	-1.37510200	-1.34585300
O	1.70760200	-1.04458000	-2.15001800
O	0.67450600	-2.70031200	-1.00988000
C	1.48391200	-3.62242600	-1.74569300
H	2.54777200	-3.42895900	-1.58478800
H	1.21615600	-4.61158900	-1.37223600
H	1.27938800	-3.55413900	-2.81768600
C	-0.01434600	0.96466400	-0.70770600
C	0.72594800	1.63866700	-1.70802000
C	-0.69527000	1.76538900	0.23794200
C	0.76393200	3.02989300	-1.75399200
H	1.27217000	1.05603200	-2.43604400
C	-0.64576200	3.15464000	0.18809000
H	-1.26028700	1.28700800	1.02589800
C	0.07989900	3.80163900	-0.81351900

H	1.33875100	3.51438800	-2.53873800
H	-1.18211000	3.73343700	0.93541700
H	0.11286300	4.88632500	-0.85824100
C	1.73434600	-0.78718200	1.54695600
C	0.74042200	-0.29925100	2.38223700
H	0.73421500	0.75629100	2.63943500
C	-3.00493000	-0.34175600	0.12061800
C	-3.41033400	0.08292300	-1.14754400
C	-3.82176300	-0.13080700	1.23325000
C	-4.62769500	0.74645200	-1.29194700
H	-2.77307800	-0.09463100	-2.00693600
C	-5.04718800	0.51976000	1.07734600
H	-3.50348100	-0.46603200	2.21559500
C	-5.44885000	0.96406300	-0.18283800
H	-4.93792500	1.08778400	-2.27513600
H	-5.68209100	0.68472100	1.94295000
H	-6.39876400	1.47632400	-0.30189800
C	-0.36512200	-1.06348200	2.74094500
H	-0.31771300	-2.14619900	2.70844100
H	-1.14711300	-0.64355400	3.36566100
H	1.70204700	-1.84805000	1.30793900
Se	-1.39417100	-1.39442800	0.31918700
C	2.91654900	-0.07942500	1.09517600
C	3.09649900	1.31138200	1.26405000
C	3.93792700	-0.80112300	0.44101800
C	4.25538400	1.93749700	0.82079100
H	2.31788400	1.90519300	1.72988000
C	5.09775700	-0.17228300	0.00141700
H	3.81422900	-1.87016900	0.29285800
C	5.26422500	1.20062500	0.19276100
H	4.37175800	3.00849800	0.95878200
H	5.87066600	-0.75162800	-0.49489300
H	6.16773900	1.69512000	-0.15145000

Zero-point correction= 0.392194 (Hartree/Particle)
Thermal correction to Energy= 0.417240
Thermal correction to Enthalpy= 0.418184
Thermal correction to Gibbs Free Energy= 0.335118
Sum of electronic and zero-point Energies= -3477.211019
Sum of electronic and thermal Energies= -3477.185973
Sum of electronic and thermal Enthalpies= -3477.185028
Sum of electronic and thermal Free Energies= -3477.268095
E(RB3LYP) = -3480.16289640 A.U.

G-tsc2

1 1

C	-2.33322200	-0.24260000	-0.39403100
C	-1.52815400	-1.14025500	-1.18175000
O	-0.27991900	-1.10674400	-1.34216100
O	-2.21590900	-2.12681800	-1.76576600
C	-1.49221100	-3.07777500	-2.57366600
H	-0.76248500	-3.61668100	-1.96825300
H	-2.25234200	-3.75878300	-2.95333300
H	-0.99089400	-2.56794400	-3.39900900
C	-1.78700000	1.08953400	-0.01380900
C	-1.17137800	1.89453600	-0.99435300
C	-1.96078600	1.63553700	1.26832300
C	-0.74956800	3.19138100	-0.69973100
H	-1.05613600	1.51058600	-2.00342300
C	-1.53415900	2.93077400	1.56474800
H	-2.45815300	1.05269500	2.03398600
C	-0.92914800	3.71583400	0.58239100
H	-0.30399700	3.80024900	-1.48134700
H	-1.69156200	3.33108100	2.56187500
H	-0.61640700	4.73092500	0.80813900
P	3.55478600	0.61609500	0.15852800
Au	1.47378000	-0.14232200	-0.52658300
C	4.79639300	-0.85110400	-0.07824400
C	4.14330700	-2.16385000	0.41698400
C	5.07633700	-1.05333700	-1.58386800
C	6.13615400	-0.64197400	0.65896900
H	3.91842900	-2.16694000	1.48194600
H	3.22293300	-2.38550800	-0.13098200
H	4.84781300	-2.98218500	0.22945800
H	5.66413400	-0.24718000	-2.02399200
H	5.65954200	-1.97366100	-1.69764800
H	4.15497800	-1.17755900	-2.16067800
H	6.79767100	-1.48114400	0.41629700
H	6.64930600	0.27223000	0.35642000
H	6.02152200	-0.63020000	1.74445500
C	4.04575300	2.11960200	-0.95920900
C	3.63435100	1.82551400	-2.42202400
C	3.24153300	3.36604300	-0.53167300
C	5.55188100	2.45111900	-0.90470400
H	4.13335000	0.96138200	-2.85637100
H	2.55407300	1.67889800	-2.51187500
H	3.90234600	2.69751300	-3.02943200
H	3.54944900	3.76470400	0.43566400
H	3.42162200	4.15189800	-1.27364900

H	2.16582700	3.17212200	-0.51199000
H	5.72592100	3.36000300	-1.49151100
H	5.90562600	2.64651600	0.10924800
H	6.17288500	1.66697400	-1.34145800
C	3.44698400	1.13853800	2.01849500
C	2.13915700	1.93298500	2.24617600
C	3.34882900	-0.11820500	2.91075400
C	4.64976900	1.98563600	2.48600000
H	2.09082000	2.86845000	1.69322200
H	1.25487300	1.34454600	1.98685200
H	2.07540700	2.17890500	3.31247700
H	4.27341500	-0.69584300	2.94562400
H	3.13954600	0.21212400	3.93404300
H	2.52936900	-0.77665800	2.60846200
H	4.54012700	2.17468200	3.55978600
H	5.60720600	1.48186100	2.34239100
H	4.69573500	2.95915100	1.99508900
C	-2.02947200	-1.77140600	1.61020500
C	-3.34071300	-1.53779500	2.12524300
H	-3.40039900	-0.73943600	2.86399700
C	-4.88673600	1.35571000	-0.24071200
C	-4.80466500	2.44680000	-1.11388100
C	-5.56554000	1.47962000	0.97588100
C	-5.38023900	3.66607800	-0.75481700
H	-4.30001300	2.34152300	-2.06815900
C	-6.14508300	2.70038700	1.32601600
H	-5.64591500	0.62785400	1.64110100
C	-6.04987400	3.79407800	0.46394900
H	-5.31429700	4.51149100	-1.43299200
H	-6.67426100	2.79338800	2.26969400
H	-6.50452900	4.74163000	0.73665000
C	-4.52617100	-2.05319700	1.70390400
H	-4.61733300	-2.81177800	0.93950100
H	-5.45389900	-1.75048500	2.17871700
H	-1.27640600	-1.08372600	1.98587600
Se	-4.20445200	-0.35740400	-0.81659300
C	-1.45824100	-3.03708800	1.15825700
C	-2.20342100	-4.20131400	0.86043400
C	-0.04885400	-3.13318200	1.08019000
C	-1.57071700	-5.38233100	0.48682300
H	-3.27994800	-4.19937700	0.95570800
C	0.58294100	-4.31639500	0.70941300
H	0.55175000	-2.26535700	1.33838600
C	-0.17627300	-5.44781300	0.40220600

H	-2.16850900	-6.26338500	0.27366300
H	1.66730000	-4.36193200	0.67352400
H	0.31149400	-6.37586200	0.12018200

Zero-point correction= 0.766116 (Hartree/Particle)
Thermal correction to Energy= 0.812898
Thermal correction to Enthalpy= 0.813842
Thermal correction to Gibbs Free Energy= 0.684453
Sum of electronic and zero-point Energies= -4426.592837
Sum of electronic and thermal Energies= -4426.546055
Sum of electronic and thermal Enthalpies= -4426.545111
Sum of electronic and thermal Free Energies= -4426.674500
E(RB3LYP) = -4430.72354984 A.U.

G-tsd1
1 1

C	-1.86609100	-0.62062000	0.37802800
C	-1.74373200	-0.47308000	1.80902000
O	-0.99198300	-1.13286900	2.52529700
O	-2.52413300	0.52108600	2.34713200
C	-2.35057500	0.73585500	3.76076000
H	-1.32452300	1.03767700	3.98365400
H	-3.04729000	1.53234900	4.02272400
H	-2.57944900	-0.17281000	4.32084000
C	-1.50025100	-1.90092200	-0.31054400
C	-1.39762900	-3.13028100	0.40326700
C	-1.32037100	-1.97047800	-1.72548500
C	-1.15189300	-4.32890500	-0.25972900
H	-1.51204600	-3.12052700	1.47914600
C	-1.09288800	-3.18546400	-2.37524400
H	-1.39697800	-1.06643100	-2.32146100
C	-1.01119200	-4.37302200	-1.65065400
H	-1.08953000	-5.24502600	0.32047200
H	-0.98229100	-3.19315000	-3.45555900
H	-0.83920100	-5.31716700	-2.15733200
P	3.07574100	-0.73007900	0.05383300
Au	0.77363200	-1.02172100	-0.10549300
C	3.57684200	0.85923900	-0.92999700
C	2.79778500	0.89916800	-2.26657200
C	3.14042300	2.11025000	-0.13989900
C	5.09079000	0.94928600	-1.21747300
H	3.04989100	0.08732000	-2.94612900
H	1.71681400	0.88384800	-2.10007300
H	3.04350400	1.83932300	-2.77340400
H	3.71586700	2.26170200	0.77417400

H	3.30361900	2.98942300	-0.77202000
H	2.07635200	2.08723100	0.10886000
H	5.28962400	1.90373200	-1.71792600
H	5.69733600	0.92706000	-0.31005700
H	5.44037700	0.16008400	-1.88534100
C	3.50436500	-0.55761900	1.93446400
C	2.45927600	0.35827200	2.61660700
C	3.37825300	-1.93352300	2.62473500
C	4.92223700	0.00012100	2.17929800
H	2.43280200	1.36848300	2.21115900
H	1.45359000	-0.06887100	2.56436800
H	2.72873600	0.43834100	3.67632100
H	4.15899600	-2.63656600	2.33125200
H	3.47822400	-1.77617400	3.70429000
H	2.39930600	-2.38962300	2.45366900
H	5.11674600	-0.01283300	3.25765800
H	5.70114100	-0.59744700	1.70202800
H	5.03068900	1.03481200	1.84822400
C	3.90821600	-2.30758300	-0.70635500
C	3.13482200	-3.56884700	-0.25271300
C	3.78898300	-2.26382200	-2.24506800
C	5.39549600	-2.45131000	-0.31979200
H	3.15174000	-3.73286800	0.82293100
H	2.09128500	-3.54165500	-0.57909900
H	3.60711900	-4.43893800	-0.72309100
H	4.40911100	-1.49260200	-2.70393100
H	4.13295100	-3.22703200	-2.63775000
H	2.75292400	-2.13073900	-2.56980200
H	5.80523800	-3.32311500	-0.84216000
H	5.99646500	-1.58741400	-0.60990500
H	5.53524400	-2.62458300	0.74853700
C	-1.32847900	3.94285600	-0.58029000
H	-1.96065400	4.19250800	-1.43356400
C	-1.75526200	2.98259000	0.26231900
H	-1.14842300	2.66967700	1.10694900
C	-4.87241500	-0.05060800	-0.34350800
C	-5.32178200	-0.47805100	0.90735100
C	-5.72970900	0.00695200	-1.44557300
C	-6.66032000	-0.84486400	1.05182500
H	-4.64254700	-0.51807300	1.75040000
C	-7.06816000	-0.35765500	-1.28568300
H	-5.36352200	0.32335100	-2.41808100
C	-7.53111100	-0.78341400	-0.03959800
H	-7.02283600	-1.17883900	2.01917800

H	-7.74211400	-0.31637800	-2.13563600
H	-8.57052500	-1.07228400	0.08107300
C	-3.08115000	2.33639600	0.13630200
H	-3.58496900	2.18215100	1.08723100
H	-3.73887300	2.83869400	-0.57641300
Se	-3.01422900	0.47055500	-0.67071300
C	-0.09147600	4.72440800	-0.47821400
C	0.65254800	4.81839900	0.71387600
C	0.36082300	5.43315700	-1.60589700
C	1.81746100	5.57873900	0.76523700
H	0.29844100	4.32171200	1.61222100
C	1.53150400	6.18784800	-1.55645100
H	-0.21190300	5.38627100	-2.52859800
C	2.26472000	6.26210500	-0.37054800
H	2.37019200	5.65523100	1.69700600
H	1.86445800	6.72676600	-2.43827800
H	3.16825500	6.86248700	-0.32433400

Zero-point correction= 0.766414 (Hartree/Particle)
Thermal correction to Energy= 0.813236
Thermal correction to Enthalpy= 0.814180
Thermal correction to Gibbs Free Energy= 0.681985
Sum of electronic and zero-point Energies= -4426.597094
Sum of electronic and thermal Energies= -4426.550272
Sum of electronic and thermal Enthalpies= -4426.549328
Sum of electronic and thermal Free Energies= -4426.681523
E(RB3LYP) = -4430.71872126 A.U.

G-tsd2
1 1

C	2.51196900	0.40151400	0.45315600
C	1.59809600	1.14293700	1.28109600
O	0.34234600	1.14763800	1.24663900
O	2.20830000	1.96454600	2.15552200
C	1.38498800	2.71784200	3.06467300
H	0.79720800	2.04568100	3.69393500
H	2.08423300	3.29014300	3.67292400
H	0.71369100	3.38471000	2.52050600
C	2.04439800	-0.79634000	-0.29412200
C	1.25349300	-1.76312700	0.35819000
C	2.45884700	-1.07115100	-1.60797500
C	0.88300400	-2.94541200	-0.28387100
H	0.96600700	-1.60439000	1.39314700
C	2.08101600	-2.24818700	-2.25457800

H	3.11221200	-0.37742200	-2.12413000
C	1.28993000	-3.19082600	-1.59689300
H	0.29690100	-3.68518300	0.25384900
H	2.42163700	-2.43501400	-3.26858300
H	1.01094900	-4.11472100	-2.09443500
P	-3.55805200	-0.66571900	0.06304900
Au	-1.44327800	0.17660900	0.49957800
C	-3.57430400	-1.48735700	-1.68840500
C	-2.78003700	-0.59546400	-2.67096000
C	-2.82837400	-2.83775500	-1.63667000
C	-4.99654100	-1.71998100	-2.23971800
H	-3.21935900	0.38897800	-2.81846000
H	-1.74517200	-0.46193500	-2.34510600
H	-2.76254500	-1.09822500	-3.64482700
H	-3.36043700	-3.60126600	-1.06781700
H	-2.73641100	-3.20933200	-2.66328200
H	-1.81617100	-2.72965400	-1.23822800
H	-4.91316100	-2.25588100	-3.19186600
H	-5.61448300	-2.32941900	-1.57821100
H	-5.52716700	-0.78851500	-2.44518900
C	-3.96127300	-1.96750100	1.44005600
C	-2.72155300	-2.86120100	1.68046400
C	-4.23151800	-1.24384300	2.77761700
C	-5.17414400	-2.85880600	1.09820600
H	-2.41781100	-3.43314100	0.80613300
H	-1.86486200	-2.27310000	2.02108400
H	-2.96971400	-3.57653700	2.47273600
H	-5.16798900	-0.68474200	2.78400400
H	-4.30647800	-2.00382500	3.56306100
H	-3.41308600	-0.57155300	3.05144400
H	-5.36755200	-3.51891700	1.95128900
H	-6.08609900	-2.28618000	0.92034400
H	-4.99554500	-3.50038500	0.23329300
C	-4.79245400	0.82494000	0.14135500
C	-4.41868100	1.74005600	1.33258500
C	-4.63527600	1.68832600	-1.12900500
C	-6.26760400	0.39154400	0.27588100
H	-4.50032300	1.25435700	2.30316800
H	-3.40462000	2.13697600	1.23132200
H	-5.11017300	2.59041600	1.33405600
H	-5.00751400	1.19821800	-2.02969900
H	-5.22878200	2.59901500	-0.99164400
H	-3.59774800	1.99423100	-1.29026900
H	-6.89475100	1.28927400	0.23713600

H	-6.59292600	-0.26566300	-0.53229000
H	-6.47622900	-0.10176900	1.22688200
C	2.55808200	2.33372700	-1.10013600
H	2.97700000	1.61534400	-1.79521300
C	3.50262100	3.13340000	-0.40638700
H	3.15076300	3.94138600	0.22844200
C	5.09747000	-1.15056400	0.30078300
C	6.02841600	-0.95786100	-0.72570500
C	4.83787400	-2.44071000	0.77835400
C	6.67951600	-2.05670000	-1.28980600
H	6.25499700	0.04220700	-1.07924200
C	5.48413900	-3.53535600	0.20397700
H	4.13649000	-2.58710200	1.59252200
C	6.40407300	-3.34519100	-0.82966000
H	7.40303100	-1.90310600	-2.08478800
H	5.27787900	-4.53534000	0.57348700
H	6.91237700	-4.19858700	-1.26809100
C	4.83350000	2.85036700	-0.42111600
H	5.24422100	2.12302600	-1.11184500
H	5.54694100	3.42681500	0.15783200
Se	4.29806100	0.37164500	1.18359000
C	1.19720800	2.75591400	-1.41182000
C	0.53745300	3.79464400	-0.72030400
C	0.53320200	2.16457300	-2.50783900
C	-0.71357800	4.24425900	-1.13143400
H	1.01768500	4.27389300	0.12632800
C	-0.71506200	2.62051200	-2.92236400
H	1.02441900	1.36453300	-3.05409300
C	-1.34163300	3.66747100	-2.23990100
H	-1.19230400	5.06145400	-0.60000000
H	-1.18932400	2.17549000	-3.79195700
H	-2.30296400	4.04288700	-2.57776000

Zero-point correction= 0.766217 (Hartree/Particle)
Thermal correction to Energy= 0.813056
Thermal correction to Enthalpy= 0.814000
Thermal correction to Gibbs Free Energy= 0.684041
Sum of electronic and zero-point Energies= -4426.599588
Sum of electronic and thermal Energies= -4426.552748
Sum of electronic and thermal Enthalpies= -4426.551804
Sum of electronic and thermal Free Energies= -4426.681764
E(RB3LYP) = -4430.72912008 A.U.

G-p1
0 1

C	0.75775900	-0.51185900	0.18204900
C	0.70560100	-1.95989200	0.68342900
O	-0.04708300	-2.36237600	1.55032000
O	1.53905200	-2.77109800	0.00486100
C	1.43712500	-4.16756100	0.32153700
H	0.46590600	-4.55930300	0.00699700
H	2.23797300	-4.65209600	-0.23627600
H	1.55624700	-4.33252600	1.39450400
C	2.13689900	-0.11406500	-0.35088100
C	3.28623800	-0.49108000	0.36537400
C	2.30872900	0.68280100	-1.49174900
C	4.55603200	-0.09550500	-0.04823700
H	3.18814200	-1.10310200	1.25491600
C	3.58234800	1.06910100	-1.91459100
H	1.44042100	1.02039800	-2.04586500
C	4.71176200	0.68332400	-1.19621600
H	5.42533000	-0.40277600	0.52592200
H	3.68414800	1.68089000	-2.80618100
H	5.70209100	0.98456100	-1.52482000
C	0.90769900	-0.08204800	3.64243200
H	0.06132400	-0.74336100	3.80131900
C	1.10247100	0.53771400	2.47821500
H	1.96917400	1.18390800	2.35638400
C	-2.27031900	-0.75497500	-0.75575000
C	-3.15205700	0.27160300	-1.11778500
C	-2.74831400	-1.86337400	-0.04634000
C	-4.50190400	0.19026600	-0.77404800
H	-2.77152300	1.13178100	-1.65765900
C	-4.09334700	-1.92483600	0.32025800
H	-2.07494800	-2.66436000	0.23183500
C	-4.97266500	-0.90418300	-0.04686300
H	-5.18048800	0.98710200	-1.06460900
H	-4.45621000	-2.78043900	0.88240800
H	-6.02146500	-0.96402300	0.22916300
C	0.16942400	0.44315700	1.28275900
H	-0.74226200	-0.05425500	1.62013200
H	1.59690900	0.04779000	4.47217800
C	-0.21616700	1.84805100	0.82196100
C	-1.55040900	2.26038200	0.94239700
C	0.72824900	2.79751100	0.40146600
C	-1.94051800	3.55878900	0.61270000
H	-2.29280300	1.55578200	1.30275800
C	0.34135400	4.09525100	0.06577700
H	1.77642000	2.53089100	0.33675500

C	-0.99570700	4.48138400	0.16419200
H	-2.98264500	3.84874300	0.71411500
H	1.09149800	4.80875300	-0.26372300
H	-1.29482200	5.49351900	-0.09271100
Se	-0.47223200	-0.65440700	-1.44504400

Zero-point correction= 0.395443 (Hartree/Particle)
Thermal correction to Energy= 0.420524
Thermal correction to Enthalpy= 0.421468
Thermal correction to Gibbs Free Energy= 0.338566
Sum of electronic and zero-point Energies= -3477.247956
Sum of electronic and thermal Energies= -3477.222875
Sum of electronic and thermal Enthalpies= -3477.221931
Sum of electronic and thermal Free Energies= -3477.304833
E(RB3LYP) = -3480.20393779 A.U.