Supporting Information

Mechanistic Understanding on the Dual Gold and Photoredox-Catalyzed Thiosulfonylation of Alkynes and Enynes: A DFT Study†

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1. Computational Methods

The Marcus Theory was applied to calculate the kinetic barrier of single electron transfer (SET). For a SET reaction below,

$$*[Ru]^{2+} + R_1 \xrightarrow{SET} [Ru]^{3+} + P_1$$

according to the Marcus-Hush equation, the reorganization energy is normally decomposed into internal energy (λ_i) and external energy ($\lambda_\circ$). The internal reorganization energy λ_i can be estimated according to the equation:

$$\lambda_{i1} = [E^D(Q_R) + E^A(Q_R)] - [E^D(Q) + E^A(Q_P)] \quad \text{Equation S1}$$

$$\lambda_{i2} = [E^{D+}(Q_R) + E^{A-}(Q_R)] - [E^{D+}(Q_P) + E^{A-}(Q_P)] \quad \text{Equation S2}$$

$$\lambda_i = (\lambda_{i1} + \lambda_{i2})/2 \quad \text{Equation S3}$$

where Q_R and Q_P are the equilibrium geometries of the reactants and products, respectively. In addition, the solvent outer-sphere reorganization energy $\lambda_\circ$ could be calculated from Equations S4 and S5.

$$\lambda_\circ = (332\ kcal/mol)\left(\frac{1}{2a_1} + \frac{1}{2a_2} - \frac{1}{R}\right)\left(\frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon}\right) \quad \text{Equation S4}$$

$$R = a_1 + a_2 \quad \text{Equation S5}$$

a_1 and a_2 are the radii of the excited-state photoredox ***Ru^{II}** and reactant **R_1**, respectively. ε_{op} and ε are the optical dielectric constant and the static dielectric constant of solvent, respectively. The radius of a molecule can be derived by calculating molecular volume via a Monte-Carlo integration as implemented in the Gaussian 09 program. Next, the $\Delta G^{\neq}$ of a single electron transfer process could be calculated from Equations S6 and S7. ΔG_r is the Gibbs energy change for a SET reaction (Equation S8).

$$\Delta G_{ET}^{\neq} = \Delta G_o^{\neq}\left(1 + \frac{\Delta G_r}{4\Delta G_o^{\neq}}\right)^2 \quad \text{Equation S6}$$

$$\Delta G_o^{\neq} = \frac{\lambda}{4} \quad \text{Equation S7}$$

$$\Delta G_r = G([Ru]^{3+}) + G(P_1) - G(*[Ru]^{2+}) - G(R_1) \quad \text{Equation S8}$$

Calculation of Redox Potentials:

For the molecules under study the oxidation potential is calculated by Nernst equation as

$$E_{1/2}^{red} = -\frac{\Delta G}{nF} - E_{SCE}$$ Equation S9

where ΔG is the Gibbs free energy difference between the reductant and the oxidant in aqueous solution, n is the number of electrons which attribute to the reaction, *F* is Faraday constant, and E_{SCE} = 4.51V (saturated calomel electrode). In the present study, only one electron transfer is considered, and n is equal to 1 for all the systems. If the employed unit of energy is eV, *F* is equal to the unit charge *e*.

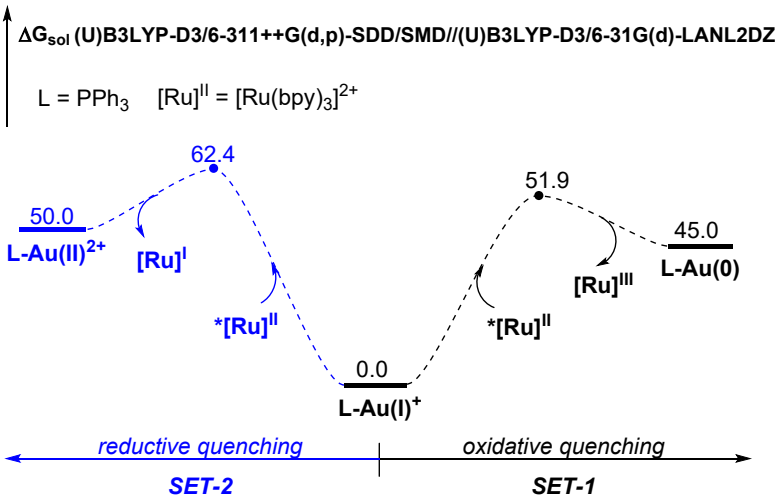

Fig. S1 Energy profiles (in kcal mol^{-1}) for the oxidative quenching and reductive quenching of *[Ru]^{II} by the Au(I) catalyst.

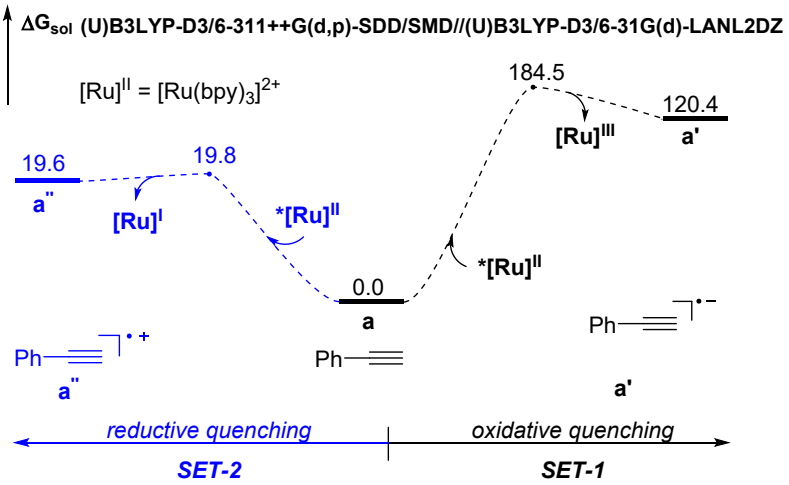

Fig. S2 Energy profiles (in kcal mol^{-1}) for the oxidative quenching and reductive quenching of *[Ru]^{II} by the substrate **a.**

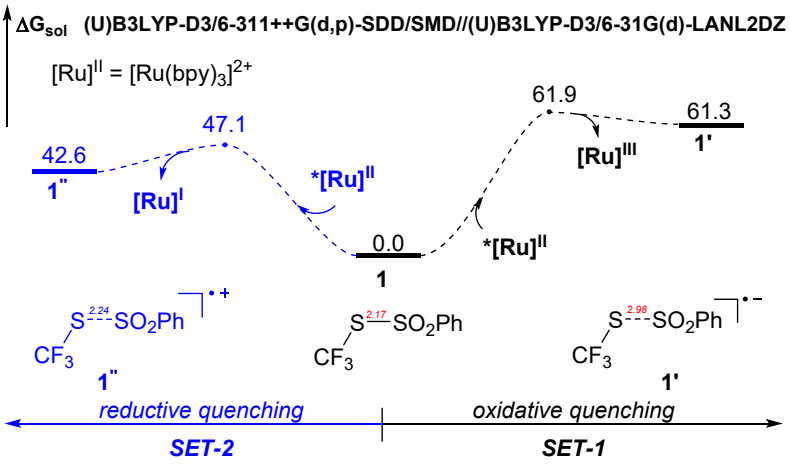

Fig. S3 Energy profiles (in kcal mol^{-1}) for the oxidative quenching and reductive quenching of *[Ru]^{II} by the substrate **1**. Bond lengths are shown in Å.

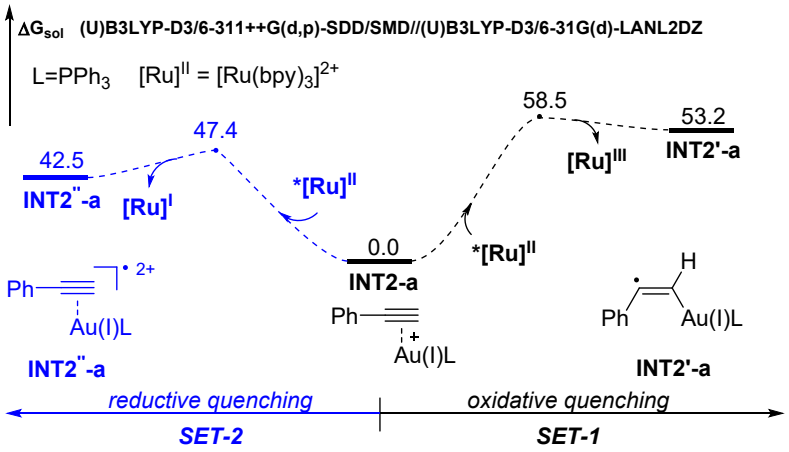

Fig. S4 Energy profiles (in kcal mol^{-1}) for the oxidative quenching and reductive quenching of *[Ru]^{II} by **INT2-a**.

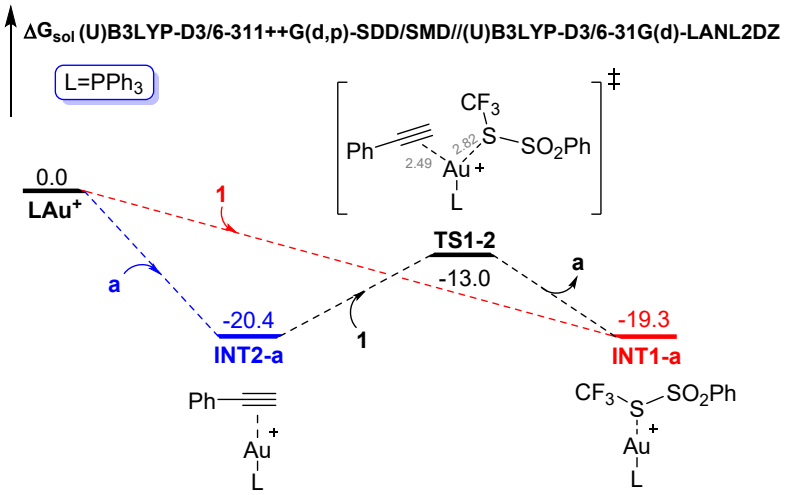

Fig. S5 Energy profiles (in kcal mol^{-1}) for the formation of **INT1-a** and **INT2-a** complexes. Bond lengths are shown in Å.

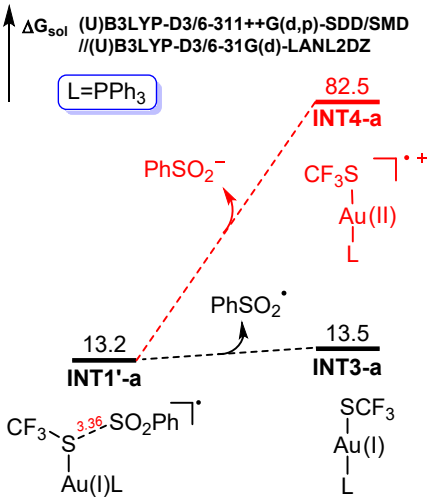

Fig. S6 Energy profiles (in kcal mol^{-1}) for the formation of benzenesulfonyl radical or benzenesulfonyl anion dissociated from **INT1′-a**. Bond lengths are shown in Å.

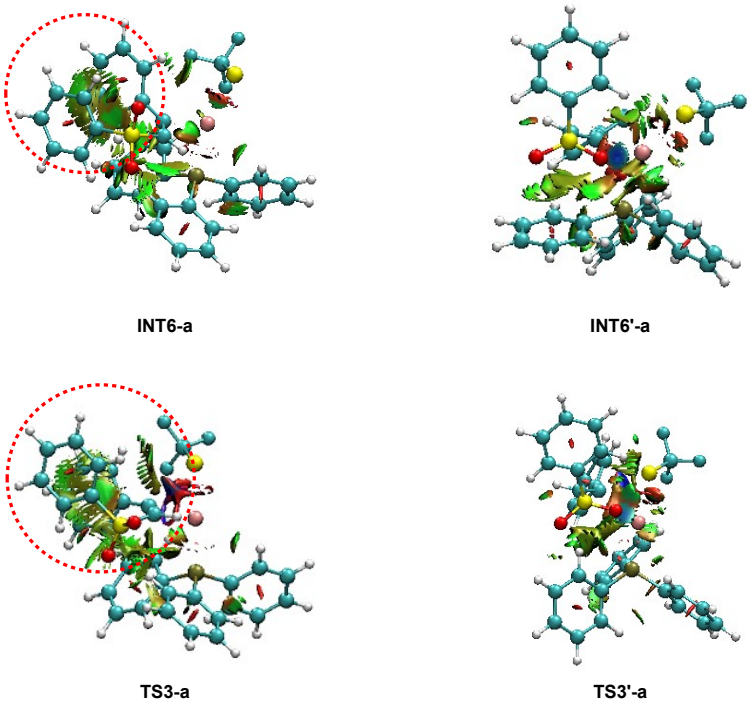

Fig. S7 Noncovalent interactions analyses (NCI) for the **INT6-a/INT6′-a** and the corresponding transition states of reductive elimination (**TS3-a/TS3′-a**).

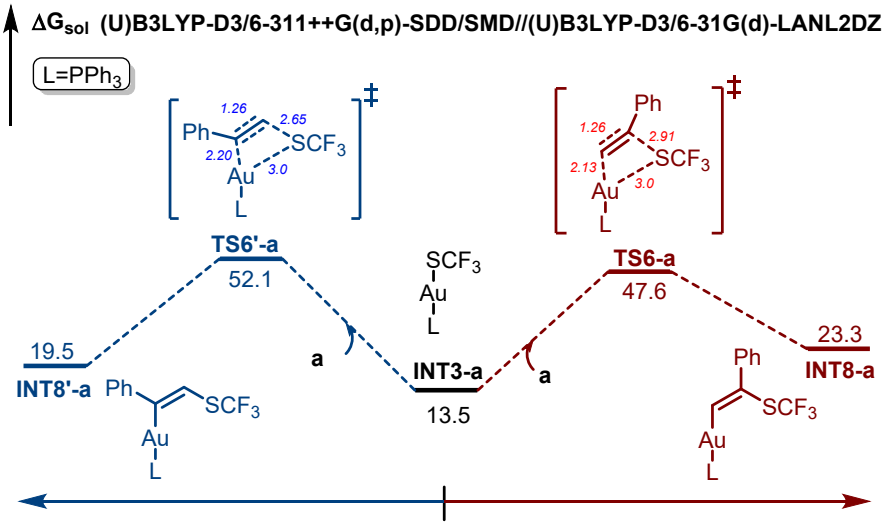

Fig. S8 Energy profiles (in kcal mol^{-1}) for the migratory insertion of phenylacetylene (**a**) to **INT3-a**. Bond lengths are shown in Å.

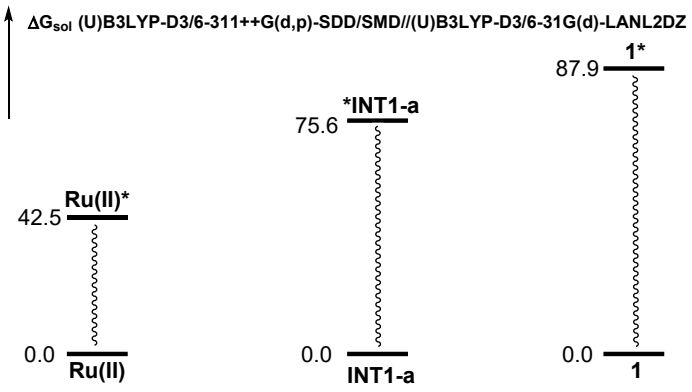

Fig. S9 Calculated singlet-triplet energy gap (in kcal mol^{-1}) for $PhSO_2SCF_3$ (**1**), **INT1-a**, and the Ru(II) photocatalyst.

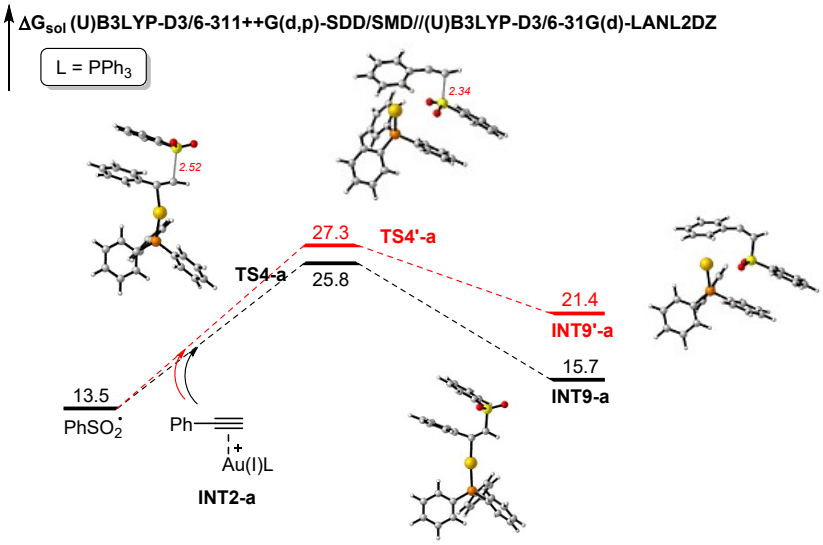

Fig. S10 Energy profile (in kcal mol^{-1}) for the attack of benzenesulfonyl radical to **INT2-a** in a *cis* manner.

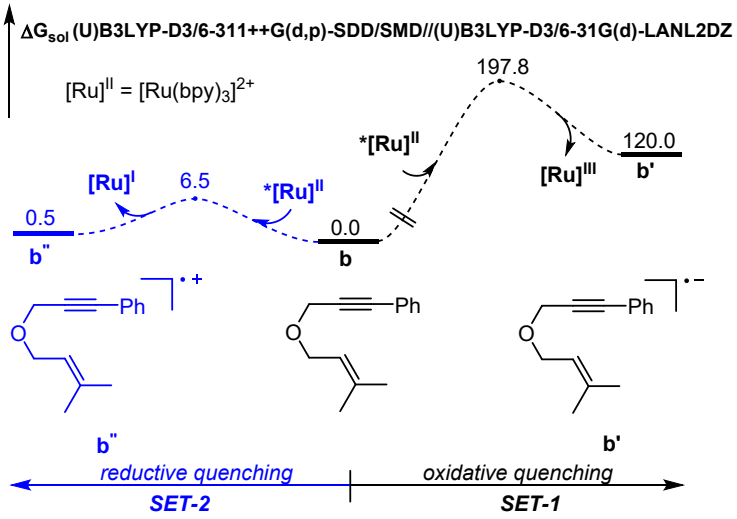

Fig. S11 Energy profiles (in kcal mol^{-1}) for the oxidative quenching and reductive quenching of *[Ru]^{II} by the substrate **b**.

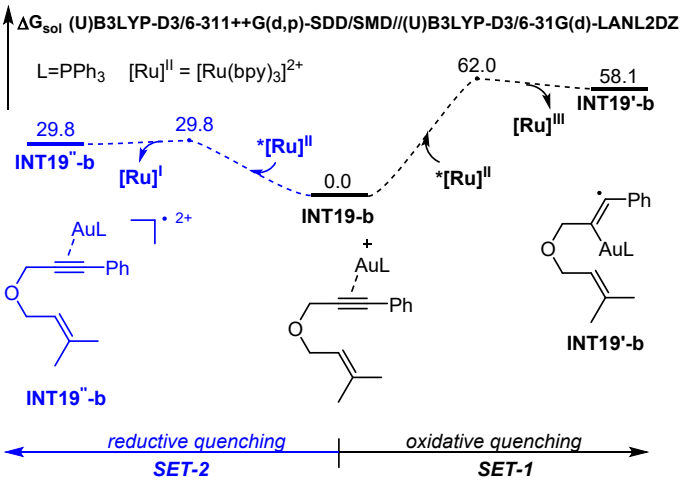

Fig. S12 Energy profiles (in kcal mol^{-1}) for the oxidative quenching and reductive quenching of *[Ru]^{II} by **INT19-b**.

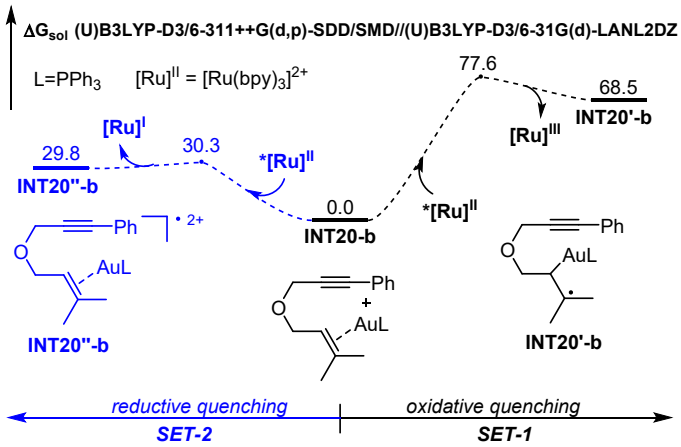

Fig. S13 Energy profiles (in kcal mol^{-1}) for the oxidative quenching and reductive quenching of *[Ru]^{II} by **INT20-b**.

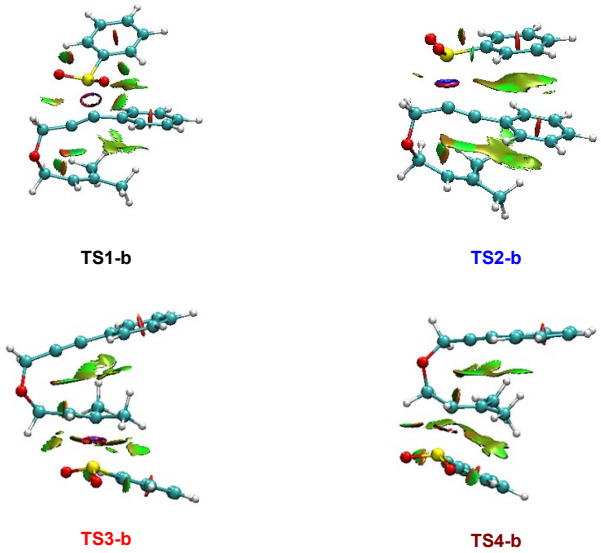

Fig. S14 Noncovalent interactions analyses (NCI) for the four transition states of **TS1-b**, **TS2-b**, **TS3-b**, and **TS4-b**.

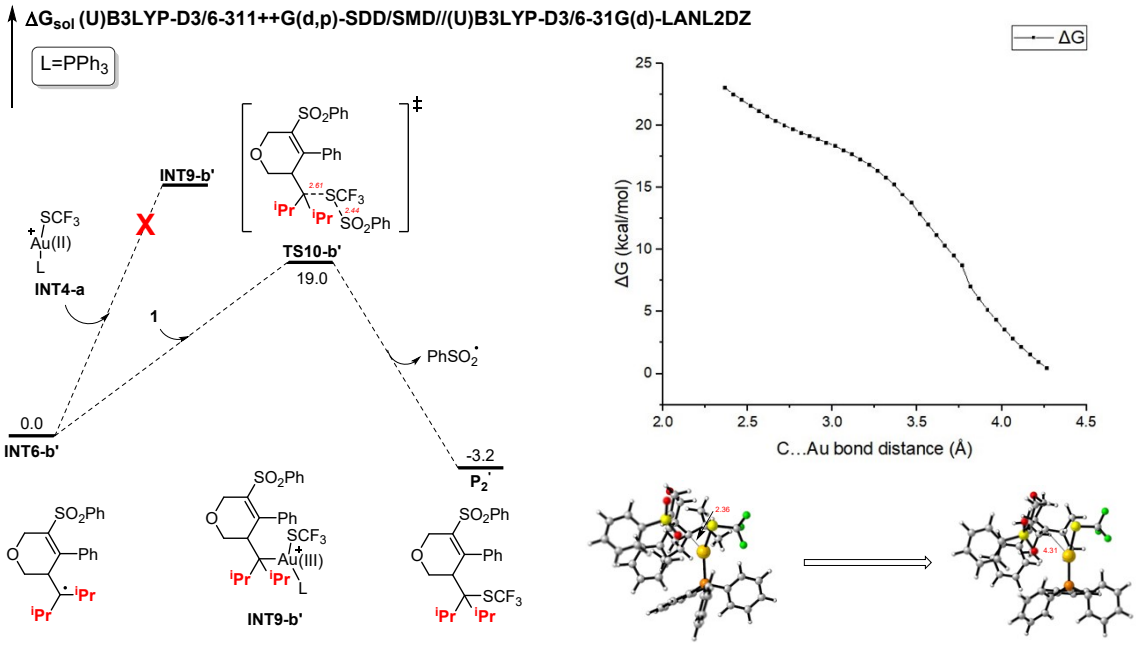

Fig. S15 Energy profiles (in kcal mol^{-1}) for the formation of product $\mathbf{P_2'}$ via a radical chain pathway for **INT6-b′**. The formation of an Au(III) intermediate with **INT4-a** could be ruled out by fixing C⋯Au bond distance partial optimization.

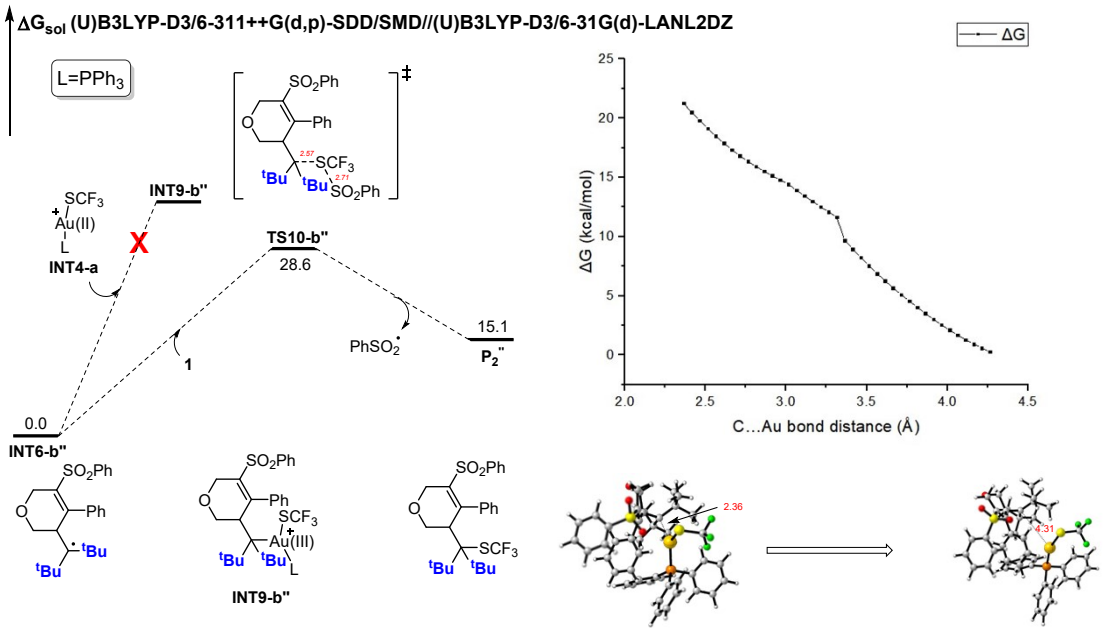

Fig. S16 Energy profiles (in kcal mol^{-1}) for the formation of product $\mathbf{P_2''}$ via a radical chain pathway for **INT6-b″**. The formation of an Au(III) intermediate with **INT4-a** could be ruled out by fixing C⋯Au bond distance partial optimization.

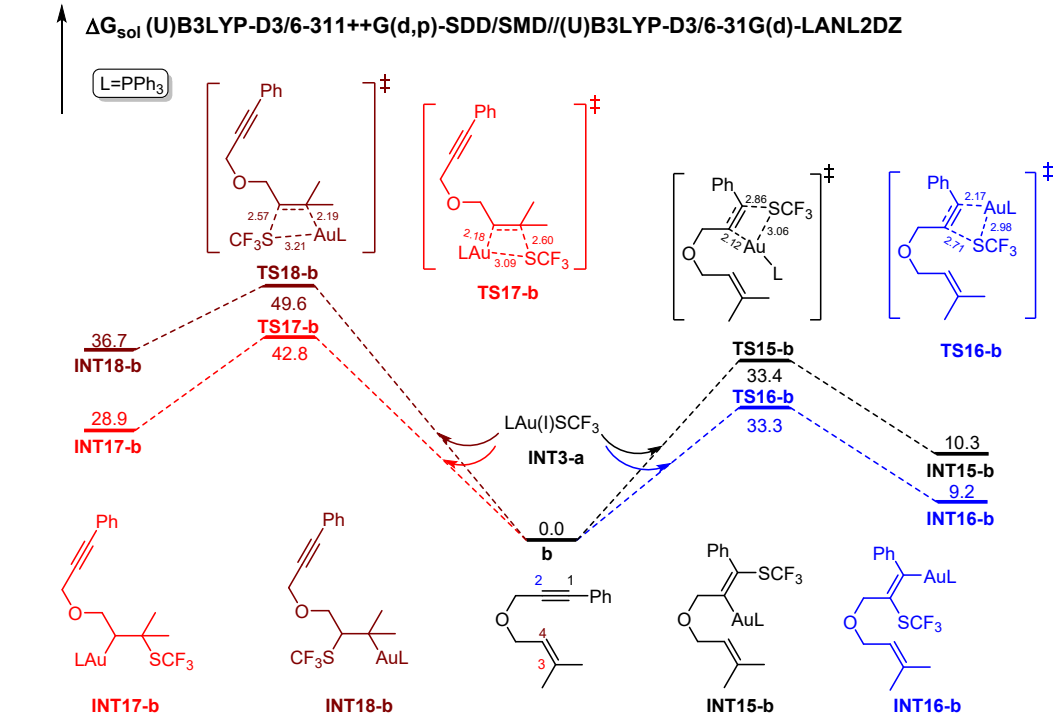

Fig. S17 Energy profiles (in kcal mol^{-1}) for the migratory insertion of 1,6-enyne (**b**) to **INT3-a**. Bond lengths are shown in Å.

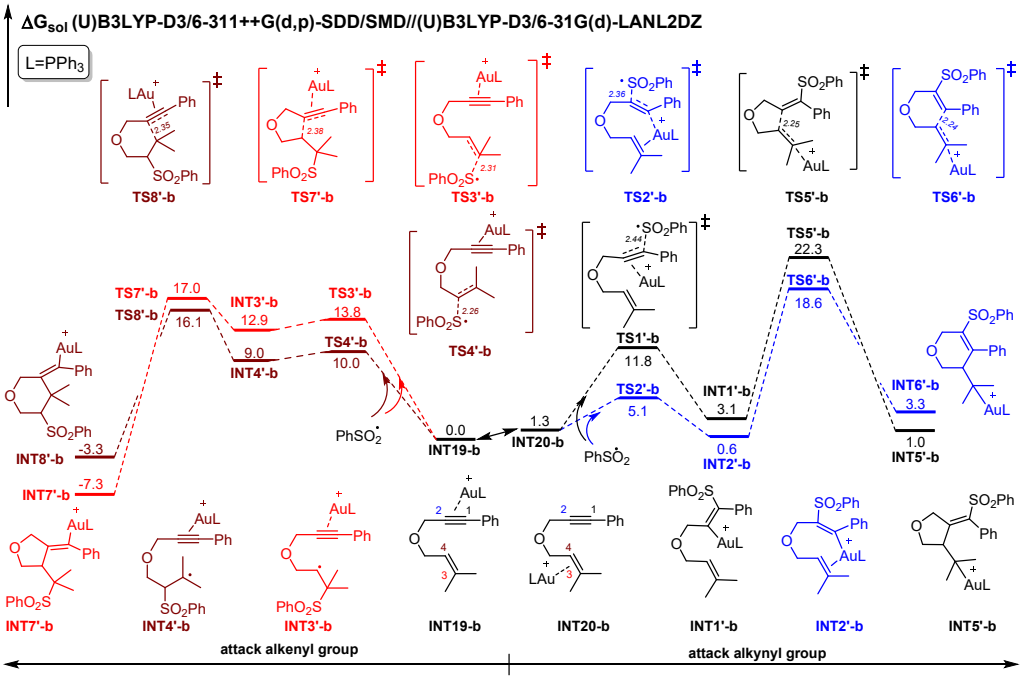

Fig. S18 Energy profiles (in kcal mol^{-1}) for the gold-catalyst involving radical chain reaction. Bond lengths are shown in Å.

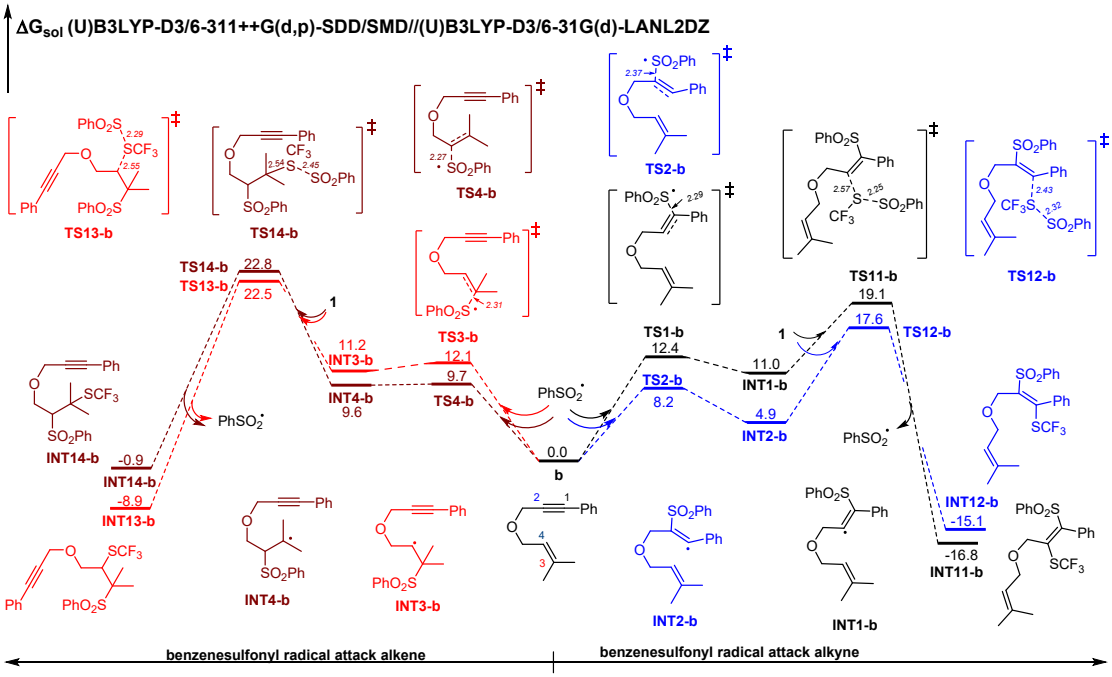

Fig. S19 Energy profiles (in kcal mol^{-1}) for the formation of acyclic products. Bond lengths are shown in Å.

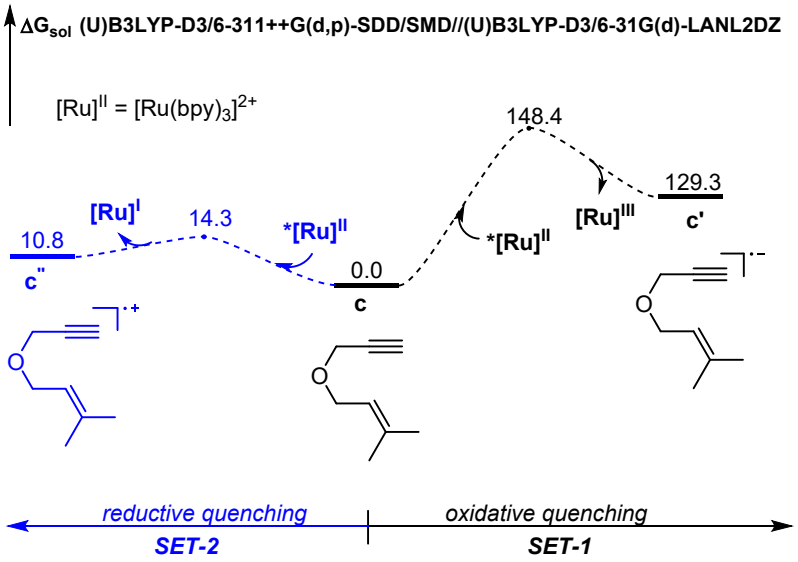

Fig. S20 Energy profiles (in kcal mol^{-1}) for the oxidative quenching and reductive quenching of *[Ru]^{II} by the substrate **c**.

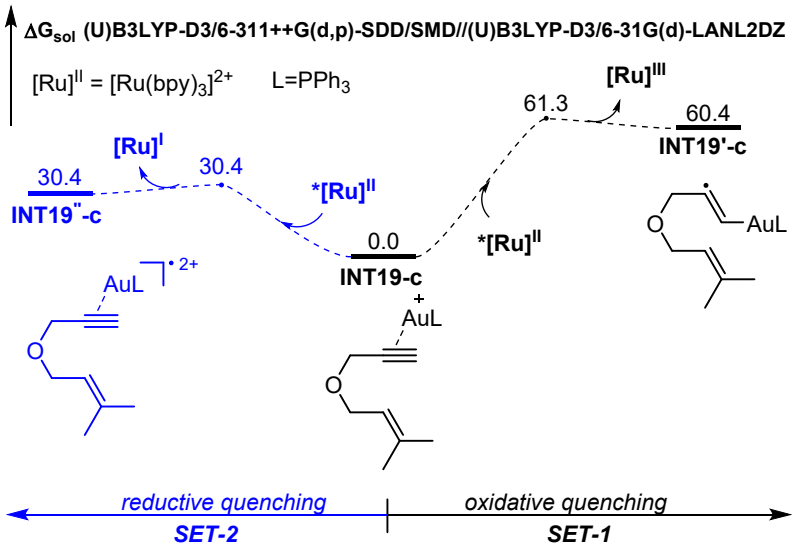

Fig. S21 Energy profiles (in kcal mol^{-1}) for the oxidative quenching and reductive quenching of *[Ru]^{II} by **INT19-c**.

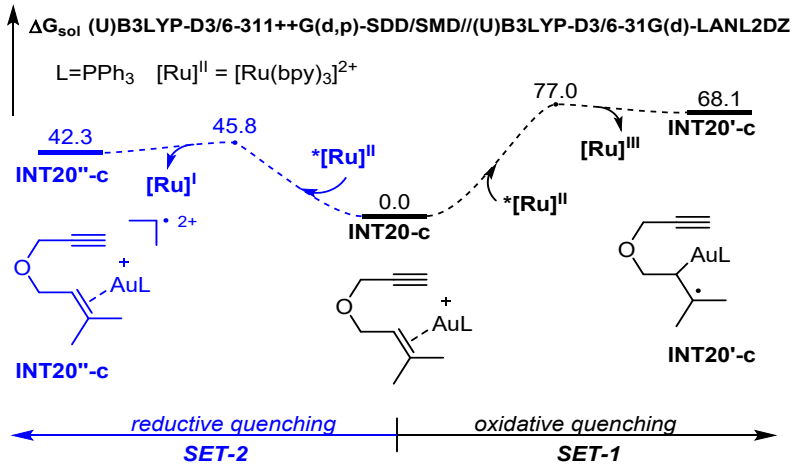

Fig. S22 Energy profiles (in kcal mol^{-1}) for the oxidative quenching and reductive quenching of *[Ru]^{II} by **INT20-c**.

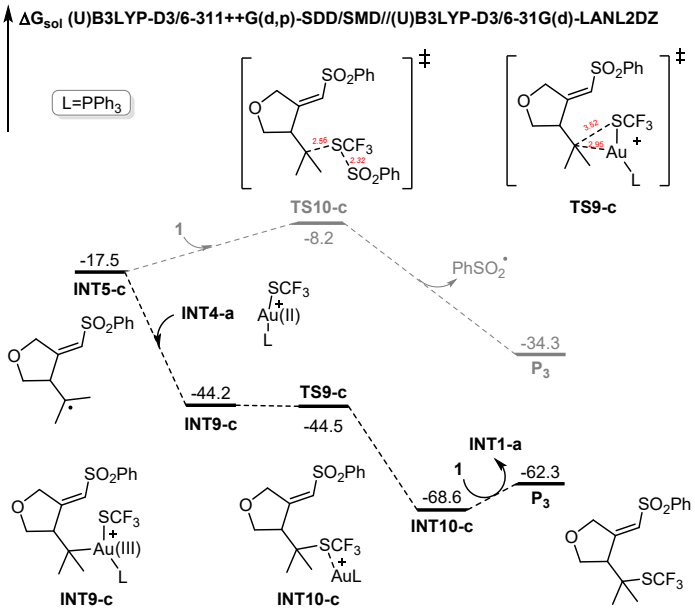

Fig. S23 Energy profiles (in kcal mol^{-1}) for the formation of product (**P$_3$**) after the formation of **INT5-c**. Bond lengths are shown in Å.

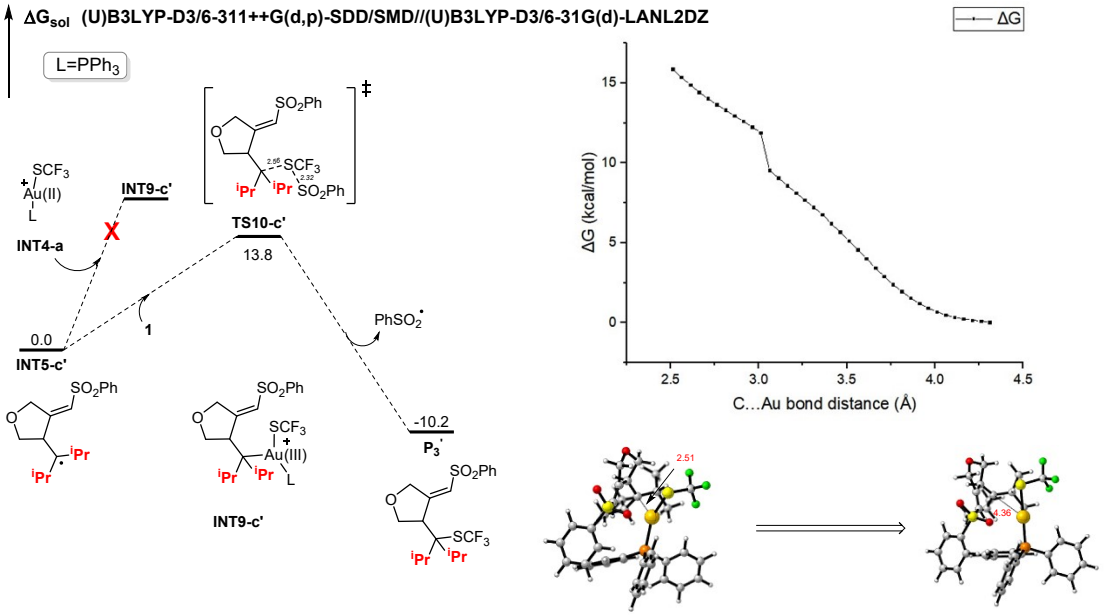

Fig. S24 Energy profiles (in kcal mol^{-1}) for the formation of product **P$_3$′** via a radical chain pathway for **INT5-c′**. The formation of an Au(III) intermediate with **INT4-a** could be ruled out by fixing C⋯Au bond distance partial optimization.

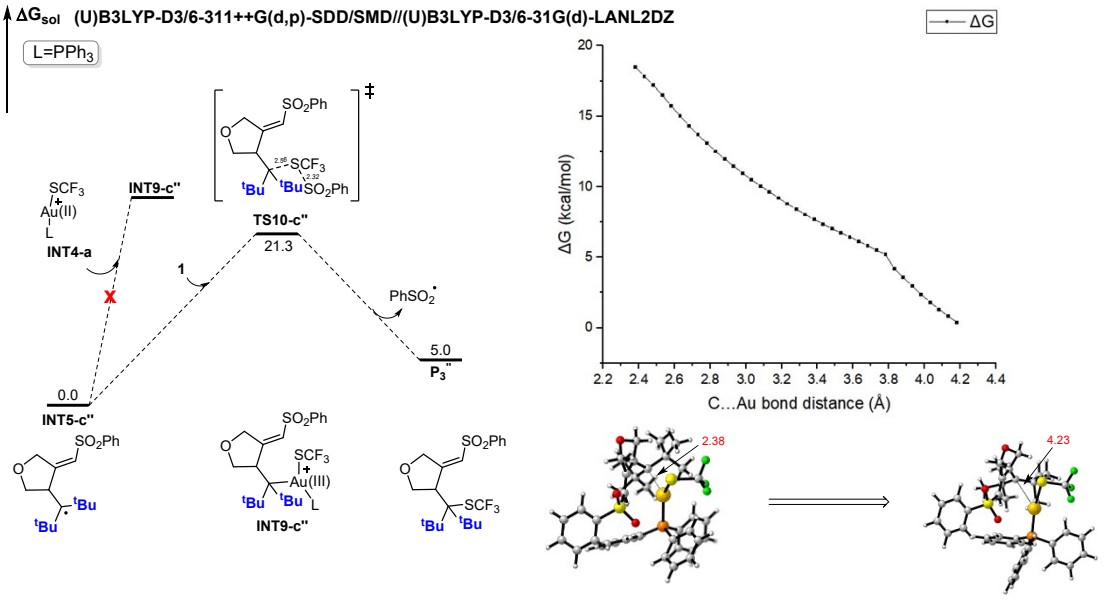

Fig. S25 Energy profiles (in kcal mol^{-1}) for the formation of product **P$_3$″** via a radical chain pathway for **INT5-c″**. The formation of an Au(III) intermediate with **INT4-a** could be ruled out by fixing C⋯Au bond distance partial optimization.

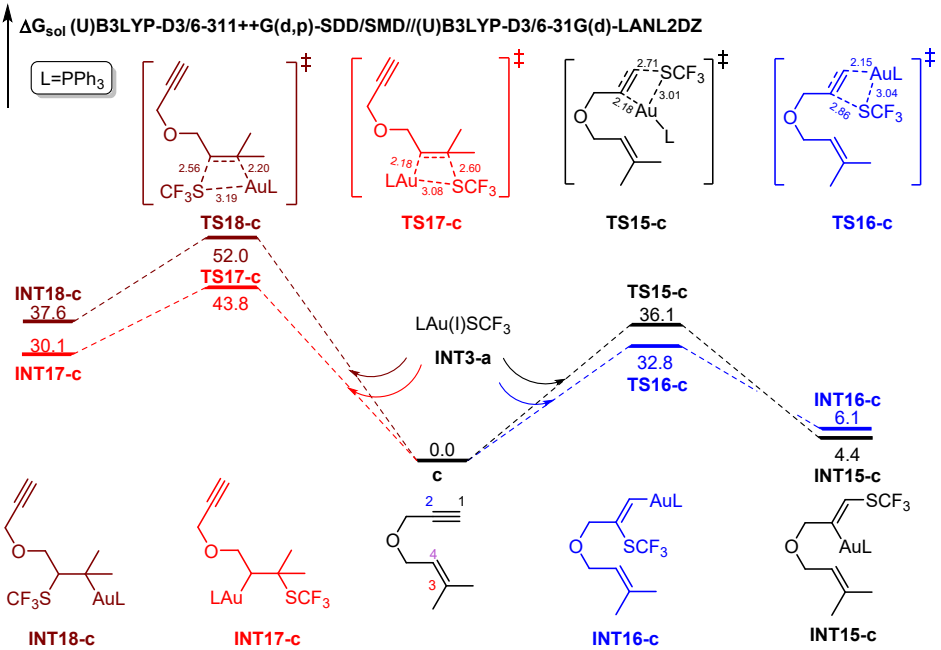

Fig. S26 Energy profiles (in kcal mol^{-1}) for the migratory insertion of 1,6-enyne (**c**) to **INT3-a**. Bond lengths are shown in Å.

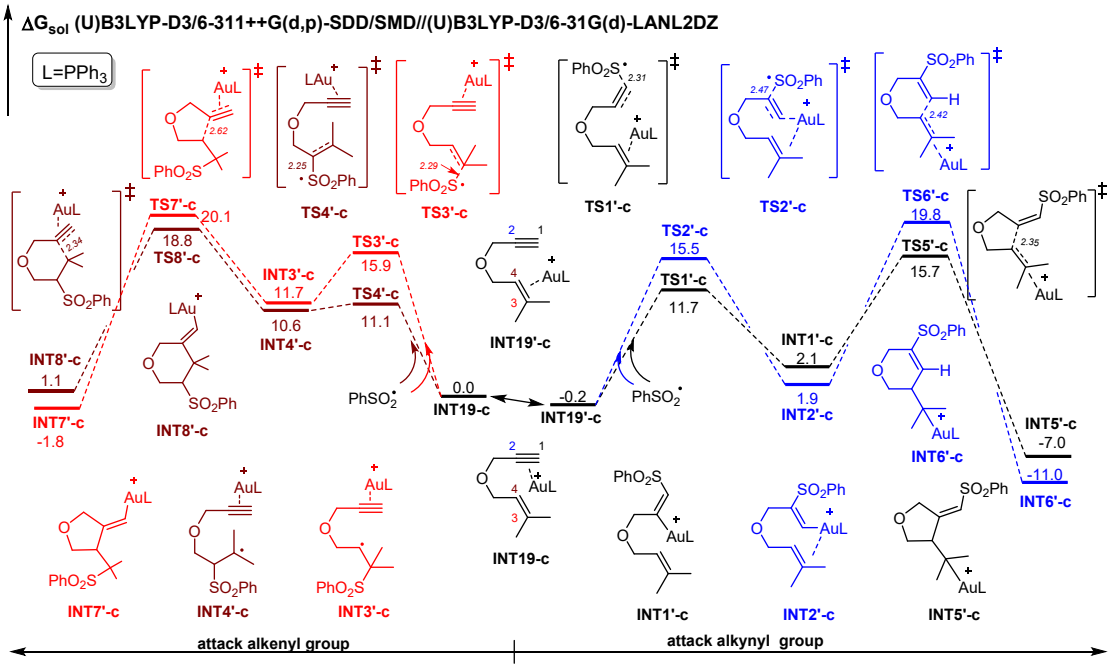

Fig. S27 Energy profiles (in kcal mol^{-1}) for the gold-catalyst involving radical chain reaction. Bond lengths are shown in Å.

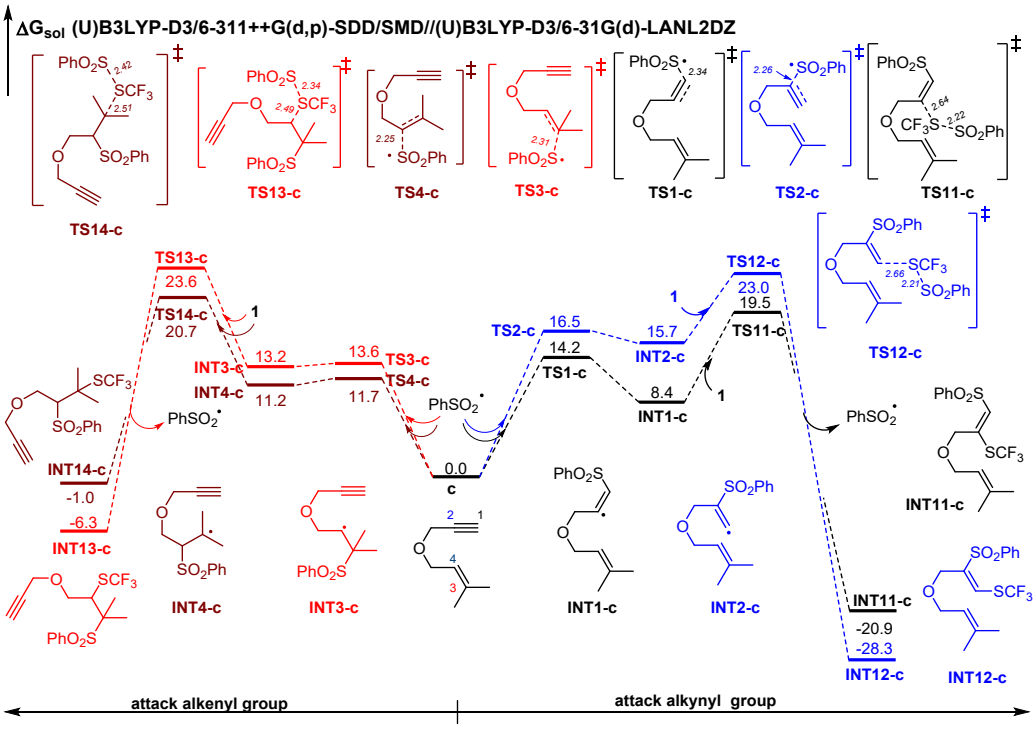

Fig. S28 Energy profiles (in kcal mol^{-1}) for the formation of acyclic products. Bond lengths are shown in Å.

3.Cartesian Coordinates and Energies

Au(I)PPh$_3$

P	-0.00003800	0.00020000	-0.22211000
C	0.01582700	1.70400100	-0.80322000
C	0.97184900	2.59351100	-0.28387500
C	-0.88293700	2.12310000	-1.79545200
C	1.03026800	3.89723300	-0.76536000
H	1.66051400	2.26451100	0.48978600
C	-0.81624100	3.43370100	-2.26793100
H	-1.62215600	1.43669000	-2.19331600
C	0.13492300	4.31726300	-1.75523500
H	1.76589700	4.58780000	-0.36591900
H	-1.50939600	3.76308000	-3.03523900
H	0.17837800	5.33746800	-2.12332200
C	-1.48325000	-0.83698900	-0.80525900
C	-2.73182400	-0.45445600	-0.28597300
C	-1.39643300	-1.82342400	-1.79891400
C	-3.88991100	-1.05497000	-0.76882800
H	-2.79155600	0.30536300	0.48872300
C	-2.56462600	-2.42015700	-2.27282900
H	-0.43220700	-2.11993300	-2.19670200
C	-3.80560300	-2.03890500	-1.76012600
H	-4.85593100	-0.76371600	-0.36937800
H	-2.50299600	-3.18403900	-3.04120400
H	-4.71071400	-2.51080600	-2.12928400
C	1.46696500	-0.86475700	-0.80582700
C	1.75939500	-2.13835400	-0.28872700
C	2.27890200	-0.29442100	-1.79749300
C	2.85899000	-2.84009500	-0.77178300
H	1.13045600	-2.57153100	0.48447300
C	3.38028600	-1.00683100	-2.27162800
H	2.05402200	0.68967100	-2.19356700
C	3.67004300	-2.27317900	-1.76108500
H	3.08931700	-3.82310300	-0.37400000
H	4.01184000	-0.57003800	-3.03848200
H	4.53166800	-2.82037100	-2.13038000
Au	0.00030000	-0.00199600	2.06856600

Zero-point correction= 0.277017 (Hartree/Particle)
Thermal correction to Energy= 0.294905
Thermal correction to Enthalpy= 0.295849
Thermal correction to Gibbs Free Energy= 0.226548
Sum of electronic and zero-point Energies= -1171.381218
Sum of electronic and thermal Energies= -1171.363330
Sum of electronic and thermal Enthalpies= -1171.362386
Sum of electronic and thermal Free Energies= -1171.431687
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1172.233795

Au(0)PPh$_3$

P	0.17704600	0.00011700	-0.00003400
C	0.89746400	-1.08816000	-1.27037400
C	0.28939400	-1.11166900	-2.53556000
C	2.02230800	-1.88883100	-1.02731100
C	0.81374000	-1.91168200	-3.54881900
H	-0.59723500	-0.50971000	-2.71546100
C	2.53822600	-2.69351500	-2.04345500
H	2.49048100	-1.88092100	-0.04837400
C	1.93789900	-2.70422600	-3.30401700
H	0.33859700	-1.92519900	-4.52535400
H	3.40980900	-3.31231600	-1.84963600
H	2.34092600	-3.33358500	-4.09228800
C	0.89677300	-0.55625000	1.57779900
C	0.28857300	-1.64059700	2.22995000
C	2.02112300	0.05463300	2.15060100
C	0.81243400	-2.11857400	3.42943300
H	-0.59777800	-2.09734200	1.79795500
C	2.53653400	-0.42350600	3.35558300
H	2.48935500	0.89883600	1.65497900
C	1.93618200	-1.51033300	3.99425600
H	0.33721400	-2.95785500	3.92876800
H	3.40777600	0.05373700	3.79525800
H	2.33883600	-1.87869700	4.93344400
C	0.89726300	1.64454500	-0.30697400
C	0.28939300	2.75168800	0.30601000
C	2.02171500	1.83481400	-1.12235500
C	0.81361800	4.02930400	0.12016000
H	-0.59693600	2.60620500	0.91764800
C	2.53749300	3.11726900	-1.31080800
H	2.48975100	0.98333200	-1.60554200
C	1.93742000	4.21398600	-0.68900700
H	0.33866800	4.88153100	0.59733300
H	3.40880800	3.25914000	-1.94391300
H	2.34037400	5.21140700	-0.83959700
Au	-2.27240100	0.00008000	-0.00044800

Zero-point correction= 0.275697 (Hartree/Particle)
Thermal correction to Energy= 0.293933
Thermal correction to Enthalpy= 0.294877
Thermal correction to Gibbs Free Energy= 0.222834
Sum of electronic and zero-point Energies= -1171.574978
Sum of electronic and thermal Energies= -1171.556742
Sum of electronic and thermal Enthalpies= -1171.555798
Sum of electronic and thermal Free Energies= -1171.627841
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1172.38809

Au(II)PPh$_3$

P	-0.00029600	0.00005800	-0.38037700
C	-0.49556500	1.65360300	-0.84630100
C	0.22455200	2.75256900	-0.30167000
C	-1.58159800	1.86291800	-1.71744700
C	-0.13694200	4.04559100	-0.64950600
H	1.05741400	2.58063200	0.37450900
C	-1.92994300	3.16532600	-2.05713900
H	-2.12856600	1.02463000	-2.13451400
C	-1.21516900	4.25416200	-1.52144200
H	0.40808300	4.89080000	-0.24292900
H	-2.74929900	3.34331000	-2.74586500
H	-1.50157700	5.26592500	-1.79105100
C	-1.18493200	-1.25547000	-0.84606200
C	-2.49609000	-1.18217600	-0.29978800
C	-0.82402800	-2.29956600	-1.71883600
C	-3.43535900	-2.14155100	-0.64758400
H	-2.76297400	-0.37575800	0.37763700
C	-1.77798700	-3.25225500	-2.05847400
H	0.17495200	-2.35337700	-2.13715000
C	-3.07770700	-3.17854100	-1.52112600

H	-4.43935100	-2.09282700	-0.23971200
H	-1.52310900	-4.05001700	-2.74838800
H	-3.81087900	-3.93231400	-1.79069700
C	1.67907000	-0.39802200	-0.84721200
C	2.27108600	-1.57086700	-0.30230200
C	2.40280200	0.43738100	-1.71922100
C	3.57142700	-1.90448300	-0.65071600
H	1.70617200	-2.20582700	0.37455800
C	3.70470800	0.08769700	-2.05948600
H	1.94997400	1.32996900	-2.13644200
C	4.29063900	-1.07543600	-1.52349400
H	4.03113800	-2.79886600	-0.24392500
H	4.26813100	0.70795600	-2.74883200
H	5.30990500	-1.33339200	-1.79356200
Au	0.00102100	-0.00008900	1.93745400

Zero-point correction= 0.275096 (Hartree/Particle)
Thermal correction to Energy= 0.293306
Thermal correction to Enthalpy= 0.294250
Thermal correction to Gibbs Free Energy= 0.224245
Sum of electronic and zero-point Energies= -1170.966237
Sum of electronic and thermal Energies= -1170.948026
Sum of electronic and thermal Enthalpies= -1170.947082
Sum of electronic and thermal Free Energies= -1171.017087
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1172.38809

$Ru(bpy)_3^{2+}$

C	-2.86874800	0.38408700	-0.57969000
C	-4.04079100	0.84856700	-1.18197400
C	-3.96169300	1.70757200	-2.27484100
C	-2.70508000	2.08812200	-2.74544200
C	-1.57500000	1.59437800	-2.10407600
H	-5.00933700	0.54705800	-0.80280900
H	-4.86644100	2.07347900	-2.74856700
H	-2.59658400	2.75578900	-3.59276800
H	-0.57651200	1.85863800	-2.43029700
C	-2.84596000	-0.52776400	0.57926800
C	-3.99330500	-1.05103200	1.18089300
C	-3.87148700	-1.90449000	2.27420600
H	-4.97566000	-0.79923100	0.80098400
C	-1.49350600	-1.67015100	2.10514100
C	-2.59750500	-2.22036800	2.74595600
H	-4.75682200	-2.31570000	2.74744600
H	-0.48310900	-1.88310000	2.43232600
H	-2.45581900	-2.88122400	3.59372300
N	-1.64678900	0.76142400	-1.05005500
N	-1.60673700	-0.84243600	1.05054200
C	0.96665400	2.72824200	0.57887700
C	1.08765200	3.98359500	1.18023600
C	0.28703300	4.30575800	2.27281700
C	-0.62465500	3.36126600	2.74411100
C	-0.70058800	2.12991100	2.10359600
H	1.79767100	4.70781800	0.80059900
H	0.37390900	5.27818700	2.74579500
H	-1.26836100	3.56976800	3.59127200
H	-1.39116600	1.36208200	2.43044100
C	1.76790300	2.29131800	-0.57971000
C	2.75687900	3.07329600	-1.18189400
C	3.46072500	2.57485300	-2.27491700
H	2.98091700	4.06260400	-0.80264500
C	2.16752600	0.56567000	-2.10445900
C	3.16067800	1.29675200	-2.74587400
H	4.23049100	3.17482300	-2.74859300
H	1.89600200	-0.43082600	-2.43082400
H	3.68408900	0.86871800	-3.59342400
N	0.07343900	1.81319200	1.04977500
N	1.48277200	1.04466500	-1.05017400
C	1.87994100	-2.20031700	0.57962100
C	2.90695700	-2.93210500	1.18120300
C	3.58509000	-2.39972900	2.27446400
C	3.22138800	-1.13859200	2.74628600
C	2.19276900	-0.45777700	2.10544400
H	3.18027500	-3.90868000	0.80126500
H	4.38406800	-2.96064400	2.74762500
H	3.72275500	-0.68541400	3.59409100
H	1.87177500	0.52365100	2.43262600
C	1.10164700	-2.67615200	-0.57928400
C	1.28554200	-3.92340300	-1.18154300
C	0.50206700	-4.28457500	-2.27435700
H	2.03106100	-4.61131900	-0.80244000
C	-0.59348200	-2.16117100	-2.10363600
C	-0.45590500	-3.38671800	-2.74498900
H	0.63766300	-5.25106600	-2.74804600
H	-1.32161100	-1.42861100	-2.42985100
H	-1.08836700	-3.62668400	-3.59229100
N	1.53273900	-0.96976800	1.05085900
N	0.16369200	-1.80676100	-1.04962800
Ru	-0.00025400	0.00007800	0.00051300

Zero-point correction= 0.486757 (Hartree/Particle)
Thermal correction to Energy= 0.515458
Thermal correction to Enthalpy= 0.516402
Thermal correction to Gibbs Free Energy= 0.426694
Sum of electronic and zero-point Energies= -1579.423359
Sum of electronic and thermal Energies= -1579.394658
Sum of electronic and thermal Enthalpies= -1579.393714
Sum of electronic and thermal Free Energies= -1579.483422
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1581.466134

***$Ru(bpy)_3^{2+}$**

C	2.97904100	-0.99827200	0.48689600
C	4.35871100	-0.96101900	0.72023500
C	4.85736600	-0.11225100	1.70652700
C	3.97096000	0.68620200	2.43012100
C	2.61416500	0.60662300	2.12631100
H	5.03869900	-1.56701900	0.13346000
H	5.92413500	-0.07089000	1.90096900
H	4.31994200	1.35693000	3.20750200
H	1.88182300	1.21485800	2.65004100
C	2.36515100	-1.87259000	-0.54140900
C	3.03264400	-2.97571700	-1.08363400
C	2.41061100	-3.75500000	-2.05481500
H	4.02359200	-3.23672500	-0.73310100
C	0.49970600	-2.32729400	-1.87528100
C	1.11940600	-3.42210300	-2.46419500
H	2.92324800	-4.61269800	-2.47775100

H	-0.50738800	-2.02868100	-2.14378200
H	0.59623400	-3.99988800	-3.21772600
N	2.12991700	-0.21519700	1.18682800
N	1.10257000	-1.56684300	-0.94157500
C	0.53078100	2.89885900	-0.50881700
C	1.09529900	4.05662700	-1.04998100
C	2.09829600	3.95069500	-2.00934400
C	2.52287200	2.68344500	-2.41088800
C	1.92747700	1.56846400	-1.83519900
H	0.75763300	5.03402400	-0.72837900
H	2.54116500	4.84443000	-2.43610600
H	3.30059200	2.55722200	-3.15558300
H	2.22217800	0.56246800	-2.10809600
C	-0.53071200	2.89883400	0.50893700
C	-1.09518700	4.05657600	1.05020000
C	-2.09819000	3.95059800	2.00955100
H	-0.75748300	5.03398700	0.72868200
C	-1.92744600	1.56837400	1.83520800
C	-2.52280600	2.68332800	2.41098700
H	-2.54102900	4.84431200	2.43638800
H	-2.22217700	0.56236600	2.10802400
H	-3.30053100	2.55706600	3.15567000
N	0.95451200	1.66601300	-0.90978600
N	-0.95448000	1.66596700	0.90980100
C	-2.97910100	-0.99826600	-0.48690900
C	-4.35876700	-0.96105000	-0.72028200
C	-4.85743800	-0.11217000	-1.70646800
C	-3.97105600	0.68644400	-2.42991200
C	-2.61426700	0.60691400	-2.12605300
H	-5.03874900	-1.56716000	-0.13361300
H	-5.92420300	-0.07084400	-1.90093900
H	-4.32005100	1.35726400	-3.20720900
H	-1.88194300	1.21526600	-2.64967300
C	-2.36518100	-1.87264000	0.54133200
C	-3.03265100	-2.97577500	1.08357200
C	-2.41055400	-3.75509300	2.05468500
H	-4.02362900	-3.23676500	0.73311200
C	-0.49964600	-2.32740400	1.87505900
C	-1.11931600	-3.42222500	2.46398400
H	-2.92317200	-4.61279600	2.47763300
H	0.50747100	-2.02880800	2.14349500
H	-0.59609600	-4.00004100	3.21745800
N	-2.13000500	-0.21502200	-1.18668200
N	-1.10257600	-1.56692100	0.94142500
Ru	-0.00001900	0.02721500	-0.00006900

Zero-point correction= 0.484396 (Hartree/Particle)
Thermal correction to Energy= 0.514313
Thermal correction to Enthalpy= 0.515257
Thermal correction to Gibbs Free Energy= 0.420057
Sum of electronic and zero-point Energies= -1579.352243
Sum of electronic and thermal Energies= -1579.322326
Sum of electronic and thermal Enthalpies= -1579.321381
Sum of electronic and thermal Free Energies= -1579.416582
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1581.391737

$Ru(bpy)_3^{3+}$

C	2.45604000	-1.54216800	0.56382800
C	3.66350700	-1.91934000	1.15345700
C	4.17765500	-1.17173000	2.21246200
C	3.47528600	-0.05188000	2.66139300
C	2.28095000	0.28174600	2.03416200
H	4.20491500	-2.78569100	0.79375600
H	5.11530900	-1.45946400	2.67714000
H	3.84289500	0.55527200	3.48124700
H	1.69890900	1.14135200	2.34316300
C	1.82800500	-2.25148500	-0.56367100
C	2.34864400	-3.40436200	-1.15333100
C	1.66850600	-4.00560700	-2.21195200
H	3.27435800	-3.83667400	-0.79384700
C	-0.00435000	-2.29931900	-2.03315500
C	0.47145400	-3.44445600	-2.66039700
H	2.06766600	-4.90152900	-2.67661100
H	-0.92850100	-1.82609200	-2.34163900
H	-0.08705700	-3.88327700	-3.47980600
N	1.77837300	-0.44780500	1.01910000
N	0.65936400	-1.71163100	-1.01861600
C	1.03628100	2.70842500	-0.56382100
C	1.77462900	3.73555000	-1.15352200
C	2.63500600	3.44695200	-2.21239800
C	2.74693400	2.12971700	-2.66105400
C	1.99298900	1.14526800	-2.03368100
H	1.68654100	4.75341300	-0.79398600
H	3.21144200	4.24044800	-2.67715300
H	3.40580900	1.86532700	-3.48075600
H	2.04466700	0.10833500	-2.34234700
C	0.10797200	2.89792500	0.56364300
C	-0.16876100	4.13225100	1.15334900
C	-1.07344000	4.20394500	2.21221200
H	0.31117400	5.03416600	0.79379200
C	-1.38471600	1.83476400	2.03360400
C	-1.69257600	3.03593900	2.66095000
H	-1.29279500	5.15988100	2.67695100
H	-1.83844900	0.90099000	2.34236800
H	-2.40232200	3.05090900	3.48068700
N	1.15264700	1.42640200	-1.01881600
N	-0.50147000	1.76406300	1.01870800
C	-2.86390000	-0.45674900	-0.56406400
C	-4.12254300	-0.33065600	-1.15381500
C	-4.30257100	0.55872900	-2.21275500
C	-3.21759700	1.31400900	-2.66144200
C	-1.98812900	1.15307300	-2.03400900
H	-4.96014600	-0.91561800	-0.79421400
H	-5.27795400	0.66141000	-2.67751000
H	-3.31789800	2.01680400	-3.48116600
H	-1.11580400	1.71606600	-2.34263700
C	-2.56407900	-1.35535400	0.56352300
C	-3.49480900	-2.21204900	1.15318300
C	-3.10477300	-3.03127500	2.21219200
H	-4.51582000	-2.24730800	0.79351100
C	-0.89720300	-2.11660700	2.03366700
C	-1.78370800	-2.98362200	2.66101200
H	-3.82307900	-3.69909700	2.67690900
H	0.13835800	-2.04296400	2.34248300
H	-1.44194500	-3.60578100	3.48079700

N	-1.81163800	0.28473600	-1.01912600
N	-1.27744200	-1.31630200	1.01871600
Ru	-0.00007600	-0.00015700	0.00003800

Zero-point correction= 0.487108 (Hartree/Particle)
Thermal correction to Energy= 0.515912
Thermal correction to Enthalpy= 0.516856
Thermal correction to Gibbs Free Energy= 0.426818
Sum of electronic and zero-point Energies= -1578.979358
Sum of electronic and thermal Energies= -1578.950553
Sum of electronic and thermal Enthalpies= -1578.949609
Sum of electronic and thermal Free Energies= -1579.039647
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1581.168783

***Ru(bpy)$_3^+$**

C	-0.09794300	2.88221100	0.59348200
C	-0.40143400	4.08473800	1.25640600
C	-1.21469700	4.07315500	2.37680500
C	-1.72822900	2.84909700	2.83481900
C	-1.38898400	1.69230000	2.15146400
H	0.00429700	5.02075600	0.89165100
H	-1.45024100	4.99912000	2.89090800
H	-2.37607200	2.79492300	3.70217400
H	-1.74991200	0.72009900	2.46582100
C	0.73576800	2.78822900	-0.59426600
C	1.29879800	3.89305600	-1.25759900
C	2.08915300	3.70068300	-2.37794200
H	1.11111600	4.89594900	-0.89321800
C	1.73030600	1.34067400	-2.15165100
C	2.31801100	2.39295800	-2.83542800
H	2.52447200	4.55100000	-2.89238800
H	1.86640300	0.31245900	-2.46550700
H	2.93769300	2.19591100	-3.70266900
N	-0.59116400	1.69125300	1.06648800
N	0.95209500	1.51730900	-1.06682200
C	-2.78293400	-0.75716800	-0.59549700
C	-4.02080500	-0.82220700	-1.25958800
C	-4.24823500	-0.04272800	-2.38101000
C	-3.22939600	0.80821900	-2.83881000
C	-2.02470100	0.82563500	-2.15420200
H	-4.79605300	-1.48542900	-0.89500700
H	-5.20195400	-0.09103200	-2.89606500
H	-3.36762800	1.44237700	-3.70695600
H	-1.20166100	1.45665800	-2.46829700
C	-2.44857000	-1.52514200	0.59330200
C	-3.33905300	-2.38820500	1.25640800
C	-2.92341700	-3.08587600	2.37774400
H	-4.35234500	-2.50473000	0.89109300
C	-0.77375600	-2.04760800	2.15274700
C	-1.60681300	-2.91877500	2.83638500
H	-3.60818500	-3.75205400	2.89203300
H	0.24857100	-1.87439500	2.46756600
H	-1.23675400	-3.45214900	3.70443700
N	-1.78977900	0.06467000	-1.06821600
N	-1.17078400	-1.35694700	1.06690200
C	2.04851800	-2.03094900	-0.59292300
C	2.72516200	-3.07009700	-1.25618100
C	2.16467800	-3.65839700	-2.37717500
C	0.91765200	-3.20363700	-2.83528600
C	0.29882600	-2.16932800	-2.15153500
H	3.68757300	-3.40831300	-0.89127500
H	2.68446900	-4.45988500	-2.89159500
H	0.43811500	-3.64185400	-3.70301400
H	-0.65981200	-1.77385000	-2.46593600
C	2.54535400	-1.35607100	0.59556000
C	3.73820500	-1.69390000	1.25930400
C	4.13323500	-0.98412700	2.38048300
H	4.34698800	-2.51254700	0.89462200
C	2.15770600	0.35586300	2.15407900
C	3.32870900	0.07170000	2.83839300
H	5.05267500	-1.24268200	2.89523800
H	1.49540700	1.15397600	2.46815400
H	3.60448400	0.65955200	3.70633300
N	0.83966400	-1.58360700	-1.06612000
N	1.75943700	-0.33426100	1.06835300
Ru	-0.00010500	-0.00042300	0.00018400

Zero-point correction= 0.481972 (Hartree/Particle)
Thermal correction to Energy= 0.510982
Thermal correction to Enthalpy= 0.511926
Thermal correction to Gibbs Free Energy= 0.420827
Sum of electronic and zero-point Energies= -1579.664118
Sum of electronic and thermal Energies= -1579.635107
Sum of electronic and thermal Enthalpies= -1579.634163
Sum of electronic and thermal Free Energies= -1579.725263
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1581.627362

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S	-0.05489400	1.31750400	0.40892100
O	0.24404800	2.66220600	-0.08469500
O	-0.57871100	1.06050500	1.74995300
C	1.37950900	0.28595700	0.15373700
C	1.57397400	-0.81846900	0.98173800
C	2.26978900	0.62326400	-0.86571400
C	2.70238100	-1.60994600	0.77502200
H	0.86065900	-1.04202000	1.76557000
C	3.39138600	-0.17975500	-1.05902600
H	2.08884500	1.49893200	-1.47886800
C	3.60478800	-1.29325500	-0.24240600
H	2.87669700	-2.47258800	1.41047200
H	4.10026500	0.06629500	-1.84342800
H	4.48096700	-1.91549900	-0.39847600
S	-1.50605800	0.61842000	-1.05057400
C	-2.16394800	-0.85876500	-0.18868900
F	-2.84646500	-0.55755800	0.91606500
F	-2.99187100	-1.46888800	-1.05104900
F	-1.19523700	-1.72752700	0.15288800

Zero-point correction= 0.117111 (Hartree/Particle)
Thermal correction to Energy= 0.130027
Thermal correction to Enthalpy= 0.130972
Thermal correction to Gibbs Free Energy= 0.075569
Sum of electronic and zero-point Energies= -1515.952462
Sum of electronic and thermal Energies= -1515.939545
Sum of electronic and thermal Enthalpies= -1515.938601
Sum of electronic and thermal Free Energies= -1515.994003

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1516.3524502

1´

S	-0.21730300	1.52631900	-0.28462400
O	-0.79886000	2.73243100	0.39651200
O	0.04453000	1.59835600	-1.76281700
C	-1.52427800	0.25826900	-0.13335100
C	-1.49621500	-0.85080900	-0.97617300
C	-2.49545300	0.38874000	0.85549300
C	-2.46838900	-1.83979400	-0.83089500
H	-0.71717700	-0.92615100	-1.72530300
C	-3.46708600	-0.60367100	0.99371100
H	-2.48119000	1.26830200	1.49041400
C	-3.45418600	-1.71793100	0.15208500
H	-2.45676100	-2.70916800	-1.48424700
H	-4.23488700	-0.50798100	1.75837500
H	-4.20897300	-2.49306300	0.26415300
S	1.72182600	0.13321100	1.49497000
C	2.41421900	-0.68364000	0.07729100
F	2.94821500	0.15803400	-0.84957700
F	3.42478800	-1.54604800	0.41007300
F	1.51695100	-1.44950700	-0.62354700

Zero-point correction= 0.113493 (Hartree/Particle)
Thermal correction to Energy= 0.127575
Thermal correction to Enthalpy= 0.128519
Thermal correction to Gibbs Free Energy= 0.067130
Sum of electronic and zero-point Energies= -1516.022706
Sum of electronic and thermal Energies= -1516.008625
Sum of electronic and thermal Enthalpies= -1516.007680
Sum of electronic and thermal Free Energies= -1516.069069
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1516.4759699

1´´

S	-0.04042200	1.41877600	0.38845200
O	0.25693600	2.70553000	-0.21131500
O	-0.68358700	1.20578500	1.67069100
C	1.33730200	0.30838300	0.18460600
C	1.51117300	-0.74512900	1.10275800
C	2.22019000	0.53843400	-0.90808800
C	2.60376900	-1.57386200	0.92925800
H	0.81785600	-0.87489800	1.92518100
C	3.30099200	-0.30890600	-1.06545100
H	2.05143700	1.37703200	-1.57533200
C	3.49340400	-1.36297000	-0.15500500
H	2.78940800	-2.38383400	1.62666100
H	3.99976200	-0.15725600	-1.88074000
H	4.34100000	-2.02986000	-0.28002200
S	-1.17395300	0.32716300	-1.20207700
C	-2.17863900	-0.87267400	-0.15338300
F	-3.00963000	-0.19603400	0.61521600
F	-2.83973200	-1.64471100	-0.99801200
F	-1.36012700	-1.60996500	0.59602800

Zero-point correction= 0.115586 (Hartree/Particle)
Thermal correction to Energy= 0.129093
Thermal correction to Enthalpy= 0.130037
Thermal correction to Gibbs Free Energy= 0.072765
Sum of electronic and zero-point Energies= -1515.616738
Sum of electronic and thermal Energies= -1515.603232
Sum of electronic and thermal Enthalpies= -1515.602288
Sum of electronic and thermal Free Energies= -1515.659560
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1516.0469005

$PhSO_2$ radical

S	1.70666700	-0.00001800	-0.25750700
O	2.19790300	-1.30371200	0.26912700
O	2.19792000	1.30373300	0.26897500
C	-0.09419000	-0.00000300	-0.08116500
C	-0.76551700	1.22188100	-0.05379400
C	-0.76553100	-1.22188400	-0.05386000
C	-2.15688800	1.21246200	0.03231600
H	-0.20532700	2.14987400	-0.07743100
C	-2.15690500	-1.21245000	0.03225500
H	-0.20535600	-2.14988000	-0.07756700
C	-2.84940900	0.00000900	0.07319300
H	-2.69919100	2.15236700	0.07011300
H	-2.69922000	-2.15235000	0.07000800
H	-3.93351400	0.00002000	0.13650500

Zero-point correction= 0.098903 (Hartree/Particle)
Thermal correction to Energy= 0.106504
Thermal correction to Enthalpy= 0.107448
Thermal correction to Gibbs Free Energy= 0.065210
Sum of electronic and zero-point Energies= -780.126193
Sum of electronic and thermal Energies= -780.118593
Sum of electronic and thermal Enthalpies= -780.117649
Sum of electronic and thermal Free Energies= -780.159887
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-780.3685129

$PhSO_2^-$

S	1.77444000	0.00000000	-0.34911700
O	2.16551800	-1.29409000	0.36106800
O	2.16551800	1.29409000	0.36106900
C	-0.08162700	0.00000000	-0.10068100
C	-0.78118800	1.20584800	-0.05220800
C	-0.78118800	-1.20584800	-0.05220700
C	-2.17510100	1.20910000	0.03432100
H	-0.20566100	2.12859400	-0.05805700
C	-2.17510100	-1.20910000	0.03432100
H	-0.20566100	-2.12859400	-0.05805700
C	-2.87667400	0.00000000	0.07348300
H	-2.71963600	2.15191500	0.08150800
H	-2.71963600	-2.15191500	0.08150800
H	-3.96345400	0.00000000	0.13970700

Zero-point correction= 0.097427 (Hartree/Particle)
Thermal correction to Energy= 0.105154
Thermal correction to Enthalpy= 0.106099
Thermal correction to Gibbs Free Energy= 0.064059
Sum of electronic and zero-point Energies= -780.202335
Sum of electronic and thermal Energies= -780.194608
Sum of electronic and thermal Enthalpies= -780.193664
Sum of electronic and thermal Free Energies= -780.235703
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-780.5079945

SCF_3 radical

S	1.48687400	-0.04466000	0.00083900

C	-0.33239000	-0.00436800	0.00005100
F	-0.85636900	-0.58798700	1.08738100
F	-0.71003900	1.28618000	-0.01640800
F	-0.85533100	-0.61588600	-1.07249900

Zero-point correction= 0.014320 (Hartree/Particle)
Thermal correction to Energy= 0.018964
Thermal correction to Enthalpy= 0.019908
Thermal correction to Gibbs Free Energy= -0.014848
Sum of electronic and zero-point Energies= -735.753957
Sum of electronic and thermal Energies= -735.749313
Sum of electronic and thermal Enthalpies= -735.748369
Sum of electronic and thermal Free Energies= -735.783125
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-735.9143674

SCF_3^-

S	1.50528300	0.00025000	-0.00007100
C	-0.24387900	0.00061200	-0.00054400
F	-0.83759800	-0.80010900	-0.96468900
F	-0.83733100	-0.43692900	1.17445300
F	-0.83854300	1.23618500	-0.20927500

Zero-point correction= 0.013842 (Hartree/Particle)
Thermal correction to Energy= 0.018267
Thermal correction to Enthalpy= 0.019211
Thermal correction to Gibbs Free Energy= -0.014388
Sum of electronic and zero-point Energies= -735.857516
Sum of electronic and thermal Energies= -735.853091
Sum of electronic and thermal Enthalpies= -735.852147
Sum of electronic and thermal Free Energies= -735.885746
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-736.0873228

INT2-a

P	1.15251700	0.13889600	0.01762200
C	1.86179900	0.30507200	1.67715000
C	2.09469200	-0.85143900	2.43639800
C	2.21877400	1.56289600	2.18300700
C	2.69050400	-0.74897200	3.69137100
H	1.81053800	-1.82507200	2.04554900
C	2.81229400	1.65722400	3.44177900
H	2.03040400	2.45921200	1.60096200
C	3.04857400	0.50486300	4.19392300
H	2.87013700	-1.64396700	4.27867800
H	3.08675700	2.63092800	3.83542400
H	3.50774600	0.58331400	5.17451300
C	0.41530400	1.74084900	-0.42916400
C	-0.88807600	2.03819100	-0.00027100
C	1.13794700	2.68122700	-1.17607000
C	-1.45959000	3.26884000	-0.31272200
H	-1.45544500	1.31001500	0.57302000
C	0.55846800	3.91255100	-1.48480000
H	2.14129800	2.45064700	-1.51912400
C	-0.73700300	4.20644400	-1.05554700
H	-2.46988400	3.48996200	0.01669700
H	1.11835600	4.63938800	-2.06496900
H	-1.18494700	5.16387200	-1.30331200
C	2.51397100	-0.17271600	-1.13718200
C	2.21813300	-0.67351300	-2.41432500
C	3.83849600	0.12196700	-0.78617300
C	3.24272100	-0.86928300	-3.33689300
H	1.19071700	-0.90658100	-2.68199700
C	4.85952700	-0.08041400	-1.71524800
H	4.07008100	0.50100900	0.20372200
C	4.56327500	-0.57366300	-2.98698800
H	3.01376500	-1.25790800	-4.32421500
H	5.88609500	0.14394100	-1.44299400
H	5.36153300	-0.73318500	-3.70521800
Au	-0.53335700	-1.45369100	-0.07334300
C	-2.21924300	-2.92764400	-0.16847400
H	-2.01856400	-3.98025900	-0.23603300
C	-2.97623600	-1.94796100	-0.10686100
C	-3.73680600	-0.75256700	-0.03146300
C	-4.09472400	-0.22774200	1.22848400
C	-4.07692000	-0.06210300	-1.21345900
C	-4.78580300	0.97619300	1.29689100
H	-3.82241400	-0.76762500	2.12920400
C	-4.76834500	1.14001900	-1.12917500
H	-3.78752900	-0.47367000	-2.17441500
C	-5.12127300	1.65811800	0.12171300
H	-5.06653300	1.38377200	2.26250100
H	-5.03302100	1.67531100	-2.03501800
H	-5.66440400	2.59643900	0.18139100

Zero-point correction= 0.387766 (Hartree/Particle)
Thermal correction to Energy= 0.413931
Thermal correction to Enthalpy= 0.414875
Thermal correction to Gibbs Free Energy= 0.324175
Sum of electronic and zero-point Energies= -1479.746327
Sum of electronic and thermal Energies= -1479.720162
Sum of electronic and thermal Enthalpies= -1479.719218
Sum of electronic and thermal Free Energies= -1479.809918
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1480.790628

INT4-a

P	-1.08819600	0.12323100	-0.07686400
C	-0.92030100	1.90079600	-0.33220400
C	0.21302000	2.39661100	-1.00017700
C	-1.93213400	2.77703700	0.09598300
C	0.32425100	3.76254700	-1.24513400
H	1.00463300	1.72262900	-1.31406100
C	-1.81016900	4.14155700	-0.15628400
H	-2.80284400	2.39475700	0.61876900
C	-0.68498500	4.63342500	-0.82415200
H	1.19999800	4.14855100	-1.75662600
H	-2.59112300	4.82119900	0.16944300
H	-0.59225900	5.69837100	-1.01270200
C	-2.09876400	-0.15658900	1.39281500
C	-1.65945000	0.40607400	2.61060300
C	-3.25816900	-0.94704400	1.35385100
C	-2.39226600	0.19286000	3.77213900
H	-0.75791500	1.01220500	2.63569800
C	-3.98361900	-1.15409600	2.52415600
H	-3.59187100	-1.38181100	0.41799900
C	-3.55225300	-0.58894100	3.73026700
H	-2.06119700	0.62890900	4.70899200
H	-4.88894200	-1.75197400	2.49781800
H	-4.12110800	-0.75915600	4.63888800

C	-1.86106500	-0.64449400	-1.51137000
C	-1.76075700	-2.03617800	-1.67967000
C	-2.57444100	0.13339600	-2.43582600
C	-2.38711000	-2.64589600	-2.76286300
H	-1.19423800	-2.63341700	-0.96997200
C	-3.19340500	-0.48703700	-3.51964600
H	-2.64190500	1.20892300	-2.31037000
C	-3.10125900	-1.87133100	-3.68255300
H	-2.31100600	-3.72016800	-2.89633600
H	-3.74524800	0.11067900	-4.23797700
H	-3.58160500	-2.34834900	-4.53105200
Au	1.00972400	-0.79086000	0.38068800
S	3.23980800	-1.51322600	-0.00994600
C	4.00439300	0.16467100	-0.08026800
F	3.56142500	0.81144900	-1.17206500
F	3.68724000	0.89929700	0.99485900
F	5.32526000	0.04765200	-0.14710300

Zero-point correction= 0.292346 (Hartree/Particle)
Thermal correction to Energy= 0.316688
Thermal correction to Enthalpy= 0.317632
Thermal correction to Gibbs Free Energy= 0.229713
Sum of electronic and zero-point Energies= -1907.182273
Sum of electronic and thermal Energies= -1907.157931
Sum of electronic and thermal Enthalpies= -1907.156987
Sum of electronic and thermal Free Energies= -1907.244905
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1908.196805

TS1-2

P	-0.78841600	1.49057800	0.29054300
C	0.07399000	2.95239900	-0.36621200
C	0.26767700	3.04688200	-1.75289800
C	0.50027400	3.99234300	0.46972500
C	0.86877000	4.17867800	-2.29877900
H	-0.05383400	2.23557800	-2.40078500
C	1.10845000	5.12214300	-0.08252700
H	0.36086800	3.92242600	1.54303600
C	1.28969900	5.21809800	-1.46385300
H	1.01200900	4.24892900	-3.37259800
H	1.43792900	5.92651100	0.56790700
H	1.75935200	6.09967700	-1.88930800
C	-0.55531400	1.45799200	2.08790900
C	0.37540800	0.57640200	2.65144400
C	-1.28439000	2.33238800	2.91083300
C	0.60143100	0.58816700	4.02750900
H	0.91336500	-0.12731900	2.02922700
C	-1.05548000	2.33622300	4.28532900
H	-2.02835100	2.99551100	2.47985200
C	-0.11035900	1.46926800	4.84300200
H	1.32855600	-0.09606100	4.45294900
H	-1.61856700	3.01085100	4.92283900
H	0.06168000	1.47582100	5.91498400
C	-2.56333500	1.79708900	0.02606100
C	-3.46753800	0.76411000	0.31778600
C	-3.03705500	3.04281700	-0.40557300
C	-4.83589900	0.98419100	0.18756100
H	-3.10501400	-0.20551900	0.64578100
C	-4.41066500	3.25175200	-0.54203300
H	-2.34255400	3.84418600	-0.63286100
C	-5.30874400	2.22661800	-0.24431200
H	-5.52950100	0.18254400	0.41621800
H	-4.77599900	4.21703500	-0.87872000
H	-6.37636600	2.39394900	-0.34932500
Au	-0.10173300	-0.44882700	-0.76825300
S	3.58813700	-1.47747900	0.70850300
O	2.96220200	-1.13189900	1.98444800
O	4.71946700	-2.39070800	0.61346500
C	3.87979000	-0.02142600	-0.25924200
C	4.70563100	-0.13387800	-1.38056700
C	3.24782000	1.17067300	0.10192600
C	4.89874900	0.99900300	-2.16963000
H	5.19242300	-1.07464400	-1.61321300
C	3.46600400	2.29303600	-0.69332100
H	2.62416000	1.21892500	0.98655500
C	4.27983200	2.20389400	-1.82570400
H	5.54063400	0.94219100	-3.04267000
H	3.00142800	3.23473100	-0.42869900
H	4.43729700	3.08430000	-2.44098200
S	1.97260700	-2.34500000	-0.58581000
C	1.15037700	-3.40399300	0.67284700
F	0.40690000	-2.68175200	1.52983400
F	0.32861200	-4.23985300	0.02236900
F	2.03437300	-4.10621900	1.37473300
C	-4.08013600	-3.11710100	0.70086600
C	-2.86879800	-2.97235000	0.03271500
C	-2.85509900	-2.46839100	-1.28309400
C	-4.06206400	-2.11947400	-1.91772500
C	-5.26745800	-2.28462600	-1.24347700
C	-5.27857900	-2.77981400	0.06362100
H	-4.09225900	-3.50271800	1.71528600
H	-1.93550100	-3.23705000	0.51410300
H	-4.04080100	-1.72720700	-2.92874700
H	-6.19890200	-2.02388100	-1.73567700
H	-6.22203000	-2.90722900	0.58577400
C	-1.62262600	-2.30147900	-1.97610300
C	-0.56598600	-2.10924400	-2.56821300
H	0.25266100	-2.19629700	-3.25112700

Zero-point correction= 0.506136 (Hartree/Particle)
Thermal correction to Energy= 0.546377
Thermal correction to Enthalpy= 0.547321
Thermal correction to Gibbs Free Energy= 0.426473
Sum of electronic and zero-point Energies= -2995.708587
Sum of electronic and thermal Energies= -2995.668345
Sum of electronic and thermal Enthalpies= -2995.667401
Sum of electronic and thermal Free Energies= -2995.788249
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2997.158054

INT1-a

P	1.78360600	-0.11433000	-0.04247600
C	2.10921800	1.67001300	0.08984100
C	1.90313500	2.29490100	1.33015500
C	2.55298700	2.41855800	-1.00705900
C	2.15651400	3.65635300	1.47341900
H	1.54840300	1.71570600	2.17868400
C	2.79811300	3.78624900	-0.85818500

H	2.71088100	1.93969300	-1.96743000
C	2.60407300	4.40369600	0.37883300
H	2.00463900	4.13505900	2.43583800
H	3.14660800	4.36484200	-1.70808300
H	2.80220400	5.46518900	0.49179400
C	1.99510400	-0.58936200	-1.77852100
C	0.87530600	-0.70475300	-2.61676000
C	3.28382300	-0.80308400	-2.29216800
C	1.04859700	-1.01668200	-3.96459600
H	-0.12790800	-0.57077100	-2.22209500
C	3.44710000	-1.11510400	-3.64051900
H	4.14956300	-0.73512400	-1.64064900
C	2.33189800	-1.21947500	-4.47615600
H	0.18081700	-1.11060200	-4.60973000
H	4.44327700	-1.28417800	-4.03709900
H	2.46360700	-1.46838000	-5.52457700
C	3.04729000	-0.96123800	0.93962900
C	2.80334200	-2.27546300	1.36644600
C	4.27240300	-0.34225600	1.22671200
C	3.78559800	-2.96847400	2.06975700
H	1.85049500	-2.75077800	1.14813000
C	5.24952600	-1.04313500	1.93356700
H	4.45821400	0.67827400	0.90792400
C	5.00760000	-2.35255100	2.35328800
H	3.59640100	-3.98437500	2.40171900
H	6.19742200	-0.56465800	2.15901600
H	5.76951900	-2.89266900	2.90660500
Au	-0.38103400	-0.55681600	0.64526300
S	-3.43682800	0.36403500	-0.76520100
O	-2.69370300	-0.19364800	-1.89131200
O	-4.88903100	0.37854100	-0.68932200
C	-2.73769700	1.90806000	-0.25554900
C	-3.42543200	2.65983800	0.70044400
C	-1.49621700	2.28763900	-0.77605700
C	-2.83490700	3.83965400	1.15062100
H	-4.39290800	2.33622500	1.06862900
C	-0.92839900	3.47169100	-0.31412400
H	-1.00200100	1.68218900	-1.52609900
C	-1.59212700	4.23711200	0.64900200
H	-3.34754700	4.44753300	1.88866300
H	0.03141600	3.79178600	-0.70203800
H	-1.13650700	5.15415600	1.00888800
S	-2.76516200	-0.85934400	1.08708200
C	-3.02809700	-2.56296400	0.38173500
F	-2.19341800	-2.81096100	-0.62917400
F	-2.80252700	-3.43779800	1.35903500
F	-4.27937000	-2.67071100	-0.05033500

Zero-point correction= 0.395221 (Hartree/Particle)
Thermal correction to Energy= 0.427960
Thermal correction to Enthalpy= 0.428904
Thermal correction to Gibbs Free Energy= 0.324705
Sum of electronic and zero-point Energies= -2687.383002
Sum of electronic and thermal Energies= -2687.350264
Sum of electronic and thermal Enthalpies= -2687.349320
Sum of electronic and thermal Free Energies= -2687.453519
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2688.637471

INT1*-a

P	1.61912300	0.50299300	-0.02753700
C	3.06946800	0.79791000	1.01882800
C	3.91084500	-0.28201400	1.32787600
C	3.37917400	2.08553300	1.47827000
C	5.06002800	-0.07100200	2.08576500
H	3.66551800	-1.28077900	0.97594700
C	4.53052500	2.28766500	2.23945300
H	2.72610100	2.92043600	1.24667200
C	5.36916600	1.21328100	2.54222100
H	5.70969500	-0.90679900	2.32558600
H	4.77004300	3.28393100	2.59784500
H	6.26206500	1.37489000	3.13814200
C	0.48572200	1.89979300	0.22447800
C	-0.32247100	1.92015800	1.37158100
C	0.46466000	2.97893700	-0.66858400
C	-1.13082300	3.02437300	1.63179000
H	-0.31642300	1.07683900	2.05688300
C	-0.35026300	4.07951600	-0.40193500
H	1.08180800	2.95931900	-1.56086800
C	-1.14165200	4.10551300	0.74781000
H	-1.75636900	3.03824500	2.51809600
H	-0.36387000	4.91739600	-1.09228500
H	-1.77483300	4.96287100	0.95102800
C	2.17014200	0.52093600	-1.75374700
C	1.32764600	-0.00906700	-2.74471400
C	3.41054200	1.07527300	-2.10084700
C	1.72778500	0.02782300	-4.07825600
H	0.36699800	-0.43329100	-2.47254800
C	3.80120400	1.10502400	-3.43947600
H	4.06528500	1.47489000	-1.33364300
C	2.96293800	0.58207800	-4.42595300
H	1.07870200	-0.38186000	-4.84592100
H	4.76196400	1.53192600	-3.70971800
H	3.27370100	0.60203200	-5.46602000
Au	0.51314600	-1.46235700	0.54320400
S	-2.80532700	-0.20890200	-0.46887300
O	-2.57021900	-0.86980100	0.86268900
O	-1.66999400	-0.02179600	-1.41638500
C	-3.54932600	1.39215500	-0.15214400
C	-3.44741600	2.36807200	-1.14407800
C	-4.27681500	1.57610500	1.02542300
C	-4.07145400	3.59355800	-0.92092100
H	-2.87423100	2.18092100	-2.04441400
C	-4.88638600	2.81209800	1.23016300
H	-4.34267400	0.78379500	1.76220900
C	-4.78713500	3.81376300	0.25922600
H	-3.99695700	4.37660200	-1.66861500
H	-5.44525700	2.98997900	2.14331800
H	-5.27755200	4.76871400	0.42069300
S	-1.03808000	-3.13603600	1.30070200
C	-1.77096900	-3.77003600	-0.27805300
F	-1.39067900	-3.05567200	-1.34472400
F	-1.35908900	-5.02838600	-0.42832200
F	-3.09842200	-3.73501000	-0.20108800

Zero-point correction= 0.392469 (Hartree/Particle)
Thermal correction to Energy= 0.426270

Thermal correction to Enthalpy= 0.427214

Thermal correction to Gibbs Free Energy= 0.317199

Sum of electronic and zero-point Energies= -2687.336487

Sum of electronic and thermal Energies= -2687.302686

Sum of electronic and thermal Enthalpies= -2687.301742

Sum of electronic and thermal Free Energies= -2687.411757

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2688.586172

INT1´´-a

P	-2.35162500	0.26319800	0.16802100
C	-3.10516000	1.35837900	-1.03312400
C	-3.24309400	0.89211400	-2.36611400
C	-3.51666400	2.65907700	-0.68095100
C	-3.82001300	1.71515300	-3.32220800
H	-2.90479800	-0.10487300	-2.63394400
C	-4.08922700	3.47291600	-1.64997900
H	-3.40807800	3.01296800	0.33835200
C	-4.23865600	3.00560500	-2.96763100
H	-3.93815700	1.36444100	-4.34191900
H	-4.43338300	4.46763000	-1.38662900
H	-4.68443200	3.65148600	-3.71750400
C	-1.96419000	1.09937000	1.70675100
C	-0.94769600	2.09018500	1.69063600
C	-2.61122600	0.75345300	2.90972600
C	-0.60987500	2.74048100	2.86857300
H	-0.42978000	2.33381400	0.76797400
C	-2.26314900	1.41553600	4.07976400
H	-3.38598600	-0.00536000	2.91935300
C	-1.26223200	2.40350300	4.06215600
H	0.16423300	3.50023500	2.86401200
H	-2.77177400	1.17736000	5.00811600
H	-0.99475100	2.91008400	4.98412800
C	-3.31238200	-1.22434500	0.43666400
C	-2.70593500	-2.27916400	1.16712600
C	-4.61493700	-1.36560700	-0.08058500
C	-3.41586600	-3.44888500	1.39603700
H	-1.69514900	-2.16720400	1.54949500
C	-5.31221100	-2.54395900	0.15430400
H	-5.07683500	-0.55730700	-0.63682100
C	-4.71497700	-3.58498400	0.88678300
H	-2.96373000	-4.25794300	1.95972100
H	-6.32500000	-2.65672900	-0.21825000
H	-5.26799000	-4.50255400	1.06116500
Au	-0.25593800	-0.35965600	-0.67544500
S	2.80164900	0.73060100	0.40761100
O	2.11925000	1.93595800	-0.05988900
O	2.44153200	0.05385900	1.64728500
C	4.53463600	0.80164600	0.15867900
C	5.34964500	-0.04950200	0.91758000
C	5.03054600	1.68729100	-0.80824500
C	6.72326400	0.01852700	0.70810500
H	4.92250400	-0.72104800	1.65251900
C	6.40776400	1.73133300	-0.99643300
H	4.36310100	2.32856000	-1.37252500
C	7.24677200	0.90004400	-0.24449600
H	7.38571200	-0.61411900	1.28908800
H	6.82788100	2.41533800	-1.72596900
H	8.31979700	0.94071800	-0.40223000
S	2.07181400	-0.74145600	-1.28067800
C	2.36596900	-2.38395800	-0.45272200
F	1.60002000	-2.52906100	0.63298700
F	2.07272200	-3.33889800	-1.32482300
F	3.64523200	-2.46323800	-0.09602800

Zero-point correction= 0.393194 (Hartree/Particle)

Thermal correction to Energy= 0.426669

Thermal correction to Enthalpy= 0.427613

Thermal correction to Gibbs Free Energy= 0.317731

Sum of electronic and zero-point Energies= -2686.998290

Sum of electronic and thermal Energies= -2686.964815

Sum of electronic and thermal Enthalpies= -2686.963871

Sum of electronic and thermal Free Energies= -2687.073753

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2688.3296629

INT1´-a

P	-1.61898700	-0.14027500	0.07708000
C	-2.22437800	1.50559800	-0.42470200
C	-2.05166500	1.88583600	-1.76403600
C	-2.82367400	2.39261700	0.47673200
C	-2.48775100	3.13469200	-2.19834700
H	-1.56056000	1.20872900	-2.45760500
C	-3.25117200	3.64825200	0.03869200
H	-2.94760100	2.10939600	1.51645500
C	-3.08565600	4.01967800	-1.29643600
H	-2.34960600	3.42299600	-3.23614500
H	-3.71106700	4.33528900	0.74300100
H	-3.41696000	4.99753100	-1.63350300
C	-1.72959000	-0.20713600	1.89168500
C	-0.55797300	-0.04889300	2.64382700
C	-2.95955400	-0.38842300	2.54311100
C	-0.61833200	-0.04582000	4.03726800
H	0.40434200	0.06570500	2.15882600
C	-3.01263300	-0.38822800	3.93583500
H	-3.86580000	-0.53874400	1.96418800
C	-1.84381400	-0.21286300	4.68317400
H	0.29926700	0.08093900	4.60291900
H	-3.96466500	-0.53181400	4.43860200
H	-1.89074900	-0.21656500	5.76837600
C	-2.86359400	-1.31716500	-0.54602900
C	-2.48072300	-2.65280400	-0.73809100
C	-4.18549100	-0.92714800	-0.80044500
C	-3.41815100	-3.59086500	-1.16659200
H	-1.45102800	-2.95089000	-0.55907400
C	-5.11821000	-1.87017800	-1.23280900
H	-4.48010800	0.10955200	-0.67030200
C	-4.73644300	-3.20080100	-1.41370600
H	-3.11647800	-4.62313400	-1.31617800
H	-6.14099100	-1.56418400	-1.43265600
H	-5.46362000	-3.93204200	-1.75442100
Au	0.52103600	-0.58874000	-0.70169900
S	3.26736200	0.86096000	1.25403100
O	2.53042600	0.86343500	2.55597700
O	4.72625000	1.15297900	1.20701200
C	2.44611000	2.08922200	0.20735100
C	3.01781400	2.38059100	-1.03000400

C	1.21893800	2.62129900	0.60099000
C	2.33722800	3.23694600	-1.89450700
H	3.96872800	1.93895800	-1.30583900
C	0.55520900	3.48526900	-0.27037100
H	0.80246000	2.36580200	1.56809400
C	1.10816700	3.78414400	-1.51646300
H	2.76636100	3.47404700	-2.86343700
H	-0.39934500	3.91166300	0.01822700
H	0.57538400	4.44237200	-2.19626300
S	2.73275900	-1.12270300	-1.40630400
C	2.91257600	-2.60927500	-0.39487100
F	2.81536300	-2.35939500	0.93640300
F	1.97327500	-3.55099900	-0.66345500
F	4.11428100	-3.17646300	-0.60298100

Zero-point correction= 0.392559 (Hartree/Particle)
Thermal correction to Energy= 0.426106
Thermal correction to Enthalpy= 0.427050
Thermal correction to Gibbs Free Energy= 0.319149
Sum of electronic and zero-point Energies= -2687.603104
Sum of electronic and thermal Energies= -2687.569558
Sum of electronic and thermal Enthalpies= -2687.568613
Sum of electronic and thermal Free Energies= -2687.676514
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2688.8406328

INT3-a

P	-2.35162500	0.26319800	0.16802100
C	-3.10516000	1.35837900	-1.03312400
C	-3.24309400	0.89211400	-2.36611400
C	-3.51666400	2.65907700	-0.68095100
C	-3.82001300	1.71515300	-3.32220800
H	-2.90479800	-0.10487300	-2.63394400
C	-4.08922700	3.47291600	-1.64997900
H	-3.40807800	3.01296800	0.33835200
C	-4.23865600	3.00560500	-2.96763100
H	-3.93815700	1.36444100	-4.34191900
H	-4.43338300	4.46763000	-1.38662900
H	-4.68443200	3.65148600	-3.71750400
C	-1.96419000	1.09937000	1.70675100
C	-0.94769600	2.09018500	1.69063600
C	-2.61122600	0.75345300	2.90972600
C	-0.60987500	2.74048100	2.86857300
H	-0.42978000	2.33381400	0.76797400
C	-2.26314900	1.41553600	4.07976400
H	-3.38598600	-0.00536000	2.91935300
C	-1.26223200	2.40350300	4.06215600
H	0.16423300	3.50023500	2.86401200
H	-2.77177400	1.17736000	5.00811600
H	-0.99475100	2.91008400	4.98412800
C	-3.31238200	-1.22434500	0.43666400
C	-2.70593500	-2.27916400	1.16712600
C	-4.61493700	-1.36560700	-0.08058500
C	-3.41586600	-3.44888500	1.39603700
H	-1.69514900	-2.16720400	1.54949500
C	-5.31221100	-2.54395900	0.15430400
H	-5.07683500	-0.55730700	-0.63682100
C	-4.71497700	-3.58498400	0.88678300
H	-2.96373000	-4.25794300	1.95972100
H	-6.32500000	-2.65672900	-0.21825000
H	-5.26799000	-4.50255400	1.06116500
Au	-0.25593800	-0.35965600	-0.67544500
S	2.80164900	0.73060100	0.40761100
O	2.11925000	1.93595800	-0.05988900
O	2.44153200	0.05385900	1.64728500
C	4.53463600	0.80164600	0.15867900
C	5.34964500	-0.04950200	0.91758000
C	5.03054600	1.68729100	-0.80824500
C	6.72326400	0.01852700	0.70810500
H	4.92250400	-0.72104800	1.65251900
C	6.40776400	1.73133300	-0.99643300
H	4.36310100	2.32856000	-1.37252500
C	7.24677200	0.90004400	-0.24449600
H	7.38571200	-0.61411900	1.28908800
H	6.82788100	2.41533800	-1.72596900
H	8.31979700	0.94071800	-0.40223000
S	2.07181400	-0.74145600	-1.28067800
C	2.36596900	-2.38395800	-0.45272200
F	1.60002000	-2.52906100	0.63298700
F	2.07272200	-3.33889800	-1.32482300
F	3.64523200	-2.46323800	-0.09602800

Zero-point correction= 0.292446 (Hartree/Particle)
Thermal correction to Energy= 0.316478
Thermal correction to Enthalpy= 0.317422
Thermal correction to Gibbs Free Energy= 0.231462
Sum of electronic and zero-point Energies= -1907.457050
Sum of electronic and thermal Energies= -1907.433018
Sum of electronic and thermal Enthalpies= -1907.432074
Sum of electronic and thermal Free Energies= -1907.518034
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1908.4492116

TS1´-a

C	-2.69542700	1.30104300	0.96740100
C	-1.75777500	0.36290500	1.39001700
C	-1.51226200	-0.78314200	0.61749400
C	-2.20965600	-0.97362800	-0.58538300
C	-3.14683700	-0.03045400	-1.00022900
C	-3.39004100	1.10777100	-0.22831800
H	-2.87860300	2.18698400	1.56828100
H	-1.19833100	0.51182100	2.30756300
H	-1.99391200	-1.84416900	-1.19391400
H	-3.68528100	-0.18314200	-1.93089600
H	-4.11795200	1.84313100	-0.55893000
C	-0.47810100	-1.71427100	1.03149300
C	-0.05588900	-2.53155700	1.88227500
H	0.69944000	-3.19211600	2.25936700
S	1.16040100	-1.40539100	-0.50227800
O	2.37096100	-2.10244400	-0.01837700
O	0.61964300	-1.65670600	-1.86086500
C	1.40854500	0.36406100	-0.32734000
C	0.60400600	1.23450300	-1.06321000
C	2.30558200	0.82281600	0.63719400
C	0.71901300	2.60421600	-0.83484100
H	-0.09362200	0.84012200	-1.79246100
C	2.41333100	2.19610400	0.85069300
H	2.91021600	0.11282700	1.19073200

C	1.61966400	3.08326300	0.11921600
H	0.10246100	3.29664100	-1.40002900
H	3.11678100	2.57365400	1.58688300
H	1.70264000	4.15192300	0.29501300

Zero-point correction= 0.209060 (Hartree/Particle)
Thermal correction to Energy= 0.224116
Thermal correction to Enthalpy= 0.225060
Thermal correction to Gibbs Free Energy= 0.163940
Sum of electronic and zero-point Energies= -1088.431242
Sum of electronic and thermal Energies= -1088.416187
Sum of electronic and thermal Enthalpies= -1088.415243
Sum of electronic and thermal Free Energies= -1088.476362
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1088.865051

TS1-a

C	3.22028900	-1.16889300	0.99177800
C	1.99701600	-1.74163100	0.66921100
C	1.31554800	-1.34368700	-0.50315100
C	1.90078600	-0.37240700	-1.34443900
C	3.12370700	0.19315100	-1.00837800
C	3.78717500	-0.19971300	0.15777300
H	3.73549200	-1.47557300	1.89734000
H	1.54425300	-2.48714700	1.31451500
H	1.37028400	-0.05922900	-2.23663600
H	3.56109500	0.94864400	-1.65431700
H	4.74296600	0.24678300	0.41571400
C	0.05006200	-1.88435100	-0.81099800
C	-1.15104100	-2.14593800	-0.94659200
H	-1.94381200	-2.76059300	-1.32558700
S	-2.49118500	-0.48666700	0.13163000
O	-3.54701800	-0.03662900	-0.81187800
O	-2.82458000	-0.89280000	1.52053600
C	-1.25559900	0.81871800	0.23515800
C	-0.38369400	0.83254300	1.32221400
C	-1.11547100	1.70073000	-0.83502900
C	0.65058900	1.76677500	1.34057800
H	-0.52097600	0.12456300	2.13175600
C	-0.08140800	2.63512800	-0.80053000
H	-1.81323000	1.65518500	-1.66404600
C	0.80229100	2.66276600	0.28110400
H	1.34383500	1.78650900	2.17567800
H	0.03605700	3.33990700	-1.61857000
H	1.61428300	3.38390000	0.29660600

Zero-point correction= 0.209469 (Hartree/Particle)
Thermal correction to Energy= 0.224462
Thermal correction to Enthalpy= 0.225406
Thermal correction to Gibbs Free Energy= 0.164735
Sum of electronic and zero-point Energies= -1088.442802
Sum of electronic and thermal Energies= -1088.427809
Sum of electronic and thermal Enthalpies= -1088.426865
Sum of electronic and thermal Free Energies= -1088.487536
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1088.879764

INT5-a

C	3.12463900	-1.29892600	0.92772700
C	1.86781600	-1.80191300	0.63281700
C	1.16973500	-1.35136000	-0.52296400
C	1.80192800	-0.40491800	-1.37661100
C	3.05709400	0.08812700	-1.06018000
C	3.72638300	-0.35130600	0.08928000
H	3.64311500	-1.64106100	1.81876800
H	1.39083300	-2.52770800	1.28309500
H	1.27163600	-0.05504900	-2.25519300
H	3.52102400	0.82579500	-1.70844400
H	4.71052700	0.03980400	0.32872200
C	-0.10577100	-1.82673200	-0.80850900
C	-1.40348100	-1.81197200	-0.78212800
H	-2.08103000	-2.52697200	-1.24526700
S	-2.34185200	-0.51498600	0.11143200
O	-3.42974400	-0.09547300	-0.78778900
O	-2.63398300	-0.99676400	1.47121200
C	-1.15175500	0.81891300	0.23452500
C	-0.30208700	0.87050300	1.33799900
C	-1.05720100	1.73484600	-0.81232200
C	0.67996100	1.85828800	1.38347100
H	-0.41292300	0.14461000	2.13552100
C	-0.07625600	2.72327800	-0.75155400
H	-1.74684900	1.66940500	-1.64697000
C	0.79424800	2.77820300	0.33959800
H	1.35875700	1.90514700	2.22926800
H	0.00916900	3.44960500	-1.55435400
H	1.56366000	3.54391100	0.37767100

Zero-point correction= 0.211834 (Hartree/Particle)
Thermal correction to Energy= 0.226457
Thermal correction to Enthalpy= 0.227401
Thermal correction to Gibbs Free Energy= 0.167897
Sum of electronic and zero-point Energies= -1088.456361
Sum of electronic and thermal Energies= -1088.441737
Sum of electronic and thermal Enthalpies= -1088.440793
Sum of electronic and thermal Free Energies= -1088.500297
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1088.891467

TS2-a

C	-1.09940200	-1.82647700	0.81663000
F	-0.70565200	-0.72670000	1.49924900
F	-2.23955900	-2.24942000	1.38080000
F	-0.16734000	-2.76984400	1.01799300
C	2.16180500	2.40825600	-2.61718800
C	2.02237900	1.04094500	-2.41333400
C	1.15820600	0.56027000	-1.40168100
C	0.41935800	1.48224000	-0.62847400
C	0.57611600	2.84485100	-0.83896100
C	1.44367800	3.31401600	-1.83099600
H	2.83631300	2.76983600	-3.38753500
H	2.59522900	0.32938700	-2.99718500
H	-0.24427800	1.11942200	0.14405800
H	0.01904700	3.54586900	-0.22482800
H	1.55728600	4.38201000	-1.99290100
C	1.07614200	-0.84419800	-1.18418500
C	1.86331100	-1.84212400	-0.86297000
H	1.62077300	-2.89919700	-0.86403900
S	3.54271600	-1.53011700	-0.21278400
O	3.87061500	-2.70994800	0.60198900
O	4.42672400	-1.09253200	-1.30599700

C	3.26113100	-0.12477000	0.86642500
C	3.81818100	1.10761700	0.53809300
C	2.42827800	-0.28924000	1.97347400
C	3.52778900	2.20963700	1.34215000
H	4.44522900	1.19253300	-0.34150500
C	2.13967400	0.82023200	2.76376200
H	1.99811600	-1.26005000	2.19372500
C	2.68820400	2.06646600	2.44738100
H	3.94689000	3.18040800	1.09600200
H	1.48541900	0.71349900	3.62368400
H	2.45620000	2.92962400	3.06471200
S	-1.30888700	-1.48846600	-0.97677300
S	-3.54999900	-0.92316300	-0.99234000
O	-3.69919700	-0.54317000	-2.40281300
O	-4.42708800	-1.91044000	-0.35050700
C	-3.51840600	0.56096300	0.00594100
C	-3.84565700	0.47848300	1.35864800
C	-3.08340200	1.74643300	-0.58717400
C	-3.74496800	1.63093400	2.13653800
H	-4.17323900	-0.46386000	1.78103400
C	-2.99150400	2.88932100	0.20484100
H	-2.82916500	1.76545500	-1.64054500
C	-3.31776800	2.83027900	1.56214600
H	-4.00157300	1.59169600	3.19063700
H	-2.66707100	3.82510200	-0.23974200
H	-3.24080800	3.72378600	2.17463500

Zero-point correction= 0.329918 (Hartree/Particle)
Thermal correction to Energy= 0.358682
Thermal correction to Enthalpy= 0.359626
Thermal correction to Gibbs Free Energy= 0.266028
Sum of electronic and zero-point Energies= -2604.418231
Sum of electronic and thermal Energies= -2604.389467
Sum of electronic and thermal Enthalpies= -2604.388523
Sum of electronic and thermal Free Energies= -2604.482121
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2605.248021

TS4-a

P	2.53312800	-0.02956300	0.09024300
C	2.87606300	0.00558500	1.87033900
C	2.28324000	-0.96270300	2.69523800
C	3.75454600	0.95174400	2.41565300
C	2.57662400	-0.98820700	4.05648600
H	1.59836200	-1.69251800	2.27111500
C	4.03975000	0.92212700	3.78104400
H	4.20874600	1.70512400	1.78058000
C	3.45380500	-0.04509600	4.59948200
H	2.11925800	-1.73853800	4.69378600
H	4.71836900	1.65605700	4.20434400
H	3.67738800	-0.06312900	5.66167400
C	2.99158100	1.58580300	-0.59495100
C	2.06137000	2.63590800	-0.56060500
C	4.27492500	1.80000000	-1.11741900
C	2.41823200	3.89433100	-1.03926800
H	1.06244800	2.46729900	-0.16621600
C	4.62363300	3.06285300	-1.59623200
H	4.99161700	0.98598200	-1.15493100
C	3.69843900	4.10775400	-1.55717400
H	1.69704400	4.70530900	-1.01589700
H	5.61601200	3.22825600	-2.00380200
H	3.97248200	5.08757700	-1.93583100
C	3.62564200	-1.26896500	-0.65601400
C	3.36809600	-1.69180000	-1.96954400
C	4.73221700	-1.77103800	0.04190600
C	4.22034900	-2.60650000	-2.58233600
H	2.50704700	-1.30312800	-2.50729100
C	5.57891900	-2.69037200	-0.57870200
H	4.92906500	-1.44921100	1.05907400
C	5.32470400	-3.10697700	-1.88630700
H	4.02146400	-2.93348400	-3.59808900
H	6.43520100	-3.08182500	-0.03846000
H	5.98429700	-3.82506100	-2.36357400
Au	0.29313400	-0.46765900	-0.34399300
C	-2.01287100	-1.58276600	-0.82235600
H	-1.74997000	-2.61860000	-0.92036200
C	-1.89136900	-0.33865200	-0.76155900
C	-2.43962900	0.99190600	-0.78475600
C	-2.27710800	1.85344800	0.31521800
C	-3.16972000	1.40949900	-1.91307600
C	-2.86359600	3.11397600	0.29281600
H	-1.72023100	1.51503900	1.18326700
C	-3.74347400	2.67713500	-1.92482200
H	-3.29873800	0.73059100	-2.74890600
C	-3.59370400	3.52803000	-0.82566200
H	-2.75470600	3.77403700	1.14747000
H	-4.31284300	2.99972000	-2.79073100
H	-4.04566600	4.51500200	-0.84113900
S	-4.48509800	-2.04972900	-0.76052200
O	-5.12318600	-1.64123900	-2.03360900
O	-4.54399600	-3.43251300	-0.23229000
C	-4.97052900	-0.89292200	0.51973000
C	-4.60714600	-1.17584400	1.83753100
C	-5.58390100	0.30403300	0.14959100
C	-4.88824400	-0.22639100	2.81810600
H	-4.13866300	-2.12186700	2.08650700
C	-5.85884700	1.24031900	1.14447600
H	-5.84113900	0.48586900	-0.88631900
C	-5.50744500	0.97842700	2.47085600
H	-4.63229900	-0.42985300	3.85312600
H	-6.34595900	2.17363100	0.88159700
H	-5.72138400	1.71401800	3.24021700

Zero-point correction= 0.486912 (Hartree/Particle)
Thermal correction to Energy= 0.522169
Thermal correction to Enthalpy= 0.523113
Thermal correction to Gibbs Free Energy= 0.407618
Sum of electronic and zero-point Energies= -2259.863839
Sum of electronic and thermal Energies= -2259.828582
Sum of electronic and thermal Enthalpies= -2259.827638
Sum of electronic and thermal Free Energies= -2259.943133
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2261.157694

INT9-a

P	2.50541100	-0.34331100	-0.03408100
C	3.40090100	0.01142900	1.50291800
C	2.79025300	-0.29618900	2.72848800

C	4.69746000	0.54403000	1.47757500
C	3.47834000	-0.08154000	3.92014500
H	1.78169900	-0.70129100	2.74647300
C	5.37860800	0.75953400	2.67581600
H	5.16840100	0.78908200	0.53128600
C	4.77184400	0.44746100	3.89381500
H	3.00507900	-0.31946300	4.86761300
H	6.38204400	1.17330100	2.65685800
H	5.30434000	0.62045200	4.82392800
C	3.29985500	0.61677200	-1.35352000
C	2.99443200	1.98183000	-1.47049000
C	4.22994000	0.02813700	-2.22091500
C	3.62614100	2.75375000	-2.44203700
H	2.26724300	2.43423700	-0.80086200
C	4.85509300	0.80744200	-3.19502700
H	4.46277700	-1.02811400	-2.13596900
C	4.55540900	2.16623900	-3.30557500
H	3.39154900	3.81000100	-2.53036500
H	5.57511700	0.35156200	-3.86745900
H	5.04265600	2.76802900	-4.06653000
C	2.75441300	-2.09874300	-0.41575100
C	1.89117900	-2.72283300	-1.32931900
C	3.81423700	-2.81812000	0.15353100
C	2.09481900	-4.05584600	-1.67764100
H	1.06564300	-2.16493400	-1.76400600
C	4.00897000	-4.15432600	-0.19718600
H	4.47830100	-2.33927600	0.86557800
C	3.15283000	-4.77187900	-1.11062100
H	1.42667200	-4.53795900	-2.38443200
H	4.82790500	-4.71247600	0.24576300
H	3.30623500	-5.81282800	-1.37800700
Au	0.21889500	0.19568700	0.16205400
C	-2.66829100	-0.33081400	0.88325700
H	-2.40369500	-1.32995800	1.21255000
C	-1.85552400	0.58490500	0.39486400
C	-2.01841200	1.94257500	-0.02419500
C	-1.95338700	2.99843800	0.93340700
C	-2.18605900	2.25577900	-1.40531000
C	-2.11867100	4.30726600	0.52430900
H	-1.81251400	2.74663500	1.97860900
C	-2.35267100	3.56937700	-1.79551600
H	-2.20880600	1.44551400	-2.12616600
C	-2.31993100	4.59888900	-0.83599900
H	-2.10443000	5.11026100	1.25369700
H	-2.51262500	3.81085200	-2.84120300
H	-2.45095800	5.62946500	-1.15067500
S	-4.42385800	0.08139100	1.16060700
O	-4.69013800	-0.25559900	2.56455500
O	-4.63654400	1.43843800	0.62798700
C	-5.27344900	-1.08244200	0.10835000
C	-5.51466100	-0.73721600	-1.22327000
C	-5.65604400	-2.31428400	0.64135800
C	-6.15759700	-1.66219600	-2.04319300
H	-5.22569800	0.24110100	-1.59141900
C	-6.29881700	-3.22817000	-0.19340500
H	-5.47439100	-2.53401500	1.68767300
C	-6.54468500	-2.90365400	-1.52963100
H	-6.36662000	-1.41191900	-3.07852300
H	-6.61510800	-4.18810000	0.20213500
H	-7.04860500	-3.61834100	-2.17306000

Zero-point correction= 0.490188 (Hartree/Particle)
Thermal correction to Energy= 0.524847
Thermal correction to Enthalpy= 0.525792
Thermal correction to Gibbs Free Energy= 0.410718
Sum of electronic and zero-point Energies= -2259.886784
Sum of electronic and thermal Energies= -2259.852125
Sum of electronic and thermal Enthalpies= -2259.851180
Sum of electronic and thermal Free Energies= -2259.966254
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2261.177013

TS4´-a

P	1.21560400	-1.04836600	0.04373600
C	1.65702100	-1.14878100	1.80278700
C	0.99590400	-0.31291200	2.71769800
C	2.62685200	-2.05615300	2.24904300
C	1.30547200	-0.39660000	4.07328900
H	0.23569300	0.37758200	2.36745900
C	2.93301400	-2.12706300	3.60863600
H	3.14111200	-2.69885900	1.54257300
C	2.27482100	-1.29964600	4.51936900
H	0.79223800	0.24566000	4.78261500
H	3.68722500	-2.82755900	3.95363300
H	2.51724100	-1.35657500	5.57622300
C	2.49555400	-1.93338600	-0.88938400
C	3.65625600	-1.25080900	-1.28140100
C	2.36027800	-3.30179100	-1.16517700
C	4.67730700	-1.93420100	-1.93805400
H	3.75412600	-0.18891000	-1.07185400
C	3.38484900	-3.97869500	-1.82663200
H	1.46061400	-3.83087600	-0.86866800
C	4.54121700	-3.29758200	-2.21173200
H	5.57423800	-1.40373100	-2.24233500
H	3.27793100	-5.03707500	-2.04314400
H	5.33472500	-3.82752200	-2.72959900
C	-0.33097400	-1.97026300	-0.19112300
C	-0.91601600	-1.98657200	-1.46609900
C	-0.93215200	-2.66330800	0.86657100
C	-2.08909700	-2.70519300	-1.67988900
H	-0.46418200	-1.42788900	-2.27947600
C	-2.11169900	-3.37470500	0.64447200
H	-0.48705000	-2.64167100	1.85504100
C	-2.68836700	-3.39845900	-0.62542800
H	-2.54333600	-2.71186600	-2.66558000
H	-2.58020800	-3.90746500	1.46608000
H	-3.61239000	-3.94290300	-0.79136200
Au	1.02111000	1.16195600	-0.60728100
C	-2.91999300	3.27244900	0.07926600
H	-3.98668800	3.38346200	0.04082700
C	-1.77310300	3.74256800	0.09380700
C	-0.36920900	3.84269700	0.03796300
C	0.38624100	4.29475200	1.13505400
C	0.30984200	3.45446700	-1.16178400
C	1.77856700	4.37241300	1.05385900
H	-0.12790900	4.58880300	2.04342800

C	1.71490000	3.54612000	-1.22768300
H	-0.27597700	3.20304700	-2.04008700
C	2.44745900	4.00118600	-0.11046900
H	2.34257900	4.72948600	1.90939400
H	2.22152400	3.33599900	-2.16503700
H	3.52784100	4.07596200	-0.17200500
S	-2.49756700	0.97241300	-0.07864700
O	-1.92109600	0.89287100	-1.44755600
O	-1.63266200	0.68889800	1.09570900
C	-3.90829400	-0.12666100	-0.00422500
C	-4.27211800	-0.66968100	1.22855000
C	-4.62082500	-0.38135400	-1.17746300
C	-5.37222200	-1.52423200	1.27488200
H	-3.68628200	-0.45007100	2.11358800
C	-5.71872600	-1.23678800	-1.11140900
H	-4.29978300	0.05539600	-2.11646800
C	-6.09205100	-1.80547700	0.11024400
H	-5.66602100	-1.97246100	2.21885200
H	-6.28111000	-1.46176700	-2.01218100
H	-6.95099300	-2.46801600	0.15512700

Zero-point correction= 0.487833 (Hartree/Particle)
Thermal correction to Energy= 0.522403
Thermal correction to Enthalpy= 0.523347
Thermal correction to Gibbs Free Energy= 0.414808
Sum of electronic and zero-point Energies= -2259.879390
Sum of electronic and thermal Energies= -2259.844820
Sum of electronic and thermal Enthalpies= -2259.843876
Sum of electronic and thermal Free Energies= -2259.952416
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2261.162574

INT9´-a

P	1.35112800	-0.95830300	0.05662500
C	1.75694100	-0.96984600	1.82773700
C	1.02899000	-0.14102100	2.69728900
C	2.76683700	-1.80221500	2.32764700
C	1.31129300	-0.15806600	4.06148600
H	0.23834300	0.49157300	2.30656900
C	3.04611600	-1.80558500	3.69471100
H	3.33395300	-2.43821100	1.65638300
C	2.32073800	-0.98610400	4.56055800
H	0.74584000	0.47802200	4.73583200
H	3.83204500	-2.44726700	4.08084000
H	2.54228300	-0.99058600	5.62348200
C	2.72237300	-1.74888200	-0.82840100
C	3.80574700	-0.96875900	-1.25754900
C	2.73648400	-3.13755200	-1.02796400
C	4.89787600	-1.57382200	-1.87592200
H	3.78828200	0.10735700	-1.10700200
C	3.83141000	-3.73596000	-1.65075700
H	1.89626200	-3.74278500	-0.70401100
C	4.91033400	-2.95672500	-2.07344300
H	5.73427200	-0.96760400	-2.20962800
H	3.83992600	-4.81004100	-1.80805900
H	5.75896100	-3.42622700	-2.56137900
C	-0.10909500	-2.01052400	-0.18357300
C	-0.55477600	-2.25239400	-1.49142300
C	-0.81686800	-2.53164700	0.90598800
C	-1.69344700	-3.02384900	-1.70404900
H	-0.02246600	-1.82620700	-2.33620300
C	-1.96312200	-3.29548200	0.68475200
H	-0.48316800	-2.33342600	1.91800100
C	-2.40130300	-3.54217300	-0.61641200
H	-2.03688400	-3.20751900	-2.71727600
H	-2.51520900	-3.69288600	1.53047400
H	-3.29930200	-4.12850400	-0.78364700
Au	0.97224100	1.22186700	-0.63024100
C	-3.12462700	2.45715100	-0.31017800
H	-4.18016200	2.58189300	-0.53363400
C	-2.19851400	3.36452400	-0.20618700
C	-0.83603800	3.64785200	-0.09429600
C	-0.27322500	4.17736000	1.09135200
C	0.03005000	3.40474200	-1.22004600
C	1.08977600	4.45669400	1.16680700
H	-0.92080400	4.36292600	1.94106000
C	1.40088000	3.70992300	-1.12445400
H	-0.41119300	3.11249400	-2.16786100
C	1.93173000	4.22913400	0.07689000
H	1.49936800	4.86085200	2.08693600
H	2.03354400	3.60612000	-2.00112100
H	2.98874100	4.46362600	0.13932200
S	-2.50566400	0.73318800	-0.22578600
O	-1.90247600	0.46725700	-1.54739700
O	-1.66968500	0.63103500	0.98705200
C	-3.92459300	-0.31996400	-0.02671500
C	-4.31225200	-0.68959600	1.26196900
C	-4.57981100	-0.78580900	-1.16755700
C	-5.39614700	-1.55376200	1.40660900
H	-3.75951100	-0.32533700	2.12044600
C	-5.66348300	-1.64735600	-1.00515700
H	-4.22782100	-0.50035700	-2.15250500
C	-6.06853100	-2.02871800	0.27701800
H	-5.71314800	-1.85990500	2.39850100
H	-6.18651500	-2.02607000	-1.87754200
H	-6.91209000	-2.70167500	0.39664000

Zero-point correction= 0.490158 (Hartree/Particle)
Thermal correction to Energy= 0.524457
Thermal correction to Enthalpy= 0.525401
Thermal correction to Gibbs Free Energy= 0.416958
Sum of electronic and zero-point Energies= -2259.892468
Sum of electronic and thermal Energies= -2259.858169
Sum of electronic and thermal Enthalpies= -2259.857225
Sum of electronic and thermal Free Energies= -2259.965668
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2261.176087

TS5-a

C	-2.15902000	3.10209800	0.97490100
F	-3.37724700	2.67578600	1.34377700
F	-1.94696700	4.30986000	1.50186600
F	-2.16533900	3.23372400	-0.36572000
C	-2.49593000	-3.07842200	2.53892400
C	-1.95584400	-2.18230700	1.62422200
C	-2.52190700	-0.89419900	1.48581000
C	-3.61306800	-0.52119100	2.30205500
C	-4.15330700	-1.43543100	3.19691900

C	-3.59675200	-2.71287700	3.32067200
H	-2.06312800	-4.06912400	2.63586800
H	-1.12766100	-2.47755900	0.99055000
H	-4.02724600	0.47598100	2.21194100
H	-5.00256700	-1.14906700	3.80888700
H	-4.01539600	-3.41984400	4.03009900
C	-2.03488800	0.06192600	0.53610800
C	-1.94648300	0.16536600	-0.80537700
H	-1.71958900	1.09407800	-1.32599300
S	-2.57230300	-1.13313600	-1.94859600
O	-2.38558500	-0.56288100	-3.28756600
O	-1.92472900	-2.39709700	-1.55128500
C	-4.30596800	-1.22941900	-1.55719300
C	-4.74304800	-2.16935000	-0.62117400
C	-5.17665200	-0.32340800	-2.16823100
C	-6.09542700	-2.19104000	-0.28494600
H	-4.04168300	-2.86689500	-0.18017000
C	-6.52560400	-0.36102200	-1.82106500
H	-4.80444200	0.37586100	-2.90908700
C	-6.98078700	-1.28860800	-0.87941000
H	-6.45672800	-2.91592800	0.43745200
H	-7.22173800	0.32716000	-2.28964000
H	-8.03326300	-1.31252200	-0.61396300
S	-0.89143300	1.90401400	1.54507000
S	1.00658500	3.25552500	1.38185200
O	2.03280200	2.20953800	1.51119000
O	0.93980600	4.40885200	2.28386300
C	0.91924200	3.80362000	-0.30930000
C	0.42637700	5.08109500	-0.57670000
C	1.26740300	2.90530700	-1.32078600
C	0.29431400	5.46994100	-1.90937400
H	0.16140300	5.74614500	0.23686300
C	1.12505000	3.30996000	-2.64560800
H	1.66658300	1.92889800	-1.07815500
C	0.63591600	4.58735700	-2.93731900
H	-0.07708400	6.46231600	-2.14357300
H	1.40417200	2.63207900	-3.44601000
H	0.52353600	4.89708000	-3.97164800
P	2.42312800	-1.20982000	-0.03787400
C	2.99550900	-0.99412400	1.66778000
C	2.05656600	-0.96437100	2.70888100
C	4.36407900	-0.89016500	1.95663600
C	2.48412500	-0.83686500	4.02798200
H	0.99490700	-1.03306100	2.48785400
C	4.78473100	-0.76175400	3.27956600
H	5.09446800	-0.89027500	1.15400500
C	3.84727200	-0.73422400	4.31373900
H	1.75427600	-0.80622000	4.83088800
H	5.84393600	-0.67573900	3.50096100
H	4.17851100	-0.62566400	5.34184200
C	3.59338300	-0.35307100	-1.13071300
C	4.05753500	0.92706500	-0.78486400
C	3.96055600	-0.92987100	-2.35450700
C	4.88738600	1.61872300	-1.66540300
H	3.76821500	1.37835800	0.15845200
C	4.79079100	-0.22742800	-3.22790700
H	3.60619700	-1.92050000	-2.62011700
C	5.25346200	1.04466700	-2.88550900
H	5.24879400	2.60646600	-1.39624200
H	5.07895600	-0.67714000	-4.17298600
H	5.90133300	1.58719300	-3.56723800
C	2.47346400	-2.97623100	-0.45438400
C	1.42845200	-3.55605500	-1.18962500
C	3.57573500	-3.75321600	-0.06440500
C	1.49502700	-4.90547700	-1.53892800
H	0.56301300	-2.96900100	-1.48368300
C	3.63194700	-5.09940300	-0.41597400
H	4.37823100	-3.31139100	0.51775100
C	2.59360800	-5.67511300	-1.15431100
H	0.68474500	-5.35086900	-2.10755300
H	4.48321100	-5.70045500	-0.11177200
H	2.64107900	-6.72556800	-1.42479500
Au	0.25147600	-0.43451300	-0.27774600

Zero-point correction= 0.608201 (Hartree/Particle)
Thermal correction to Energy= 0.656819
Thermal correction to Enthalpy= 0.657763
Thermal correction to Gibbs Free Energy= 0.514514
Sum of electronic and zero-point Energies= -3775.845385
Sum of electronic and thermal Energies= -3775.796768
Sum of electronic and thermal Enthalpies= -3775.795823
Sum of electronic and thermal Free Energies= -3775.939072
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-3777.026655

INT6-a

P	2.18539900	-0.49869600	0.24771300
C	2.02788900	-0.36415400	2.04358500
C	0.95167200	-0.98998600	2.69837100
C	2.90557500	0.45638200	2.76931700
C	0.75387000	-0.78908100	4.06181300
H	0.26190600	-1.62635500	2.15967300
C	2.70212900	0.64698000	4.13548900
H	3.74242800	0.93765300	2.27517900
C	1.62653300	0.03236800	4.78032600
H	-0.09081800	-1.26497800	4.54849100
H	3.38518900	1.27801600	4.69515300
H	1.46757200	0.19335600	5.84190600
C	3.82560800	0.06640400	-0.26947400
C	4.06831100	1.44818600	-0.37167400
C	4.83925800	-0.85220100	-0.57766800
C	5.32369800	1.90358000	-0.76850300
H	3.28429600	2.16371500	-0.13395900
C	6.09103800	-0.38609500	-0.97630300
H	4.65043800	-1.91828300	-0.50824700
C	6.33320300	0.98659500	-1.07196300
H	5.51082000	2.96971100	-0.84652800
H	6.87773800	-1.09530400	-1.21335500
H	7.30909400	1.34252800	-1.38687300
C	1.97222200	-2.21696800	-0.26541200
C	1.64775400	-2.47089200	-1.60814600
C	2.13255400	-3.28266900	0.63220900
C	1.48885700	-3.78138300	-2.04931300
H	1.51389600	-1.64507600	-2.30214800
C	1.95927600	-4.59271000	0.18459600
H	2.38528500	-3.09137000	1.66939200

C	1.63848700	-4.84196900	-1.15176200
H	1.23633200	-3.97418500	-3.08697000
H	2.08009900	-5.41757400	0.87966000
H	1.50656500	-5.86365200	-1.49443800
Au	0.66483000	0.94346000	-0.90581800
S	-0.55316900	2.63954000	-2.05399300
C	-1.05077400	3.59476600	-0.58678700
F	-2.23643100	3.17702200	-0.09136800
F	-0.15844300	3.49387100	0.43704300
F	-1.17037000	4.88640800	-0.89677400
C	-2.90507600	-1.69133200	-2.76915200
C	-2.29971700	-0.69785600	-2.01465200
C	-1.56846400	-1.04900900	-0.85940200
C	-1.41773500	-2.40519700	-0.49868100
C	-2.02611700	-3.38971600	-1.26753700
C	-2.76677700	-3.03610000	-2.39890800
H	-3.48332900	-1.42537200	-3.64778800
H	-2.38480400	0.34841700	-2.28774400
H	-0.86021300	-2.66778400	0.39080100
H	-1.92111900	-4.43203100	-0.98519100
H	-3.23625300	-3.80974800	-2.99899700
C	-1.02475900	-0.02782300	-0.00823700
C	-1.28866900	0.47345300	1.17548800
H	-0.74302400	1.25278200	1.69312900
S	-2.66394100	-0.18786100	2.18936100
O	-2.28628300	-1.55816000	2.57517800
O	-2.89255300	0.85240800	3.19502300
C	-4.02335400	-0.26770900	1.04196200
C	-4.52416300	0.92679300	0.51933300
C	-4.52285200	-1.51485700	0.67020200
C	-5.55121400	0.85922000	-0.41906700
H	-4.11818700	1.88069300	0.83549200
C	-5.55538000	-1.56364000	-0.26544800
H	-4.10360900	-2.41500400	1.10305900
C	-6.06251400	-0.38227400	-0.81059400
H	-5.95678000	1.77400700	-0.83909400
H	-5.96169400	-2.52363000	-0.56762500
H	-6.86490000	-0.42664800	-1.54070100

Zero-point correction= 0.508348 (Hartree/Particle)
Thermal correction to Energy= 0.548165
Thermal correction to Enthalpy= 0.549109
Thermal correction to Gibbs Free Energy= 0.429107
Sum of electronic and zero-point Energies= -2995.716379
Sum of electronic and thermal Energies= -2995.676562
Sum of electronic and thermal Enthalpies= -2995.675618
Sum of electronic and thermal Free Energies= -2995.795620
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2996.749891

TS3-a

P	2.34333200	0.44328100	0.18925100
C	2.30030200	2.13555400	-0.45430600
C	1.09055000	2.84708400	-0.39422600
C	3.42924700	2.71733800	-1.04584900
C	1.01159500	4.13262700	-0.92138000
H	0.20959600	2.41443800	0.06384800
C	3.34096200	4.00627200	-1.57444300
H	4.36503200	2.17098600	-1.09531600
C	2.13747400	4.71119800	-1.51553900
H	0.06938600	4.66806300	-0.86889100
H	4.21504000	4.45771900	-2.03328000
H	2.07547600	5.71151000	-1.93275400
C	4.02223300	-0.20528200	-0.00316000
C	4.37068900	-0.86510100	-1.19169900
C	4.97891100	-0.01625000	1.00487100
C	5.67300000	-1.32692500	-1.37210500
H	3.62784500	-1.01442300	-1.97142800
C	6.27851100	-0.48420900	0.81766100
H	4.70807800	0.48696700	1.92758300
C	6.62513900	-1.13736100	-0.36765300
H	5.94179700	-1.83889500	-2.29058700
H	7.01953400	-0.34152500	1.59788400
H	7.63764800	-1.50324900	-0.50696700
C	1.96654400	0.49285200	1.96457000
C	1.65053800	-0.71529400	2.60738100
C	1.96501100	1.69342900	2.68627600
C	1.34700200	-0.72076100	3.96587200
H	1.63318000	-1.64431900	2.04324100
C	1.64665500	1.68156900	4.04613200
H	2.20050900	2.62894100	2.19023900
C	1.34122200	0.47838100	4.68519000
H	1.10540400	-1.65614300	4.46071600
H	1.64340800	2.61237500	4.60473100
H	1.09992600	0.47362200	5.74387200
Au	0.75601100	-0.92575300	-0.87967300
S	-0.86870900	-2.29696200	-1.99500400
C	-0.95116300	-3.65495800	-0.77048900
F	-0.14550100	-4.66516500	-1.10716800
F	-0.59856600	-3.24846300	0.47492500
F	-2.20551700	-4.12899300	-0.69393000
C	-3.56749800	-1.61410700	2.01519400
C	-2.97449600	-1.37489300	0.78694900
C	-1.94463100	-0.41321600	0.68767300
C	-1.49563900	0.27228400	1.83958900
C	-2.09941900	0.02011200	3.06381900
C	-3.12930200	-0.92175200	3.15298400
H	-4.36804800	-2.34156600	2.09541500
H	-3.29291000	-1.90805600	-0.09974300
H	-0.70513300	1.00626000	1.75613600
H	-1.76159900	0.55177500	3.94651600
H	-3.59237800	-1.12294600	4.11429900
C	-1.41238900	-0.04345400	-0.57973000
C	-1.55853300	0.90386900	-1.47266400
H	-1.02851100	1.02127600	-2.41017600
S	-2.70193300	2.30867900	-1.14948800
O	-2.92727400	2.87871000	-2.47978000
O	-2.11148400	3.10224500	-0.06036500
C	-4.18387500	1.53136700	-0.54140600
C	-4.93325000	0.74075200	-1.41607300
C	-4.54706700	1.72290700	0.79096500
C	-6.07528900	0.11085600	-0.92692600
H	-4.63402200	0.63033800	-2.45319500
C	-5.69790200	1.09228600	1.26160600
H	-3.93696800	2.34735800	1.43240900
C	-6.45410500	0.28625800	0.40805500

H	-6.67536200	-0.50592300	-1.58815400
H	-6.00258200	1.23146700	2.29393800
H	-7.34880800	-0.20293200	0.78084400

Zero-point correction= 0.507835 (Hartree/Particle)
Thermal correction to Energy= 0.547034
Thermal correction to Enthalpy= 0.547978
Thermal correction to Gibbs Free Energy= 0.429675
Sum of electronic and zero-point Energies= -2995.711242
Sum of electronic and thermal Energies= -2995.672044
Sum of electronic and thermal Enthalpies= -2995.671100
Sum of electronic and thermal Free Energies= -2995.789402
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2996.738142

INT7-a

P	2.34312100	0.33801500	0.02934100
C	2.44054100	0.34903700	-1.77838900
C	1.27214200	0.17579900	-2.53463400
C	3.66206400	0.60133800	-2.42146000
C	1.31349600	0.27855300	-3.92279100
H	0.32587800	-0.03879500	-2.05163900
C	3.69959800	0.69159300	-3.81263800
H	4.57187600	0.72089000	-1.84160700
C	2.52932400	0.53564600	-4.56087400
H	0.39502000	0.15782200	-4.48689800
H	4.64419400	0.88189800	-4.31255700
H	2.56717900	0.60979800	-5.64329400
C	3.94821800	-0.18478800	0.68373700
C	4.25154700	-1.55465400	0.71736800
C	4.89749600	0.75870500	1.10074700
C	5.50302300	-1.97557300	1.15943900
H	3.51188500	-2.28448200	0.39828100
C	6.14808500	0.32756400	1.54418100
H	4.66148100	1.81759800	1.08285200
C	6.45051700	-1.03483500	1.57316500
H	5.73761600	-3.03495000	1.18712500
H	6.88363200	1.05649300	1.86954200
H	7.42356000	-1.36571500	1.92262600
C	2.06104000	2.04485600	0.58353500
C	1.68978200	2.26817700	1.91893000
C	2.25387700	3.12875300	-0.28282400
C	1.53064000	3.57002800	2.38704700
H	1.53394800	1.42556500	2.58789400
C	2.08837400	4.43133300	0.19279500
H	2.53095800	2.95825600	-1.31763100
C	1.73230600	4.65253400	1.52445600
H	1.24885000	3.74163500	3.42121200
H	2.23723200	5.27085100	-0.47892900
H	1.60734900	5.66694500	1.89047100
Au	0.60173400	-1.01837600	0.71592100
S	-1.43101700	-2.35484300	1.16514300
C	-1.13921800	-3.80980200	0.04118600
F	-0.36339400	-3.50280100	-1.01042500
F	-0.51998400	-4.72890800	0.77538000
F	-2.29837300	-4.27435400	-0.40403400
C	-5.68294000	0.16855600	1.52645300
C	-4.78528200	-0.55020400	0.73852200
C	-3.40925200	-0.45061700	0.98966800
C	-2.93978200	0.36337200	2.03180600
C	-3.84229500	1.08808100	2.80349600
C	-5.21430400	0.98669800	2.55521000
H	-6.74797400	0.08921700	1.33308300
H	-5.13898100	-1.17422200	-0.07447100
H	-1.87146600	0.46393300	2.20497600
H	-3.47774500	1.73469600	3.59521600
H	-5.91661000	1.54700000	3.16463700
C	-2.46974500	-1.21877300	0.15381600
C	-2.27082100	-1.10945800	-1.16134800
H	-1.58781300	-1.72890400	-1.72940000
S	-2.95011400	0.19616900	-2.20883500
O	-1.93419200	0.28808300	-3.27125400
O	-4.35781200	-0.07514300	-2.51310500
C	-2.84199400	1.65708800	-1.18469100
C	-4.01872800	2.28123500	-0.77783300
C	-1.58394200	2.12535500	-0.79758800
C	-3.93070500	3.39455100	0.05785900
H	-4.97469800	1.88967400	-1.10339500
C	-1.51012900	3.23172900	0.04398000
H	-0.68006400	1.64499300	-1.15213200
C	-2.68263700	3.86110500	0.47304900
H	-4.83777500	3.89082900	0.38727800
H	-0.54250500	3.60799600	0.35344200
H	-2.62070600	4.72442600	1.12886100

Zero-point correction= 0.509975 (Hartree/Particle)
Thermal correction to Energy= 0.549284
Thermal correction to Enthalpy= 0.550228
Thermal correction to Gibbs Free Energy= 0.431819
Sum of electronic and zero-point Energies= -2995.749754
Sum of electronic and thermal Energies= -2995.710446
Sum of electronic and thermal Enthalpies= -2995.709501
Sum of electronic and thermal Free Energies= -2995.827910
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2997.200642

P_1

S	2.49200800	1.12182600	1.01352400
C	3.09169500	0.30124600	-0.50390400
F	2.25785800	0.49010800	-1.54898000
F	4.27991700	0.83912400	-0.80831100
F	3.24966500	-1.02696800	-0.37642000
C	-2.46250800	2.07676300	1.61858000
C	-1.35119400	1.26117300	1.82325100
C	-0.30225000	1.25744400	0.89179300
C	-0.37237100	2.09201300	-0.23446700
C	-1.49426700	2.88601800	-0.44400100
C	-2.54013300	2.88294700	0.48314400
H	-3.26798200	2.07777500	2.34683800
H	-1.29585800	0.61630000	2.69197000
H	0.43868300	2.08661400	-0.95337000
H	-1.55325600	3.51039100	-1.33043500
H	-3.41020700	3.51295900	0.32170700
C	0.85324400	0.36262000	1.09588600
C	0.79589600	-0.96181900	1.30396400
H	1.66774600	-1.56501200	1.52917500
S	-0.64372200	-2.00239600	1.00723700
O	-0.06155500	-3.32324400	0.72454500

O	-1.65080800	-1.83871800	2.06750500
C	-1.30383500	-1.32653300	-0.51593000
C	-2.58489900	-0.78395300	-0.52573200
C	-0.49255700	-1.33001700	-1.65187900
C	-3.06392200	-0.21882900	-1.70726100
H	-3.17415800	-0.78995800	0.38321900
C	-0.97975900	-0.75650600	-2.82314700
H	0.50429300	-1.75573900	-1.61147700
C	-2.26249900	-0.20144100	-2.84924700
H	-4.05767600	0.21764100	-1.73015300
H	-0.35993500	-0.74184100	-3.71445800
H	-2.63613700	0.24855900	-3.76450700

Zero-point correction= 0.231714 (Hartree/Particle)
Thermal correction to Energy= 0.251212
Thermal correction to Enthalpy= 0.252156
Thermal correction to Gibbs Free Energy= 0.182033
Sum of electronic and zero-point Energies= -1824.326752
Sum of electronic and thermal Energies= -1824.307254
Sum of electronic and thermal Enthalpies= -1824.306310
Sum of electronic and thermal Free Energies= -1824.376432
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1824.736272

INT6´-a

P	1.29213400	-1.21044300	0.54157100
C	2.72074300	-0.98111600	-0.52932200
C	3.15152400	0.32766500	-0.80963800
C	3.39606500	-2.07953300	-1.08648700
C	4.23886500	0.53115600	-1.65309500
H	2.63790100	1.18093900	-0.37898000
C	4.48627200	-1.86341000	-1.92712100
H	3.07281200	-3.09070400	-0.86624000
C	4.90176700	-0.56198900	-2.21694300
H	4.56146400	1.54239400	-1.87718500
H	5.01002000	-2.71206600	-2.35552200
H	5.74604700	-0.39936400	-2.87978800
C	0.54764400	-2.82079000	0.25565700
C	0.37998800	-3.27978100	-1.06267700
C	0.06988800	-3.58768300	1.32991900
C	-0.25512500	-4.49300000	-1.29890900
H	0.75885200	-2.69748400	-1.89266000
C	-0.56970500	-4.79880700	1.08121100
H	0.19558900	-3.24481400	2.34927200
C	-0.73822700	-5.24935300	-0.22836400
H	-0.38252900	-4.84500900	-2.31747200
H	-0.94001900	-5.38853800	1.91330900
H	-1.24621100	-6.18975200	-0.41646500
C	1.74434600	-0.99558500	2.27598500
C	0.71642900	-0.87402100	3.23438100
C	3.09008500	-0.86736800	2.65311600
C	1.04884700	-0.64982100	4.56724800
H	-0.32476200	-0.95189500	2.93397900
C	3.40575200	-0.64262300	3.99128200
H	3.87641300	-0.94599200	1.91024700
C	2.38977700	-0.53296200	4.94479200
H	0.26199700	-0.55708500	5.30874600
H	4.44510700	-0.55116500	4.29003800
H	2.64358300	-0.35108600	5.98439700
Au	-0.05069300	0.77123700	0.45678400
S	-0.77654000	2.79463000	1.42614700
C	0.48383900	3.92799900	0.76671600
F	1.69662500	3.33642500	0.59631100
F	0.13336600	4.42510700	-0.44045000
F	0.65210100	4.95776500	1.59891400
C	1.59224400	2.34454800	-3.54654900
C	0.70266600	1.92864900	-2.56288900
C	0.29850200	0.58053600	-2.49892900
C	0.80640700	-0.33529700	-3.44132300
C	1.70306300	0.08713100	-4.41670600
C	2.10317000	1.42512300	-4.46765400
H	1.88895900	3.38753900	-3.59315700
H	0.31518500	2.64099700	-1.84529400
H	0.48384100	-1.36954700	-3.40709600
H	2.08931900	-0.62627600	-5.13772700
H	2.80590600	1.75172000	-5.22792700
C	-0.59830900	0.11094200	-1.45435000
C	-1.69902300	-0.62588400	-1.55528600
S	-2.67109900	-1.33528100	-0.21582700
O	-1.99236600	-1.05347800	1.07045100
C	-4.15841900	-0.36204500	-0.28438000
C	-4.17038700	0.90341000	0.31003000
C	-5.26623000	-0.88076700	-0.95674100
C	-5.33099700	1.66762100	0.22114100
H	-3.29823900	1.27623200	0.83427400
C	-6.42190600	-0.10369300	-1.03109100
H	-5.22159400	-1.87359600	-1.39043600
C	-6.45147400	1.16515000	-0.44788300
H	-5.36255800	2.65141400	0.67817600
H	-7.29848100	-0.49069300	-1.54060200
H	-7.35380200	1.76545100	-0.51099100
O	-2.96832700	-2.71554300	-0.61256500
H	-2.14157600	-0.84022200	-2.52639800

Zero-point correction= 0.508963 (Hartree/Particle)
Thermal correction to Energy= 0.548497
Thermal correction to Enthalpy= 0.549441
Thermal correction to Gibbs Free Energy= 0.430725
Sum of electronic and zero-point Energies= -2995.721811
Sum of electronic and thermal Energies= -2995.682276
Sum of electronic and thermal Enthalpies= -2995.681332
Sum of electronic and thermal Free Energies= -2995.800048
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2997.178274

TS3´-a

P	-2.10334700	0.71940500	0.06133500
C	-2.00537400	2.23052400	-0.92715000
C	-0.80030500	2.56632300	-1.55753600
C	-3.12485800	3.06835800	-1.05606700
C	-0.71112900	3.73000000	-2.31862600
H	0.07427600	1.94065500	-1.43711700
C	-3.03275700	4.22391500	-1.82928500
H	-4.05128900	2.82570900	-0.54418700
C	-1.82849800	4.55479800	-2.45865300
H	0.23665600	3.99317300	-2.77625800
H	-3.89605900	4.87434400	-1.92960800
H	-1.75997000	5.46500500	-3.04645300

C	-3.16322800	1.06694300	1.49190000
C	-2.62685600	1.83226300	2.54094500
C	-4.48745900	0.61343400	1.55459100
C	-3.41842200	2.14626100	3.64238700
H	-1.59875100	2.18306800	2.49117000
C	-5.27222200	0.93172300	2.66356400
H	-4.89984300	0.01640100	0.74801200
C	-4.74018300	1.69522000	3.70412800
H	-3.00432500	2.73703700	4.45329900
H	-6.29844700	0.58141300	2.71413100
H	-5.35396000	1.93703100	4.56627200
C	-2.92073300	-0.57432400	-0.91712200
C	-2.85011400	-1.90056800	-0.46043700
C	-3.60619500	-0.27653100	-2.10182900
C	-3.47312500	-2.91662600	-1.17895800
H	-2.29998300	-2.13688100	0.44592100
C	-4.22419600	-1.30184100	-2.81987700
H	-3.65565700	0.74608000	-2.46113500
C	-4.15997400	-2.61833200	-2.35933200
H	-3.41610500	-3.94068300	-0.82378800
H	-4.75828800	-1.06987900	-3.73628000
H	-4.64390000	-3.41242300	-2.91986800
Au	-0.04039100	-0.10395000	0.81471300
S	1.90164000	-1.24909000	1.63461500
C	1.19235300	-2.91324700	1.92628600
F	0.95648300	-3.08558700	3.22985200
F	0.02923500	-3.11862500	1.26495400
F	2.05013900	-3.87225700	1.53351600
C	0.56774600	-4.11008500	-2.28396800
C	1.16101300	-3.14960600	-1.47548700
C	0.79079500	-1.79863700	-1.61750100
C	-0.19463200	-1.43091600	-2.56302300
C	-0.77436200	-2.40016300	-3.36889400
C	-0.40080600	-3.73982500	-3.22473800
H	0.85855900	-5.15062700	-2.18340300
H	1.90815700	-3.42931700	-0.74464600
H	-0.47878600	-0.38901900	-2.65745600
H	-1.52765700	-2.11540700	-4.09459800
H	-0.86527600	-4.49913600	-3.84629700
C	1.42602400	-0.73777300	-0.88481600
C	2.26103100	0.21653900	-1.25399900
H	2.66795800	0.19482000	-2.26350400
S	2.78774400	1.67555400	-0.34650900
O	2.17223100	1.63158200	0.99363200
O	2.52156000	2.78924500	-1.26679100
C	4.54050800	1.43952900	-0.18588100
C	5.36919400	1.88508300	-1.21925600
C	5.04048500	0.80246500	0.95282300
C	6.74204400	1.67488100	-1.10568600
H	4.94699000	2.40260900	-2.07367100
C	6.41603700	0.60168600	1.04833200
H	4.37056100	0.49201800	1.74601900
C	7.26098400	1.03252600	0.02183200
H	7.40623100	2.01961100	-1.89159400
H	6.82839100	0.11572500	1.92663400
H	8.33171200	0.87383500	0.10469200

Zero-point correction= 0.507689 (Hartree/Particle)
Thermal correction to Energy= 0.546861
Thermal correction to Enthalpy= 0.547805
Thermal correction to Gibbs Free Energy= 0.429297
Sum of electronic and zero-point Energies= -2995.709512
Sum of electronic and thermal Energies= -2995.670340
Sum of electronic and thermal Enthalpies= -2995.669396
Sum of electronic and thermal Free Energies= -2995.787904
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2997.160593

INT7′-a

P	2.45585800	-0.61083200	-0.08473700
C	2.31522200	-2.29886700	-0.72134400
C	1.06956300	-2.74359500	-1.18793200
C	3.43409900	-3.14318100	-0.77667700
C	0.94407200	-4.02728800	-1.71261200
H	0.19440400	-2.10506600	-1.13615900
C	3.29973500	-4.42593300	-1.30689400
H	4.39502200	-2.80475100	-0.40233100
C	2.05851900	-4.86742700	-1.77288000
H	-0.02806100	-4.36497500	-2.05653600
H	4.16262300	-5.08336300	-1.34814400
H	1.95951700	-5.87107400	-2.17512800
C	3.88574900	-0.53623300	1.02349900
C	3.73284600	-0.94609400	2.35664100
C	5.14025200	-0.12650800	0.55077600
C	4.83419600	-0.95269400	3.20910900
H	2.75759900	-1.25760800	2.72165000
C	6.23749700	-0.13408500	1.41219500
H	5.25692000	0.19903100	-0.47788400
C	6.08546800	-0.54651000	2.73724800
H	4.71605900	-1.26808400	4.24098400
H	7.20911600	0.18541600	1.04852600
H	6.94126800	-0.54704800	3.40522000
C	2.79149000	0.49572700	-1.48766400
C	2.64351000	1.88040000	-1.30700900
C	3.20217700	-0.01032900	-2.72765100
C	2.92030000	2.75103400	-2.35847200
H	2.30820900	2.27190000	-0.35018500
C	3.46935100	0.86818500	-3.77894000
H	3.30774900	-1.08064100	-2.87085200
C	3.33123300	2.24501700	-3.59557600
H	2.81242100	3.82155800	-2.21350200
H	3.78522900	0.47532100	-4.74030800
H	3.54268300	2.92450500	-4.41558800
Au	0.48735800	0.07583800	0.90090100
S	-1.71777300	0.97388200	1.53490100
C	-1.24579000	2.72354800	1.95783900
F	-0.75307500	2.62912900	3.19739800
F	-0.30940900	3.24652600	1.16493900
F	-2.31048700	3.52315400	1.96869800
C	-2.72749600	4.59087800	-1.63205500
C	-2.96308600	3.43725000	-0.88511000
C	-2.05574900	2.37404400	-0.95034500
C	-0.91672500	2.46725300	-1.76347000
C	-0.68547200	3.62511600	-2.50143000
C	-1.58958500	4.68772100	-2.43551500
H	-3.43537900	5.41244600	-1.58802200

H	-3.84770100	3.35866600	-0.26197600
H	-0.21791000	1.63742300	-1.80861200
H	0.19774800	3.69027000	-3.12873900
H	-1.41106400	5.58920100	-3.01348500
C	-2.27647800	1.10857500	-0.20535100
C	-2.77336300	0.04016600	-0.84079200
H	-3.08617600	0.13194700	-1.87629000
S	-2.81433500	-1.63524100	-0.23547100
O	-2.21525600	-1.59835700	1.11818400
O	-2.21509200	-2.45650500	-1.29802600
C	-4.54006400	-2.02640500	-0.09367000
C	-5.19398100	-2.59209500	-1.19101700
C	-5.20163400	-1.73354900	1.10208300
C	-6.55602400	-2.86689400	-1.08200800
H	-4.64069600	-2.82720300	-2.09355500
C	-6.56275300	-2.01590400	1.19294600
H	-4.65458300	-1.31785400	1.94114100
C	-7.23612200	-2.57675600	0.10372200
H	-7.08394000	-3.31314300	-1.91855700
H	-7.09617600	-1.80614800	2.11445500
H	-8.29653800	-2.79549700	0.18238300

Zero-point correction= 0.509596 (Hartree/Particle)
Thermal correction to Energy= 0.549079
Thermal correction to Enthalpy= 0.550024
Thermal correction to Gibbs Free Energy= 0.428175
Sum of electronic and zero-point Energies= -2995.754909
Sum of electronic and thermal Energies= -2995.715425
Sum of electronic and thermal Enthalpies= -2995.714481
Sum of electronic and thermal Free Energies= -2995.836330
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2997.201315

P_1'

S	-0.27613400	0.59556500	-1.57916000
C	-0.45391300	2.01067100	-0.43151200
F	0.31274600	3.00259400	-0.91340300
F	-1.70989900	2.47299300	-0.33030500
F	-0.03612200	1.70572200	0.80621000
C	-3.86190400	-0.95677300	1.80841200
C	-2.56180900	-1.01339600	1.31318800
C	-2.28209600	-0.59898300	0.00100500
C	-3.32595900	-0.10540500	-0.79657300
C	-4.62498400	-0.05619100	-0.30008700
C	-4.89728000	-0.48182900	1.00182600
H	-4.06408400	-1.27195500	2.82775700
H	-1.74914200	-1.35246900	1.94791900
H	-3.11364800	0.22786000	-1.80666800
H	-5.42686500	0.31674600	-0.93020900
H	-5.91072500	-0.43374000	1.38927600
C	-0.90049900	-0.70145100	-0.51355800
C	-0.12338100	-1.76096300	-0.23133600
H	-0.51842200	-2.62561800	0.29311400
S	1.62665500	-1.95513700	-0.57701100
O	1.88030500	-1.82175900	-2.01892500
O	1.99892000	-3.17589900	0.15442800
C	2.36565600	-0.55173600	0.25903500
C	2.35115200	-0.52172800	1.65415300
C	2.90476600	0.48983600	-0.49268900
C	2.86895900	0.59377800	2.30761400
H	1.94738900	-1.36064300	2.21132600
C	3.42425700	1.59963400	0.17293000
H	2.90317900	0.42173500	-1.57393200
C	3.39833600	1.65419900	1.56727200
H	2.86240200	0.63576300	3.39257700
H	3.84339800	2.42243000	-0.39806800
H	3.79603800	2.52455400	2.08103900

Zero-point correction= 0.231425 (Hartree/Particle)
Thermal correction to Energy= 0.251035
Thermal correction to Enthalpy= 0.251979
Thermal correction to Gibbs Free Energy= 0.180845
Sum of electronic and zero-point Energies= -1824.323988
Sum of electronic and thermal Energies= -1824.304377
Sum of electronic and thermal Enthalpies= -1824.303433
Sum of electronic and thermal Free Energies= -1824.374567
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1824.917227

a′

C	-1.51116700	-1.21016200	0.00243400
C	-0.13196200	-1.22358800	-0.00130900
C	0.64331200	-0.00002100	-0.00089400
C	-0.13198400	1.22360700	-0.00135000
C	-1.51113200	1.21016300	0.00241400
C	-2.24549200	-0.00002900	0.00650900
H	-2.04756800	-2.16114200	0.00078600
H	0.40675400	-2.16926600	-0.00716500
H	0.40688800	2.16922600	-0.00715400
H	-2.04760300	2.16110200	0.00085500
H	-3.33279300	0.00002500	0.01026900
C	2.02735800	0.00019700	0.02133700
C	3.27863600	-0.00018800	-0.12554600
H	4.10890800	0.00017900	0.58083200

Zero-point correction= 0.104995 (Hartree/Particle)
Thermal correction to Energy= 0.111786
Thermal correction to Enthalpy= 0.112730
Thermal correction to Gibbs Free Energy= 0.073690
Sum of electronic and zero-point Energies= -308.282580
Sum of electronic and thermal Energies= -308.275788
Sum of electronic and thermal Enthalpies= -308.274844
Sum of electronic and thermal Free Energies= -308.313884
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-308.5382918

a′′

C	-3.20833900	-0.00001600	-0.00003600
H	-4.28086600	-0.00006600	-0.00005300
C	-1.98221200	0.00000900	0.00005500
C	-0.59466300	0.00010800	0.00004100
C	0.12048000	-1.24723000	-0.00000700
C	0.12058100	1.24732200	-0.00000600
C	1.49454600	-1.23596200	-0.00003500
H	-0.44177900	-2.17439300	0.00002400
C	1.49464600	1.23587500	-0.00003600
H	-0.44153300	2.17457500	0.00002800
C	2.18575900	-0.00008200	0.00002300
H	2.05368700	-2.16525500	-0.00008000
H	2.05388900	2.16510600	-0.00008300

H	3.27181800	-0.00012000	0.00017900

Zero-point correction= 0.109078 (Hartree/Particle)
Thermal correction to Energy= 0.115735
Thermal correction to Enthalpy= 0.116680
Thermal correction to Gibbs Free Energy= 0.077725
Sum of electronic and zero-point Energies= -308.007287
Sum of electronic and thermal Energies= -308.000630
Sum of electronic and thermal Enthalpies= -307.999686
Sum of electronic and thermal Free Energies= -308.038640
(U) B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-308.2383602

INT2´-a

P	1.17460800	0.08080500	0.00927500
C	1.97168900	0.26936000	1.64034000
C	2.25648600	-0.89294000	2.37199000
C	2.31439600	1.52151100	2.16815400
C	2.89373400	-0.80344400	3.60844400
H	1.96691800	-1.86148100	1.97324600
C	2.94790300	1.60648800	3.40831100
H	2.07902100	2.42475900	1.61437800
C	3.24050600	0.44603700	4.12738100
H	3.10985000	-1.70711100	4.17076100
H	3.20837200	2.57968500	3.81455600
H	3.73022700	0.51555100	5.09446800
C	0.38091600	1.68961500	-0.34146400
C	-0.96921700	1.85752900	0.00447400
C	1.07837100	2.74671900	-0.94406800
C	-1.60910500	3.07209300	-0.23940900
H	-1.52775200	1.03911600	0.44868100
C	0.43423600	3.96030700	-1.18425100
H	2.11667200	2.61630900	-1.23323100
C	-0.90779400	4.12357800	-0.83238800
H	-2.65764700	3.17803200	0.01913200
H	0.97838200	4.77515900	-1.65353700
H	-1.40835500	5.06739700	-1.02994100
C	2.55199700	-0.03919700	-1.18315600
C	2.27497200	-0.57046600	-2.45178000
C	3.85011400	0.39383700	-0.88205000
C	3.28176600	-0.65062300	-3.41201400
H	1.27232100	-0.92387400	-2.67721500
C	4.85613300	0.30657300	-1.84521300
H	4.07334500	0.79255100	0.10237200
C	4.57326300	-0.21230300	-3.10983600
H	3.06064800	-1.06305500	-4.39209300
H	5.86141800	0.64137100	-1.60573000
H	5.35902600	-0.28164400	-3.85661500
Au	-0.48467000	-1.61205200	-0.09568200
C	-2.24984800	-2.69745700	-0.15457300
H	-2.28868500	-3.78359700	-0.21470200
C	-3.28945300	-1.92065700	-0.10140200
C	-3.92124000	-0.67614900	-0.01806200
C	-4.21342800	-0.08301400	1.24457700
C	-4.28350000	0.04730100	-1.19071700
C	-4.81719900	1.16418000	1.31908200
H	-3.94003400	-0.62154400	2.14658300
C	-4.88897300	1.29143300	-1.09736500
H	-4.06128300	-0.38955900	-2.15911200
C	-5.16449800	1.86255500	0.15356400
H	-5.02149400	1.60180800	2.29298200
H	-5.14672700	1.82979600	-2.00582700
H	-5.64772800	2.83316200	0.21922900

Zero-point correction= 0.386303 (Hartree/Particle)
Thermal correction to Energy= 0.412189
Thermal correction to Enthalpy= 0.413133
Thermal correction to Gibbs Free Energy= 0.323276
Sum of electronic and zero-point Energies= -1479.918102
Sum of electronic and thermal Energies= -1479.892217
Sum of electronic and thermal Enthalpies= -1479.891273
Sum of electronic and thermal Free Energies= -1479.981129
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1480.934665

INT2´´-a

P	1.58518600	-0.00940900	0.24002400
C	2.01747500	-1.72915200	0.50429800
C	1.90891100	-2.61734400	-0.59542200
C	2.43807300	-2.19882800	1.76491200
C	2.25196100	-3.95216500	-0.43481600
H	1.56561700	-2.25207900	-1.55903800
C	2.77465900	-3.53847900	1.91163900
H	2.52388700	-1.51802100	2.60443800
C	2.67975500	-4.41495400	0.81760300
H	2.18138300	-4.63629100	-1.27375900
H	3.12497200	-3.90586200	2.87061500
H	2.94268800	-5.46046500	0.94393400
C	1.48785800	0.89443500	1.78550500
C	0.49674400	0.50538200	2.72133500
C	2.34967300	1.97430600	2.06324000
C	0.40081800	1.17165200	3.93466200
H	-0.17637300	-0.31571800	2.49157200
C	2.23869100	2.63520900	3.28010200
H	3.10839100	2.26987400	1.34728100
C	1.26660900	2.23862800	4.21340300
H	-0.34632800	0.87241400	4.66205000
H	2.91420400	3.45104000	3.51551100
H	1.18739800	2.76289600	5.16052000
C	2.69644400	0.78112100	-0.92372900
C	2.34934800	2.06767600	-1.40779700
C	3.86959300	0.14073900	-1.37077400
C	3.18927400	2.71193400	-2.30475400
H	1.43351900	2.54684600	-1.07373400
C	4.69904900	0.79635100	-2.27185600
H	4.13519200	-0.84238500	-0.99847000
C	4.36042600	2.07641000	-2.74137900
H	2.93566600	3.70012000	-2.67353600
H	5.61707900	0.32315900	-2.60439800
H	5.01359800	2.57839900	-3.44815400
Au	-0.57479000	0.03635300	-0.76794800
C	-2.32132300	0.09275000	-1.95285800
H	-2.13202400	0.14678700	-3.02024900
C	-3.41581700	0.05963800	-1.32460800
C	-4.59588600	0.02171600	-0.60232700
C	-5.21648300	-1.23026300	-0.32138800
C	-5.21995800	1.23769200	-0.19802600
C	-6.42743600	-1.25450800	0.34650900

H	-4.73400900	-2.14634100	-0.64490000
C	-6.43094800	1.19182000	0.46864500
H	-4.74006200	2.18279900	-0.42850200
C	-7.03159900	-0.04871800	0.73810500
H	-6.91406900	-2.19967000	0.56158700
H	-6.92034500	2.10946800	0.77657200
H	-7.98520500	-0.07600800	1.25684400

Zero-point correction= 0.386745 (Hartree/Particle)
Thermal correction to Energy= 0.413154
Thermal correction to Enthalpy= 0.414099
Thermal correction to Gibbs Free Energy= 0.320949
Sum of electronic and zero-point Energies= -1479.365015
Sum of electronic and thermal Energies= -1479.338606
Sum of electronic and thermal Enthalpies= -1479.337661
Sum of electronic and thermal Free Energies= -1479.430811
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1480.484752

INT10-a

P	-0.14657300	2.16155700	0.29438200
C	-0.68552000	1.64397200	1.95234900
C	0.20003100	0.86673400	2.71968600
C	-1.98502700	1.88916100	2.41108100
C	-0.21918500	0.34544500	3.94046900
H	1.20121000	0.66361300	2.35149000
C	-2.39791300	1.35604000	3.63400500
H	-2.66923600	2.48461400	1.81620500
C	-1.52025400	0.58415100	4.39631600
H	0.46550500	-0.25247500	4.53412500
H	-3.40424200	1.54946800	3.99226100
H	-1.84578500	0.17247700	5.34685600
C	-1.44376600	3.19430600	-0.43283700
C	-2.55873500	2.56982700	-1.01152500
C	-1.35948300	4.59352900	-0.40459700
C	-3.58779100	3.33228700	-1.55818000
H	-2.61415700	1.49047100	-1.03846600
C	-2.39467500	5.35316900	-0.95072500
H	-0.49476900	5.08185500	0.03239600
C	-3.50349900	4.72729700	-1.52608200
H	-4.43160300	2.82871500	-2.01964900
H	-2.33066900	6.43675100	-0.93247500
H	-4.29864500	5.32754800	-1.95755500
C	1.34132300	3.17434500	0.48192300
C	2.16552800	3.36239000	-0.63717700
C	1.66364300	3.77902900	1.70534200
C	3.30453500	4.15590500	-0.53253600
H	1.92893300	2.87301700	-1.57637100
C	2.80714600	4.57120900	1.80144500
H	1.03006500	3.63026100	2.57320400
C	3.62639100	4.75889800	0.68617500
H	3.94497800	4.29333300	-1.39786600
H	3.05791400	5.04038400	2.74779300
H	4.51837600	5.37257900	0.76766500
Au	0.22508800	0.09603900	-0.79062400
C	1.99005400	-2.58377400	0.46524600
F	1.43340800	-1.84784500	1.43363300
F	1.20783700	-3.63358100	0.21794100
F	3.17929900	-3.01316400	0.90294800
C	-1.89615900	-4.50283200	0.36380900
C	-1.80249800	-3.49456400	-0.58606300
C	-1.73537200	-2.14208200	-0.17394800
C	-1.74269100	-1.83275200	1.20621300
C	-1.84163600	-2.84969300	2.14254000
C	-1.91311600	-4.18566700	1.72753200
H	-1.96096500	-5.53861600	0.04545500
H	-1.80501100	-3.72222800	-1.64678200
H	-1.69884700	-0.79752400	1.51937000
H	-1.86650900	-2.60202300	3.19884900
H	-1.98480300	-4.97885800	2.46547100
C	-1.63719000	-1.11300700	-1.16760200
C	-2.42824900	-0.64561400	-2.11364200
H	-2.15510500	0.07559300	-2.87825100
S	-4.21458400	-0.99850600	-2.20597800
O	-4.78782500	0.27950600	-2.66253900
O	-4.42690000	-2.24891900	-2.94627700
C	-4.69983400	-1.25812500	-0.50213500
C	-4.95761400	-2.55547800	-0.06394200
C	-4.79202400	-0.15761300	0.35223800
C	-5.29689500	-2.75626600	1.27374000
H	-4.88965500	-3.38074400	-0.76257000
C	-5.12828900	-0.37315100	1.68664600
H	-4.61848100	0.84434800	-0.02287300
C	-5.37468500	-1.66979100	2.14677500
H	-5.49868200	-3.76059100	1.63206600
H	-5.21144900	0.47062100	2.36419700
H	-5.63865400	-1.83178200	3.18757100
S	2.18234900	-1.64952100	-1.11559000
S	3.68837200	-0.09815300	-0.49296000
O	3.62510900	0.78561700	-1.65479000
O	3.31007100	0.32834000	0.85369400
C	5.23606300	-0.95387800	-0.45251500
C	5.73561300	-1.38425000	0.77893100
C	5.90071400	-1.17340900	-1.66247500
C	6.95832000	-2.05117800	0.79045400
H	5.18782500	-1.18935000	1.69284300
C	7.11939200	-1.84559000	-1.62640800
H	5.48203100	-0.81458000	-2.59592200
C	7.64307800	-2.28310700	-0.40576700
H	7.37666300	-2.38811700	1.73315100
H	7.66164500	-2.02378800	-2.54906600
H	8.59363600	-2.80683100	-0.38702700

Zero-point correction= 0.609247 (Hartree/Particle)
Thermal correction to Energy= 0.658364
Thermal correction to Enthalpy= 0.659308
Thermal correction to Gibbs Free Energy= 0.516175
Sum of electronic and zero-point Energies= -3775.858750
Sum of electronic and thermal Energies= -3775.809633
Sum of electronic and thermal Enthalpies= -3775.808688
Sum of electronic and thermal Free Energies= -3775.951822
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-3777.040147

INT11-a

P	-2.26834000	0.28102100	0.05656100
C	-2.21209700	0.87047800	1.77922000
C	-1.15957100	1.69752600	2.20131500

C	-3.13800600	0.39735000	2.72001000
C	-1.02748100	2.03873000	3.54521600
H	-0.43203900	2.06748300	1.49303600
C	-3.00639900	0.74865200	4.06358000
H	-3.95508900	-0.24366700	2.40572900
C	-1.95087200	1.56311500	4.47864500
H	-0.18750200	2.65435100	3.84969000
H	-3.72765600	0.37928800	4.78674000
H	-1.84492400	1.82224000	5.52796300
C	-3.99130500	-0.25279400	-0.21973600
C	-4.29630900	-1.62002900	-0.19432700
C	-5.01410500	0.68585500	-0.41870000
C	-5.61580500	-2.04450500	-0.35569600
H	-3.49959600	-2.34579300	-0.05324700
C	-6.32899800	0.25665600	-0.58556600
H	-4.77975600	1.74525100	-0.45130000
C	-6.63105200	-1.10749700	-0.55189200
H	-5.84652700	-3.10535900	-0.33540500
H	-7.11819600	0.98570700	-0.74440500
H	-7.65700500	-1.43855700	-0.68417600
C	-2.00825100	1.72783600	-1.01703200
C	-1.53432900	1.50356800	-2.31827400
C	-2.27599400	3.03596100	-0.59172100
C	-1.34004100	2.57442400	-3.18597700
H	-1.29503700	0.49388300	-2.63891100
C	-2.07224800	4.10646500	-1.46312500
H	-2.62507600	3.21772300	0.41947700
C	-1.60675000	3.87677400	-2.75868800
H	-0.95532600	2.39371500	-4.18442800
H	-2.27386800	5.11933600	-1.12688900
H	-1.44176400	4.71314400	-3.43175000
Au	-0.67421900	-1.41377100	-0.41686800
S	0.41144700	-3.43669800	-1.10235500
C	1.97648200	-3.37718600	-0.21451300
F	2.85391900	-2.46575900	-0.72404500
F	1.86302000	-3.07654900	1.10250000
F	2.59160600	-4.57466000	-0.29235200
C	2.38127300	1.09225300	-3.16890000
C	1.98422900	0.28183300	-2.11152100
C	1.49847600	0.85963100	-0.92036000
C	1.39555600	2.26457600	-0.83294400
C	1.78537900	3.06373400	-1.90122400
C	2.28099800	2.48391300	-3.07140500
H	2.76965400	0.63691000	-4.07539100
H	2.05564400	-0.79672600	-2.17956200
H	1.04338200	2.71805100	0.08471600
H	1.70158500	4.14337100	-1.81904500
H	2.58617100	3.11154600	-3.90400900
C	1.06357300	0.02571000	0.17256800
C	1.34630600	-0.05225400	1.45931200
H	0.85699400	-0.70135300	2.17807100
S	2.62418500	0.94681100	2.25615500
O	2.17832000	2.35773300	2.31351300
O	2.98174600	0.24458400	3.49926000
C	3.97893800	0.84171000	1.09071700
C	4.49253600	-0.42051100	0.79248100
C	4.43807000	1.99464400	0.45991600
C	5.48629000	-0.52580200	-0.17720000
H	4.09337300	-1.30261100	1.27928500
C	5.44047900	1.87713700	-0.50270000
H	3.99612200	2.95174200	0.70975900
C	5.95824700	0.62070200	-0.82258500
H	5.88111100	-1.50294800	-0.43704100
H	5.80493700	2.76411700	-1.01206400
H	6.72799600	0.53216900	-1.58394100

Zero-point correction= 0.506872 (Hartree/Particle)
Thermal correction to Energy= 0.546895
Thermal correction to Enthalpy= 0.547839
Thermal correction to Gibbs Free Energy= 0.426735
Sum of electronic and zero-point Energies= -2995.933482
Sum of electronic and thermal Energies= -2995.893459
Sum of electronic and thermal Enthalpies= -2995.892515
Sum of electronic and thermal Free Energies= -2996.013618
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2996.943071

TS6-a

P	-1.82588100	-0.10357700	-0.03752400
C	-3.18395600	-1.23830600	-0.48852100
C	-3.10504500	-2.57720700	-0.07969500
C	-4.31002300	-0.79513400	-1.19542700
C	-4.14726300	-3.45853100	-0.36249100
H	-2.22134700	-2.91972500	0.45188900
C	-5.34783600	-1.68240400	-1.48185600
H	-4.37051400	0.23705600	-1.52450900
C	-5.26924500	-3.01230200	-1.06446700
H	-4.07934300	-4.49459100	-0.04368000
H	-6.21592400	-1.33479000	-2.03455000
H	-6.07747600	-3.70153400	-1.29188400
C	-1.93740900	1.29087000	-1.20129800
C	-1.18323200	1.24736900	-2.38093300
C	-2.76754900	2.39087200	-0.94123300
C	-1.27319400	2.29081600	-3.30103400
H	-0.50109900	0.42359300	-2.55563100
C	-2.85347500	3.43017300	-1.86608800
H	-3.33469300	2.43673800	-0.01690300
C	-2.10764500	3.37978800	-3.04627100
H	-0.67324900	2.26017300	-4.20528800
H	-3.49474000	4.28268500	-1.66120400
H	-2.16810000	4.19625900	-3.76035900
C	-2.29984500	0.60012300	1.57998900
C	-1.35177500	1.38146900	2.26018100
C	-3.56762600	0.39792100	2.13839300
C	-1.68129200	1.95838300	3.48455900
H	-0.36751100	1.53884500	1.83220500
C	-3.88717300	0.97504200	3.36898400
H	-4.30158100	-0.20726200	1.61674400
C	-2.94670400	1.75515700	4.04195200
H	-0.94585400	2.56396400	4.00602900
H	-4.87118400	0.81278700	3.79972300
H	-3.19699900	2.20231800	4.99983300
Au	0.26233300	-1.11392100	0.07988300
S	2.18756400	0.67976000	-1.36161800
C	2.03377500	1.83109700	-0.02894600
F	0.89306100	2.58362000	-0.07280300

F	1.98677900	1.23516600	1.23039200
F	3.05934800	2.71639500	0.06732500
C	2.06036500	-2.14945900	0.56161200
C	3.12929600	-1.53626200	0.28414100
H	1.96367600	-3.06690800	1.13209600
C	4.44392800	-1.03873000	0.14995800
C	5.30666700	-1.59284500	-0.81935500
C	4.92544200	-0.05131200	1.03780400
C	6.62697000	-1.16748000	-0.89309700
H	4.92129500	-2.34255500	-1.50194800
C	6.24386500	0.37021300	0.94614600
H	4.23887600	0.39458900	1.74667000
C	7.09615500	-0.18579800	-0.01494400
H	7.29117600	-1.59316600	-1.63909600
H	6.61125600	1.13970800	1.61808100
H	8.12645500	0.15131200	-0.08279600

Zero-point correction= 0.401967 (Hartree/Particle)
Thermal correction to Energy= 0.433503
Thermal correction to Enthalpy= 0.434447
Thermal correction to Gibbs Free Energy= 0.331365
Sum of electronic and zero-point Energies= -2215.736152
Sum of electronic and thermal Energies= -2215.704617
Sum of electronic and thermal Enthalpies= -2215.703673
Sum of electronic and thermal Free Energies= -2215.806754
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2216.921539

INT8-a

P	-2.01006700	-0.21269600	-0.03502400
C	-3.23626600	-1.27546500	-0.86657900
C	-3.06434100	-2.66479000	-0.78417600
C	-4.34192300	-0.75306400	-1.55142700
C	-3.99799400	-3.52160100	-1.36596200
H	-2.19501800	-3.06694700	-0.27090500
C	-5.26981900	-1.61359700	-2.13722800
H	-4.47007400	0.32137800	-1.63373600
C	-5.10086500	-2.99676200	-2.04250100
H	-3.85885500	-4.59660500	-1.29953600
H	-6.12246400	-1.20405900	-2.67117100
H	-5.82391500	-3.66430100	-2.50235700
C	-2.02383400	1.39540300	-0.90099600
C	-1.00162200	1.67653300	-1.81815500
C	-3.00187400	2.36509700	-0.63413100
C	-0.96206100	2.91104400	-2.46504300
H	-0.22258700	0.94327100	-2.00182700
C	-2.96415100	3.59405500	-1.29132300
H	-3.77654600	2.16524300	0.10009900
C	-1.94381300	3.86842100	-2.20534500
H	-0.15499100	3.12747500	-3.15825200
H	-3.72266400	4.34231900	-1.07989700
H	-1.90810200	4.83253800	-2.70446900
C	-2.72355700	0.17864900	1.60120600
C	-1.93854900	0.95147700	2.47298300
C	-3.98982600	-0.25627000	2.00579600
C	-2.42503100	1.28989800	3.73263900
H	-0.95543500	1.28692400	2.15364300
C	-4.46939000	0.08128300	3.27372400
H	-4.59821300	-0.85563300	1.33638200
C	-3.69059500	0.85295800	4.13581300
H	-1.81530300	1.88910400	4.40246800
H	-5.45228900	-0.26056300	3.58533800
H	-4.06590700	1.11270100	5.12147900
Au	0.21829600	-0.99104100	0.14243500
S	2.72366700	0.89374800	-1.22677500
C	2.26240100	2.15779700	-0.00888100
F	1.16745700	1.86151800	0.72688400
F	3.24022500	2.43995700	0.87562600
F	1.98185400	3.28371600	-0.69581800
C	2.22005900	-1.32426500	0.31803200
C	3.18301600	-0.52764600	-0.19014800
H	2.59221200	-2.14669600	0.93239100
C	4.64103800	-0.77799000	-0.05037300
C	5.12157200	-2.09901300	-0.06374400
C	5.56798800	0.26407100	0.11263500
C	6.47770700	-2.37028900	0.10364500
H	4.42216700	-2.91313800	-0.22739300
C	6.92420100	-0.00826100	0.28057900
H	5.21899600	1.28971300	0.12281200
C	7.38682100	-1.32536700	0.27836200
H	6.82645600	-3.39932300	0.08263800
H	7.62226700	0.81366200	0.41489300
H	8.44563200	-1.53490600	0.40213400

Zero-point correction= 0.405863 (Hartree/Particle)
Thermal correction to Energy= 0.436777
Thermal correction to Enthalpy= 0.437721
Thermal correction to Gibbs Free Energy= 0.336004
Sum of electronic and zero-point Energies= -2215.785335
Sum of electronic and thermal Energies= -2215.754420
Sum of electronic and thermal Enthalpies= -2215.753476
Sum of electronic and thermal Free Energies= -2215.855194
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2216.964799

TS6´-a

P	1.35572300	0.58167000	0.00559600
C	1.38580500	2.36102000	-0.40599000
C	0.32813300	3.15691400	0.06321500
C	2.41207200	2.94595400	-1.15635500
C	0.30668600	4.52260500	-0.20724800
H	-0.47803700	2.69875400	0.62944700
C	2.38071600	4.31481000	-1.43258700
H	3.22783100	2.33607500	-1.52939300
C	1.33258300	5.10357200	-0.95848700
H	-0.51433100	5.13142500	0.16030600
H	3.17626300	4.76195400	-2.02157400
H	1.31048200	6.16718300	-1.17754900
C	2.68302600	-0.20849800	-0.95825500
C	2.34511000	-0.99150500	-2.06987800
C	4.03025500	-0.05185400	-0.59623800
C	3.35050500	-1.59511300	-2.82598500
H	1.30185000	-1.15400600	-2.31933000
C	5.02918600	-0.65422600	-1.35781800
H	4.29194400	0.52897800	0.28314300
C	4.68960800	-1.42384000	-2.47427200
H	3.08270700	-2.21040500	-3.67941000
H	6.07092800	-0.53209400	-1.07565100

H	5.47014000	-1.89996400	-3.06079300
C	1.90460900	0.48177800	1.74161600
C	1.66205300	-0.70826000	2.44439700
C	2.58643700	1.53617200	2.36309700
C	2.11078200	-0.83938600	3.75729100
H	1.11886400	-1.51978600	1.97046800
C	3.02932200	1.39735600	3.67909400
H	2.76384100	2.46152100	1.82435400
C	2.79359100	0.21100100	4.37558500
H	1.91928100	-1.76071700	4.29917600
H	3.55489800	2.21752100	4.15978000
H	3.13633000	0.10674800	5.40105000
Au	-0.73741900	-0.31089000	-0.33399500
S	-0.85339100	-3.10488700	-1.29995600
C	-0.83049600	-3.81951800	0.32987500
F	0.11357500	-4.77502000	0.48798200
F	-0.59372200	-2.90771000	1.33921600
F	-2.01952400	-4.39570900	0.66899700
C	-4.07832500	3.12803100	-0.28842400
C	-3.28626200	2.01010300	-0.54025000
C	-3.74343500	0.72373500	-0.21104800
C	-5.00871200	0.58456100	0.38559500
C	-5.79112200	1.70614500	0.64910800
C	-5.33053600	2.98113000	0.31143900
H	-3.71366400	4.11571400	-0.55683600
H	-2.30816000	2.11897600	-0.99754300
H	-5.36344000	-0.40712000	0.64818600
H	-6.76371900	1.58448500	1.11749100
H	-5.94381200	3.85386900	0.51665900
C	-2.92435800	-0.45722700	-0.47740500
C	-3.01177600	-1.69770800	-0.67095900
H	-3.40139500	-2.68620900	-0.77141700

Zero-point correction= 0.401985 (Hartree/Particle)
Thermal correction to Energy= 0.433681
Thermal correction to Enthalpy= 0.434625
Thermal correction to Gibbs Free Energy= 0.329265
Sum of electronic and zero-point Energies= -2215.724838
Sum of electronic and thermal Energies= -2215.693143
Sum of electronic and thermal Enthalpies= -2215.692199
Sum of electronic and thermal Free Energies= -2215.797558
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2216.582989

INT8´-a

P	1.67344400	0.30223400	-0.03128800
C	2.58524800	0.61060200	-1.58126900
C	2.04389500	1.52577900	-2.49598400
C	3.80316000	-0.01995600	-1.86916100
C	2.72342400	1.81886200	-3.67727200
H	1.08803900	1.99654400	-2.28231900
C	4.47736200	0.27342700	-3.05474800
H	4.21608700	-0.74293200	-1.17283500
C	3.94045200	1.19354300	-3.95726900
H	2.29818800	2.52664300	-4.38267600
H	5.41905000	-0.22087000	-3.27553800
H	4.46542300	1.41664400	-4.88164400
C	2.23612600	-1.32907800	0.56400400
C	1.48316000	-2.45679500	0.20560100
C	3.37329300	-1.47999700	1.36997200
C	1.86586400	-3.72247900	0.64582600
H	0.59327300	-2.34008700	-0.40399800
C	3.75675200	-2.74989800	1.80123600
H	3.94691300	-0.60786600	1.66837900
C	3.00358000	-3.87002600	1.44140700
H	1.25895100	-4.58259800	0.38290600
H	4.63731300	-2.86318200	2.42719300
H	3.29797800	-4.85563200	1.79062100
C	2.34556100	1.50166600	1.17037900
C	1.59778900	1.75631200	2.32994000
C	3.57406200	2.14785000	0.98249700
C	2.08211800	2.63608200	3.29584600
H	0.63783900	1.26565000	2.46740500
C	4.05232100	3.03261000	1.95017000
H	4.15051800	1.96440000	0.08147200
C	3.30964600	3.27574300	3.10657900
H	1.49858200	2.82857900	4.19135500
H	5.00391100	3.53385000	1.79799600
H	3.68308700	3.96699800	3.85659200
Au	-0.68225800	0.33185700	-0.25515900
S	-2.32671500	-2.44210800	-1.19992000
C	-2.15219100	-3.28579500	0.40049100
F	-1.53888500	-2.53693200	1.33779300
F	-3.32311100	-3.68315100	0.92730800
F	-1.39007200	-4.38726700	0.20030100
C	-4.10304500	3.33064300	1.16743000
C	-3.26822200	2.25690300	0.86747200
C	-3.61195100	1.32557100	-0.12830900
C	-4.80818400	1.53207800	-0.83969700
C	-5.63603100	2.61572500	-0.55228300
C	-5.29148700	3.51638200	0.45733600
H	-3.82149500	4.03003900	1.95017800
H	-2.33685900	2.12024800	1.41051600
H	-5.07122300	0.84762100	-1.64053900
H	-6.54993400	2.76072400	-1.12236100
H	-5.93609100	4.36212700	0.68002200
C	-2.72982500	0.17342200	-0.41344700
C	-3.28964000	-1.01552700	-0.71705600
H	-4.36619700	-1.17911500	-0.72392300

Zero-point correction= 0.405800 (Hartree/Particle)
Thermal correction to Energy= 0.436792
Thermal correction to Enthalpy= 0.437736
Thermal correction to Gibbs Free Energy= 0.335861
Sum of electronic and zero-point Energies= -2215.788907
Sum of electronic and thermal Energies= -2215.757916
Sum of electronic and thermal Enthalpies= -2215.756972
Sum of electronic and thermal Free Energies= -2215.858847
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2216.970835

TS7-a

P	-0.24676800	2.01954200	0.44174100
C	-0.61732100	1.41646400	2.10834100
C	0.25126300	0.44988100	2.64791700
C	-1.74366400	1.83318300	2.82961000
C	-0.01984200	-0.09808700	3.89838600
H	1.12937500	0.13422400	2.09167900

C	-2.01183000	1.26755800	4.07761400
H	-2.40566800	2.58952100	2.42337600
C	-1.15585800	0.30108000	4.60916500
H	0.65025600	-0.84372900	4.31448200
H	-2.88543600	1.58925200	4.63604600
H	-1.36877700	-0.13501700	5.58046000
C	-1.58646300	3.06778900	-0.16938700
C	-2.91291200	2.60051200	-0.16129000
C	-1.29521600	4.32501000	-0.72396900
C	-3.93073900	3.37664100	-0.70820200
H	-3.14597400	1.63398100	0.26620100
C	-2.32212000	5.09791000	-1.26343700
H	-0.27745000	4.69765700	-0.72970200
C	-3.63543400	4.62449100	-1.26230700
H	-4.94470600	2.99336500	-0.73210200
H	-2.09306000	6.07040500	-1.68758700
H	-4.42904900	5.22407100	-1.69677200
C	1.26860700	3.00011500	0.51982000
C	1.99323400	3.23433000	-0.65865300
C	1.72631100	3.50828400	1.74414200
C	3.16299800	3.98730600	-0.61356000
H	1.66147800	2.80831000	-1.60123000
C	2.89898700	4.25964400	1.77932400
H	1.17439700	3.31659400	2.65780000
C	3.61543800	4.49949400	0.60434400
H	3.73101000	4.14985000	-1.52293600
H	3.25493600	4.65532400	2.72541300
H	4.53308800	5.07853200	0.63940400
Au	0.29390000	0.06991700	-0.82723800
C	1.98285500	-2.70240000	-0.51214300
F	1.43684700	-2.32110300	0.66325300
F	1.30553800	-3.77309900	-0.94516400
F	3.24672600	-3.08269100	-0.26102600
C	-1.66668800	-4.22473100	0.16243600
C	-1.62132000	-3.09305100	-0.64017900
C	-1.81314300	-1.81721400	-0.06601100
C	-2.02686800	-1.69721300	1.32454700
C	-2.07148600	-2.83667100	2.11399500
C	-1.88654600	-4.09944600	1.53874700
H	-1.52574800	-5.20537300	-0.28038500
H	-1.44764300	-3.17128400	-1.70790200
H	-2.18631000	-0.72003100	1.76090100
H	-2.25272400	-2.74252700	3.17965700
H	-1.91558800	-4.98718300	2.16320800
C	-1.75583400	-0.65242100	-0.91043000
C	-2.57348300	-0.03463200	-1.73501600
H	-2.33740100	0.83913300	-2.33326100
S	-4.30451800	-0.54027400	-2.02587200
O	-5.00409100	0.73273800	-2.25546800
O	-4.29380300	-1.61199100	-3.02727200
C	-4.86320300	-1.22132000	-0.47057300
C	-4.92776600	-2.60626800	-0.32550400
C	-5.22469300	-0.35272100	0.56104800
C	-5.34095100	-3.13206400	0.89775900
H	-4.66030800	-3.24666400	-1.15739100
C	-5.62959500	-0.89131500	1.78061800
H	-5.21654900	0.71912100	0.39979000
C	-5.68181100	-2.27799300	1.94861500
H	-5.39640400	-4.20788800	1.02863400
H	-5.92149200	-0.23201900	2.59220700
H	-6.00316400	-2.69370200	2.89882700
S	1.96980300	-1.38175500	-1.77833000
S	3.89336000	0.07364700	-0.53798300
O	4.14466800	1.10683600	-1.56114000
O	3.14800500	0.38350700	0.70595800
C	5.40616100	-0.76624800	-0.12722200
C	5.48553800	-1.45949700	1.08389800
C	6.43162100	-0.78338800	-1.07681900
C	6.65740900	-2.15586700	1.36551900
H	4.65906900	-1.43340900	1.78397400
C	7.59495100	-1.48720000	-0.77425000
H	6.32367300	-0.24213700	-2.00984900
C	7.70599300	-2.17108900	0.43996000
H	6.75382100	-2.68716800	2.30692900
H	8.41408700	-1.50131000	-1.48588600
H	8.61364800	-2.72215300	0.66538700

Zero-point correction= 0.608476 (Hartree/Particle)
Thermal correction to Energy= 0.656941
Thermal correction to Enthalpy= 0.657885
Thermal correction to Gibbs Free Energy= 0.516469
Sum of electronic and zero-point Energies= -3775.850089
Sum of electronic and thermal Energies= -3775.801624
Sum of electronic and thermal Enthalpies= -3775.800680
Sum of electronic and thermal Free Energies= -3775.942096
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-3777.5524784

b

C	0.11209700	-1.38851000	-0.12885600
C	-1.04249500	-1.75419700	-0.14617400
C	-2.47112300	-2.08823700	-0.13541800
H	-2.66509200	-2.95051700	-0.78368400
H	-2.76237200	-2.37888600	0.88881600
O	-3.32399900	-1.06194500	-0.61423000
C	-3.30323900	0.14453300	0.16501200
H	-4.32402200	0.53889700	0.08560700
H	-3.12518800	-0.09336300	1.22123900
C	-2.32969900	1.15790700	-0.36554500
H	-2.51098400	1.43416700	-1.40410600
C	-1.30500900	1.73718800	0.27468100
C	-0.43754800	2.75568400	-0.42220400
H	-0.45700100	3.71874800	0.10682100
H	0.60931700	2.42550500	-0.43757000
H	-0.75947700	2.92765200	-1.45394800
C	-0.89115800	1.43991700	1.69236600
H	-1.50018900	0.67085100	2.17102700
H	0.15168300	1.09838700	1.71057500
H	-0.93978700	2.34692500	2.31016900
C	1.44488100	-0.88337800	-0.12997000
C	2.32833700	-1.16463600	0.92820800
C	1.88219200	-0.05939300	-1.18454200
C	3.61509700	-0.63279400	0.92897500
H	1.99183200	-1.79808500	1.74274200
C	3.16865500	0.47196100	-1.17349900
H	1.19808500	0.15889000	-1.99784400

C	4.03898900	0.18754300	-0.11851900
H	4.28865400	-0.85689200	1.75125500
H	3.49409000	1.10888500	-1.99111900
H	5.04258100	0.60286900	-0.11322800

Zero-point correction= 0.262503 (Hartree/Particle)
Thermal correction to Energy= 0.277819
Thermal correction to Enthalpy= 0.278763
Thermal correction to Gibbs Free Energy= 0.217915
Sum of electronic and zero-point Energies= -618.050746
Sum of electronic and thermal Energies= -618.035430
Sum of electronic and thermal Enthalpies= -618.034485
Sum of electronic and thermal Free Energies= -618.095334
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-618.4906998

b´

C	-0.16605400	-1.45801400	-0.02519400
C	-1.32650800	-1.90081000	-0.03990600
C	-2.77501500	-1.88587900	-0.01754500
H	-3.20799300	-2.60929700	-0.72376000
H	-3.12576500	-2.17755400	0.99017500
O	-3.49519400	-0.65798500	-0.38727700
C	-3.05946500	0.51186800	0.29596400
H	-3.96327400	1.13814100	0.38240500
H	-2.73555300	0.26863900	1.31738600
C	-1.99473800	1.25703000	-0.45905600
H	-2.19731000	1.32263600	-1.52882400
C	-0.85440500	1.78772200	0.00578900
C	0.12990800	2.44670700	-0.92640600
H	0.38932000	3.46252300	-0.58927800
H	1.06142500	1.86562900	-0.96193900
H	-0.26519800	2.51612800	-1.94629800
C	-0.42024200	1.76257100	1.44732500
H	-1.07544900	1.15513200	2.07667500
H	0.59380700	1.35175600	1.52848300
H	-0.39763400	2.78155300	1.86613700
C	1.15157600	-1.02711700	-0.02463700
C	1.89474200	-0.81217900	1.19964200
C	1.86054300	-0.72182600	-1.24758800
C	3.19122200	-0.33852000	1.18529800
H	1.40506300	-1.04015100	2.14411100
C	3.15586100	-0.24784400	-1.23516000
H	1.33786600	-0.86567200	-2.19072000
C	3.86330400	-0.04326900	-0.02386200
H	3.70938500	-0.19401700	2.13467800
H	3.64581600	-0.02780000	-2.18484200
H	4.88267200	0.33359200	-0.02415100

Zero-point correction= 0.256955 (Hartree/Particle)
Thermal correction to Energy= 0.272658
Thermal correction to Enthalpy= 0.273602
Thermal correction to Gibbs Free Energy= 0.212768
Sum of electronic and zero-point Energies= -618.035164
Sum of electronic and thermal Energies= -618.019461
Sum of electronic and thermal Enthalpies= -618.018517
Sum of electronic and thermal Free Energies= -618.079352
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-618.524261

b´´

C	0.25726300	-0.96169300	0.39393600
C	-0.94696200	-1.20413800	0.50505600
C	-2.25611300	-1.81576200	0.80917800
H	-2.11667900	-2.89500100	0.93778200
H	-2.63765300	-1.40336800	1.75667600
O	-3.18567700	-1.64930600	-0.23864400
C	-3.44308000	-0.26328500	-0.45943700
H	-4.17676500	-0.22981600	-1.27154800
H	-3.89413200	0.19043600	0.43174100
C	-2.17950000	0.42540100	-0.88360900
H	-1.73050600	0.02067300	-1.78788400
C	-1.60123100	1.54651900	-0.32737500
C	-0.35198200	2.10714900	-0.92570200
H	-0.47455000	3.17687500	-1.13890500
H	0.47355300	2.03373200	-0.20293300
H	-0.05652700	1.59536000	-1.84404300
C	-2.13954600	2.26267500	0.87036000
H	-2.91513900	1.71277100	1.40416300
H	-1.32832300	2.50152900	1.56800000
H	-2.56583800	3.22606400	0.55672200
C	1.59616100	-0.60398300	0.22087300
C	2.27810800	0.12090300	1.23765400
C	2.28147800	-0.96424900	-0.97125500
C	3.60357400	0.47510800	1.05585800
H	1.74908700	0.37908700	2.14886500
C	3.60597800	-0.59926900	-1.13690300
H	1.75484100	-1.52564800	-1.73539300
C	4.26759100	0.11823800	-0.12788500
H	4.13062700	1.02428300	1.82883100
H	4.13511800	-0.87151600	-2.04396500
H	5.30786600	0.39730200	-0.26346400

Zero-point correction= 0.261709 (Hartree/Particle)
Thermal correction to Energy= 0.277226
Thermal correction to Enthalpy= 0.278170
Thermal correction to Gibbs Free Energy= 0.216715
Sum of electronic and zero-point Energies= -617.786038
Sum of electronic and thermal Energies= -617.770521
Sum of electronic and thermal Enthalpies= -617.769577
Sum of electronic and thermal Free Energies= -617.831033
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-618.2538133

INT19´-b

P	-1.71519500	0.44628100	-0.00286300
C	-1.76205200	0.28674000	1.81595500
C	-0.96099700	1.16311600	2.56639200
C	-2.47748800	-0.72357700	2.46904600
C	-0.89454900	1.04024300	3.95122900
H	-0.38184900	1.93101000	2.06061500
C	-2.39828000	-0.85018700	3.85802700
H	-3.09021100	-1.41131200	1.89625400
C	-1.61125400	0.03012500	4.60009000
H	-0.27268400	1.72218400	4.52367500
H	-2.95242200	-1.63975500	4.35741900
H	-1.54920400	-0.07268300	5.67952000
C	-2.90421200	-0.78849500	-0.63403200
C	-2.41374700	-1.95336100	-1.24430400
C	-4.28840200	-0.60514000	-0.49730200

C	-3.30461000	-2.92895300	-1.69513500
H	-1.34432100	-2.09122100	-1.38110800
C	-5.17172100	-1.58280900	-0.95069500
H	-4.67200800	0.30370800	-0.04359000
C	-4.68004900	-2.74735000	-1.54701700
H	-2.91890900	-3.82670400	-2.16919800
H	-6.24254300	-1.43487900	-0.84365800
H	-5.37052900	-3.50716000	-1.90215000
C	-2.46299400	2.07328800	-0.35067200
C	-2.14325700	2.69644400	-1.56571300
C	-3.34706900	2.70007600	0.53887000
C	-2.71738300	3.92351900	-1.89440800
H	-1.43850000	2.22021800	-2.24215600
C	-3.91483700	3.93032400	0.20772300
H	-3.57949100	2.23189000	1.49036800
C	-3.60368100	4.54085500	-1.00900600
H	-2.46471500	4.40214300	-2.83598300
H	-4.59735100	4.41336900	0.90118500
H	-4.04462200	5.50051300	-1.26297800
Au	0.45862900	-0.03229000	-0.79049500
C	3.37747000	-0.16149900	-0.98220600
C	2.30755000	-0.80810100	-1.32118800
C	2.26083800	-2.14915600	-2.03786400
H	2.21948700	-1.95853000	-3.11589500
H	3.17150200	-2.73224700	-1.83064500
O	1.10951900	-2.95051600	-1.77877200
C	1.16982200	-3.73464000	-0.58118600
H	0.38233700	-4.48556500	-0.71206300
H	2.13070300	-4.26590600	-0.54597400
C	0.92638300	-2.94703900	0.67490700
H	-0.10541300	-2.63218000	0.82832500
C	1.84495500	-2.54015500	1.56428700
C	1.45663600	-1.62564100	2.69552300
H	1.81670400	-2.00151300	3.66260000
H	1.91302900	-0.63613500	2.54691400
H	0.37513900	-1.48455100	2.75549900
C	3.31656700	-2.84345100	1.46720200
H	3.54219400	-3.68873600	0.81333500
H	3.84644400	-1.97062400	1.06289100
H	3.73911000	-3.05687700	2.45669200
C	4.19714800	0.85410100	-0.50207000
C	4.70821100	1.86020700	-1.37682200
C	4.57956800	0.92223000	0.87199900
C	5.54234800	2.85968400	-0.90121900
H	4.42657900	1.82575700	-2.42477300
C	5.41446100	1.93011800	1.32914700
H	4.19475700	0.17455600	1.55801000
C	5.90818100	2.90567600	0.45185000
H	5.91475800	3.61632200	-1.58736800
H	5.68551700	1.96283300	2.38163700
H	6.56525800	3.68971100	0.81639800

Zero-point correction= 0.538588 (Hartree/Particle)
Thermal correction to Energy= 0.573392
Thermal correction to Enthalpy= 0.574336
Thermal correction to Gibbs Free Energy= 0.464558
Sum of electronic and zero-point Energies= -1789.659104
Sum of electronic and thermal Energies= -1789.624299
Sum of electronic and thermal Enthalpies= -1789.623355
Sum of electronic and thermal Free Energies= -1789.733134
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1790.922466

INT19´´-b

P	-1.60142900	0.57589600	0.09935400
C	-2.02367300	0.55747000	1.84960900
C	-1.09690600	1.09375400	2.76734700
C	-3.21206800	-0.02875500	2.31054800
C	-1.37792500	1.06774800	4.13051400
H	-0.16716100	1.53202300	2.41351600
C	-3.47805600	-0.05923700	3.67962500
H	-3.92424500	-0.45068700	1.61005500
C	-2.56718100	0.48904900	4.58719700
H	-0.67266500	1.49383600	4.83690700
H	-4.40096300	-0.50431100	4.03717200
H	-2.78361100	0.46655200	5.65047500
C	-2.90269000	-0.15493900	-0.91331700
C	-2.64813800	-1.26450300	-1.73641000
C	-4.17438700	0.44899200	-0.91050700
C	-3.67168300	-1.78221700	-2.52990200
H	-1.65757400	-1.70599600	-1.78696300
C	-5.18987600	-0.08349100	-1.69955800
H	-4.36676800	1.32593800	-0.29917200
C	-4.94003900	-1.19933500	-2.50567500
H	-3.47572000	-2.63527600	-3.17143600
H	-6.17333900	0.37517900	-1.69280200
H	-5.73408300	-1.60635900	-3.12352900
C	-1.35456600	2.27752200	-0.46084200
C	-1.00344100	2.45294600	-1.82122000
C	-1.49410500	3.39257300	0.38274900
C	-0.80087800	3.73211200	-2.32398600
H	-0.92124200	1.58982000	-2.47645000
C	-1.29298200	4.66902900	-0.13386600
H	-1.78229400	3.26567700	1.41993600
C	-0.94181200	4.84061600	-1.48095100
H	-0.54516700	3.87029500	-3.36938800
H	-1.42297700	5.53562200	0.50627800
H	-0.79125300	5.84101500	-1.87414800
Au	0.47761400	-0.43792400	-0.36004800
C	3.17804600	-0.47810900	-0.89816400
C	2.28103900	-1.22382200	-1.34789600
C	1.93899200	-2.31770900	-2.32286100
H	1.84113800	-1.88163300	-3.32037400
H	2.75798600	-3.04921200	-2.33984500
O	0.70411400	-2.95352100	-2.05418400
C	0.69053900	-3.68734800	-0.82853400
H	0.09647000	-4.58865500	-1.02016200
H	1.70228200	-4.00853600	-0.56196500
C	0.01717400	-2.94244000	0.30235200
H	-1.05855200	-2.81720700	0.19549800
C	0.55317100	-2.72106700	1.56488600
C	-0.32839200	-2.30942600	2.69722700
H	-0.27544600	-3.07365800	3.48584600
H	0.02477200	-1.37778300	3.15435100
H	-1.37096900	-2.18555900	2.40266600
C	1.99438900	-2.95503600	1.89643800

H	2.64641200	-2.94877700	1.02222900
H	2.34697300	-2.20478300	2.61203100
H	2.09902200	-3.92997200	2.39468100
C	4.13395600	0.39097800	-0.35675300
C	4.32300700	1.67742300	-0.92349200
C	4.94421300	-0.03348100	0.72686300
C	5.30327300	2.51361400	-0.41168300
H	3.70448800	1.98723700	-1.75938600
C	5.92101000	0.81432100	1.22565100
H	4.79997700	-1.02393300	1.14568800
C	6.10006700	2.08346300	0.65809300
H	5.45975000	3.49608600	-0.84415300
H	6.55103800	0.49398000	2.04860800
H	6.87025600	2.74064100	1.04988300

Zero-point correction= 0.540289 (Hartree/Particle)
Thermal correction to Energy= 0.575198
Thermal correction to Enthalpy= 0.576142
Thermal correction to Gibbs Free Energy= 0.466080
Sum of electronic and zero-point Energies= -1789.135332
Sum of electronic and thermal Energies= -1789.100423
Sum of electronic and thermal Enthalpies= -1789.099479
Sum of electronic and thermal Free Energies= -1789.209541
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1790.504579

INT20-b

C	-5.49751700	1.12253000	0.04062400
C	-4.88344600	2.16690100	0.09011400
C	-4.15696400	3.43690400	0.16187800
H	-4.75236000	4.23700700	-0.28941100
H	-3.98610800	3.70682500	1.21612200
O	-2.91917800	3.46268700	-0.54852500
C	-1.87706300	2.68064000	0.00692700
H	-0.95064800	3.17605700	-0.29784900
H	-1.91567300	2.68398800	1.10397600
C	-1.91635000	1.26925000	-0.56022300
H	-1.94303600	1.25331500	-1.65076600
C	-2.31644000	0.10967200	0.08270200
C	-2.68370000	-1.11124300	-0.71943100
H	-2.25332500	-2.02137300	-0.28880200
H	-3.77513700	-1.22355100	-0.68725800
H	-2.37715900	-1.02824500	-1.76517200
C	-2.57532900	0.00431000	1.56075500
H	-2.27299200	0.88985600	2.12068300
H	-3.65048100	-0.15082600	1.70755400
H	-2.06121100	-0.86768100	1.97931300
C	-6.17811200	-0.13136800	-0.00305600
C	-6.51827800	-0.79739700	1.19034000
C	-6.49141500	-0.73058900	-1.23864400
C	-7.15221600	-2.03623100	1.14469800
H	-6.29289200	-0.32787900	2.14298500
C	-7.12214200	-1.97145200	-1.27386900
H	-6.23915900	-0.21159200	-2.15785100
C	-7.45259700	-2.62706500	-0.08498900
H	-7.41672200	-2.53980100	2.06956200
H	-7.36291800	-2.42529000	-2.23040400
H	-7.94841100	-3.59239600	-0.11702300
P	2.41900600	-0.21249500	0.00403800
C	2.69942700	-1.45156900	1.30009100
C	1.81682800	-2.53802700	1.40120800
C	3.79945900	-1.35742800	2.16283700
C	2.03994200	-3.52754600	2.35521200
H	0.96314600	-2.60790900	0.73157800
C	4.01361300	-2.35059300	3.11957300
H	4.48010900	-0.51568500	2.08936800
C	3.13750700	-3.43275600	3.21583900
H	1.35806200	-4.36875400	2.43183200
H	4.86415200	-2.27645000	3.78995900
H	3.30678300	-4.20180000	3.96311800
C	3.40626900	1.24949000	0.42663900
C	2.90792000	2.15288600	1.37824000
C	4.66569700	1.46051400	-0.15055500
C	3.67036900	3.25573200	1.75460900
H	1.92931200	1.98901300	1.82252000
C	5.42151600	2.57057200	0.22842100
H	5.05020700	0.76642500	-0.89056000
C	4.92649600	3.46544000	1.17834400
H	3.28449600	3.95400900	2.49072600
H	6.39553000	2.73631800	-0.22115100
H	5.51673100	4.32935600	1.46775400
C	3.07579000	-0.88823100	-1.54507900
C	2.65978900	-0.32628800	-2.76184400
C	4.02042900	-1.92377200	-1.53516800
C	3.19374500	-0.79331800	-3.96044200
H	1.92371700	0.47365400	-2.76810100
C	4.54751400	-2.38867600	-2.74035200
H	4.33818300	-2.36386900	-0.59560700
C	4.13648700	-1.82509300	-3.94960500
H	2.87154500	-0.35828400	-4.90129100
H	5.27696500	-3.19253800	-2.73357500
H	4.54716600	-2.19207000	-4.88512400
Au	0.15515300	0.32074600	-0.17688900

Zero-point correction= 0.540800 (Hartree/Particle)
Thermal correction to Energy= 0.575857
Thermal correction to Enthalpy= 0.576802
Thermal correction to Gibbs Free Energy= 0.463998
Sum of electronic and zero-point Energies= -1789.488474
Sum of electronic and thermal Energies= -1789.453417
Sum of electronic and thermal Enthalpies= -1789.452473
Sum of electronic and thermal Free Energies= -1789.565276
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1790.782199

INT20´-b

C	5.65588800	0.93213500	-0.01893900
C	4.93501700	1.90587900	-0.08162900
C	4.16051400	3.15388400	-0.12985400
H	4.85001100	3.99818400	0.00699500
H	3.70647600	3.26785100	-1.12710200
O	3.18046400	3.28063500	0.88175700
C	1.87889300	2.76918000	0.55390800
H	1.22840800	3.19784400	1.31964500
H	1.56701500	3.17955700	-0.41831200
C	1.77751500	1.24955000	0.57779000
H	2.11035400	0.88798700	1.55626800
C	2.38043100	0.47680700	-0.50101200

C	2.87165400	-0.91180000	-0.23427400
H	2.13960600	-1.67611000	-0.55388800
H	3.79875300	-1.11909800	-0.78504200
H	3.07223800	-1.07450000	0.82973800
C	2.21698600	0.84238700	-1.94619900
H	1.83153100	1.85624500	-2.08809300
H	3.17234800	0.76230100	-2.48506900
H	1.51205300	0.15974200	-2.45442100
C	6.44217300	-0.25347000	0.05241900
C	7.12324500	-0.73546700	-1.08219900
C	6.54159100	-0.97107300	1.26053300
C	7.87965600	-1.90178800	-1.00690300
H	7.04752800	-0.18560300	-2.01498500
C	7.29831200	-2.13735500	1.32602000
H	6.01597900	-0.60190700	2.13524800
C	7.97040900	-2.60778300	0.19506400
H	8.39959700	-2.26236900	-1.89020000
H	7.36420400	-2.68223400	2.26370500
H	8.56044600	-3.51813900	0.25004500
P	-2.48873900	-0.23484200	0.02454300
C	-2.55029200	-1.02944600	-1.61850300
C	-1.40542000	-1.71611700	-2.05440200
C	-3.67677100	-0.96790600	-2.45010700
C	-1.39685400	-2.34699400	-3.29693200
H	-0.52267300	-1.74469800	-1.42106000
C	-3.66114800	-1.59627600	-3.69593000
H	-4.56007800	-0.42772400	-2.12452600
C	-2.52438900	-2.28753600	-4.11959300
H	-0.50703200	-2.87525800	-3.62677700
H	-4.53715400	-1.54396000	-4.33628000
H	-2.51431500	-2.77282900	-5.09133800
C	-3.85071300	0.97937600	0.01000700
C	-3.57908000	2.26043700	-0.49436800
C	-5.14098600	0.67313500	0.46295800
C	-4.59172900	3.21569000	-0.56162200
H	-2.57251300	2.50321100	-0.82448100
C	-6.14998500	1.63493300	0.39958600
H	-5.35311200	-0.31249800	0.86492200
C	-5.87795300	2.90411000	-0.11467100
H	-4.37481900	4.20533500	-0.95304700
H	-7.14800200	1.39282000	0.75374200
H	-6.66487300	3.65149900	-0.16072400
C	-3.01465300	-1.52715300	1.19908800
C	-2.68589700	-1.35550500	2.55269100
C	-3.73096700	-2.66380500	0.79954400
C	-3.08527400	-2.30125600	3.49533700
H	-2.11016300	-0.48577300	2.85797200
C	-4.12343800	-3.61049700	1.74627500
H	-3.97648800	-2.80716100	-0.24796300
C	-3.80438200	-3.42941400	3.09351400
H	-2.82673300	-2.16292500	4.54112300
H	-4.67678400	-4.49049100	1.43077900
H	-4.10917200	-4.16937600	3.82801800
Au	-0.30037200	0.67400600	0.46376400

Zero-point correction= 0.537326 (Hartree/Particle)
Thermal correction to Energy= 0.572815
Thermal correction to Enthalpy= 0.573759
Thermal correction to Gibbs Free Energy= 0.457809
Sum of electronic and zero-point Energies= -1789.632324
Sum of electronic and thermal Energies= -1789.596835
Sum of electronic and thermal Enthalpies= -1789.595891
Sum of electronic and thermal Free Energies= -1789.711841
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1790.896511

INT20´´-b

C	-5.56138000	0.86679400	-0.05884500
C	-4.82847800	1.80840400	0.22551700
C	-4.05781000	3.01712800	0.53005300
H	-4.72453200	3.87703500	0.37104100
H	-3.77904600	3.02453200	1.59566300
O	-2.94168600	3.21957500	-0.30633300
C	-1.76062500	2.53157300	0.09642700
H	-0.96413600	2.97991300	-0.50021900
H	-1.54419500	2.72211900	1.15487900
C	-1.87979700	1.05065400	-0.20921700
H	-2.02522700	0.83498600	-1.26842700
C	-2.19768300	0.03538200	0.68133200
C	-2.64098500	-1.30835600	0.16510600
H	-2.13049700	-2.12621900	0.68357600
H	-3.71357400	-1.42472900	0.37272500
H	-2.48422200	-1.41353200	-0.91120200
C	-2.27267000	0.20910500	2.17533700
H	-1.87251800	1.16012000	2.52811400
H	-3.32262600	0.13476800	2.48769800
H	-1.73813600	-0.60040000	2.68315100
C	-6.41455700	-0.19292400	-0.37832300
C	-7.35648800	-0.66630900	0.58682100
C	-6.36660300	-0.78554900	-1.67767600
C	-8.21856800	-1.69089000	0.25378300
H	-7.38720700	-0.20229100	1.56647400
C	-7.23544700	-1.80964700	-1.99309700
H	-5.65552700	-0.40728000	-2.40379400
C	-8.16320500	-2.26489200	-1.03292200
H	-8.94299500	-2.05246000	0.97558900
H	-7.21536100	-2.26050800	-2.97944700
H	-8.84841900	-3.06673000	-1.29026800
P	2.56940000	-0.25487900	0.06742500
C	2.99677700	-1.42226000	1.37730400
C	2.24071800	-2.60286200	1.50512500
C	4.08560800	-1.18194400	2.22942300
C	2.58467500	-3.54141100	2.47188500
H	1.39869300	-2.78424400	0.84181500
C	4.41876500	-2.12669800	3.19884600
H	4.66946500	-0.27328900	2.13026000
C	3.67159300	-3.30210400	3.32107400
H	2.00980000	-4.45679400	2.56856000
H	5.26418800	-1.94860900	3.85546000
H	3.93629200	-4.03361600	4.07795100
C	3.46617800	1.28913000	0.33690500
C	3.06169400	2.13508300	1.38716000
C	4.57077100	1.62740000	-0.46028200
C	3.76968700	3.30419300	1.64356700
H	2.20520300	1.86897000	2.00147600
C	5.27025700	2.80431600	-0.19841100

H	4.88345700	0.97577800	-1.26898200
C	4.87182400	3.64081600	0.84877100
H	3.46544100	3.95565800	2.45640400
H	6.12857600	3.06706800	-0.80817300
H	5.42012600	4.55634800	1.04670500
C	3.06103600	-0.95008600	-1.52392500
C	2.58859200	-0.34446700	-2.70368100
C	3.93687800	-2.04512800	-1.59039200
C	3.00401200	-0.82581300	-3.94050600
H	1.90945800	0.50246000	-2.64757000
C	4.34336200	-2.52274000	-2.83507100
H	4.30216400	-2.51121600	-0.68165700
C	3.87902500	-1.91639800	-4.00650700
H	2.64719300	-0.35768200	-4.85217500
H	5.02595400	-3.36443400	-2.89179300
H	4.19918600	-2.29343300	-4.97263300
Au	0.26823400	0.17047900	0.09364900

Zero-point correction= 0.539208 (Hartree/Particle)
Thermal correction to Energy= 0.574648
Thermal correction to Enthalpy= 0.575593
Thermal correction to Gibbs Free Energy= 0.459667
Sum of electronic and zero-point Energies= -1789.131930
Sum of electronic and thermal Energies= -1789.096489
Sum of electronic and thermal Enthalpies= -1789.095545
Sum of electronic and thermal Free Energies= -1789.211470
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1790.495524

TS2-b

C	-0.52180100	-0.29028500	-0.44830300
C	-0.43894600	-1.52496100	-0.39525900
C	-1.07959300	-2.86936600	-0.35269700
H	-0.59886400	-3.51940300	-1.09123500
H	-0.89306100	-3.30727400	0.64094600
O	-2.45261200	-2.87359400	-0.66687100
C	-3.29689000	-2.16691500	0.25024600
H	-4.23009700	-2.74478700	0.27144300
H	-2.86972400	-2.19823300	1.26075000
C	-3.57334000	-0.76500800	-0.21630000
H	-3.77646300	-0.70087900	-1.28467000
C	-3.62076600	0.35832900	0.51308500
C	-3.93887900	1.68410900	-0.13003700
H	-4.82416700	2.14484800	0.32998500
H	-3.10775700	2.38835300	0.00593400
H	-4.12602500	1.58113600	-1.20289700
C	-3.36127500	0.42736100	1.99574800
H	-2.97941200	-0.50754300	2.41273900
H	-2.63500300	1.22013100	2.21481600
H	-4.28018300	0.68511000	2.54007300
C	-0.41720000	1.11269300	-0.47752700
C	-0.23923700	1.84017400	0.71977600
C	-0.49211900	1.81441800	-1.70109000
C	-0.13711200	3.22516200	0.68804600
H	-0.16228800	1.29877000	1.65547600
C	-0.39181800	3.19964800	-1.71958800
H	-0.63064200	1.25426600	-2.61986300
C	-0.21481500	3.91060700	-0.52806800
H	0.00837400	3.77448600	1.61361700
H	-0.45262500	3.73084300	-2.66497300
H	-0.13651700	4.99359900	-0.54787000
S	1.83089100	-2.16505000	-0.16148700
O	1.98404500	-2.98801800	1.06861000
O	2.37583400	-2.63060900	-1.46324700
C	2.53639500	-0.54509200	0.17877400
C	2.78972900	0.31159100	-0.89106800
C	2.67968100	-0.13389400	1.50274200
C	3.20405300	1.61520200	-0.62360000
H	2.66171900	-0.04323000	-1.90782600
C	3.10601500	1.16916600	1.75653700
H	2.46835300	-0.83114100	2.30610400
C	3.35852100	2.04287400	0.69636000
H	3.39753700	2.29866800	-1.44460500
H	3.23614100	1.50417500	2.78155100
H	3.67470300	3.06178900	0.89971300

Zero-point correction= 0.362030 (Hartree/Particle)
Thermal correction to Energy= 0.385955
Thermal correction to Enthalpy= 0.386899
Thermal correction to Gibbs Free Energy= 0.304770
Sum of electronic and zero-point Energies= -1398.189527
Sum of electronic and thermal Energies= -1398.165602
Sum of electronic and thermal Enthalpies= -1398.164657
Sum of electronic and thermal Free Energies= -1398.246787
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.867746

TS1-b

C	-0.46226600	-0.40902200	-0.39531000
C	-1.29849700	-1.26277400	-0.03967500
C	-1.95462100	-2.53785000	0.25614700
H	-1.42657300	-3.33915000	-0.27589400
H	-1.86808100	-2.73939000	1.33796000
O	-3.30869100	-2.60781100	-0.15438900
C	-4.14770400	-1.63899000	0.48500500
H	-5.16506600	-1.99441700	0.28469200
H	-3.99338400	-1.66907800	1.57291300
C	-3.96071200	-0.26080400	-0.08166500
H	-4.05088500	-0.22513900	-1.16684900
C	-3.71454400	0.88715000	0.57069400
C	-3.57925000	2.18527100	-0.18422400
H	-4.33790000	2.90969700	0.14386400
H	-2.60035600	2.64385600	0.00243100
H	-3.68786900	2.04104300	-1.26290100
C	-3.53796200	1.00951300	2.06171700
H	-3.55433500	0.04983600	2.58276500
H	-2.58346400	1.50302700	2.28536100
H	-4.32536700	1.64074600	2.49546300
C	-0.10995700	0.99379200	-0.47563200
C	0.06219200	1.73214800	0.70607100
C	0.09292300	1.61444800	-1.71713300
C	0.40739100	3.07947900	0.64492000
H	-0.06967000	1.23524000	1.66154600
C	0.43635500	2.96362300	-1.77063700
H	-0.00635800	1.03017900	-2.62484500
C	0.59158200	3.69902500	-0.59351300
H	0.53809200	3.64482100	1.56311200
H	0.58553300	3.44131400	-2.73449300

H	0.86139200	4.75012000	-0.64071300
S	1.41969300	-1.50190400	-1.11119400
O	1.22098600	-2.94217000	-0.81432000
O	1.82266100	-1.04734400	-2.46752500
C	2.61742000	-0.84919900	0.06060600
C	3.23141700	0.37306400	-0.21568700
C	2.79413300	-1.50389400	1.27935200
C	4.05948300	0.94025800	0.75109300
H	3.06003200	0.86036200	-1.16856100
C	3.62993000	-0.92780300	2.23504700
H	2.29573700	-2.45075400	1.45624800
C	4.25769000	0.29243100	1.97269000
H	4.54864900	1.88889400	0.55079900
H	3.79254400	-1.43152300	3.18348000
H	4.90257600	0.74019800	2.72341000

Zero-point correction= 0.361492 (Hartree/Particle)
Thermal correction to Energy= 0.385643
Thermal correction to Enthalpy= 0.386587
Thermal correction to Gibbs Free Energy= 0.302177
Sum of electronic and zero-point Energies= -1398.181957
Sum of electronic and thermal Energies= -1398.157806
Sum of electronic and thermal Enthalpies= -1398.156862
Sum of electronic and thermal Free Energies= -1398.241272
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.858531

TS3-b

C	3.44583000	-0.63634200	0.42275400
C	3.20572200	-1.81311500	0.59132800
C	2.85906500	-3.22389000	0.80131000
H	3.72030000	-3.86246900	0.57673000
H	2.60454900	-3.37361600	1.86422000
O	1.80927800	-3.70471500	-0.02422200
C	0.56662200	-3.02514700	0.17689200
H	-0.20398800	-3.71677400	-0.18657400
H	0.38425900	-2.87156200	1.24785500
C	0.49701400	-1.74868300	-0.60087200
H	0.78830700	-1.83639500	-1.64499000
C	-0.06732000	-0.54137400	-0.17441100
C	0.12020600	0.66913500	-1.06654400
H	-0.62522300	1.44172900	-0.85175900
H	1.11016100	1.10455400	-0.88694700
H	0.04502800	0.39698200	-2.12267900
C	-0.19059000	-0.23392200	1.30521600
H	-0.60765100	-1.06948000	1.87096300
H	0.80676300	-0.00841400	1.70238900
H	-0.82571700	0.64091300	1.47093700
C	3.67674000	0.75296700	0.20153300
C	3.47460200	1.68488500	1.23696000
C	4.07333100	1.21567900	-1.06747700
C	3.66061000	3.04436200	1.00416700
H	3.17075000	1.32874900	2.21622000
C	4.25431300	2.57720100	-1.29233800
H	4.22664900	0.49709700	-1.86597900
C	4.04836900	3.49486300	-0.25961800
H	3.50054400	3.75490500	1.80992600
H	4.55631500	2.92397700	-2.27630900
H	4.18970300	4.55663400	-0.43905500
S	-2.27821400	-1.04894900	-0.63241500
O	-2.40855200	-1.14079500	-2.10786200
O	-2.60047900	-2.21249200	0.23547400
C	-3.31259000	0.32440800	-0.08876500
C	-3.77631900	0.34933700	1.22744600
C	-3.55004900	1.38102200	-0.96968100
C	-4.50609500	1.45440500	1.66325100
H	-3.58291200	-0.49606500	1.87861000
C	-4.28041500	2.48062100	-0.52102800
H	-3.18620600	1.31933500	-1.98958100
C	-4.75404900	2.51873300	0.79273300
H	-4.88603300	1.48293500	2.68037800
H	-4.48488400	3.30499100	-1.19796700
H	-5.32125300	3.37829600	1.13800500

Zero-point correction= 0.362039 (Hartree/Particle)
Thermal correction to Energy= 0.385851
Thermal correction to Enthalpy= 0.386795
Thermal correction to Gibbs Free Energy= 0.303902
Sum of electronic and zero-point Energies= -1398.181157
Sum of electronic and thermal Energies= -1398.157345
Sum of electronic and thermal Enthalpies= -1398.156401
Sum of electronic and thermal Free Energies= -1398.239294
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.860776

TS4-b

C	2.98528500	1.01345400	-0.79015100
C	2.12967600	1.77217600	-1.19266600
C	1.11679900	2.71571700	-1.67923400
H	1.61262300	3.61942200	-2.05273500
H	0.57098500	2.26950200	-2.52600200
O	0.20626900	3.16881600	-0.68795400
C	-0.90025500	2.30993100	-0.42836700
H	-1.61601000	2.93136600	0.11392300
H	-1.37074900	1.99954100	-1.37186400
C	-0.52532000	1.11038600	0.42409400
H	-0.06705500	1.40736000	1.36839800
C	-0.06372000	-0.11227600	-0.09372100
C	0.65391100	-1.07450400	0.80168300
H	0.09269000	-2.01573600	0.89079600
H	1.63666300	-1.33220100	0.38464600
H	0.79810900	-0.67156500	1.80704800
C	-0.33357400	-0.59098900	-1.48845700
H	-0.94968100	0.09393500	-2.07362000
H	0.61717800	-0.73507800	-2.02089400
H	-0.84375400	-1.56290100	-1.47338100
S	-2.48979900	0.65513600	1.43289500
O	-2.16543000	-0.04238400	2.70104600
O	-3.39046100	1.83948200	1.41571900
C	-3.20363800	-0.57181700	0.32297900
C	-3.88540700	-0.13662900	-0.81274400
C	-2.96301600	-1.92344100	0.56168100
C	-4.33200400	-1.08306900	-1.73393300
H	-4.07141100	0.92277000	-0.95569700
C	-3.41605100	-2.86214800	-0.36573100
H	-2.44103900	-2.22029900	1.46480100
C	-4.09196300	-2.44189200	-1.51360500
H	-4.87094700	-0.76208300	-2.62053400

H	-3.24386100	-3.92031300	-0.19145600
H	-4.43898100	-3.17550600	-2.23551600
C	3.95379600	0.09024700	-0.29759500
C	4.32168300	-1.03438100	-1.06036700
C	4.53773900	0.27855300	0.96901000
C	5.25018500	-1.94519300	-0.56486300
H	3.87193800	-1.18002600	-2.03750400
C	5.46294400	-0.63905100	1.45765800
H	4.25271200	1.14438400	1.55771800
C	5.82240400	-1.75201400	0.69436600
H	5.52728700	-2.80916700	-1.16205800
H	5.90521200	-0.48555900	2.43773300
H	6.54499200	-2.46569000	1.07916100

Zero-point correction= 0.362332 (Hartree/Particle)
Thermal correction to Energy= 0.386196
Thermal correction to Enthalpy= 0.387140
Thermal correction to Gibbs Free Energy= 0.303605
Sum of electronic and zero-point Energies= -1398.183928
Sum of electronic and thermal Energies= -1398.160064
Sum of electronic and thermal Enthalpies= -1398.159120
Sum of electronic and thermal Free Energies= -1398.242655
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.86427

INT2-b

C	-0.52634600	-0.37265700	-0.49804500
C	-0.24209500	-1.62883400	-0.36070900
C	-1.15598200	-2.85049100	-0.33257900
H	-0.75803600	-3.58751000	-1.03875100
H	-1.10098700	-3.29599500	0.67207200
O	-2.48187800	-2.61289000	-0.72052600
C	-3.29294900	-1.90126900	0.22076900
H	-4.26052900	-2.42190100	0.22079900
H	-2.87363700	-1.99237900	1.23060200
C	-3.48055100	-0.47120000	-0.19800900
H	-3.62149900	-0.35532400	-1.27175000
C	-3.53431300	0.62234000	0.57584700
C	-3.75983100	1.98282000	-0.03156600
H	-4.64639200	2.46797000	0.40004700
H	-2.90538400	2.64139500	0.17112600
H	-3.89414800	1.92581300	-1.11553500
C	-3.36160700	0.61927400	2.07231700
H	-3.05704400	-0.35149200	2.47116700
H	-2.60892100	1.36147500	2.36818500
H	-4.29645500	0.90644900	2.57305400
C	-0.32660300	1.00173300	-0.56471700
C	-0.18687900	1.77035200	0.62320300
C	-0.28095600	1.67378700	-1.81589200
C	0.01359000	3.14009500	0.55164700
H	-0.20949800	1.26128600	1.57976400
C	-0.08568300	3.04541400	-1.86679600
H	-0.39589000	1.09373700	-2.72564800
C	0.06408200	3.78820400	-0.68872900
H	0.13720400	3.71120400	1.46747500
H	-0.04830900	3.54542900	-2.83047900
H	0.21832900	4.86184900	-0.73710100
S	1.52543100	-2.14312400	-0.19030900
O	1.58973400	-3.04759900	0.97395700
O	2.00800900	-2.59030000	-1.50853300
C	2.36793200	-0.62076800	0.23226000
C	2.79695200	0.22396500	-0.79011900
C	2.51873300	-0.28698100	1.57720100
C	3.37475000	1.44587200	-0.45240000
H	2.67031600	-0.07562800	-1.82438300
C	3.10845300	0.93354200	1.90255700
H	2.18424100	-0.97971200	2.34178200
C	3.52556800	1.80018500	0.88982400
H	3.70130300	2.12285400	-1.23556600
H	3.24053900	1.20899100	2.94469400
H	3.97339500	2.75546300	1.14782400

Zero-point correction= 0.363646 (Hartree/Particle)
Thermal correction to Energy= 0.387407
Thermal correction to Enthalpy= 0.388351
Thermal correction to Gibbs Free Energy= 0.306811
Sum of electronic and zero-point Energies= -1398.199590
Sum of electronic and thermal Energies= -1398.175830
Sum of electronic and thermal Enthalpies= -1398.174885
Sum of electronic and thermal Free Energies= -1398.256426
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.875117

TS6-b

C	-0.89250100	-0.29878500	-0.49007900
C	-0.57121300	-1.56509800	-0.38931700
C	-1.49888100	-2.74855800	-0.17923700
H	-1.26806100	-3.53345800	-0.90542800
H	-1.31574600	-3.17181600	0.82086400
O	-2.86054800	-2.43946900	-0.35516500
C	-3.35108100	-1.42464300	0.50952100
H	-4.42206900	-1.63530800	0.62430000
H	-2.89032600	-1.50938300	1.50386600
C	-3.17063700	-0.04930300	-0.08577400
H	-3.31324300	-0.03006500	-1.16439100
C	-3.27080400	1.13482000	0.58751400
C	-3.35504700	2.43354200	-0.16358900
H	-4.28083100	2.97222400	0.08655500
H	-2.52040400	3.09571500	0.10093500
H	-3.33079000	2.27921200	-1.24594400
C	-3.25762400	1.24727500	2.08669400
H	-3.02064300	0.30495800	2.58709500
H	-2.52579000	1.99914700	2.41174700
H	-4.23407900	1.58629000	2.46221200
C	-0.25927400	0.95933500	-0.70845800
C	-0.02334000	1.84213100	0.36742000
C	0.11320500	1.35600900	-2.01021200
C	0.59085700	3.06842100	0.14784500
H	-0.29227500	1.53174500	1.37112100
C	0.72066300	2.58968300	-2.21932600
H	-0.05605500	0.67235200	-2.83552500
C	0.96222900	3.45069600	-1.14507900
H	0.78893500	3.72804100	0.98795200
H	1.01403100	2.87919100	-3.22446800
H	1.43934600	4.41173700	-1.31334500
S	1.18419900	-2.08225100	-0.52609100
O	1.29307300	-3.35061400	0.22095100
O	1.59681300	-2.00780000	-1.93858400

C	2.09586800	-0.82598200	0.37331300
C	2.84622000	0.10742800	-0.33664600
C	2.01395500	-0.80069600	1.76530000
C	3.52105300	1.10281700	0.36821900
H	2.87870500	0.05338800	-1.41809600
C	2.68818700	0.20196500	2.45902600
H	1.43900000	-1.55761300	2.28859000
C	3.43681000	1.15320300	1.76030200
H	4.10154600	1.84451300	-0.17141800
H	2.63648000	0.23789200	3.54326000
H	3.95850500	1.93474900	2.30533900

Zero-point correction= 0.363505 (Hartree/Particle)
Thermal correction to Energy= 0.386282
Thermal correction to Enthalpy= 0.387226
Thermal correction to Gibbs Free Energy= 0.309327
Sum of electronic and zero-point Energies= -1398.196040
Sum of electronic and thermal Energies= -1398.173263
Sum of electronic and thermal Enthalpies= -1398.172319
Sum of electronic and thermal Free Energies= -1398.250218
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.870159

INT6-b

C	-1.17742100	-0.03563000	-0.41864100
C	-0.95709700	-1.35625100	-0.32528700
C	-2.07169500	-2.37141700	-0.16149200
H	-1.91116900	-3.21819700	-0.83399000
H	-2.08490700	-2.76924700	0.86544300
O	-3.32301100	-1.81099200	-0.50284500
C	-3.55327600	-0.61904700	0.22409100
H	-4.58859500	-0.32554500	0.03427400
H	-3.44316500	-0.81268300	1.30250200
C	-2.59688400	0.51231100	-0.20788300
H	-2.92440600	0.88784800	-1.18654800
C	-2.64060900	1.64784400	0.77857700
C	-2.99081900	3.03533100	0.35209300
H	-3.68185200	3.51575100	1.06034100
H	-2.09728500	3.68109900	0.30465800
H	-3.45341500	3.05516300	-0.64032000
C	-2.28776800	1.40394000	2.21443500
H	-1.69338000	0.49203100	2.34506100
H	-1.71167200	2.24165800	2.63194200
H	-3.18174900	1.30361200	2.85250400
C	-0.13760500	0.95107700	-0.81682100
C	0.33707400	1.93460100	0.06222700
C	0.35374500	0.91953400	-2.12944600
C	1.28861200	2.85933500	-0.36025400
H	0.00197200	1.94437600	1.09148700
C	1.29967600	1.85250000	-2.55313800
H	0.00447900	0.14799100	-2.80632700
C	1.76909600	2.82509400	-1.67059000
H	1.66415400	3.60028900	0.33960100
H	1.67224000	1.81342900	-3.57270800
H	2.50994100	3.54868900	-1.99895200
S	0.66816600	-2.12438800	-0.43247900
O	0.52839900	-3.38463500	0.32124800
O	1.13489000	-2.15196600	-1.82950000
C	1.76008000	-1.05037700	0.50012400
C	2.80564600	-0.40894100	-0.15607400
C	1.54060400	-0.89217600	1.86884400
C	3.64178900	0.43237900	0.57664200
H	2.93367600	-0.55359800	-1.22189200
C	2.37625200	-0.04209200	2.58881800
H	0.73188200	-1.42737700	2.35585800
C	3.42330400	0.62090800	1.94174900
H	4.45488500	0.94983400	0.07700900
H	2.21741300	0.09789600	3.65399700
H	4.07185700	1.28439500	2.50665900

Zero-point correction= 0.366424 (Hartree/Particle)
Thermal correction to Energy= 0.388862
Thermal correction to Enthalpy= 0.389806
Thermal correction to Gibbs Free Energy= 0.313603
Sum of electronic and zero-point Energies= -1398.234609
Sum of electronic and thermal Energies= -1398.212171
Sum of electronic and thermal Enthalpies= -1398.211227
Sum of electronic and thermal Free Energies= -1398.287431
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.870159

INT1-b

C	-0.17376300	-0.53322000	-0.50675000
C	-1.14407100	-1.31150700	-0.10087900
C	-1.55817300	-2.70041800	0.16294300
H	-1.07074100	-3.39427700	-0.52979100
H	-1.23123600	-2.96224800	1.18556700
O	-2.95680400	-2.90412600	0.02355600
C	-3.73106600	-1.90569900	0.68285300
H	-4.76032100	-2.27925300	0.62521600
H	-3.45862300	-1.84389600	1.74711900
C	-3.62021300	-0.57572800	-0.01098100
H	-3.67017800	-0.65632900	-1.09634400
C	-3.61178800	0.65952400	0.53265500
C	-3.63121900	1.88263800	-0.34475900
H	-4.52994200	2.48539700	-0.15035400
H	-2.76733400	2.52572900	-0.13992200
H	-3.61821100	1.62128300	-1.40646200
C	-3.58145200	0.93685900	2.01145200
H	-3.43573900	0.03886500	2.61651200
H	-2.77481300	1.64321500	2.24464400
H	-4.51755000	1.41150800	2.33690300
C	-0.15946000	0.95045100	-0.47513200
C	-0.19226700	1.60640400	0.76241200
C	-0.07600400	1.70534800	-1.65224800
C	-0.15623100	2.99818600	0.82500400
H	-0.23763400	1.01335800	1.67022500
C	-0.04240800	3.09793300	-1.58691500
H	-0.02734000	1.19489000	-2.60735000
C	-0.08263600	3.74733500	-0.35121700
H	-0.17996800	3.49674700	1.78999300
H	0.01472300	3.67711300	-2.50406700
H	-0.05314600	4.83227400	-0.30503100
S	1.38134600	-1.30474300	-1.11993600
O	1.28412800	-2.75883100	-0.89727400
O	1.66795700	-0.76407600	-2.46128500
C	2.60457800	-0.64787700	0.01433800
C	3.16876600	0.60263900	-0.24058300

C	2.91489300	-1.37465500	1.16365900
C	4.06630200	1.13421400	0.68370500
H	2.90811000	1.13791600	-1.14614000
C	3.81787800	-0.83377400	2.07768600
H	2.46389600	-2.34869200	1.31901500
C	4.38815500	0.41893900	1.83942700
H	4.51551700	2.10567300	0.50055300
H	4.07889200	-1.39053300	2.97280500
H	5.08893900	0.83786900	2.55589800

Zero-point correction= 0.363628 (Hartree/Particle)
Thermal correction to Energy= 0.387346
Thermal correction to Enthalpy= 0.388290
Thermal correction to Gibbs Free Energy= 0.306562
Sum of electronic and zero-point Energies= -1398.191117
Sum of electronic and thermal Energies= -1398.167399
Sum of electronic and thermal Enthalpies= -1398.166455
Sum of electronic and thermal Free Energies= -1398.248182
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.865044

TS5-b

C	-0.19106100	-0.53443000	-0.53086200
C	-1.17414500	-1.30636900	-0.14185300
C	-1.57853700	-2.70078000	0.11318300
H	-1.12451500	-3.38446200	-0.61098300
H	-1.20905300	-2.98222400	1.11569200
O	-2.98383700	-2.89478900	0.03136300
C	-3.71686700	-1.87875400	0.70786700
H	-4.75739400	-2.22218200	0.66972600
H	-3.42206500	-1.82544500	1.76680200
C	-3.58064700	-0.55075600	0.01338000
H	-3.64966500	-0.62862300	-1.07110700
C	-3.56905500	0.68635400	0.55886200
C	-3.59443500	1.90950900	-0.31760600
H	-4.49547700	2.50821000	-0.12078800
H	-2.73309500	2.55648300	-0.11456700
H	-3.58284800	1.64890600	-1.37947000
C	-3.52842400	0.96037800	2.03764900
H	-4.46301900	1.43254400	2.37125100
H	-3.37659200	0.06109700	2.63931000
H	-2.72153600	1.66779300	2.26697600
C	-0.16035500	0.94892700	-0.49937200
C	-0.16685300	1.60523800	0.73833900
C	-0.07942900	1.70233500	-1.67742400
C	-0.10835100	2.99629800	0.80024800
H	-0.20891200	1.01292100	1.64677800
C	-0.02378800	3.09430300	-1.61307500
H	-0.04918400	1.19086600	-2.63282600
C	-0.03833400	3.74416500	-0.37704700
H	-0.11171800	3.49521500	1.76534300
H	0.03128900	3.67255800	-2.53093500
H	0.00867400	4.82851900	-0.33146700
S	1.36678300	-1.31663600	-1.12109700
O	1.25914100	-2.76943200	-0.89355200
O	1.67196900	-0.78294900	-2.46120000
C	2.58082600	-0.66194800	0.02428100
C	3.15674200	0.58316300	-0.23076000
C	2.87109600	-1.38355500	1.18207000
C	4.04554200	1.11457500	0.70199800
H	2.91120100	1.11459200	-1.14281100
C	3.76548700	-0.84294900	2.10469800
H	2.41159800	-2.35362300	1.33741500
C	4.34724300	0.40446200	1.86631300
H	4.50350500	2.08195500	0.51889800
H	4.01092300	-1.39582100	3.00661500
H	5.04122900	0.82324200	2.58946800

Zero-point correction= 0.363478 (Hartree/Particle)
Thermal correction to Energy= 0.386342
Thermal correction to Enthalpy= 0.387286
Thermal correction to Gibbs Free Energy= 0.308466
Sum of electronic and zero-point Energies= -1398.191263
Sum of electronic and thermal Energies= -1398.168399
Sum of electronic and thermal Enthalpies= -1398.167455
Sum of electronic and thermal Free Energies= -1398.246275
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.864996

INT5-b

C	-0.43876800	-0.45903700	-0.52483400
C	-1.62164400	-1.01642600	-0.23460500
C	-2.02661300	-2.48102200	-0.22148700
H	-1.75184600	-3.02672000	-1.12362600
H	-1.55996700	-2.99466400	0.63327500
O	-3.44757400	-2.47929200	-0.10985900
C	-3.79350600	-1.34133700	0.65799900
H	-4.85480900	-1.13188300	0.50763800
H	-3.61294500	-1.51727300	1.73108100
C	-2.87108400	-0.20669500	0.13989300
H	-3.30029100	0.16460200	-0.80013500
C	-2.67426700	0.93429500	1.08400600
C	-3.11628800	2.31791900	0.73928300
H	-3.87190900	2.69728000	1.44707300
H	-2.27322600	3.02467900	0.78058000
H	-3.54346000	2.37436200	-0.26673200
C	-2.09174800	0.69047400	2.44060000
H	-2.86620900	0.64599200	3.22524600
H	-1.52912400	-0.24890600	2.48673700
H	-1.41024400	1.50265900	2.72675000
C	-0.18448600	1.00477500	-0.59142300
C	0.44519800	1.68398800	0.46066100
C	-0.54351200	1.71564900	-1.74408700
C	0.68291600	3.05397000	0.37374000
H	0.74449500	1.13390900	1.34619700
C	-0.30320000	3.08630000	-1.83171300
H	-1.00347700	1.18258100	-2.56996200
C	0.30826200	3.75875800	-0.77251700
H	1.16645500	3.56975200	1.19846900
H	-0.58853800	3.62741200	-2.72924600
H	0.49670500	4.82639500	-0.84123400
S	0.95049400	-1.47739400	-1.05886700
O	0.67448300	-2.88359800	-0.71069800
O	1.27822100	-1.09535900	-2.44283200
C	2.28731500	-0.91240900	-0.00756500
C	3.14350100	0.08472200	-0.47107300
C	2.40246800	-1.44292200	1.27770000
C	4.13823000	0.56500500	0.37959700

H	3.02012100	0.46863500	-1.47727800
C	3.39786600	-0.95196300	2.12084400
H	1.72891700	-2.23108100	1.59699200
C	4.26049100	0.05230100	1.67263200
H	4.81406600	1.34169900	0.03466400
H	3.50539200	-1.35584700	3.12312800
H	5.03417100	0.43264100	2.33345300

Zero-point correction= 0.365536 (Hartree/Particle)
Thermal correction to Energy= 0.388303
Thermal correction to Enthalpy= 0.389247
Thermal correction to Gibbs Free Energy= 0.311016
Sum of electronic and zero-point Energies= -1398.235031
Sum of electronic and thermal Energies= -1398.212263
Sum of electronic and thermal Enthalpies= -1398.211319
Sum of electronic and thermal Free Energies= -1398.289551
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.908738

TS9-b

C	-2.26930000	-3.02728500	1.93487600
H	-2.16440300	-3.47102500	2.92893400
H	-1.66639200	-3.59917200	1.22238000
C	-1.80647700	-1.55390500	1.96582900
H	-2.25596400	-1.07740900	2.85996800
C	-0.34175000	-1.40425400	2.25007500
C	0.49203800	-2.58980300	2.57247600
H	1.55700600	-2.35929900	2.51273600
H	0.27366700	-2.81392700	3.63523900
H	0.26656800	-3.48462700	2.00060700
C	0.16122200	-0.10840200	2.76227100
H	-0.20801800	0.74774200	2.20010400
H	-0.25687100	0.00232700	3.77860800
H	1.24645300	-0.08024000	2.84425600
S	-0.32158300	-2.70983500	-1.01861900
C	0.79425900	-4.09380300	-0.65293400
F	1.98375800	-3.71112200	-0.10850600
F	0.23345100	-4.93958000	0.25543600
F	1.06555100	-4.81347100	-1.74310300
P	2.51601600	0.91383000	-0.11581300
C	2.08100700	2.19126800	-1.33529900
C	1.44626000	1.79046900	-2.52183300
C	2.37428300	3.54655500	-1.12781400
C	1.09637800	2.73734000	-3.48235200
H	1.21729600	0.74182000	-2.69255100
C	2.01923100	4.49059800	-2.09167000
H	2.86186600	3.86729100	-0.21336300
C	1.37725500	4.08906500	-3.26515300
H	0.59950200	2.42039000	-4.39379100
H	2.24418700	5.53956100	-1.92497300
H	1.09850100	4.82727400	-4.01078800
C	4.19182200	0.32982900	-0.50984500
C	4.48264100	-1.04175500	-0.48282300
C	5.20144900	1.25444300	-0.82050600
C	5.77772200	-1.48302800	-0.75734200
H	3.70188800	-1.76355600	-0.26190600
C	6.49106500	0.80652900	-1.09393000
H	4.97754800	2.31609700	-0.85720300
C	6.77989400	-0.56114600	-1.06106000
H	5.99863000	-2.54567600	-0.74132500
H	7.26999900	1.52214400	-1.33794000
H	7.78566100	-0.90655200	-1.27954200
C	2.63356300	1.73488100	1.50375500
C	3.64158700	1.36148300	2.40441300
C	1.64162600	2.64291400	1.90710900
C	3.65287800	1.89102600	3.69593800
H	4.41642000	0.66680100	2.09656900
C	1.66197200	3.17036600	3.19640700
H	0.85106800	2.92785400	1.22266200
C	2.66434900	2.79326000	4.09429900
H	4.43947700	1.60404800	4.38701600
H	0.89331100	3.87548700	3.49841600
H	2.67897800	3.20615100	5.09829700
Au	1.00724400	-0.88435700	-0.31848200
C	-2.40633300	-0.72744800	0.78935000
C	-3.30506300	-1.33791900	0.00363300
C	-3.81947100	-2.73851700	0.24271800
H	-4.89049600	-2.77762800	0.04341700
H	-3.32554600	-3.45149600	-0.43422200
O	-3.62935900	-3.10686200	1.59628800
S	-4.06382200	-0.52717600	-1.44255800
C	-2.11200400	0.73141800	0.72672200
C	-2.61306000	1.55803400	1.74734800
C	-1.40326300	1.31649100	-0.33202400
C	-2.41488900	2.93540400	1.70833500
H	-3.19009200	1.12099400	2.55787300
C	-1.20417600	2.69844800	-0.36902800
H	-1.07384400	0.70226900	-1.15883600
C	-1.70789200	3.50938000	0.64753800
H	-2.82917000	3.56142600	2.49244800
H	-0.66999100	3.13624600	-1.20518100
H	-1.56339000	4.58504200	0.60866300
O	-5.11195700	-1.45771900	-1.88203800
O	-2.99204400	-0.11533500	-2.36282300
C	-4.84225700	0.93364000	-0.76651000
C	-4.48072900	2.18700700	-1.25303200
C	-5.81546600	0.77581100	0.22301300
C	-5.09962900	3.31639600	-0.71756700
H	-3.72649700	2.26422800	-2.02645900
C	-6.41837300	1.91230900	0.75619800
H	-6.09957800	-0.21463400	0.56398800
C	-6.05861100	3.17980200	0.28738300
H	-4.83138900	4.30171800	-1.08569000
H	-7.17680900	1.81024800	1.52607200
H	-6.53610600	4.06249700	0.70197700

Zero-point correction= 0.662497 (Hartree/Particle)
Thermal correction to Energy= 0.708770
Thermal correction to Enthalpy= 0.709714
Thermal correction to Gibbs Free Energy= 0.578192
Sum of electronic and zero-point Energies= -3305.481124
Sum of electronic and thermal Energies= -3305.434851
Sum of electronic and thermal Enthalpies= -3305.433907
Sum of electronic and thermal Free Energies= -3305.565429
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-3307.187422

INT9-b

C	0.01579900	0.87889300	-2.26659000
C	0.92927400	1.95237800	-2.80281100
H	1.96823300	1.61518300	-2.80059300
H	0.64633200	2.12115500	-3.85561800
H	0.85675700	2.90141500	-2.27712700
C	0.33232200	-0.48278300	-2.80683200
H	-0.16669200	-1.28805500	-2.27029400
H	-0.05347300	-0.50118600	-3.83929100
H	1.40307600	-0.67324700	-2.85928200
S	-0.30333400	2.75238900	0.82336800
C	1.20894300	3.75628500	0.85415200
F	2.21249900	3.16362600	1.54816000
F	1.70966000	3.98321200	-0.39333600
F	0.96640100	4.94174100	1.41418300
P	2.38923800	-0.95131400	0.06335100
C	2.04159200	-1.74145000	1.66450500
C	1.62661700	-0.91540300	2.72397100
C	2.15392600	-3.12375100	1.86192300
C	1.30325300	-1.47251600	3.95823500
H	1.55880700	0.16237800	2.59132900
C	1.83486800	-3.67467000	3.10393700
H	2.47941600	-3.76824200	1.05321000
C	1.40150100	-2.85445400	4.14730000
H	0.97500200	-0.82997200	4.76889900
H	1.92458400	-4.74608900	3.25435200
H	1.14733600	-3.28852800	5.10928300
C	4.01108800	-0.14876300	0.20344000
C	4.20631800	1.15477400	-0.27605100
C	5.07618900	-0.84556500	0.79781400
C	5.46194000	1.75262200	-0.17031800
H	3.38040500	1.71376400	-0.70436400
C	6.32762400	-0.24325900	0.89559900
H	4.92264600	-1.84779000	1.18642800
C	6.52077600	1.05427200	0.41123600
H	5.60820500	2.76504100	-0.53310400
H	7.15030400	-0.78128300	1.35594200
H	7.49621400	1.52297800	0.49648900
C	2.52167300	-2.25669800	-1.18243700
C	3.61720100	-2.30267600	-2.05652000
C	1.46542200	-3.17169500	-1.33085400
C	3.65467900	-3.26295500	-3.06874500
H	4.43566000	-1.59970600	-1.94411400
C	1.51406100	-4.12791400	-2.34062500
H	0.60877100	-3.13047800	-0.66741100
C	2.60649800	-4.17360000	-3.21241800
H	4.50593600	-3.30089400	-3.74118600
H	0.69719000	-4.83483200	-2.44923700
H	2.64068900	-4.91907000	-4.00085300
Au	0.78877100	0.82323500	-0.03384000
C	-1.48180200	1.20264800	-2.15521700
H	-1.90588100	0.65069200	-3.01259900
C	-1.77923100	2.69728400	-2.39018100
H	-1.21573100	3.31435700	-1.67992100
H	-1.49972100	2.98169900	-3.40729700
C	-2.25928500	0.66513100	-0.92875200
C	-3.19856300	1.45372700	-0.38103200
C	-3.58115700	2.80946400	-0.93009600
H	-4.66598600	2.91947500	-0.92047600
H	-3.16136000	3.60952500	-0.30157100
O	-3.15861200	2.94333500	-2.27252900
S	-4.16890000	0.98265300	1.08644300
O	-5.22359600	2.00121800	1.17939100
O	-3.24442300	0.75877100	2.20973200
C	-4.92100900	-0.57652200	0.63680000
C	-5.75407500	-0.61982200	-0.48339800
C	-4.68130500	-1.70090200	1.42198000
C	-6.33533900	-1.83438800	-0.83911200
H	-5.94788400	0.27865600	-1.06057400
C	-5.27775600	-2.90885300	1.06070100
H	-4.03528700	-1.62169700	2.28777100
C	-6.09481900	-2.97666500	-0.06894200
H	-6.98546800	-1.88825100	-1.70678200
H	-5.10306200	-3.79561500	1.66195900
H	-6.55543800	-3.91994300	-0.34673000
C	-2.04255900	-0.75196800	-0.50936400
C	-2.45486600	-1.78639800	-1.36519300
C	-1.47889600	-1.08581900	0.73162000
C	-2.31642000	-3.11977600	-0.98579500
H	-2.92239500	-1.54250700	-2.31486400
C	-1.32013900	-2.42307900	1.10167800
H	-1.23643200	-0.30315200	1.43859700
C	-1.74341500	-3.44186000	0.24861800
H	-2.67033000	-3.90572100	-1.64579600
H	-0.88464600	-2.65878500	2.06715000
H	-1.64109200	-4.48122300	0.54664800

Zero-point correction= 0.663736 (Hartree/Particle)
Thermal correction to Energy= 0.710491
Thermal correction to Enthalpy= 0.711435
Thermal correction to Gibbs Free Energy= 0.577467
Sum of electronic and zero-point Energies= -3305.481856
Sum of electronic and thermal Energies= -3305.435101
Sum of electronic and thermal Enthalpies= -3305.434157
Sum of electronic and thermal Free Energies= -3305.568125
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-3307.187716

INT10-b

O	-4.51946000	-2.77591100	-0.91270200
C	-3.59941200	-3.37966200	-0.04142700
H	-4.16865200	-4.06449500	0.59009600
H	-2.88551400	-3.97285400	-0.63243400
C	-2.83643600	-2.35109500	0.84378100
H	-3.36384100	-2.25793600	1.80168400
C	-1.43412500	-2.91720100	1.25786900
C	-1.56396700	-4.38041900	1.71217100
H	-0.61612500	-4.75325400	2.10344300
H	-2.29227100	-4.40747400	2.53039700
H	-1.90523000	-5.05962700	0.93097000
C	-0.72636800	-2.12665300	2.36231500
H	-0.56093600	-1.08415400	2.10111100
H	-1.35009600	-2.14996700	3.26293900
H	0.23426400	-2.58893000	2.59808900
S	-0.42224000	-2.82592200	-0.36698100
C	0.91688000	-4.07939300	-0.14411000
F	1.54504900	-3.96450200	1.03460900

F	0.43420800	-5.31729600	-0.24836500
F	1.80605300	-3.87804100	-1.12406800
P	2.54352200	0.89173600	-0.13432200
C	1.77125900	2.50173000	-0.45045600
C	0.82441400	2.60103700	-1.47912200
C	2.09880100	3.62821300	0.31961200
C	0.20348700	3.82240300	-1.73441900
H	0.54468700	1.72924000	-2.06044400
C	1.47459900	4.84747300	0.05580200
H	2.82586400	3.54961700	1.12134500
C	0.52657400	4.94404500	-0.96679400
H	-0.53941200	3.88335500	-2.52279900
H	1.72611700	5.72024300	0.65054800
H	0.03912700	5.89418900	-1.16362900
C	3.90640700	0.68119100	-1.30907400
C	4.35807000	-0.61251800	-1.61138200
C	4.53612200	1.79777900	-1.87713800
C	5.44160400	-0.78480300	-2.46969700
H	3.86012700	-1.47762000	-1.18115900
C	5.61802900	1.61603400	-2.73824200
H	4.17959300	2.79809800	-1.65330000
C	6.07082800	0.32845200	-3.03283500
H	5.78901600	-1.78566000	-2.70603500
H	6.10313900	2.47959200	-3.18233900
H	6.91028900	0.19139900	-3.70742500
C	3.25151100	0.95992900	1.53674700
C	4.62553000	1.14008500	1.73804400
C	2.38549900	0.85546800	2.63742600
C	5.12906400	1.21744300	3.03787800
H	5.29610800	1.21651700	0.88854800
C	2.89542200	0.93968800	3.93006800
H	1.31913400	0.72068400	2.48041100
C	4.26767100	1.11793400	4.13106400
H	6.19467300	1.35348700	3.19389100
H	2.22505800	0.86187600	4.78062100
H	4.66404500	1.17663600	5.14006800
Au	1.01734500	-0.84917400	-0.26255400
C	-2.79618900	-0.94784400	0.22056900
C	-3.18966900	-0.79800500	-1.06040000
C	-3.84300800	-1.93138300	-1.82349400
H	-4.58455100	-1.53212000	-2.51455000
H	-3.10692700	-2.50182800	-2.41328400
C	-2.43574000	0.17073700	1.13874200
C	-1.38044700	1.05620000	0.87940600
C	-3.17245400	0.33760100	2.32236000
C	-1.04571800	2.05701200	1.79120000
H	-0.85235800	0.99289700	-0.06076100
C	-2.85227500	1.35052100	3.22395200
H	-4.01961800	-0.30965500	2.52854300
C	-1.77660700	2.20454100	2.96959400
H	-0.22912100	2.73352700	1.56076200
H	-3.44540200	1.47346800	4.12496500
H	-1.52365400	2.98838500	3.67711900
S	-3.18197400	0.77642200	-1.96509900
O	-4.00287200	0.54519000	-3.16184500
O	-1.77986700	1.21565200	-2.11936100
C	-4.04262500	1.92462500	-0.90133700
C	-3.39428100	3.07079400	-0.44819900
C	-5.36559900	1.63723200	-0.55817300
C	-4.08798200	3.94436300	0.38838200
H	-2.36751100	3.26032000	-0.73543100
C	-6.04466700	2.51535200	0.28265900
H	-5.85264400	0.74622000	-0.94126000
C	-5.40500000	3.66462100	0.75685000
H	-3.59687700	4.84016500	0.75545700
H	-7.07272500	2.30797700	0.56225600
H	-5.93880900	4.34633200	1.41200100

Zero-point correction= 0.666635 (Hartree/Particle)
Thermal correction to Energy= 0.712714
Thermal correction to Enthalpy= 0.713658
Thermal correction to Gibbs Free Energy= 0.581619
Sum of electronic and zero-point Energies= -3305.531418
Sum of electronic and thermal Energies= -3305.485339
Sum of electronic and thermal Enthalpies= -3305.484395
Sum of electronic and thermal Free Energies= -3305.616434
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-3307.229495

P_2

C	-0.10427100	0.37614400	-0.59662200
C	-0.70351900	1.56938500	-0.44191400
C	0.03141200	2.89490800	-0.43502500
H	-0.49498100	3.62725500	-1.05065100
H	0.06554100	3.29975800	0.58964900
O	1.32498000	2.76252800	-0.97408200
C	2.02342300	1.68936400	-0.37628400
H	3.05442800	1.77672400	-0.71064600
H	2.00288000	1.78701800	0.71900600
C	1.42871900	0.33786700	-0.80912700
H	1.56039500	0.27220400	-1.89967500
C	2.21079000	-0.88383500	-0.21328400
C	1.86337700	-2.21362400	-0.91065900
H	2.54165500	-2.99794600	-0.56498900
H	0.84303100	-2.52096800	-0.69115600
H	1.96261400	-2.12979600	-1.99847000
C	2.05913700	-1.02209200	1.30285400
H	1.00783700	-1.20476600	1.53436300
H	2.63856200	-1.86950200	1.67509500
H	2.37482100	-0.12836300	1.84302000
C	-0.91467100	-0.86671000	-0.76799200
C	-1.27299100	-1.67755000	0.31658000
C	-1.31893600	-1.23838400	-2.05571000
C	-1.98954500	-2.85421300	0.11579100
H	-1.01976500	-1.37032200	1.32457400
C	-2.04167600	-2.41393200	-2.25691400
H	-1.07743000	-0.59374300	-2.89442100
C	-2.36919700	-3.23019300	-1.17363900
H	-2.26631300	-3.46597400	0.96885400
H	-2.35120500	-2.68898200	-3.26093300
H	-2.92934100	-4.14726200	-1.33176200
S	-2.49624000	1.84017400	-0.46275000
O	-2.67507100	3.16514300	0.15852600
O	-2.98588200	1.58951200	-1.82864700
C	-3.27468000	0.65242200	0.62725700
C	-4.17759100	-0.25850000	0.08797400

C	-3.01140200	0.71105800	1.99614000
C	-4.81852300	-1.15255400	0.94420800
H	-4.34579500	-0.27087400	-0.98237200
C	-3.64470200	-0.19865800	2.83935600
H	-2.32718500	1.45630800	2.38871700
C	-4.54598300	-1.12926700	2.31264300
H	-5.52102400	-1.87478300	0.53980200
H	-3.44752000	-0.17443300	3.90695400
H	-5.04171900	-1.83313400	2.97497700
S	4.03647300	-0.70143200	-0.72542000
C	4.93384700	-0.07318300	0.72266300
F	4.99267300	-0.95346000	1.74179400
F	6.19296900	0.16667600	0.32033800
F	4.44063000	1.07384000	1.23949300

Zero-point correction= 0.387165 (Hartree/Particle)
Thermal correction to Energy= 0.413986
Thermal correction to Enthalpy= 0.414930
Thermal correction to Gibbs Free Energy= 0.329029
Sum of electronic and zero-point Energies= -2134.082620
Sum of electronic and thermal Energies= -2134.055798
Sum of electronic and thermal Enthalpies= -2134.054854
Sum of electronic and thermal Free Energies= -2134.140756
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2134.918776

INT19-b

P	-1.56365200	0.47611900	0.01785900
C	-1.77089900	0.19335700	1.80190100
C	-1.06459800	1.01128300	2.69835900
C	-2.54728800	-0.86709700	2.28462900
C	-1.14750100	0.77432800	4.06752700
H	-0.45646200	1.83038700	2.32413000
C	-2.61875500	-1.10387000	3.65929800
H	-3.09447400	-1.50058000	1.59476800
C	-1.92214300	-0.28596400	4.54921300
H	-0.60662800	1.41238100	4.75957600
H	-3.22231900	-1.92568600	4.03183400
H	-1.98159300	-0.47177300	5.61713100
C	-2.78592500	-0.55914200	-0.83635000
C	-2.37842600	-1.71950100	-1.51148600
C	-4.14581900	-0.21383000	-0.78845700
C	-3.33230200	-2.53350600	-2.12336600
H	-1.32684300	-1.98455800	-1.57344600
C	-5.09036700	-1.03285500	-1.40223900
H	-4.46199700	0.69299100	-0.28227900
C	-4.68459500	-2.19348600	-2.06735300
H	-3.01479400	-3.42845200	-2.64951700
H	-6.14136900	-0.76349600	-1.36717600
H	-5.42363900	-2.82734900	-2.54777400
C	-1.98085000	2.21428600	-0.29217700
C	-1.44012300	2.85078000	-1.41892400
C	-2.87671200	2.90208700	0.53987900
C	-1.80245400	4.16292300	-1.71633600
H	-0.73953400	2.31858500	-2.05682000
C	-3.23182300	4.21628600	0.23739400
H	-3.28418900	2.41892400	1.42208900
C	-2.69772700	4.84530500	-0.88904900
H	-1.38290100	4.65418000	-2.58870000
H	-3.92305100	4.74899900	0.88308100
H	-2.97496600	5.86933400	-1.11952000
Au	0.58054600	-0.12143900	-0.62249200
C	3.03807200	-0.24187900	-0.99165000
C	2.38004600	-1.19850200	-1.42057500
C	2.09771200	-2.48710600	-2.12220700
H	2.06390600	-2.27570500	-3.19552300
H	2.94008300	-3.16940000	-1.93536900
O	0.87071600	-3.09621100	-1.80139800
C	0.86892100	-3.86409700	-0.57624600
H	0.02680200	-4.55004500	-0.69931800
H	1.78490900	-4.46479800	-0.53416800
C	0.67658000	-3.02906100	0.65715500
H	-0.34633000	-2.69892900	0.83438900
C	1.61597600	-2.66582900	1.54911600
C	1.25278200	-1.80205200	2.72874200
H	1.60373300	-2.25002900	3.66681400
H	1.73715600	-0.81814900	2.65052900
H	0.17628000	-1.63946800	2.80277900
C	3.07250800	-3.03498300	1.46249700
H	3.31346100	-3.68481800	0.61924900
H	3.68793600	-2.13018400	1.37026000
H	3.39491900	-3.53978800	2.38139200
C	3.78973400	0.86034700	-0.49398300
C	4.25588900	1.84935600	-1.38260100
C	4.07396000	0.96062900	0.88294100
C	5.00432300	2.91557900	-0.89578400
H	4.03063400	1.76521400	-2.44063500
C	4.81838400	2.03409400	1.35766100
H	3.70291500	0.19916400	1.56058400
C	5.28475500	3.00932500	0.47060600
H	5.36936500	3.67479900	-1.57986100
H	5.03898500	2.11186600	2.41745100
H	5.86789200	3.84477700	0.84542200

Zero-point correction= 0.541050 (Hartree/Particle)
Thermal correction to Energy= 0.575887
Thermal correction to Enthalpy= 0.576831
Thermal correction to Gibbs Free Energy= 0.468237
Sum of electronic and zero-point Energies= -1789.501531
Sum of electronic and thermal Energies= -1789.466694
Sum of electronic and thermal Enthalpies= -1789.465750
Sum of electronic and thermal Free Energies= -1789.574344
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1790.789092

INT3-b

C	3.31804800	0.66747800	-0.45815800
C	2.99242900	1.82211200	-0.63969600
C	2.60712400	3.21880900	-0.88227000
H	3.48890200	3.86508300	-0.80973600
H	2.21683700	3.30693100	-1.91052600
O	1.67374400	3.74864800	0.04328900
C	0.38690800	3.12240400	-0.02410200
H	-0.28751200	3.81959300	0.48997300
H	0.04659100	3.06036600	-1.06594600
C	0.37232000	1.79252900	0.65236000
H	0.79233000	1.76216000	1.65324000
C	-0.36661100	0.59256100	0.18494400

C	0.03395800	-0.65486100	0.97658900
H	-0.56235500	-1.52280900	0.67949000
H	1.08526000	-0.88026500	0.77707900
H	-0.09284100	-0.49038000	2.04974000
C	-0.29344300	0.35011400	-1.32705700
H	-0.70066000	1.18927100	-1.89450000
H	0.75546300	0.21304800	-1.60485800
H	-0.84679000	-0.55284400	-1.60093900
C	3.64017900	-0.70070700	-0.22131800
C	3.46375700	-1.66221600	-1.23454800
C	4.10753800	-1.11494100	1.04051100
C	3.74815200	-3.00199700	-0.98808700
H	3.10298300	-1.34400100	-2.20750200
C	4.38638100	-2.45746600	1.27899800
H	4.24082700	-0.37416400	1.82218800
C	4.20851900	-3.40417500	0.26766500
H	3.60845600	-3.73531200	-1.77711200
H	4.74372700	-2.76645400	2.25703000
H	4.42737600	-4.45090700	0.45746300
S	-2.18122800	0.98892300	0.61095000
O	-2.27728200	1.07010500	2.08110900
O	-2.57207400	2.13596200	-0.23568700
C	-3.16250400	-0.42229800	0.08452100
C	-3.68226700	-0.44763900	-1.21047000
C	-3.38032800	-1.47057300	0.97997700
C	-4.42415400	-1.55528500	-1.61843900
H	-3.52016900	0.39880200	-1.86845400
C	-4.12334500	-2.57318000	0.56052800
H	-2.98926000	-1.40221000	1.98902600
C	-4.63926800	-2.61709100	-0.73673300
H	-4.84046200	-1.58639600	-2.62096900
H	-4.30603600	-3.39378600	1.24793500
H	-5.21847600	-3.47767100	-1.05880600

Zero-point correction= 0.363813 (Hartree/Particle)
Thermal correction to Energy= 0.387407
Thermal correction to Enthalpy= 0.388351
Thermal correction to Gibbs Free Energy= 0.306748
Sum of electronic and zero-point Energies= -1398.186334
Sum of electronic and thermal Energies= -1398.162740
Sum of electronic and thermal Enthalpies= -1398.161796
Sum of electronic and thermal Free Energies= -1398.243398
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.864939

TS7-b

C	3.12342600	0.72012600	-0.32932900
C	2.52777500	1.79309900	-0.40529100
C	2.35209800	3.21851100	-0.77379200
H	3.29083400	3.76018000	-0.62157900
H	2.09757000	3.26986700	-1.84694800
O	1.37573100	3.88561200	-0.00265000
C	0.14487700	3.16175800	-0.04474500
H	-0.55499900	3.73864600	0.57032400
H	-0.25488600	3.14210300	-1.06750800
C	0.34446200	1.78312800	0.50473300
H	0.69127800	1.74855200	1.53406800
C	-0.40084300	0.57901200	0.03472200
C	0.06933200	-0.68694300	0.75473600
H	-0.52485800	-1.55658400	0.45908000
H	1.11090300	-0.88167900	0.48985300
H	0.00189900	-0.56548100	1.83898400
C	-0.41654000	0.39366900	-1.48526900
H	-0.85103900	1.25457900	-1.99691600
H	0.61454200	0.26398300	-1.82639800
H	-0.98770900	-0.49731800	-1.76212200
S	-2.19525600	0.90884400	0.58714800
O	-2.18590600	0.98856900	2.06085500
O	-2.69690800	2.03707800	-0.22525100
C	-3.15477500	-0.54141200	0.13113600
C	-3.75619500	-0.59239100	-1.12730500
C	-3.27850900	-1.59018100	1.04360900
C	-4.48461800	-1.72714700	-1.48147300
H	-3.66705400	0.25506200	-1.79782500
C	-4.00946200	-2.71971200	0.67814400
H	-2.82462600	-1.50214700	2.02439500
C	-4.60625200	-2.78956100	-0.58281900
H	-4.96357000	-1.77881500	-2.45473700
H	-4.11942800	-3.54138100	1.37959300
H	-5.17552900	-3.67121900	-0.86279700
C	3.66185500	-0.57930200	-0.16592600
C	4.29252900	-0.94840500	1.04205900
C	3.56724700	-1.53268800	-1.20331900
C	4.80609100	-2.23033100	1.20253400
H	4.36506300	-0.21818600	1.84146700
C	4.08590600	-2.81110400	-1.03217800
H	3.08358100	-1.25241900	-2.13375200
C	4.70610300	-3.16591600	0.16903400
H	5.28655500	-2.50297800	2.13777300
H	4.00607200	-3.53565900	-1.83753200
H	5.10911000	-4.16595800	0.29900800

Zero-point correction= 0.363837 (Hartree/Particle)
Thermal correction to Energy= 0.386478
Thermal correction to Enthalpy= 0.387422
Thermal correction to Gibbs Free Energy= 0.308806
Sum of electronic and zero-point Energies= -1398.183047
Sum of electronic and thermal Energies= -1398.160406
Sum of electronic and thermal Enthalpies= -1398.159462
Sum of electronic and thermal Free Energies= -1398.238079
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.860288

INT7-b

C	2.70561400	0.52135100	-0.01588900
C	1.90308100	1.54119700	-0.05026500
C	2.29087200	2.95558500	-0.50875500
H	3.23795700	3.29933100	-0.08594400
H	2.36321000	2.98159100	-1.60955500
O	1.25245400	3.79573800	-0.04524700
C	0.05134800	3.04124800	-0.15865000
H	-0.71638300	3.53476200	0.43601800
H	-0.28654100	3.00392900	-1.20307900
C	0.42136300	1.63222600	0.36857400
H	0.38000800	1.66655700	1.46274500
C	-0.45701200	0.44180800	-0.09110900
C	-0.09356300	-0.82956600	0.68327900
H	-0.73721900	-1.66614500	0.39838000

H	0.93849200	-1.10484900	0.45480900
H	-0.17675200	-0.67021200	1.76189300
C	-0.42651300	0.20098700	-1.60106400
H	-0.77318100	1.07190100	-2.16034100
H	0.60099200	-0.02433400	-1.90058200
H	-1.05305800	-0.65471300	-1.86960700
S	-2.19948600	0.91687400	0.39484400
O	-2.18453600	1.18522300	1.84645000
O	-2.67685300	1.94203500	-0.55457200
C	-3.20384200	-0.54998000	0.12625300
C	-3.78143000	-0.75578500	-1.12725900
C	-3.40887800	-1.43908200	1.18168300
C	-4.56296000	-1.89244000	-1.33092300
H	-3.63540400	-0.02260300	-1.91253100
C	-4.19401500	-2.57083900	0.96669000
H	-2.97175500	-1.22881500	2.15137200
C	-4.76392200	-2.79920600	-0.28793300
H	-5.02203200	-2.06491800	-2.29972600
H	-4.36619600	-3.27019100	1.77929100
H	-5.37521800	-3.68215200	-0.45049500
C	3.60119500	-0.52203100	-0.01361500
C	4.39855400	-0.81109100	1.14029200
C	3.75295100	-1.37070200	-1.15735500
C	5.28343300	-1.87475200	1.13587300
H	4.29332700	-0.17895200	2.01609200
C	4.64445700	-2.42878700	-1.13646500
H	3.15698400	-1.16521800	-2.04117000
C	5.41699700	-2.69298500	0.00412800
H	5.88031500	-2.07651100	2.02114100
H	4.74550300	-3.05997000	-2.01520000
H	6.11382800	-3.52536200	0.01100400

Zero-point correction= 0.366853 (Hartree/Particle)
Thermal correction to Energy= 0.389084
Thermal correction to Enthalpy= 0.390029
Thermal correction to Gibbs Free Energy= 0.312617
Sum of electronic and zero-point Energies= -1398.223469
Sum of electronic and thermal Energies= -1398.201238
Sum of electronic and thermal Enthalpies= -1398.200294
Sum of electronic and thermal Free Energies= -1398.277706
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.899884

INT4-b

C	2.94082500	0.96945500	-0.85198000
C	2.00060600	1.63800700	-1.22477800
C	0.90064300	2.49237300	-1.68113300
H	1.31214000	3.40295700	-2.13303600
H	0.32134700	1.97362200	-2.46055300
O	0.04060300	2.94008000	-0.64096500
C	-1.05466100	2.09652200	-0.32642800
H	-1.74381300	2.72839900	0.23723800
H	-1.55953000	1.76413200	-1.24399200
C	-0.66340400	0.89593500	0.55075700
H	-0.04167600	1.27116700	1.37286200
C	-0.03314600	-0.27925600	-0.08289900
C	0.90418600	-1.12103300	0.72115400
H	0.36125500	-1.89888800	1.28076800
H	1.63617000	-1.62294100	0.07833900
H	1.45318400	-0.52700900	1.45891800
C	-0.41595300	-0.77522800	-1.44324300
H	-1.26486100	-0.24421000	-1.88108300
H	0.43552800	-0.68765200	-2.13648000
H	-0.68387600	-1.84034400	-1.41378400
S	-2.19336900	0.36349600	1.55328800
O	-1.73273100	-0.64785100	2.52287800
O	-2.91469000	1.57196100	2.00262600
C	-3.22882500	-0.47940300	0.35101300
C	-4.07639700	0.27242100	-0.46281000
C	-3.13322200	-1.86448400	0.22829500
C	-4.82822000	-0.38144800	-1.43844400
H	-4.15491300	1.34431400	-0.31604400
C	-3.89268700	-2.50846500	-0.74774400
H	-2.48036100	-2.41478200	0.89668400
C	-4.73131000	-1.76749500	-1.58338500
H	-5.49535200	0.18839400	-2.07832600
H	-3.83215600	-3.58747900	-0.85451100
H	-5.31893000	-2.27274100	-2.34441400
C	4.00996600	0.14470900	-0.39536300
C	4.40837900	-0.98289600	-1.13747900
C	4.66707000	0.43473100	0.81460500
C	5.43836300	-1.79775100	-0.67697800
H	3.90106600	-1.20707400	-2.07051400
C	5.69342900	-0.38793000	1.26947600
H	4.35934300	1.30364600	1.38727300
C	6.08274100	-1.50479100	0.52695800
H	5.73797900	-2.66550300	-1.25763100
H	6.19141800	-0.15697600	2.20671000
H	6.88419600	-2.14430100	0.88509500

Zero-point correction= 0.363754 (Hartree/Particle)
Thermal correction to Energy= 0.387618
Thermal correction to Enthalpy= 0.388562
Thermal correction to Gibbs Free Energy= 0.305856
Sum of electronic and zero-point Energies= -1398.186964
Sum of electronic and thermal Energies= -1398.163100
Sum of electronic and thermal Enthalpies= -1398.162156
Sum of electronic and thermal Free Energies= -1398.244863
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.866636

TS8-b

C	2.85463400	0.73206200	-0.82438400
C	1.73811300	1.17777100	-1.09827500
C	0.85392200	2.13067700	-1.80590400
H	1.46733900	2.90127200	-2.28367200
H	0.29215400	1.60677600	-2.59545000
O	-0.03916800	2.83094200	-0.95469300
C	-1.12871500	2.05591900	-0.49431100
H	-1.79506500	2.75461900	0.01392600
H	-1.66686300	1.60985300	-1.34340500
C	-0.68097200	0.97320300	0.49856400
H	-0.12267000	1.47031300	1.30154900
C	0.12853800	-0.15015000	-0.05334500
C	0.97853200	-0.91958400	0.91416200
H	0.36248700	-1.61643200	1.49845200
H	1.74394300	-1.49767300	0.38705000
H	1.48218200	-0.25772300	1.62536000

C	-0.34891700	-0.93140600	-1.24905300
H	-1.02002500	-0.36738300	-1.90198900
H	0.50867000	-1.26537900	-1.84475200
H	-0.89205100	-1.83535600	-0.93890300
S	-2.18790500	0.41936300	1.49934800
O	-1.72554200	-0.57801100	2.48226700
O	-2.88758300	1.64417900	1.93554600
C	-3.26851500	-0.43617000	0.34402200
C	-4.09738500	0.30708500	-0.49692600
C	-3.26353500	-1.82997400	0.32015100
C	-4.91421700	-0.36555500	-1.40509600
H	-4.11665900	1.38871900	-0.42088000
C	-4.09022600	-2.49261100	-0.58611300
H	-2.62798500	-2.37142100	1.01220400
C	-4.90588200	-1.76146100	-1.45256500
H	-5.56484800	0.19888600	-2.06629900
H	-4.10044900	-3.57812400	-0.61359000
H	-5.54606700	-2.28125600	-2.15941300
C	4.02144000	0.06715200	-0.38665800
C	4.53740200	-1.03415200	-1.10623500
C	4.69623500	0.49304300	0.77942900
C	5.68396200	-1.68546700	-0.66707900
H	4.02382100	-1.36343800	-2.00404100
C	5.83978400	-0.16887700	1.21004500
H	4.30459500	1.33990100	1.33364000
C	6.33972500	-1.25891600	0.49147700
H	6.06887400	-2.53193200	-1.22879200
H	6.34578100	0.16576800	2.11115300
H	7.23412000	-1.77220600	0.83188800

Zero-point correction= 0.364307 (Hartree/Particle)
Thermal correction to Energy= 0.386860
Thermal correction to Enthalpy= 0.387805
Thermal correction to Gibbs Free Energy= 0.309180
Sum of electronic and zero-point Energies= -1398.180237
Sum of electronic and thermal Energies= -1398.157683
Sum of electronic and thermal Enthalpies= -1398.156739
Sum of electronic and thermal Free Energies= -1398.235363
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.858447

INT8-b

C	2.71183900	0.03913200	-0.68672500
C	1.43305200	0.16314400	-0.90423700
C	0.90927900	0.72590700	-2.21497600
H	1.72943400	1.08281400	-2.83906900
H	0.35440000	-0.04809700	-2.77312400
O	0.05911700	1.84068700	-1.97764500
C	-1.06430000	1.46524700	-1.20884000
H	-1.68142200	2.35896500	-1.10250800
H	-1.64439100	0.69449300	-1.73824000
C	-0.63646000	0.96093800	0.18263100
H	-0.13830100	1.79610400	0.68969900
C	0.35552400	-0.23744800	0.13887300
C	1.01999200	-0.45989800	1.50496900
H	0.28119500	-0.73876500	2.25579400
H	1.77057900	-1.25247900	1.42720100
H	1.53038600	0.44872900	1.84125600
C	-0.30581300	-1.55045700	-0.32581000
H	-0.88710400	-1.43605700	-1.24544400
H	0.47061600	-2.29980300	-0.50780300
H	-0.97192400	-1.93883400	0.44741200
S	-2.14612000	0.81586100	1.24693400
O	-1.82644800	0.05351900	2.46649800
O	-2.65926000	2.19537500	1.33349700
C	-3.37813900	-0.14044200	0.34488900
C	-4.15421700	0.48733600	-0.63107500
C	-3.58993100	-1.47355300	0.69452700
C	-5.12612600	-0.25299300	-1.30239500
H	-4.01377300	1.54171200	-0.83961900
C	-4.56878300	-2.20331300	0.02171800
H	-3.00939900	-1.91351700	1.49722200
C	-5.32732800	-1.59726300	-0.98171300
H	-5.73420000	0.22330600	-2.06547400
H	-4.74439900	-3.24146600	0.28698700
H	-6.08810500	-2.16941300	-1.50463800
C	4.01867300	-0.15134200	-0.30856300
C	4.69066200	-1.39011500	-0.56139700
C	4.75715000	0.88926000	0.34109100
C	6.00899800	-1.56518000	-0.17950300
H	4.14431300	-2.18774800	-1.05470800
C	6.07455900	0.68861900	0.71294700
H	4.26089900	1.83408900	0.53769000
C	6.71397000	-0.53396700	0.45878700
H	6.50089200	-2.51383600	-0.37657600
H	6.61724100	1.48886200	1.20864100
H	7.74811000	-0.68116900	0.75436300

Zero-point correction= 0.367808 (Hartree/Particle)
Thermal correction to Energy= 0.389652
Thermal correction to Enthalpy= 0.390596
Thermal correction to Gibbs Free Energy= 0.314062
Sum of electronic and zero-point Energies= -1398.218159
Sum of electronic and thermal Energies= -1398.196315
Sum of electronic and thermal Enthalpies= -1398.195371
Sum of electronic and thermal Free Energies= -1398.271905
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1398.896458

TS10-b

C	2.07510800	-0.55719500	-0.46330600
C	2.89751700	-1.59938800	-0.27333800
C	2.42195500	-3.02785500	-0.09905800
H	3.02242600	-3.70718000	-0.70813200
H	2.54762100	-3.33804900	0.95095300
O	1.08549900	-3.17810200	-0.51872300
C	0.24140700	-2.20328100	0.05879500
H	-0.77837800	-2.49553400	-0.18363900
H	0.35543100	-2.20094400	1.15246900
C	0.54590300	-0.80979400	-0.52329900
H	0.30700400	-0.85254200	-1.59585100
C	-0.29957400	0.30722600	0.06940400
C	-0.53970800	1.51972000	-0.78975100
H	-1.36372100	2.12046500	-0.39426600
H	0.35671400	2.15200600	-0.81054000
H	-0.77420600	1.24617800	-1.82332100
C	-0.25514600	0.56837800	1.54914500
H	0.54494400	1.29128700	1.76337000

H	-1.18738600	1.02297700	1.89660700
H	-0.06722200	-0.32776400	2.14149300
C	2.57482200	0.81325300	-0.76853700
C	2.74619400	1.77187400	0.23833800
C	2.85123100	1.16159500	-2.09562500
C	3.16437100	3.06180800	-0.07673600
H	2.59044300	1.49303600	1.27410600
C	3.27274100	2.45347300	-2.41093600
H	2.75126500	0.41165600	-2.87328100
C	3.42175400	3.40828300	-1.40451500
H	3.30571500	3.78971700	0.71637500
H	3.48751100	2.71110000	-3.44387600
H	3.74899800	4.41404600	-1.65180700
S	4.70123200	-1.51466300	-0.39395000
O	5.17639600	-2.71466200	0.31810800
O	5.06464000	-1.29272600	-1.80328500
C	5.25234600	-0.09372500	0.54616700
C	5.88983700	0.94711300	-0.12214200
C	5.07900600	-0.08737300	1.93052800
C	6.34736600	2.03668100	0.61718200
H	5.99723800	0.90147100	-1.19932300
C	5.52698000	1.01354600	2.65658300
H	4.60727700	-0.93042500	2.42485300
C	6.15874000	2.07386300	1.99941800
H	6.84040000	2.86092300	0.11110200
H	5.39624500	1.04020200	3.73430200
H	6.51041700	2.92836200	2.57042300
C	-3.14074600	-1.08478300	1.27445000
F	-3.47757300	-0.05196600	2.07702400
F	-4.20029200	-1.90991300	1.23101200
F	-2.14030000	-1.74906100	1.89004300
S	-2.63566600	-0.52432700	-0.38556600
S	-4.82675400	-0.54208500	-1.40108800
O	-5.49289400	-1.85592000	-1.37406300
O	-4.50484900	0.14091100	-2.66612700
C	-5.75173000	0.58616700	-0.36198500
C	-6.57365900	0.06989400	0.63869400
C	-5.55934900	1.95676500	-0.53600500
C	-7.23782600	0.96271700	1.47832800
H	-6.69073900	-1.00202100	0.74353900
C	-6.22979800	2.83510800	0.31234600
H	-4.91041500	2.31478800	-1.32728600
C	-7.06455900	2.33896300	1.31720900
H	-7.89065000	0.58265000	2.25820100
H	-6.10360700	3.90637300	0.18769400
H	-7.58226700	3.02866000	1.97737600

Zero-point correction= 0.484997 (Hartree/Particle)
Thermal correction to Energy= 0.521380
Thermal correction to Enthalpy= 0.522324
Thermal correction to Gibbs Free Energy= 0.411057
Sum of electronic and zero-point Energies= -2914.189795
Sum of electronic and thermal Energies= -2914.153413
Sum of electronic and thermal Enthalpies= -2914.152468
Sum of electronic and thermal Free Energies= -2914.263736
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2915.265625

TS2´-b

C	-1.80158300	-0.80089800	-0.39132600
C	-2.04607100	-1.67090100	0.45888900
C	-1.63665800	-2.82283200	1.30852700
H	-1.79234800	-2.55670200	2.35838300
H	-2.28414000	-3.68446200	1.09017700
O	-0.26832200	-3.17939100	1.19112100
C	0.07606300	-4.01312000	0.08699600
H	0.98143800	-4.53688400	0.39543000
H	-0.71081600	-4.76468600	-0.07332800
C	0.29304100	-3.25520500	-1.20819000
H	-0.60986200	-2.86896800	-1.67569100
C	1.43914900	-3.26478200	-1.97931800
C	1.40690700	-2.71947900	-3.38684300
H	2.26948700	-2.07474400	-3.58353600
H	1.46411300	-3.55750900	-4.09450900
H	0.49193900	-2.15741700	-3.59030200
C	2.71812200	-3.96207400	-1.59088100
H	2.79359500	-4.17375400	-0.52337400
H	2.78318700	-4.91409100	-2.13492500
H	3.58531400	-3.36512500	-1.88994300
C	-1.77134300	0.29079200	-1.28796500
C	-1.75500400	0.07867500	-2.68566000
C	-1.76575400	1.61335900	-0.79295700
C	-1.73671500	1.16216100	-3.55723000
H	-1.77861100	-0.93667300	-3.06916900
C	-1.75428500	2.68614800	-1.67448000
H	-1.80388200	1.77655800	0.27456800
C	-1.73848600	2.46861500	-3.05560800
H	-1.73271600	0.99085000	-4.62940400
H	-1.76211500	3.69825400	-1.28247600
H	-1.73307200	3.31207800	-3.73911600
S	-4.18926000	-1.34850400	1.40463000
O	-5.09210500	-2.43472700	0.95559400
O	-3.95934000	-1.07620500	2.84808800
C	-4.68117100	0.18347000	0.61734800
C	-4.53145300	1.38296600	1.31225300
C	-5.09490300	0.14133100	-0.71455300
C	-4.82265900	2.57554000	0.65136500
H	-4.20768100	1.36920500	2.34565300
C	-5.37045200	1.34249700	-1.36503100
H	-5.20646300	-0.81145000	-1.22064600
C	-5.23198700	2.55488800	-0.68422700
H	-4.72998100	3.52009400	1.17879800
H	-5.69466100	1.33252000	-2.40074100
H	-5.44904000	3.48736500	-1.19627400
P	1.94039200	0.75345200	0.46210100
C	2.32734000	2.03794900	-0.75890400
C	1.61453300	2.06817500	-1.96615000
C	3.29548900	3.01611400	-0.48807100
C	1.86253600	3.08007700	-2.89100200
H	0.86866500	1.30901500	-2.17835700
C	3.53941500	4.02373000	-1.42089700
H	3.85751500	2.98482400	0.44004400
C	2.82385700	4.05654500	-2.62014500
H	1.30596000	3.10195900	-3.82254800
H	4.29139700	4.77872900	-1.21368700
H	3.02036100	4.84006100	-3.34564700

C	3.42065800	0.51733500	1.48556200
C	4.46614200	-0.27761700	0.99140000
C	3.54631100	1.14645400	2.73130600
C	5.63254700	-0.43300600	1.73584300
H	4.36269600	-0.76986200	0.02771000
C	4.71643200	0.98213900	3.47399500
H	2.73596600	1.75461600	3.11960300
C	5.75724500	0.19587400	2.97811000
H	6.44101900	-1.04787000	1.35264100
H	4.81168900	1.46620100	4.44094700
H	6.66442000	0.06798000	3.56053500
C	0.63285700	1.39904200	1.54503500
C	-0.14866200	0.48864100	2.27242700
C	0.37592400	2.77397900	1.63354100
C	-1.19476200	0.94872900	3.07014100
H	0.05094500	-0.57571600	2.19712500
C	-0.66419400	3.23063900	2.44351200
H	0.97021800	3.47812800	1.06063800
C	-1.45209600	2.32033200	3.15271500
H	-1.82428300	0.24080400	3.59903400
H	-0.86423900	4.29552400	2.51323000
H	-2.26835800	2.67947900	3.77245000
Au	1.24942700	-1.22998900	-0.53170200

Zero-point correction= 0.641515 (Hartree/Particle)
Thermal correction to Energy= 0.684617
Thermal correction to Enthalpy= 0.685561
Thermal correction to Gibbs Free Energy= 0.559197
Sum of electronic and zero-point Energies= -2569.639026
Sum of electronic and thermal Energies= -2569.595925
Sum of electronic and thermal Enthalpies= -2569.594981
Sum of electronic and thermal Free Energies= -2569.721345
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.1752592

INT2´-b

C	1.41319200	-0.87358600	0.28479200
C	1.93821100	-1.69150900	-0.59475500
C	1.28422900	-2.85945400	-1.32830200
H	1.02180000	-2.55769900	-2.34531800
H	2.01125200	-3.67835000	-1.40548900
O	0.09006800	-3.31225400	-0.72507200
C	0.26314100	-3.89701500	0.57519700
H	-0.01300000	-4.95582200	0.50522200
H	1.31054200	-3.83957700	0.88270600
C	-0.60023000	-3.18405600	1.60038600
H	-0.11118900	-2.90579300	2.53347000
C	-1.98519300	-3.19126300	1.58391500
C	-2.77165600	-2.74075700	2.78845200
H	-3.60905800	-2.09489200	2.50511000
H	-3.20405700	-3.62429700	3.27852400
H	-2.14994900	-2.21434500	3.51733100
C	-2.77806400	-3.83349200	0.47516100
H	-2.18067200	-4.01508300	-0.41845900
H	-3.17560600	-4.79208200	0.83821100
H	-3.63946500	-3.21578500	0.20107200
C	1.72416100	0.23264900	1.13197400
C	1.87004200	0.03461100	2.52669500
C	1.82014500	1.54475600	0.61307200
C	2.12424900	1.11246300	3.36499400
H	1.79094300	-0.97115000	2.92733900
C	2.08105600	2.61151300	1.46053900
H	1.72307900	1.70014300	-0.45116800
C	2.22981500	2.40523500	2.83660700
H	2.24660000	0.94883200	4.43128800
H	2.17310100	3.61055300	1.04671800
H	2.43101600	3.24532300	3.49403400
S	3.69428000	-1.60665800	-1.13478500
O	4.38849300	-2.70293800	-0.44224000
O	3.60856300	-1.56900600	-2.60633700
C	4.36152600	-0.05445200	-0.57189100
C	4.34845700	1.03385000	-1.44433300
C	4.89375300	0.03033700	0.71557500
C	4.87167000	2.24803800	-1.00337000
H	3.94563400	0.91847500	-2.44311000
C	5.40423600	1.25277300	1.14569900
H	4.91216200	-0.84551800	1.35407600
C	5.39027800	2.35721400	0.28908900
H	4.88042000	3.10547600	-1.66910100
H	5.81966600	1.34209700	2.14419900
H	5.79647000	3.30540500	0.62822500
P	-1.80518100	0.86264900	-0.40150500
C	-2.09346700	2.21216700	0.77642100
C	-1.34361400	2.26099800	1.96043300
C	-3.02861600	3.21988600	0.49510000
C	-1.51703800	3.32132200	2.84793400
H	-0.62904000	1.47641100	2.18522800
C	-3.19807800	4.27593000	1.38943900
H	-3.62350400	3.17306700	-0.41195700
C	-2.44174800	4.32828200	2.56321100
H	-0.93183200	3.35675700	3.76153700
H	-3.92360700	5.05398700	1.17325700
H	-2.57963600	5.15054200	3.25872400
C	-3.38095400	0.55964600	-1.25548700
C	-4.38235800	-0.15156600	-0.57560800
C	-3.61690100	1.03214500	-2.55245900
C	-5.61214400	-0.37942800	-1.18651600
H	-4.19444400	-0.51903400	0.43030400
C	-4.85023500	0.79408000	-3.16238700
H	-2.84346400	1.57754500	-3.08316500
C	-5.84535700	0.09119500	-2.48269800
H	-6.38720500	-0.92567800	-0.65763600
H	-5.03073400	1.15776600	-4.16918100
H	-6.80199300	-0.09348100	-2.96148200
C	-0.62821100	1.46437500	-1.65044700
C	0.05064300	0.51514800	-2.42971700
C	-0.32575100	2.82524800	-1.78920500
C	1.03972100	0.91772200	-3.32407800
H	-0.18425000	-0.53848200	-2.31900300
C	0.65993700	3.22635000	-2.69251200
H	-0.83809000	3.56234200	-1.18001300
C	1.34798000	2.27571500	-3.45052100
H	1.58361900	0.17363300	-3.89736600
H	0.89600000	4.28093700	-2.79710500
H	2.12341500	2.59202100	-4.14184000
Au	-0.98283100	-1.09451000	0.60811100

Zero-point correction= 0.643670 (Hartree/Particle)
Thermal correction to Energy= 0.686283
Thermal correction to Enthalpy= 0.687227
Thermal correction to Gibbs Free Energy= 0.562791
Sum of electronic and zero-point Energies= -2569.652069
Sum of electronic and thermal Energies= -2569.609457
Sum of electronic and thermal Enthalpies= -2569.608512
Sum of electronic and thermal Free Energies= -2569.732948
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.185961

TS6´-b

C	3.33946900	-0.34610900	-0.20958700
C	3.72908400	-1.59492300	-0.21480900
C	2.92970200	-2.85110600	0.06679900
H	3.12377400	-3.59994200	-0.70464600
H	3.27007200	-3.27474100	1.02343300
O	1.53399100	-2.64179700	0.07425600
C	1.11214700	-1.58043500	0.90159800
H	0.09677700	-1.83192500	1.22641700
H	1.73384600	-1.49798600	1.80310900
C	1.11920400	-0.27568200	0.11129800
H	1.05144400	-0.41516800	-0.96618700
C	0.75996700	0.98441400	0.63250000
C	0.88196200	2.21618400	-0.24680100
H	0.11982600	2.96248000	0.00146700
H	1.85913000	2.68735700	-0.08151800
H	0.80131700	1.97291100	-1.30996100
C	0.87922100	1.25260400	2.11995700
H	0.62078900	0.38580000	2.73361500
H	1.91379000	1.54076700	2.35592800
H	0.23724000	2.08639300	2.42012200
C	3.86833100	0.95440300	-0.44338500
C	4.28503800	1.76525500	0.63792300
C	3.97062100	1.45210600	-1.76210800
C	4.80340900	3.03067600	0.40010600
H	4.23656100	1.36761000	1.64578000
C	4.48755800	2.72239700	-1.98632100
H	3.66901400	0.81844900	-2.58942600
C	4.89971800	3.51580100	-0.90972000
H	5.14384700	3.63923300	1.23186100
H	4.57826800	3.09542000	-3.00176500
H	5.30409200	4.50677300	-1.09137000
S	5.48255500	-1.99821100	-0.65463000
O	5.74140700	-3.28735700	0.00515000
O	5.60582200	-1.84061100	-2.11010400
C	6.46665600	-0.73546200	0.13611700
C	7.05139500	0.25493500	-0.65099900
C	6.62405000	-0.77323500	1.52261800
C	7.80546900	1.24617500	-0.02447400
H	6.90949100	0.24055200	-1.72500100
C	7.37464700	0.22784000	2.13586700
H	6.18267900	-1.57816400	2.10098000
C	7.96044400	1.23558800	1.36319800
H	8.26961000	2.02572800	-0.62006200
H	7.51599800	0.21442400	3.21214500
H	8.54886700	2.00996500	1.84617400
P	-3.72114400	-0.01643000	-0.03670200
C	-4.63167300	1.51489000	-0.37911100
C	-4.06085700	2.46454100	-1.24033200
C	-5.90375600	1.73610400	0.16600400
C	-4.76419500	3.62317200	-1.56032700
H	-3.07179800	2.29349200	-1.65761000
C	-6.60032100	2.90149300	-0.15601100
H	-6.34418100	1.00605700	0.83713200
C	-6.03337500	3.84225700	-1.01728500
H	-4.32211700	4.35698900	-2.22706300
H	-7.58450100	3.07408300	0.26827700
H	-6.57780800	4.74878300	-1.26306100
C	-4.45378200	-0.76047600	1.44716300
C	-4.06301500	-0.28391500	2.70801500
C	-5.42437400	-1.76644300	1.34670300
C	-4.64811600	-0.80506300	3.85937400
H	-3.30555000	0.49212800	2.78396500
C	-6.00258000	-2.28686400	2.50514100
H	-5.72313000	-2.14090500	0.37313900
C	-5.61689800	-1.80760100	3.75802800
H	-4.34586900	-0.43528800	4.83425000
H	-6.75212100	-3.06823000	2.42736000
H	-6.06735600	-2.21738300	4.65678000
C	-4.02571000	-1.15029800	-1.42017400
C	-3.15603700	-2.23494200	-1.61335400
C	-5.13246900	-0.97811000	-2.26306200
C	-3.40019800	-3.14649600	-2.63767300
H	-2.29263300	-2.36282500	-0.96550600
C	-5.36799100	-1.89375700	-3.28904500
H	-5.80144300	-0.13577900	-2.12011000
C	-4.50538100	-2.97539200	-3.47590200
H	-2.72610300	-3.98418600	-2.78649600
H	-6.22371300	-1.75950200	-3.94338300
H	-4.69059700	-3.68324200	-4.27792200
Au	-1.43867300	0.36289500	0.23939000

Zero-point correction= 0.642424 (Hartree/Particle)
Thermal correction to Energy= 0.684666
Thermal correction to Enthalpy= 0.685610
Thermal correction to Gibbs Free Energy= 0.557013
Sum of electronic and zero-point Energies= -2569.616184
Sum of electronic and thermal Energies= -2569.573943
Sum of electronic and thermal Enthalpies= -2569.572999
Sum of electronic and thermal Free Energies= -2569.701596
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.1514943

INT6´-b

C	2.74195600	-0.19605700	-0.13452100
C	3.18148200	-1.45734900	-0.24848300
C	2.34343300	-2.69497800	-0.00251300
H	2.38155300	-3.36470500	-0.86518200
H	2.75786500	-3.24865100	0.85191500
O	0.97195900	-2.39633600	0.21849200
C	0.79868600	-1.24636000	1.01402700
H	-0.26167300	-1.21129500	1.27942300
H	1.38152100	-1.31621500	1.94434200
C	1.23210200	-0.01130400	0.19805300
H	0.73482900	-0.09202200	-0.78078100
C	0.79588500	1.31405900	0.79462300

C	0.91593400	2.54966200	-0.06369700
H	0.25265900	3.35384700	0.27651300
H	1.94383000	2.94000200	0.01683500
H	0.72923800	2.34664200	-1.12157400
C	0.97108700	1.52809200	2.27568000
H	0.62428200	0.68341700	2.87715600
H	2.04491900	1.66017000	2.48944600
H	0.46435600	2.43597800	2.61646200
C	3.58216600	0.99707800	-0.40947000
C	4.16753400	1.71352700	0.64564100
C	3.77277100	1.43456400	-1.72596000
C	4.91878500	2.85791500	0.38880800
H	4.07619300	1.34192000	1.66116700
C	4.52330200	2.58288200	-1.98035600
H	3.35291200	0.85973400	-2.54426700
C	5.09018500	3.29993200	-0.92541000
H	5.38349600	3.39337300	1.21073600
H	4.67079900	2.91214300	-3.00439800
H	5.67646500	4.19134800	-1.12672500
S	4.84739000	-1.89471000	-0.82666000
O	5.02200700	-3.29089200	-0.39534600
O	4.93338800	-1.52814300	-2.24811700
C	5.99600900	-0.88141000	0.09133600
C	6.77930300	0.04098800	-0.59762800
C	6.10841600	-1.06778200	1.47042500
C	7.68804500	0.81510600	0.12282700
H	6.66011100	0.15061500	-1.66871100
C	7.01077600	-0.27868100	2.17985400
H	5.51071500	-1.82204500	1.97203200
C	7.79688000	0.66186200	1.50610000
H	8.30621700	1.54056800	-0.39635700
H	7.11445200	-0.40718500	3.25290500
H	8.50394600	1.26961200	2.06278600
P	-3.51238800	-0.05728200	-0.05807400
C	-4.89089500	1.06771300	-0.38198100
C	-4.65184400	2.24428000	-1.10967600
C	-6.18812000	0.75338300	0.04756600
C	-5.71088800	3.09380500	-1.41776200
H	-3.64278600	2.48900800	-1.43102100
C	-7.24191500	1.61344900	-0.26158500
H	-6.37155800	-0.15294400	0.61496700
C	-7.00510200	2.77900000	-0.99253800
H	-5.52767800	4.00344900	-1.98089600
H	-8.24689100	1.37266800	0.07044100
H	-7.82819600	3.44667800	-1.22747300
C	-4.00038100	-1.20784600	1.25115100
C	-3.93354700	-0.78799900	2.58904900
C	-4.47331700	-2.48983300	0.93679500
C	-4.34830100	-1.64510000	3.60498400
H	-3.55783900	0.20318200	2.82955100
C	-4.88355300	-3.34302900	1.96144600
H	-4.51710200	-2.81765300	-0.09644100
C	-4.82175500	-2.92271000	3.29114700
H	-4.29728100	-1.32124800	4.63975100
H	-5.24790100	-4.33651600	1.71976200
H	-5.13815400	-3.59182800	4.08529900
C	-3.19212100	-1.02267100	-1.55850000
C	-2.04331800	-1.83125500	-1.61216300
C	-4.07515500	-0.97974600	-2.64591100
C	-1.78799000	-2.59353700	-2.74814000
H	-1.35072500	-1.87737400	-0.77752700
C	-3.80807900	-1.74622300	-3.78131600
H	-4.96119200	-0.35517400	-2.60666700
C	-2.66801200	-2.54946400	-3.83415900
H	-0.90024500	-3.21690900	-2.78454500
H	-4.49166400	-1.71309900	-4.62387300
H	-2.46286800	-3.14056900	-4.72131800
Au	-1.52152500	1.01170700	0.52097800

Zero-point correction= 0.645090 (Hartree/Particle)
Thermal correction to Energy= 0.686948
Thermal correction to Enthalpy= 0.687892
Thermal correction to Gibbs Free Energy= 0.561215
Sum of electronic and zero-point Energies= -2569.643835
Sum of electronic and thermal Energies= -2569.601977
Sum of electronic and thermal Enthalpies= -2569.601033
Sum of electronic and thermal Free Energies= -2569.727710
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.1800683

TS1´-b

P	-2.50738300	0.46236600	-0.22098800
C	-2.67923100	0.61194500	1.58313100
C	-1.57746200	1.10279000	2.30349300
C	-3.82348500	0.17778400	2.25960400
C	-1.62895100	1.16436900	3.69215100
H	-0.68639400	1.43096200	1.77842200
C	-3.86399600	0.23466300	3.65512700
H	-4.67382900	-0.20473300	1.70489600
C	-2.77138100	0.72469700	4.37056000
H	-0.77643400	1.54762500	4.24467900
H	-4.75118700	-0.10489700	4.18056300
H	-2.80718000	0.76447700	5.45490000
C	-4.08432900	-0.12897500	-0.88447400
C	-4.23730700	-1.49274300	-1.17110300
C	-5.15943300	0.75407000	-1.06630800
C	-5.46471200	-1.97321900	-1.62525500
H	-3.39529400	-2.16793500	-1.04579600
C	-6.38237500	0.26701600	-1.52342900
H	-5.03735300	1.81260100	-0.85822300
C	-6.53550400	-1.09422500	-1.80037600
H	-5.58239000	-3.02866200	-1.85005100
H	-7.21421700	0.94929700	-1.66813800
H	-7.48909900	-1.46835200	-2.16000500
C	-2.21984900	2.14890000	-0.84325500
C	-1.60132300	2.30986400	-2.09220600
C	-2.58738500	3.27599000	-0.09691600
C	-1.35772200	3.58757600	-2.59103900
H	-1.30469700	1.43443700	-2.66404800
C	-2.33580200	4.55401500	-0.59871900
H	-3.05350600	3.15756000	0.87561100
C	-1.72203000	4.71120600	-1.84260200
H	-0.88190900	3.70808000	-3.55952600
H	-2.62010000	5.42551600	-0.01692900
H	-1.52859200	5.70680700	-2.23041600
Au	-0.62567300	-0.83315700	-0.60321200

C	2.01075700	-0.35957700	-0.16373200
C	1.55026900	-1.23923200	-0.95112800
C	1.83408600	-2.38537500	-1.86663800
H	1.97343600	-1.98007400	-2.87445500
H	2.77793600	-2.84964600	-1.54460400
O	0.80023300	-3.33487900	-1.96729400
C	0.64609200	-4.16417500	-0.80104000
H	0.26478900	-5.11509900	-1.18411400
H	1.62830000	-4.35376300	-0.35437300
C	-0.33422900	-3.60038500	0.19288700
H	-1.37775300	-3.66287600	-0.11682900
C	-0.07224300	-3.12931600	1.43355300
C	-1.19112900	-2.68057200	2.33937400
H	-1.23376600	-3.31665100	3.23325400
H	-1.02764600	-1.65468200	2.68908700
H	-2.16438200	-2.72075600	1.84219300
C	1.30384700	-3.01715400	2.02903300
H	2.10637100	-3.32491500	1.35791400
H	1.49779700	-1.98012000	2.32797600
H	1.37413400	-3.62132500	2.94226400
C	1.89680100	0.93044300	0.47602700
C	1.48641400	2.03009000	-0.30535600
C	2.10627600	1.09971300	1.85677200
C	1.26542400	3.26664600	0.28893200
H	1.30910500	1.88930900	-1.36534600
C	1.90562200	2.34996600	2.43846600
H	2.43005100	0.26072200	2.45956000
C	1.47966000	3.43065500	1.66144400
H	0.91432900	4.09603900	-0.31597200
H	2.07293900	2.47715800	3.50361200
H	1.31046000	4.39796400	2.12450800
S	4.24470300	-1.10278700	0.48480700
O	4.33041700	-1.04178300	1.96250800
O	4.49196000	-2.36695400	-0.24974500
C	5.25179200	0.19559500	-0.22286100
C	5.70784000	0.04631900	-1.53420800
C	5.45550200	1.36197400	0.51770500
C	6.42419800	1.09596200	-2.10631300
H	5.52926300	-0.87711200	-2.07343700
C	6.17113600	2.40081600	-0.07406500
H	5.08093100	1.44073600	1.53127500
C	6.65128200	2.26857200	-1.38012900
H	6.80957900	0.99585000	-3.11598500
H	6.35869800	3.31095700	0.48667200
H	7.20771200	3.08281600	-1.83388900

Zero-point correction= 0.640386 (Hartree/Particle)
Thermal correction to Energy= 0.683883
Thermal correction to Enthalpy= 0.684828
Thermal correction to Gibbs Free Energy= 0.554056
Sum of electronic and zero-point Energies= -2569.628350
Sum of electronic and thermal Energies= -2569.584853
Sum of electronic and thermal Enthalpies= -2569.583909
Sum of electronic and thermal Free Energies= -2569.714680
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.1594176

INT1´-b

P	-2.48865500	0.47517900	-0.21932700
C	-2.85628200	0.45736300	1.56337600
C	-1.94493400	1.08510800	2.42898400
C	-3.94057100	-0.25481800	2.08941200
C	-2.13051600	1.01250700	3.80634400
H	-1.09149400	1.62107000	2.02566600
C	-4.11356200	-0.33297700	3.47388300
H	-4.64657300	-0.74291900	1.42574300
C	-3.21308500	0.29960700	4.33162400
H	-1.42616500	1.50458600	4.47042600
H	-4.95607200	-0.88500000	3.87898900
H	-3.35320100	0.23854500	5.40646300
C	-3.91818100	-0.22634700	-1.08452200
C	-3.78906100	-1.46325900	-1.73174400
C	-5.14803900	0.45032600	-1.10207500
C	-4.88767400	-2.02609800	-2.38204900
H	-2.82938400	-1.97341400	-1.73909200
C	-6.24090000	-0.11735200	-1.75229900
H	-5.24535100	1.41636400	-0.61542500
C	-6.11140900	-1.35530800	-2.38967200
H	-4.78547000	-2.98145700	-2.88730100
H	-7.19179100	0.40609600	-1.76772600
H	-6.96495000	-1.79222100	-2.89882400
C	-2.34468400	2.22653800	-0.69668500
C	-1.65740000	2.53070600	-1.88204400
C	-2.87158100	3.26094700	0.08676700
C	-1.49771200	3.85686500	-2.27756000
H	-1.24372900	1.72891900	-2.48881000
C	-2.70282900	4.58862300	-0.30989000
H	-3.39540200	3.03416500	1.00937100
C	-2.01571300	4.88783400	-1.48765700
H	-0.96642400	4.08724000	-3.19592100
H	-3.10863900	5.38832500	0.30214200
H	-1.88451400	5.92179700	-1.79166200
Au	-0.40160600	-0.62983300	-0.56160400
C	2.46057100	-0.62633700	-0.11485500
C	1.54000100	-1.36112700	-0.75592200
C	1.64554000	-2.64009100	-1.54237400
H	2.03165800	-2.39684600	-2.53754700
H	2.33772300	-3.35907100	-1.09262500
O	0.36798900	-3.23435500	-1.75268900
C	-0.10982500	-3.96552300	-0.62229100
H	-0.97566700	-4.52016700	-0.99097600
H	0.65101600	-4.69260400	-0.31050500
C	-0.53901100	-3.09978700	0.54186900
H	-1.59009600	-2.81369800	0.56145300
C	0.20020200	-2.82696700	1.67223000
C	-0.38018300	-1.97925300	2.76377500
H	-0.28001100	-2.48323300	3.73289200
H	0.18101500	-1.03916700	2.83975700
H	-1.42993100	-1.73491800	2.59340000
C	1.58253000	-3.34243000	1.92420200
H	1.98785600	-3.94777100	1.11445700
H	2.28270100	-2.51883800	2.10763300
H	1.57728500	-3.95128400	2.83800800
C	2.08720700	0.60644000	0.62378300
C	1.41264100	1.63620600	-0.07376400
C	2.34454100	0.77346400	1.99586200

C	0.97546400	2.78374800	0.59171500
H	1.29508800	1.55393900	-1.14935900
C	1.91284900	1.92407000	2.65115400
H	2.88220800	0.00053700	2.53265500
C	1.22442400	2.92801800	1.95550500
H	0.45254200	3.55764400	0.03935200
H	2.11198000	2.04116400	3.71224000
H	0.89597200	3.82177900	2.47737700
S	4.19206100	-1.14182300	-0.02556800
O	4.44378300	-1.44557800	1.39939100
O	4.40971300	-2.16558500	-1.05943000
C	5.09393100	0.33299300	-0.46280100
C	5.28609500	0.61644500	-1.81685400
C	5.55124200	1.18231000	0.54566400
C	5.95183500	1.79020600	-2.16480300
H	4.94095900	-0.08085400	-2.57262300
C	6.21645400	2.35219100	0.18145700
H	5.40189900	0.91710400	1.58560200
C	6.41165400	2.65573700	-1.16805700
H	6.12155300	2.02406900	-3.21105500
H	6.58832500	3.02199900	0.95036200
H	6.93275600	3.56706300	-1.44514600

Zero-point correction= 0.643895 (Hartree/Particle)
Thermal correction to Energy= 0.686173
Thermal correction to Enthalpy= 0.687118
Thermal correction to Gibbs Free Energy= 0.562396
Sum of electronic and zero-point Energies= -2569.648389
Sum of electronic and thermal Energies= -2569.606110
Sum of electronic and thermal Enthalpies= -2569.605166
Sum of electronic and thermal Free Energies= -2569.729888
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.181622

TS5´-b

C	-4.11350700	-0.58147900	0.49854100
C	-3.12529100	-1.38301500	0.19209900
C	-2.87101700	-2.83651900	-0.00711300
H	-3.36636800	-3.42923800	0.76532600
H	-3.28622900	-3.13494900	-0.98323000
O	-1.48342800	-3.12567400	0.05234200
C	-0.75340700	-2.14758200	-0.64851100
H	0.29089000	-2.46629000	-0.58874700
H	-1.03827100	-2.11175800	-1.71024300
C	-0.95767000	-0.78847200	0.01874800
H	-0.91306200	-0.82820500	1.10733900
C	-0.78897100	0.47501300	-0.58039800
C	-0.95866200	1.73937400	0.24157200
H	-0.18779200	2.47835300	-0.00606100
H	-1.92207400	2.20395700	0.01063000
H	-0.92192500	1.54020700	1.31564400
C	-0.93544500	0.67300800	-2.07351800
H	-0.34632200	1.53070600	-2.41298600
H	-0.64169200	-0.19924700	-2.66056000
H	-1.98832700	0.89817200	-2.29340300
C	-4.16821700	0.89732300	0.50571600
C	-4.34992900	1.58272600	-0.70347700
C	-4.12658000	1.60895700	1.71078200
C	-4.45305700	2.97311000	-0.71136800
H	-4.43184700	1.01824700	-1.62728700
C	-4.22780700	3.00015000	1.69835100
H	-4.02908800	1.06836300	2.64578900
C	-4.38596100	3.68355000	0.48999100
H	-4.59526500	3.49945900	-1.65038600
H	-4.18970000	3.55036000	2.63357200
H	-4.46961700	4.76615700	0.48565700
S	-5.71909400	-1.36533200	1.02738400
O	-5.65460200	-2.79724000	0.69474900
O	-5.95523500	-0.90651800	2.40373000
C	-6.89293700	-0.57187800	-0.05636800
C	-7.48302600	0.62714400	0.34676500
C	-7.14052900	-1.13938500	-1.30770600
C	-8.34807600	1.27263900	-0.53475300
H	-7.26815800	1.03302000	1.32834100
C	-8.00899900	-0.48205100	-2.17755000
H	-6.67829600	-2.08309000	-1.57601600
C	-8.60650000	0.72151600	-1.79245800
H	-8.82233400	2.20302300	-0.23882800
H	-8.22666200	-0.91226400	-3.15012900
H	-9.28254300	1.22874000	-2.47417800
P	3.81927000	0.03984700	0.00619900
C	4.50653000	1.71781700	0.03332300
C	3.84362300	2.71111600	0.77062300
C	5.70458700	2.01618200	-0.62981800
C	4.38285200	3.99261000	0.84959300
H	2.91235300	2.47846700	1.28082000
C	6.23591700	3.30394800	-0.54944700
H	6.21568100	1.25083700	-1.20452900
C	5.57815500	4.28941200	0.18836400
H	3.87025500	4.76033400	1.42076100
H	7.16240200	3.53618900	-1.06523100
H	5.99393100	5.29058600	0.24609100
C	4.58833200	-0.84432000	-1.37766300
C	4.08598400	-0.64781100	-2.67330200
C	5.69459700	-1.67990300	-1.17169700
C	4.69434200	-1.27737900	-3.75628200
H	3.22423600	-0.00389800	-2.82975500
C	6.29567400	-2.31056900	-2.26162600
H	6.08037400	-1.83777200	-0.16994200
C	5.79816900	-2.10994500	-3.55022500
H	4.30570100	-1.12494400	-4.75832700
H	7.15051300	-2.96029500	-2.10219400
H	6.26700300	-2.60530400	-4.39482000
C	4.33203100	-0.78562300	1.53720400
C	3.65547200	-1.94638600	1.94325200
C	5.41437900	-0.30394800	2.28648300
C	4.06705500	-2.62524200	3.08734600
H	2.81177600	-2.31474100	1.36541200
C	5.81809600	-0.98798200	3.43357100
H	5.93452100	0.59682100	1.97773300
C	5.14750700	-2.14528200	3.83303300
H	3.54256100	-3.52230000	3.40105100
H	6.65467400	-0.61418700	4.01560600
H	5.46291400	-2.67197400	4.72836700
Au	1.50382400	0.07122200	-0.19217000

Zero-point correction= 0.641754 (Hartree/Particle)

Thermal correction to Energy= 0.684388
Thermal correction to Enthalpy= 0.685332
Thermal correction to Gibbs Free Energy= 0.553927
Sum of electronic and zero-point Energies= -2569.607396
Sum of electronic and thermal Energies= -2569.564762
Sum of electronic and thermal Enthalpies= -2569.563818
Sum of electronic and thermal Free Energies= -2569.695222
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.142578

INT5´-b

C	-3.91036400	-0.58980300	0.60450000
C	-2.73840800	-1.23509700	0.66566000
C	-2.49760200	-2.74122000	0.65854600
H	-3.21934500	-3.30993200	1.24048200
H	-2.50780400	-3.12999800	-0.37128300
O	-1.21705400	-2.90202700	1.25775100
C	-0.43208900	-1.83280600	0.80452800
H	0.44886700	-1.75207800	1.44521000
H	-0.10350900	-1.99849400	-0.23686600
C	-1.35648700	-0.57289100	0.87424900
H	-1.31367000	-0.17533200	1.89396000
C	-0.97768900	0.53004600	-0.09756300
C	-1.00547900	1.95967800	0.38706600
H	-0.42116800	2.63010300	-0.25414000
H	-2.04183300	2.33003000	0.34820400
H	-0.66425200	2.05714000	1.42153000
C	-1.31291800	0.31373700	-1.55169100
H	-0.77405500	1.00421700	-2.20809200
H	-1.12502500	-0.71264200	-1.87954000
H	-2.38695400	0.50912100	-1.69475400
C	-4.10594700	0.86478100	0.81561700
C	-4.43407300	1.73118200	-0.23808400
C	-3.99085400	1.37953300	2.11518600
C	-4.60504500	3.09502700	-0.00025700
H	-4.56683400	1.33605600	-1.23978200
C	-4.16700000	2.74256400	2.35170200
H	-3.77857900	0.70076300	2.93508900
C	-4.46742200	3.60360400	1.29383100
H	-4.85537300	3.75719000	-0.82350100
H	-4.07887300	3.13026800	3.36204500
H	-4.60675300	4.66445800	1.47849800
S	-5.45405300	-1.55547400	0.52942100
O	-5.14874200	-2.86033300	-0.08211000
O	-6.06355800	-1.46069300	1.86371600
C	-6.46387000	-0.63508800	-0.61885600
C	-7.35609200	0.31705100	-0.12646600
C	-6.30227800	-0.86270900	-1.98704700
C	-8.10001200	1.06879800	-1.03478400
H	-7.45772300	0.45513200	0.94392900
C	-7.04861400	-0.10022200	-2.88435500
H	-5.62039400	-1.63336900	-2.33023400
C	-7.94072600	0.86532000	-2.40772200
H	-8.80320500	1.81164000	-0.67162400
H	-6.94545800	-0.26675100	-3.95218000
H	-8.52196100	1.45439500	-3.11080600
P	3.68900200	0.03894900	-0.13881600
C	4.58524800	1.35888700	0.71651000
C	4.04934400	1.88782800	1.90149500
C	5.81847900	1.81840800	0.23344600
C	4.75196000	2.86266500	2.60443300
H	3.08921800	1.53459700	2.26874000
C	6.51295000	2.79949800	0.94172300
H	6.23141500	1.41319600	-0.68426900
C	5.98278600	3.31964800	2.12353900
H	4.33878700	3.27105700	3.52133000
H	7.46731600	3.15721400	0.56832500
H	6.52575000	4.08491100	2.66945500
C	4.37528500	-0.12442700	-1.80534300
C	3.96555000	0.77390200	-2.80292900
C	5.33931600	-1.10238300	-2.08879700
C	4.52696300	0.69881900	-4.07487600
H	3.21198300	1.52518000	-2.58134600
C	5.89365600	-1.17249500	-3.36706100
H	5.65182300	-1.80060700	-1.31939900
C	5.48969100	-0.27493300	-4.35700200
H	4.21062600	1.39291100	-4.84711400
H	6.63893900	-1.92987100	-3.58873900
H	5.92128900	-0.33591200	-5.35123000
C	3.99040400	-1.51141200	0.74872200
C	3.21779300	-2.63738300	0.41935800
C	4.98024300	-1.60117400	1.73663100
C	3.43820500	-3.84557500	1.07423200
H	2.44948000	-2.56514900	-0.34556700
C	5.19351600	-2.81627800	2.38915000
H	5.57652300	-0.73230600	1.99394600
C	4.42478300	-3.93405200	2.06148000
H	2.83756500	-4.71375700	0.82228300
H	5.95916800	-2.88681300	3.15533200
H	4.59033500	-4.87502200	2.57677500
Au	1.39328000	0.43392500	-0.18140000

Zero-point correction= 0.644742 (Hartree/Particle)
Thermal correction to Energy= 0.686786
Thermal correction to Enthalpy= 0.687730
Thermal correction to Gibbs Free Energy= 0.559647
Sum of electronic and zero-point Energies= -2569.644442
Sum of electronic and thermal Energies= -2569.602398
Sum of electronic and thermal Enthalpies= -2569.601453
Sum of electronic and thermal Free Energies= -2569.729536
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.1821838

TS3´-b

C	-0.34933100	3.07576800	-1.34801300
C	-0.23563400	2.17382400	-2.19013100
C	0.08920800	1.55318300	-3.51016300
H	-0.69700900	1.83669100	-4.21630000
H	1.03936800	1.98243200	-3.86142000
O	0.13560800	0.14647800	-3.51698000
C	1.34660500	-0.41863000	-2.96467600
H	1.33738500	-1.45624600	-3.30919700
H	2.21337200	0.07591700	-3.41473700
C	1.38300400	-0.37443700	-1.46772400
H	0.77543200	-1.11746200	-0.95937600
C	2.32305200	0.31069100	-0.68252600
C	2.03119200	0.44153500	0.79848000

H	2.93623300	0.67251200	1.36778700
H	1.32157800	1.26551200	0.95510300
H	1.58375200	-0.46661700	1.20145200
C	3.16962600	1.42389200	-1.26391500
H	3.58334600	1.17259600	-2.24226400
H	2.55938000	2.33039100	-1.36823800
H	4.00401700	1.66069800	-0.59711100
S	3.86843200	-1.40299200	-0.63528200
O	3.15805900	-2.55894100	-0.03910500
O	4.39876800	-1.45679200	-2.01749000
C	5.19384600	-0.92730200	0.47117900
C	6.28830900	-0.22930900	-0.04432100
C	5.05741100	-1.18991800	1.83697600
C	7.28230400	0.19683900	0.83584800
H	6.36430200	-0.05674900	-1.11218600
C	6.05905300	-0.75546100	2.70311800
H	4.19505400	-1.74031400	2.19702200
C	7.16610800	-0.06261400	2.20412000
H	8.15070000	0.72392100	0.45308500
H	5.98133600	-0.96330400	3.76591700
H	7.94365400	0.27196800	2.88399700
P	-2.13447900	-1.01370300	0.39686600
C	-0.90686200	-1.60004500	1.60339000
C	-0.74138700	-0.89998100	2.81008200
C	-0.04447200	-2.65652300	1.28325300
C	0.26749800	-1.27331000	3.69390900
H	-1.40106300	-0.07307200	3.05665100
C	0.97391600	-3.01653100	2.16826800
H	-0.15504300	-3.19188400	0.34664200
C	1.12627500	-2.33044800	3.37289100
H	0.38711400	-0.73865200	4.63127800
H	1.65398500	-3.81653200	1.89959300
H	1.91419600	-2.61593700	4.06353300
C	-2.40323100	-2.37109100	-0.77918100
C	-1.92993600	-2.27387600	-2.09587400
C	-3.04946300	-3.54100000	-0.34926700
C	-2.09384100	-3.34850100	-2.97089800
H	-1.44086900	-1.36950000	-2.44539000
C	-3.21023600	-4.60720900	-1.23006800
H	-3.42921500	-3.61556400	0.66490200
C	-2.73006900	-4.51282800	-2.53969400
H	-1.72691900	-3.27018000	-3.98956100
H	-3.71182200	-5.51040500	-0.89691900
H	-2.85735000	-5.34653600	-3.22336400
C	-3.68112100	-0.71758000	1.29640000
C	-4.58409900	0.23303500	0.79890200
C	-4.01043800	-1.46856000	2.43519800
C	-5.81166300	0.42350000	1.43043900
H	-4.32382300	0.81794900	-0.07922500
C	-5.23896800	-1.26977200	3.06365000
H	-3.30764300	-2.19254400	2.83475500
C	-6.13909100	-0.32728200	2.56178500
H	-6.50946500	1.15944900	1.04334500
H	-5.49172600	-1.84925500	3.94613700
H	-7.09391500	-0.17458200	3.05534600
Au	-1.27178900	0.83412300	-0.71630700
C	-0.44896400	4.08860400	-0.35412400
C	0.63982700	4.33641700	0.50661400
C	-1.63079100	4.84691600	-0.23139300
C	0.54295000	5.33225500	1.47160800
H	1.54558100	3.74811300	0.40523100
C	-1.71557900	5.83808600	0.73956100
H	-2.46260300	4.64942200	-0.89963400
C	-0.63198900	6.08105400	1.58960100
H	1.38161700	5.52746200	2.13216800
H	-2.62375400	6.42448700	0.83423900
H	-0.70314600	6.85720400	2.34528500

Zero-point correction= 0.641186 (Hartree/Particle)
Thermal correction to Energy= 0.684249
Thermal correction to Enthalpy= 0.685193
Thermal correction to Gibbs Free Energy= 0.556759
Sum of electronic and zero-point Energies= -2569.623264
Sum of electronic and thermal Energies= -2569.580202
Sum of electronic and thermal Enthalpies= -2569.579257
Sum of electronic and thermal Free Energies= -2569.707691
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.1589885

INT3´-b

C	-0.21262400	3.06485300	-1.38431600
C	-0.18477700	2.17667100	-2.24761200
C	0.02000900	1.55560000	-3.58988700
H	-0.84039300	1.80642300	-4.21709400
H	0.91791300	2.00775600	-4.03749600
O	0.10966800	0.15069100	-3.58770400
C	1.34979800	-0.36170200	-3.05470300
H	1.42146300	-1.37671400	-3.45979600
H	2.18467800	0.21698600	-3.46229100
C	1.36902100	-0.41030400	-1.55893900
H	0.73516700	-1.16384200	-1.10085300
C	2.48194800	0.08610000	-0.70409800
C	2.01414300	0.41711200	0.71704900
H	2.86368800	0.65728600	1.36268300
H	1.35697800	1.29282100	0.68475700
H	1.46114200	-0.41169100	1.15737200
C	3.30887600	1.22558600	-1.30213700
H	3.79954600	0.93587900	-2.23320600
H	2.65206400	2.07900300	-1.50228000
H	4.08139000	1.54636200	-0.59754800
S	3.60201200	-1.45614100	-0.60398200
O	2.80248500	-2.50934400	0.05214900
O	4.13422200	-1.65004000	-1.96587800
C	4.95633400	-1.03284200	0.48285400
C	6.12618300	-0.50338700	-0.06572500
C	4.81203100	-1.23695500	1.85776900
C	7.17303300	-0.16210500	0.79005800
H	6.21456900	-0.39067400	-1.14050100
C	5.86613600	-0.88936200	2.70071300
H	3.89871600	-1.67511800	2.24499400
C	7.04073400	-0.35047300	2.16808300
H	8.09428100	0.24058000	0.38091900
H	5.77678300	-1.04770800	3.77103500
H	7.86024000	-0.08564100	2.82925300
P	-2.13439200	-0.94149000	0.40424000
C	-0.97129300	-1.46717400	1.69774900

C	-0.84325300	-0.68230400	2.85681100
C	-0.11603500	-2.55612900	1.49134200
C	0.12093800	-1.00415600	3.80725200
H	-1.49730800	0.17069900	3.01352200
C	0.85476000	-2.86763700	2.44588700
H	-0.18794600	-3.15060700	0.58785000
C	0.97057900	-2.09753300	3.60217600
H	0.21244600	-0.40321700	4.70685800
H	1.52776800	-3.69817600	2.26590000
H	1.72252600	-2.34454400	4.34578900
C	-2.35819000	-2.35029700	-0.71840700
C	-1.91359600	-2.28217700	-2.04669800
C	-2.95698700	-3.52591100	-0.23734900
C	-2.05755800	-3.39067800	-2.88217900
H	-1.46090500	-1.37489600	-2.43550900
C	-3.09727000	-4.62631300	-1.07831900
H	-3.31355600	-3.57906700	0.78667800
C	-2.64507700	-4.56026500	-2.39976200
H	-1.71180700	-3.33521600	-3.90966900
H	-3.56047000	-5.53434500	-0.70517700
H	-2.75566200	-5.42085700	-3.05228800
C	-3.72171600	-0.59575500	1.21164500
C	-4.60085300	0.32029500	0.61628900
C	-4.10363400	-1.27845800	2.37642700
C	-5.85674500	0.54432100	1.17709100
H	-4.30021500	0.85191800	-0.28265000
C	-5.36025400	-1.04614600	2.93389300
H	-3.42017000	-1.97515100	2.85101000
C	-6.23633500	-0.13831400	2.33506300
H	-6.53616600	1.25318100	0.71412900
H	-5.65378900	-1.57255400	3.83678800
H	-7.21327200	0.04056500	2.77347900
Au	-1.21441400	0.85517300	-0.74586400
C	-0.20383900	4.05120100	-0.35969000
C	0.98570900	4.31195600	0.35073600
C	-1.37920800	4.76668900	-0.05305500
C	0.99336800	5.27813000	1.35042900
H	1.88638700	3.75888500	0.10718100
C	-1.35858200	5.72705000	0.95141200
H	-2.28911500	4.55928400	-0.60672500
C	-0.17552300	5.98318100	1.65221200
H	1.90938500	5.48397700	1.89478200
H	-2.26195400	6.27973000	1.18820000
H	-0.16454400	6.73594500	2.43435000

Zero-point correction= 0.643142 (Hartree/Particle)
Thermal correction to Energy= 0.685950
Thermal correction to Enthalpy= 0.686894
Thermal correction to Gibbs Free Energy= 0.559685
Sum of electronic and zero-point Energies= -2569.628666
Sum of electronic and thermal Energies= -2569.585857
Sum of electronic and thermal Enthalpies= -2569.584913
Sum of electronic and thermal Free Energies= -2569.712122
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.1632191

TS7′-b

C	-0.06496700	3.03037900	-0.73719800
C	-0.28033300	2.33843900	-1.76810300
C	-0.19285600	2.15127600	-3.26166900
H	0.15137600	3.08317100	-3.71830000
H	0.54267800	1.36044000	-3.47961500
O	-1.44088100	1.85068700	-3.82394200
C	-2.05509300	0.74684500	-3.15887600
H	-2.98980900	0.55396500	-3.69765600
H	-1.42412700	-0.15058400	-3.24053700
C	-2.32214900	1.11620600	-1.73518200
H	-2.85155500	2.05838800	-1.61163700
C	-2.54506800	0.12681600	-0.64238500
C	-2.38035100	0.75980600	0.74293000
H	-2.67347500	0.05941000	1.53071700
H	-1.33104300	1.03024000	0.89857300
H	-2.98081100	1.66726600	0.83884500
C	-1.76597300	-1.18051500	-0.77906000
H	-2.02918900	-1.72155500	-1.69006800
H	-0.69379000	-0.96924300	-0.80965900
H	-1.95244200	-1.83535500	0.07629900
S	-4.39914400	-0.29515600	-0.84967000
O	-5.13766000	0.94733200	-0.56417700
O	-4.51272500	-0.97471400	-2.15426500
C	-4.78805300	-1.48401500	0.43134800
C	-4.63743500	-2.84644500	0.16318400
C	-5.24127500	-1.02232400	1.66928200
C	-4.93404400	-3.76484900	1.16931600
H	-4.32268600	-3.16997700	-0.82257000
C	-5.53408300	-1.95235000	2.66612600
H	-5.38581300	0.04058800	1.82753200
C	-5.37558600	-3.31823800	2.41774600
H	-4.83507000	-4.82838000	0.97511100
H	-5.89895900	-1.61238700	3.63038200
H	-5.61105800	-4.03843200	3.19550800
C	-0.27668600	3.78273200	0.45046000
C	-1.51311300	4.44661300	0.61022400
C	0.69937200	3.86946700	1.46387100
C	-1.75873400	5.17761000	1.76647200
H	-2.26137500	4.37893200	-0.17243600
C	0.43583000	4.59663500	2.61865100
H	1.65313100	3.36776200	1.33179800
C	-0.78996500	5.25174800	2.77239000
H	-2.70890900	5.68838100	1.88579500
H	1.18842600	4.66031500	3.39808700
H	-0.98887700	5.82300700	3.67365300
P	2.35806800	-0.84111900	0.16453200
C	1.68403900	-2.29698000	-0.68956900
C	1.58368800	-2.25599800	-2.09008100
C	1.20820800	-3.40786600	0.01576900
C	1.01205300	-3.32266100	-2.77701500
H	1.94678400	-1.38871300	-2.63610100
C	0.63128000	-4.47242500	-0.68013300
H	1.27921300	-3.43956500	1.09766300
C	0.53021700	-4.42999900	-2.07081600
H	0.93597100	-3.29074000	-3.85942100
H	0.26103400	-5.33364400	-0.13268500
H	0.07700500	-5.25771700	-2.60742700
C	2.18039800	-1.12138800	1.94758400
C	0.92837200	-0.90362400	2.54487800

C	3.25626600	-1.58097400	2.71833300
C	0.75477200	-1.15447700	3.90348500
H	0.09573500	-0.54372700	1.94773700
C	3.07542200	-1.82390100	4.08052700
H	4.22619900	-1.74378800	2.26026900
C	1.82889400	-1.61265000	4.67195600
H	-0.21390300	-0.98659600	4.36395900
H	3.90997400	-2.17592100	4.67873000
H	1.69406700	-1.80089800	5.73257900
C	4.12177400	-0.74221000	-0.22860400
C	4.76657700	0.50278300	-0.18827400
C	4.85000700	-1.90385100	-0.52575500
C	6.13559400	0.58280500	-0.43440600
H	4.19710000	1.40221600	0.03053400
C	6.21942000	-1.81488100	-0.77306900
H	4.34886900	-2.86569300	-0.56962800
C	6.86093700	-0.57509800	-0.72642800
H	6.63425900	1.54649800	-0.40634300
H	6.78372200	-2.71225500	-1.00657400
H	7.92634500	-0.50995200	-0.92428800
Au	1.12914300	1.00573100	-0.53000600

Zero-point correction= 0.641539 (Hartree/Particle)
Thermal correction to Energy= 0.684063
Thermal correction to Enthalpy= 0.685008
Thermal correction to Gibbs Free Energy= 0.555359
Sum of electronic and zero-point Energies= -2569.613047
Sum of electronic and thermal Energies= -2569.570523
Sum of electronic and thermal Enthalpies= -2569.569579
Sum of electronic and thermal Free Energies= -2569.699228
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.152401

INT7′-b

C	-0.50500800	2.34524500	-0.35205300
C	-1.12995800	1.76518200	-1.42282300
C	-0.51127900	1.56250400	-2.79588300
H	0.23152900	2.32133800	-3.05262900
H	-0.04115100	0.56306500	-2.85891000
O	-1.62324000	1.67861900	-3.65097900
C	-2.67822600	0.93532300	-3.03586800
H	-3.62511900	1.29784200	-3.43342700
H	-2.58594000	-0.12651300	-3.27791600
C	-2.53145500	1.19574300	-1.50470100
H	-3.24996700	1.95588700	-1.17863200
C	-2.74872700	-0.03794100	-0.56287500
C	-2.62304900	0.34335300	0.91368000
H	-2.93313000	-0.48851800	1.55103400
H	-1.57848400	0.56406200	1.14934700
H	-3.22778500	1.21922800	1.16056300
C	-1.85886900	-1.24000900	-0.88517100
H	-1.98681300	-1.59977600	-1.90658600
H	-0.80565300	-0.97717600	-0.73747100
H	-2.08347500	-2.06683900	-0.20541100
S	-4.54099800	-0.48579500	-0.88004700
O	-5.31454300	0.72843000	-0.55950200
O	-4.60830900	-1.09845500	-2.21898700
C	-4.95327200	-1.75016500	0.31752200
C	-4.72537900	-3.08879600	-0.00947600
C	-5.52780600	-1.37490000	1.53364900
C	-5.06094600	-4.07207000	0.92052700
H	-4.32350900	-3.34684000	-0.98280400
C	-5.86059800	-2.36919000	2.45259200
H	-5.72717500	-0.32839100	1.73541000
C	-5.62190600	-3.71203000	2.14847900
H	-4.89938600	-5.11842700	0.68096700
H	-6.31682700	-2.09737300	3.39928000
H	-5.88783600	-4.48236000	2.86595600
C	-1.02421300	3.25649000	0.61817300
C	-2.10482100	4.11737600	0.28448100
C	-0.46001200	3.35224000	1.91630300
C	-2.61844100	4.99903700	1.22222300
H	-2.51671800	4.08718600	-0.71859600
C	-0.98797400	4.22682200	2.85246900
H	0.38336200	2.71699500	2.17094800
C	-2.06818000	5.05175900	2.50991900
H	-3.44546000	5.64971500	0.95716200
H	-0.55982800	4.27938900	3.84834300
H	-2.47368500	5.74282700	3.24234500
P	2.79084500	-0.57422200	0.14305600
C	2.04426600	-1.92888500	-0.82446900
C	1.85614800	-1.72689900	-2.20262700
C	1.54747500	-3.08611200	-0.21534500
C	1.17650300	-2.67667900	-2.96016100
H	2.24510500	-0.82981500	-2.67775800
C	0.86196600	-4.03290900	-0.98049400
H	1.68893700	-3.24643300	0.84813100
C	0.67230200	-3.82897300	-2.34734400
H	1.03853200	-2.52036600	-4.02567900
H	0.48014300	-4.93149200	-0.50552900
H	0.13781100	-4.56648300	-2.93810400
C	2.99331700	-1.17439000	1.84386400
C	1.89301700	-1.11702000	2.71404700
C	4.20689500	-1.71825200	2.28510100
C	2.00443500	-1.61313300	4.01105600
H	0.95385600	-0.68950800	2.37142200
C	4.31378700	-2.20511500	3.58795200
H	5.06231300	-1.75506400	1.61870100
C	3.21586800	-2.15512300	4.44873100
H	1.15198400	-1.57000000	4.68200900
H	5.25602300	-2.62130300	3.93049200
H	3.30467100	-2.53364800	5.46235300
C	4.43158400	-0.25769500	-0.55290100
C	4.97223000	1.03303200	-0.45856800
C	5.17483200	-1.29072700	-1.14406000
C	6.25430600	1.28531400	-0.94346500
H	4.38945300	1.83352700	-0.01058500
C	6.45566000	-1.02974400	-1.62891200
H	4.75120500	-2.28645900	-1.23085200
C	6.99485900	0.25500200	-1.52760100
H	6.67176300	2.28475300	-0.87229200
H	7.03058600	-1.82748300	-2.08879700
H	7.99102500	0.45477400	-1.91015500
Au	1.21323600	1.15862000	-0.06389200

Zero-point correction= 0.645829 (Hartree/Particle)
Thermal correction to Energy= 0.687392

Thermal correction to Enthalpy= 0.688336

Thermal correction to Gibbs Free Energy= 0.562609

Sum of electronic and zero-point Energies= -2569.661801

Sum of electronic and thermal Energies= -2569.620237

Sum of electronic and thermal Enthalpies= -2569.619293

Sum of electronic and thermal Free Energies= -2569.745020

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.1983378

TS4´-b

C	0.84282200	3.03649100	1.14827800
C	0.16421900	2.34906200	1.91978700
C	-0.77985400	1.93679700	2.99661000
H	-0.29711000	2.15098500	3.95604100
H	-1.68385100	2.55692900	2.92562000
O	-1.09533100	0.56122600	3.00137700
C	-2.27857100	0.18634500	2.28101700
H	-2.43896600	-0.85944400	2.54467500
H	-3.13414900	0.76588400	2.64730400
C	-2.09591200	0.32910600	0.78494400
H	-1.22665100	-0.22272500	0.43114100
C	-2.38414400	1.50344500	0.07205900
C	-1.75502500	1.74024900	-1.26744200
H	-2.50818500	1.70076700	-2.06692200
H	-1.31404900	2.74572600	-1.31018600
H	-0.97822400	1.00724100	-1.50086400
C	-3.41449600	2.50771700	0.49440300
H	-3.90575300	2.26257300	1.43770400
H	-2.96276000	3.50591500	0.58898300
H	-4.19866800	2.59331700	-0.26995200
S	-3.41367800	-1.31574800	-0.02158000
O	-2.71477500	-1.77706100	-1.24922800
O	-3.78724800	-2.26987700	1.05293800
C	-4.89047800	-0.43481200	-0.52725200
C	-5.87380800	-0.17792300	0.42877600
C	-4.96304900	0.08000000	-1.82142300
C	-6.96119100	0.61856100	0.07204400
H	-5.79296300	-0.61061500	1.42032900
C	-6.05663900	0.87532200	-2.16480700
H	-4.18685200	-0.15924500	-2.53973200
C	-7.04790800	1.14898900	-1.21837000
H	-7.74303200	0.82064500	0.79751700
H	-6.13901100	1.27489600	-3.17095300
H	-7.89591800	1.77017100	-1.48991400
C	1.62525200	3.87305400	0.29462400
C	2.39298600	4.90902200	0.85954300
C	1.63316000	3.67013400	-1.09987300
C	3.14449900	5.73856600	0.03286600
H	2.38800200	5.05518500	1.93457900
C	2.39881400	4.49876200	-1.91258100
H	1.05044300	2.86070100	-1.52632400
C	3.15036200	5.53434600	-1.34952300
H	3.73067900	6.54178300	0.46756800
H	2.40857800	4.33939800	-2.98609700
H	3.74324800	6.18128600	-1.98853900
P	1.72396100	-1.39871700	-0.15224200
C	0.53319600	-2.63176100	0.43171400
C	0.00692500	-2.50907700	1.72858900
C	0.14057300	-3.70184800	-0.38567400
C	-0.90832700	-3.44863900	2.19561300
H	0.29367400	-1.67204200	2.35895800
C	-0.77837700	-4.63509900	0.09093700
H	0.52811300	-3.79079200	-1.39495600
C	-1.30573400	-4.50708000	1.37603400
H	-1.32687600	-3.34464400	3.19142000
H	-1.09481200	-5.45191900	-0.54967200
H	-2.03954200	-5.22141900	1.73444400
C	3.40611300	-1.97281700	0.20192600
C	4.41827200	-1.03735700	0.46006100
C	3.70545000	-3.34250200	0.16875000
C	5.72660200	-1.47050200	0.67112700
H	4.18003600	0.02252800	0.49791700
C	5.01429500	-3.76805500	0.38720400
H	2.92009500	-4.06866300	-0.01515100
C	6.02366100	-2.83447700	0.63517400
H	6.50967600	-0.74602200	0.87195200
H	5.24563400	-4.82844500	0.36787400
H	7.04128200	-3.17125500	0.80745200
C	1.54940100	-1.27350600	-1.95753800
C	2.68145900	-1.11228200	-2.76709000
C	0.26387400	-1.24630300	-2.52390800
C	2.52782000	-0.92259300	-4.14066100
H	3.67469600	-1.14193100	-2.33082700
C	0.12421000	-1.05938700	-3.89795600
H	-0.62240300	-1.39914200	-1.91509600
C	1.25177900	-0.89374000	-4.70650500
H	3.40610300	-0.80600800	-4.76817600
H	-0.86974900	-1.05435500	-4.33486100
H	1.13668400	-0.75131700	-5.77677400
Au	1.21832200	0.65475000	0.79991000

Zero-point correction= 0.641008 (Hartree/Particle)

Thermal correction to Energy= 0.684318

Thermal correction to Enthalpy= 0.685262

Thermal correction to Gibbs Free Energy= 0.555969

Sum of electronic and zero-point Energies= -2569.629425

Sum of electronic and thermal Energies= -2569.586116

Sum of electronic and thermal Enthalpies= -2569.585172

Sum of electronic and thermal Free Energies= -2569.714465

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.1641386

INT4´-b

C	0.69160100	3.10892100	1.02415600
C	-0.06019200	2.34272600	1.64144100
C	-1.07554300	1.91716200	2.64565100
H	-0.67349700	2.15074200	3.63765200
H	-1.98681900	2.51055600	2.49985200
O	-1.34995200	0.53133900	2.63630800
C	-2.50326200	0.10371000	1.91368200
H	-2.66233100	-0.92664800	2.23166900
H	-3.37536400	0.69929900	2.20936900
C	-2.29449200	0.12626000	0.39454500
H	-1.33654100	-0.36435600	0.19045100
C	-2.38124500	1.42389000	-0.31049300
C	-1.63488200	1.61560800	-1.59251900
H	-2.22286000	1.26319000	-2.45439600

H	-1.42085500	2.67724200	-1.76478400
H	-0.69010500	1.06271200	-1.61877100
C	-3.38760300	2.47411500	0.04974600
H	-4.03915600	2.19326500	0.88014700
H	-2.88834400	3.42055200	0.31150300
H	-4.04071200	2.69992200	-0.80436100
S	-3.42054000	-1.17141600	-0.41520900
O	-2.88285300	-1.34743500	-1.78090000
O	-3.54420100	-2.32044100	0.50056200
C	-5.01073800	-0.36617100	-0.54743400
C	-5.85155800	-0.35292900	0.56705100
C	-5.35275800	0.27274900	-1.73905500
C	-7.05921000	0.33944100	0.48644100
H	-5.57351600	-0.89372400	1.46550000
C	-6.56611600	0.95701700	-1.80773800
H	-4.68421900	0.21553600	-2.59070800
C	-7.41128500	0.99651800	-0.69579300
H	-7.72973300	0.35651500	1.33988500
H	-6.85462300	1.45318200	-2.72917500
H	-8.35412900	1.53164300	-0.75412300
C	1.55759700	3.97794300	0.30237100
C	2.81253400	4.32448800	0.84337000
C	1.16205100	4.49448800	-0.94737500
C	3.65372800	5.17873900	0.13973400
H	3.10692200	3.92235900	1.80736100
C	2.01228100	5.34805600	-1.64075900
H	0.19617400	4.21896800	-1.35589000
C	3.25546400	5.68958500	-1.09965600
H	4.61869300	5.44971800	0.55578200
H	1.70861700	5.74838700	-2.60263900
H	3.91595200	6.35646400	-1.64518800
P	1.64529800	-1.40148600	-0.24279300
C	0.46512700	-2.61590200	0.40630100
C	0.00404100	-2.46972800	1.72534000
C	0.03588400	-3.70317400	-0.36934700
C	-0.87596500	-3.40687800	2.25948700
H	0.31410100	-1.61673000	2.32165800
C	-0.85158400	-4.63143500	0.17309600
H	0.37698400	-3.81378500	-1.39288400
C	-1.30767300	-4.48406900	1.48304800
H	-1.23675600	-3.28726400	3.27631600
H	-1.19569000	-5.46256300	-0.43397300
H	-2.01139600	-5.20038700	1.89451900
C	3.32042100	-1.92419600	0.21254800
C	4.31535300	-0.96030400	0.42826200
C	3.63218700	-3.28876200	0.29862000
C	5.61901400	-1.36075500	0.71778000
H	4.06730000	0.09642000	0.37035600
C	4.93622400	-3.68133700	0.59457800
H	2.85967000	-4.03540400	0.14427000
C	5.92847800	-2.71994900	0.80165500
H	6.38922900	-0.61427000	0.88518700
H	5.17708000	-4.73731900	0.66693900
H	6.94235400	-3.03063400	1.03446800
C	1.53182200	-1.42906000	-2.05481100
C	2.69169400	-1.43348400	-2.84099700
C	0.26610400	-1.37653400	-2.66183800
C	2.58380800	-1.38494000	-4.23115800
H	3.66968400	-1.48083400	-2.37360500
C	0.17109100	-1.33303900	-4.05076600
H	-0.64595900	-1.39490600	-2.07421300
C	1.32687800	-1.33349400	-4.83633900
H	3.48281900	-1.39416000	-4.83972300
H	-0.81067900	-1.30613200	-4.51322800
H	1.24788900	-1.30014700	-5.91875800
Au	1.07127700	0.68430600	0.60175500

Zero-point correction= 0.642338 (Hartree/Particle)
Thermal correction to Energy= 0.685738
Thermal correction to Enthalpy= 0.686682
Thermal correction to Gibbs Free Energy= 0.556571
Sum of electronic and zero-point Energies= -2569.633184
Sum of electronic and thermal Energies= -2569.589783
Sum of electronic and thermal Enthalpies= -2569.588839
Sum of electronic and thermal Free Energies= -2569.718951
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.166335

TS8′-b

C	0.24153400	2.70498100	-1.26930600
C	0.91364900	1.74253100	-1.73644000
C	1.43859300	1.09941600	-2.98407200
H	0.76557900	1.33545700	-3.81270100
H	2.42506400	1.53315000	-3.20510400
O	1.49790800	-0.30590100	-2.91691500
C	2.55296900	-0.83035700	-2.12110300
H	2.54692900	-1.90570200	-2.29649300
H	3.51773400	-0.42454600	-2.45343900
C	2.30774500	-0.56000900	-0.63284900
H	1.30347900	-0.93491200	-0.40178200
C	2.43504000	0.85731800	-0.17628500
C	1.79828600	1.22798200	1.13223400
H	2.49209100	1.03270000	1.96143200
H	1.54671100	2.29331400	1.15894200
H	0.89163800	0.65202100	1.33925500
C	3.63222800	1.68828800	-0.55528700
H	4.08645000	1.39910600	-1.50509800
H	3.35780900	2.74778300	-0.61514500
H	4.41563700	1.60932800	0.21061200
S	3.28250500	-1.78502900	0.41863100
O	2.66856300	-1.73257200	1.76002200
O	3.33269500	-3.05190300	-0.33373100
C	4.93793900	-1.12536800	0.53740500
C	5.79975900	-1.26548800	-0.55199800
C	5.31870800	-0.45827400	1.70190000
C	7.06902700	-0.69354600	-0.47846100
H	5.49043400	-1.83092500	-1.42466600
C	6.59449200	0.10219400	1.76469500
H	4.62919500	-0.39896900	2.53665400
C	7.46134900	-0.00687200	0.67400500
H	7.75548400	-0.79411500	-1.31319800
H	6.91376500	0.61757200	2.66512800
H	8.45235800	0.43327600	0.72720500
C	-0.20456400	3.82704000	-0.52362700
C	0.73750900	4.78486100	-0.08387100
C	-1.57243600	4.01281300	-0.22298300

C	0.31524500	5.88913600	0.64615800
H	1.78733500	4.64894800	-0.32202100
C	-1.97758700	5.11367800	0.52210800
H	-2.29962100	3.29272800	-0.58550100
C	-1.03830000	6.05355400	0.95812100
H	1.04312800	6.62237500	0.97883400
H	-3.02961900	5.24817000	0.75313300
H	-1.36056800	6.91558200	1.53350600
P	-2.28423500	-0.89310100	0.21125000
C	-1.54227900	-2.54231400	0.06294400
C	-0.32784100	-2.79340500	0.72423300
C	-2.11546400	-3.52237900	-0.75618200
C	0.30945500	-4.02001400	0.55861700
H	0.12285300	-2.04615100	1.37058100
C	-1.47020300	-4.75037100	-0.91352300
H	-3.05429700	-3.33118300	-1.26515600
C	-0.26063200	-4.99702000	-0.26319700
H	1.25408100	-4.20071600	1.05781800
H	-1.91497000	-5.51199000	-1.54657200
H	0.24158700	-5.95023900	-0.39567400
C	-3.95713800	-0.96255300	-0.48278500
C	-4.14567200	-0.67389300	-1.84265300
C	-5.04598500	-1.35045000	0.31087800
C	-5.41549900	-0.78492100	-2.40665600
H	-3.30141100	-0.36675700	-2.45441600
C	-6.31413100	-1.45229800	-0.25892900
H	-4.90517300	-1.56311300	1.36561100
C	-6.49886100	-1.17272100	-1.61488700
H	-5.55999300	-0.56318200	-3.45941900
H	-7.15813800	-1.74783100	0.35643600
H	-7.48864800	-1.25227100	-2.05376700
C	-2.39918700	-0.51641300	1.98258300
C	-2.32089600	0.81642300	2.41453400
C	-2.58992000	-1.54523500	2.91743000
C	-2.44255300	1.11632000	3.76988900
H	-2.15849400	1.61484200	1.69544700
C	-2.71090600	-1.23701500	4.27185400
H	-2.62731000	-2.57907400	2.58943400
C	-2.63804800	0.09091200	4.69796400
H	-2.37731400	2.14790400	4.10174200
H	-2.85447900	-2.03449800	4.99413300
H	-2.72643500	0.32585600	5.75419300
Au	-0.90791500	0.66388400	-0.81793100

Zero-point correction= 0.642709 (Hartree/Particle)
Thermal correction to Energy= 0.684826
Thermal correction to Enthalpy= 0.685771
Thermal correction to Gibbs Free Energy= 0.559991
Sum of electronic and zero-point Energies= -2569.624766
Sum of electronic and thermal Energies= -2569.582648
Sum of electronic and thermal Enthalpies= -2569.581704
Sum of electronic and thermal Free Energies= -2569.707484
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.1584737

INT8´-b

C	0.43739100	2.49370300	-1.02307400
C	1.31009000	1.46732200	-1.21620300
C	1.29438300	0.69215800	-2.52616700
H	0.48343900	1.03076100	-3.17094800
H	2.25108700	0.87664800	-3.04164600
O	1.10882900	-0.69548900	-2.31382300
C	2.12248100	-1.25088300	-1.48599400
H	1.87946800	-2.30578400	-1.36884500
H	3.09730700	-1.16229400	-1.98464300
C	2.14049600	-0.56970600	-0.10930200
H	1.16633800	-0.75615000	0.36094400
C	2.34470100	0.98132800	-0.17163400
C	2.09838700	1.63045500	1.19704700
H	2.79657600	1.23555900	1.93360500
H	2.22048600	2.71377500	1.13794800
H	1.08473600	1.41982900	1.55484700
C	3.73923900	1.40738200	-0.69642800
H	4.05480700	0.85365100	-1.58354200
H	3.73511000	2.47340200	-0.94228100
H	4.49217400	1.25164000	0.07682900
S	3.20115100	-1.56823500	1.03853400
O	3.09804300	-0.97832900	2.38365800
O	2.77505000	-2.95619700	0.79250900
C	4.90370400	-1.42183400	0.50609800
C	5.33992300	-2.15270600	-0.60110000
C	5.77134500	-0.61313500	1.24190900
C	6.66921900	-2.03051500	-1.00459200
H	4.66260100	-2.82698400	-1.11316300
C	7.10008500	-0.50707600	0.83291300
H	5.40724600	-0.09746300	2.12368700
C	7.54367500	-1.20469100	-0.29356800
H	7.02569100	-2.59220800	-1.86223500
H	7.79011400	0.11182500	1.39769200
H	8.57903400	-1.11823500	-0.60845500
C	0.37880900	3.79154100	-0.46648700
C	1.47203800	4.68219100	-0.65630200
C	-0.76382600	4.26359900	0.23118900
C	1.42983400	5.96711800	-0.13854700
H	2.33646600	4.34330200	-1.21793300
C	-0.78753400	5.54635700	0.75573000
H	-1.61581800	3.60254800	0.35949400
C	0.30538000	6.40387700	0.57419600
H	2.27229100	6.63546300	-0.28639100
H	-1.66050600	5.88920800	1.30203600
H	0.27740100	7.41088700	0.97798800
P	-2.49876500	-0.76928000	0.11031600
C	-1.46839100	-1.80753700	1.18818800
C	-0.78829300	-1.18971900	2.25268300
C	-1.27762500	-3.17105000	0.93293200
C	0.07756600	-1.93190900	3.04990500
H	-0.93040000	-0.12888500	2.44485200
C	-0.40548700	-3.90729500	1.73635400
H	-1.79357500	-3.64916000	0.10734700
C	0.27487700	-3.29033600	2.78512700
H	0.62663400	-1.44824100	3.84980700
H	-0.24441500	-4.96028400	1.52886400
H	0.97813000	-3.85902500	3.38380600
C	-3.03618400	-1.79490500	-1.28411800
C	-2.11603300	-2.06232500	-2.31159900
C	-4.32400600	-2.34436000	-1.32645600

C	-2.48946900	-2.88626400	-3.37086800
H	-1.11649400	-1.63566400	-2.27865300
C	-4.68916000	-3.16288700	-2.39584900
H	-5.03458500	-2.13341200	-0.53404600
C	-3.77477700	-3.43413600	-3.41491300
H	-1.77967300	-3.09598800	-4.16517600
H	-5.68802300	-3.58643700	-2.43212300
H	-4.06384400	-4.07034800	-4.24585800
C	-3.96323900	-0.25940600	1.04425400
C	-4.66197800	0.88908100	0.64340200
C	-4.42340500	-1.02202500	2.12674600
C	-5.82117000	1.26607700	1.31791300
H	-4.29990800	1.47977500	-0.19445700
C	-5.58239400	-0.63551300	2.79984800
H	-3.87654800	-1.90497200	2.44203900
C	-6.28025100	0.50451800	2.39608600
H	-6.36304300	2.15399100	1.00734200
H	-5.93807000	-1.22333000	3.64030100
H	-7.18054200	0.80302700	2.92433100
Au	-1.08641100	0.96103400	-0.57480100

Zero-point correction= 0.646695 (Hartree/Particle)
Thermal correction to Energy= 0.688015
Thermal correction to Enthalpy= 0.688960
Thermal correction to Gibbs Free Energy= 0.565908
Sum of electronic and zero-point Energies= -2569.663171
Sum of electronic and thermal Energies= -2569.621851
Sum of electronic and thermal Enthalpies= -2569.620906
Sum of electronic and thermal Free Energies= -2569.743958
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2571.1953266

TS11-b

C	1.53575500	0.26826500	-1.01335700
C	1.03206900	-0.94143300	-1.04775200
C	1.40782600	-2.35519300	-1.23898100
H	2.39314600	-2.40207900	-1.72656200
H	1.49896800	-2.80758400	-0.24110700
O	0.43020200	-3.02685300	-2.01270100
C	0.32217000	-4.42243300	-1.68872500
H	-0.33715800	-4.82471400	-2.46330700
H	1.29951700	-4.91123400	-1.79612100
C	-0.27571900	-4.62288600	-0.32713600
H	-1.31115700	-4.29805500	-0.24439800
C	0.33878000	-5.06570000	0.78133200
C	-0.39641600	-5.12686200	2.09660600
H	-0.36239400	-6.13922600	2.52070600
H	0.07718300	-4.46140000	2.83154500
H	-1.44155700	-4.82708400	1.99528200
C	1.77352700	-5.52575200	0.84887600
H	2.31005700	-5.42703500	-0.09689400
H	2.32148600	-4.95376600	1.60981500
H	1.82503700	-6.57861400	1.15690300
C	0.86586400	1.53674900	-0.63499300
C	0.39544300	1.70260300	0.67382800
C	0.76292200	2.59535900	-1.54657700
C	-0.17694300	2.90911700	1.06644200
H	0.48938700	0.88403900	1.37723300
C	0.19983400	3.80591800	-1.14512400
H	1.14275600	2.46991100	-2.55388600
C	-0.26603400	3.96641100	0.16041700
H	-0.55121100	3.02380000	2.07900300
H	0.12441600	4.62410800	-1.85581300
H	-0.70577300	4.90971600	0.46915500
S	3.34613100	0.49397600	-1.36776600
O	3.99108800	-0.82881600	-1.43382900
O	3.47853300	1.45007900	-2.47974900
C	3.88825800	1.30100700	0.13798200
C	3.85420400	2.69289100	0.21693500
C	4.26217000	0.50856100	1.22316300
C	4.20538800	3.30330500	1.41942800
H	3.55593600	3.27451500	-0.64710700
C	4.61342600	1.13214700	2.41914600
H	4.28652200	-0.57069500	1.11871100
C	4.58076500	2.52531300	2.51684200
H	4.18459400	4.38588900	1.49950000
H	4.91480000	0.53221500	3.27257800
H	4.85134300	3.00657100	3.45223300
S	-3.66389000	-0.30660700	-0.60770200
O	-4.00905200	-0.36893800	-2.03215900
O	-4.40065700	-1.05906200	0.41660700
C	-3.64022400	1.41627700	-0.12090800
C	-3.86831000	1.74809300	1.21361000
C	-3.42807800	2.38165500	-1.10372900
C	-3.90030000	3.09623900	1.56582900
H	-4.03266400	0.96704700	1.94568900
C	-3.46532400	3.72405800	-0.73472200
H	-3.25598200	2.08239800	-2.13111700
C	-3.70478700	4.07960100	0.59411000
H	-4.08863000	3.37757500	2.59752300
H	-3.30735000	4.49149400	-1.48580900
H	-3.73718200	5.12857300	0.87425800
S	-1.50701900	-0.93995400	-0.63728200
C	-1.38449400	-1.36457100	1.14053600
F	-2.14002300	-2.42037300	1.46620400
F	-0.10767900	-1.66418100	1.45265900
F	-1.75887300	-0.34419400	1.94137600

Zero-point correction= 0.481572 (Hartree/Particle)
Thermal correction to Energy= 0.519517
Thermal correction to Enthalpy= 0.520461
Thermal correction to Gibbs Free Energy= 0.403855
Sum of electronic and zero-point Energies= -2914.156487
Sum of electronic and thermal Energies= -2914.118542
Sum of electronic and thermal Enthalpies= -2914.117598
Sum of electronic and thermal Free Energies= -2914.234204
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2915.226361

INT11-b

C	0.61625100	-0.33930000	-0.51904200
C	-0.72262900	-0.32386200	-0.41802500
C	-1.65576500	-1.49298900	-0.19647900
H	-1.10803500	-2.37976100	0.12328800
H	-2.37154700	-1.21333100	0.58145200
O	-2.31706600	-1.74421700	-1.43088000
C	-3.71742600	-2.03197400	-1.28369600
H	-4.01082600	-2.43773700	-2.25709600

H	-3.86151900	-2.82449000	-0.53803800
C	-4.50440600	-0.79478300	-0.96847000
H	-4.51018600	-0.06028000	-1.77208500
C	-5.10045800	-0.46470000	0.18692500
C	-5.75794800	0.88268700	0.34956400
H	-6.80191200	0.78137000	0.67489900
H	-5.23914700	1.46864600	1.11923800
H	-5.74042300	1.45777200	-0.58079000
C	-5.15744600	-1.33778600	1.41416100
H	-4.66564500	-2.30434700	1.28516800
H	-4.68177800	-0.82597600	2.26110400
H	-6.19912100	-1.52593600	1.70619000
C	1.48569400	0.81468200	-0.86334700
C	1.85919800	1.74033000	0.11846500
C	2.01104400	0.92427700	-2.15686100
C	2.74617600	2.76738200	-0.19191400
H	1.45789900	1.64415900	1.12011100
C	2.89630900	1.95690600	-2.46353700
H	1.73586900	0.19023900	-2.90642200
C	3.26864700	2.87642500	-1.48213400
H	3.03283200	3.48034500	0.57553400
H	3.29672400	2.04002500	-3.46972800
H	3.96324100	3.67650000	-1.72173300
S	1.60255600	-1.88347300	-0.34374600
O	0.91327500	-2.85620100	0.52033200
O	2.03851100	-2.25560000	-1.69924900
C	3.02543900	-1.28493900	0.56587100
C	4.16362300	-0.88348300	-0.13107800
C	2.93523900	-1.18584000	1.95402000
C	5.23435500	-0.35349500	0.58528100
H	4.19320300	-0.97741600	-1.20997900
C	4.01325900	-0.65310900	2.65890800
H	2.04042100	-1.52689200	2.46340400
C	5.15625600	-0.23315500	1.97462300
H	6.12730100	-0.03056900	0.05893700
H	3.96274400	-0.56892700	3.74028000
H	5.99183000	0.18613800	2.52758100
S	-1.57019100	1.22927300	-0.81130500
C	-1.98648700	1.78564500	0.86869500
F	-2.79511800	2.85152000	0.74775100
F	-2.63219600	0.86005100	1.61141500
F	-0.91280500	2.16090700	1.59264400

Zero-point correction= 0.383568 (Hartree/Particle)
Thermal correction to Energy= 0.412206
Thermal correction to Enthalpy= 0.413151
Thermal correction to Gibbs Free Energy= 0.320386
Sum of electronic and zero-point Energies= -2134.063354
Sum of electronic and thermal Energies= -2134.034715
Sum of electronic and thermal Enthalpies= -2134.033771
Sum of electronic and thermal Free Energies= -2134.126535
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2134.896778

TS12-b

C	-1.14705900	0.42364200	-0.97113400
C	-1.63954900	1.58358700	-0.59221900
C	-1.01303400	2.95385500	-0.65403600
H	-1.80700900	3.71481700	-0.67488800
H	-0.43525600	3.12062000	0.26205900
O	-0.19837400	3.04453200	-1.80181200
C	0.76756000	4.10767400	-1.70056600
H	1.09516000	4.27359300	-2.73090700
H	0.27360300	5.02638400	-1.35639800
C	1.93182700	3.71868400	-0.83676300
H	2.60163500	2.99320500	-1.29215300
C	2.18357900	4.09076700	0.42774300
C	3.36692500	3.52021500	1.16877700
H	4.07045500	4.31378400	1.45552800
H	3.04108300	3.03754000	2.09924900
H	3.90335400	2.77548900	0.57428400
C	1.35266900	5.06410200	1.22469800
H	0.52331000	5.49539100	0.65995000
H	0.93407700	4.56915000	2.11143400
H	1.97591600	5.88931000	1.59393100
C	-1.61706300	-0.86965800	-1.33679200
C	-1.12489500	-2.05997900	-0.75636200
C	-2.61961200	-0.95585100	-2.33318900
C	-1.64984000	-3.28722300	-1.13473300
H	-0.35703000	-2.00714300	0.00180400
C	-3.13128000	-2.19237700	-2.70603100
H	-2.99656200	-0.04111200	-2.77639200
C	-2.65195300	-3.36154200	-2.10827800
H	-1.27612700	-4.19333400	-0.66661700
H	-3.90708600	-2.24557100	-3.46405200
H	-3.05348000	-4.32673900	-2.40320500
S	-3.31116300	1.59661800	0.18430700
O	-3.27287300	2.68899900	1.17274700
O	-4.34757100	1.57074000	-0.86229700
C	-3.35929000	0.03448600	1.06161900
C	-4.24746900	-0.95149100	0.64176000
C	-2.46552800	-0.17252600	2.11209800
C	-4.23210300	-2.18599500	1.28971700
H	-4.91346800	-0.75161900	-0.18909500
C	-2.45313000	-1.41307800	2.74427200
H	-1.77984000	0.61225100	2.40937100
C	-3.33409400	-2.41690200	2.33270800
H	-4.91088500	-2.97013400	0.96896900
H	-1.75353500	-1.59731100	3.55379500
H	-3.31692700	-3.38448600	2.82605500
S	3.35209000	-0.67497800	-1.00701500
O	3.35821000	-0.89982700	-2.45967800
O	4.44459000	0.04400200	-0.33092700
C	3.08680000	-2.24023400	-0.18095500
C	3.57818400	-2.42524000	1.10972100
C	2.29700800	-3.19505000	-0.82355100
C	3.27996200	-3.61735400	1.76900800
H	4.17921900	-1.65289600	1.57481600
C	2.00486500	-4.37826000	-0.14889100
H	1.92498900	-3.00811300	-1.82441100
C	2.49361600	-4.58719600	1.14388000
H	3.66021300	-3.78669200	2.77173300
H	1.39918100	-5.13772500	-0.63406500
H	2.26065200	-5.51074900	1.66568300
S	1.26998800	0.31253500	-0.76859200
C	1.22170700	0.36299500	1.06416200

F	2.45104500	0.46514600	1.59457600
F	0.50527600	1.40996400	1.51323000
F	0.65979300	-0.74650700	1.59886900

Zero-point correction= 0.482270 (Hartree/Particle)
Thermal correction to Energy= 0.519818
Thermal correction to Enthalpy= 0.520762
Thermal correction to Gibbs Free Energy= 0.408132
Sum of electronic and zero-point Energies= -2914.163887
Sum of electronic and thermal Energies= -2914.126339
Sum of electronic and thermal Enthalpies= -2914.125395
Sum of electronic and thermal Free Energies= -2914.238025
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2915.23313

INT12-b

C	0.16691300	-0.04421700	0.94068500
C	-0.19973600	1.08786700	0.30350400
C	-1.60197000	1.63449600	0.17544300
H	-1.56650500	2.62831900	-0.28682500
H	-2.18691900	0.99158500	-0.48862000
O	-2.18833400	1.70222000	1.46374500
C	-3.62220900	1.76608200	1.39581700
H	-3.92912800	2.04660100	2.40767500
H	-3.92736100	2.57608400	0.71925800
C	-4.22135200	0.44386000	1.01122200
H	-4.16753600	-0.31504400	1.78949200
C	-4.71682500	0.08286600	-0.18293300
C	-5.18799500	-1.32909700	-0.42312000
H	-6.23476900	-1.34613800	-0.75467600
H	-4.59519500	-1.80056000	-1.21741500
H	-5.09865200	-1.94676600	0.47498400
C	-4.83692800	0.99145100	-1.38003100
H	-4.50636700	2.01401200	-1.18748200
H	-4.24192700	0.59714000	-2.21474000
H	-5.87698100	1.03153800	-1.72961300
C	1.53799000	-0.36681600	1.38671800
C	2.13314100	-1.60965100	1.11655500
C	2.25399600	0.59089500	2.12255700
C	3.43583700	-1.86489700	1.52812700
H	1.58203300	-2.35646200	0.55956000
C	3.55387800	0.32293700	2.54723100
H	1.78952700	1.54273500	2.34927100
C	4.15083300	-0.89996200	2.24360100
H	3.89616900	-2.81964400	1.29159500
H	4.09649000	1.07146500	3.11691600
H	5.16587300	-1.10718600	2.57061400
S	1.02566300	2.07011000	-0.63049800
O	0.24785000	2.61570600	-1.75828700
O	1.78939700	2.98087000	0.23733200
C	2.13325600	0.82824800	-1.29627200
C	3.48945900	0.89637600	-0.99544200
C	1.60228500	-0.17993300	-2.10200100
C	4.33798700	-0.08495500	-1.50681800
H	3.85505400	1.68797900	-0.35249500
C	2.45826600	-1.15961000	-2.59693600
H	0.53924900	-0.21055100	-2.31407500
C	3.82321600	-1.11148400	-2.29924400
H	5.39769900	-0.05395600	-1.27311800
H	2.06072700	-1.96080100	-3.21243400
H	4.48627700	-1.88049500	-2.68493500
S	-1.10635300	-1.25756700	1.36870600
C	-1.38560300	-1.99284000	-0.27260400
F	-2.33209500	-2.93388000	-0.12601100
F	-1.80996100	-1.12439600	-1.21657000
F	-0.28734900	-2.58512400	-0.79219100

Zero-point correction= 0.383836 (Hartree/Particle)
Thermal correction to Energy= 0.412125
Thermal correction to Enthalpy= 0.413069
Thermal correction to Gibbs Free Energy= 0.323574
Sum of electronic and zero-point Energies= -2134.066327
Sum of electronic and thermal Energies= -2134.038038
Sum of electronic and thermal Enthalpies= -2134.037094
Sum of electronic and thermal Free Energies= -2134.126589
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2134.897264

TS13-b

C	-3.85205600	-2.59263300	-0.27777600
C	-2.74976100	-3.09554600	-0.23714600
C	-1.36878200	-3.57136100	-0.17030700
H	-1.33136700	-4.66388200	-0.10974800
H	-0.84061500	-3.28215200	-1.08976600
O	-0.64583900	-3.12261400	0.98147100
C	-0.78585200	-1.74772800	1.29050100
H	-1.84967500	-1.48210200	1.40134600
H	-0.32062400	-1.62297700	2.27355600
C	-0.15987200	-0.83334300	0.27844200
H	-0.19713200	-1.16126800	-0.75617300
C	-0.16234900	0.65313000	0.45818300
C	0.70925500	1.36714000	-0.57915100
H	0.60494900	2.45242200	-0.49720800
H	1.75622200	1.11252400	-0.40471700
H	0.44503100	1.06058700	-1.59414800
C	0.14896000	1.11488800	1.88358400
H	-0.55878100	0.70713800	2.60829900
H	1.15756900	0.78416500	2.15325400
H	0.12251000	2.20635900	1.95034900
C	-5.15165600	-2.00680200	-0.34002600
C	-5.31953800	-0.72276400	-0.89102800
C	-6.27303900	-2.70052300	0.14968300
C	-6.58781800	-0.15203200	-0.94577100
H	-4.45048700	-0.19016300	-1.26028400
C	-7.53702800	-2.12099400	0.08768800
H	-6.13825600	-3.68964000	0.57586400
C	-7.69789900	-0.84603600	-0.45920000
H	-6.71028800	0.84091800	-1.36945400
H	-8.39796200	-2.66376800	0.46777000
H	-8.68535600	-0.39504200	-0.50480100
S	-1.97569100	1.15750900	0.07965600
O	-2.24744100	0.74095900	-1.31189800
O	-2.82080700	0.67627600	1.18992100
C	-2.02407400	2.95321100	0.12474000
C	-2.28386400	3.59303500	1.33757800
C	-1.81374700	3.67034700	-1.05388700
C	-2.31633100	4.98651900	1.36908300
H	-2.47923700	3.00261900	2.22567700

C	-1.85102400	5.06315900	-1.00918100
H	-1.64587800	3.13731800	-1.98308400
C	-2.09579900	5.71842400	0.20005900
H	-2.52251300	5.49984800	2.30336600
H	-1.69639500	5.63623900	-1.91842100
H	-2.12421500	6.80373000	0.22959300
S	4.43882700	-0.94738700	1.27412800
O	4.20120900	-0.32305700	2.58497600
O	5.37963700	-2.06186800	1.09898400
C	4.85105800	0.33873200	0.10008700
C	5.51187800	-0.00253000	-1.07878900
C	4.43188400	1.64215100	0.36894600
C	5.76514400	1.00107000	-2.01261000
H	5.81906800	-1.02702300	-1.25132200
C	4.69181900	2.63310100	-0.57548300
H	3.92824300	1.86576900	1.30264200
C	5.35340300	2.31189400	-1.76352400
H	6.28340900	0.75813900	-2.93506400
H	4.38147100	3.65556100	-0.38272100
H	5.55039100	3.08761500	-2.49753700
S	2.27241900	-1.44649400	0.71579700
C	2.51745200	-1.99488400	-1.01144700
F	1.54986200	-2.85718500	-1.36512700
F	2.47309900	-0.96623300	-1.88313800
F	3.69868300	-2.60839100	-1.18036900

Zero-point correction= 0.482369 (Hartree/Particle)
Thermal correction to Energy= 0.519903
Thermal correction to Enthalpy= 0.520847
Thermal correction to Gibbs Free Energy= 0.405962
Sum of electronic and zero-point Energies= -2914.148589
Sum of electronic and thermal Energies= -2914.111055
Sum of electronic and thermal Enthalpies= -2914.110110
Sum of electronic and thermal Free Energies= -2914.224996
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2915.223025

INT13-b

C	-1.62991100	-2.88707100	-0.15520300
C	-0.44489500	-3.13130000	-0.08513300
C	1.00436400	-3.28788200	0.02530500
H	1.28562400	-4.34525400	0.06014600
H	1.48686000	-2.85584200	-0.86199300
O	1.56378200	-2.73067300	1.22082900
C	1.16541700	-1.40757000	1.51479800
H	0.07634500	-1.31552100	1.48526700
H	1.49335700	-1.22896400	2.54257900
C	1.80298500	-0.36914800	0.56810400
H	1.62897100	-0.67293500	-0.46591200
C	1.26443800	1.08479500	0.72072600
C	1.96618800	2.05553600	-0.23508300
H	1.55419800	3.06225900	-0.13720700
H	3.02853400	2.09682700	0.01265900
H	1.87151900	1.72889900	-1.27298000
C	1.30644400	1.59214400	2.16216700
H	0.69609900	0.98070600	2.82946100
H	2.34344400	1.57898000	2.51572300
H	0.95137300	2.62546400	2.21835400
C	-3.02184600	-2.59185900	-0.25837900
C	-3.44450500	-1.41095100	-0.89685700
C	-3.98283900	-3.46784000	0.27745800
C	-4.80210900	-1.12002900	-0.99190900
H	-2.69661700	-0.73856000	-1.30135100
C	-5.33839100	-3.16802400	0.17575200
H	-3.65278800	-4.37654000	0.77088000
C	-5.75169700	-1.99432300	-0.45813400
H	-5.12146600	-0.20531300	-1.48371300
H	-6.07393700	-3.85037100	0.59250500
H	-6.81028700	-1.76191400	-0.53493900
S	-0.53659300	1.00458100	0.17345900
O	-0.53603000	0.37924500	-1.16609100
O	-1.34866700	0.44437500	1.27054800
C	-1.06806600	2.70874600	-0.02951700
C	-1.58335100	3.39073600	1.07347400
C	-0.99069300	3.30197700	-1.28976800
C	-2.00727900	4.70907600	0.91055500
H	-1.67097900	2.88349800	2.02764500
C	-1.42223500	4.61874500	-1.44047100
H	-0.61310700	2.72938500	-2.12947300
C	-1.92240000	5.32157400	-0.34164600
H	-2.41303700	5.25338700	1.75785900
H	-1.37306300	5.09396100	-2.41546500
H	-2.25666500	6.34761800	-0.46417400
S	3.64058100	-0.42797100	0.83457900
C	4.18573600	-0.83802700	-0.84246100
F	3.73203600	-2.03526100	-1.26637000
F	3.79210500	0.06292800	-1.76782700
F	5.52663700	-0.87821500	-0.84351500

Zero-point correction= 0.384917 (Hartree/Particle)
Thermal correction to Energy= 0.413101
Thermal correction to Enthalpy= 0.414045
Thermal correction to Gibbs Free Energy= 0.322800
Sum of electronic and zero-point Energies= -2134.049941
Sum of electronic and thermal Energies= -2134.021757
Sum of electronic and thermal Enthalpies= -2134.020813
Sum of electronic and thermal Free Energies= -2134.112058
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2134.88672

TS14-b

C	-2.79289000	-1.42820200	-1.86134700
C	-1.68554200	-1.32595900	-2.34537700
C	-0.29881400	-1.02836500	-2.71094300
H	0.21191400	-1.90088500	-3.12611700
H	-0.27699300	-0.22483100	-3.46216500
O	0.48086100	-0.67228300	-1.56529100
C	-0.02351300	0.38953300	-0.77171100
H	-1.10596300	0.42929200	-0.88117600
H	0.19466400	0.14488900	0.26758700
C	0.61921100	1.72897200	-1.15738900
H	0.63773700	1.80461700	-2.24961100
C	1.97495300	2.04817500	-0.59567800
C	2.82979300	2.93452400	-1.45454800
H	2.40810600	3.95205500	-1.43948100
H	3.85519300	2.98591600	-1.08515600
H	2.84694000	2.59551400	-2.49532700
C	2.11957600	2.21113000	0.89090500

H	1.53376300	1.47904100	1.45344300
H	3.16407600	2.12409200	1.19622700
H	1.78220400	3.21878900	1.17153100
S	-0.66499100	3.07670600	-0.78701100
O	0.03726700	4.32136300	-0.42671700
O	-1.60112600	3.02536700	-1.92548400
C	-1.57994200	2.51575100	0.66332300
C	-2.73220300	1.75079400	0.46928500
C	-1.12412100	2.83233900	1.94224500
C	-3.42216400	1.26509800	1.57764700
H	-3.07968600	1.54792900	-0.53641000
C	-1.82486100	2.34658900	3.04621300
H	-0.25125500	3.46145500	2.06716600
C	-2.96453800	1.55971100	2.86421200
H	-4.31301400	0.66223700	1.42986000
H	-1.48442300	2.59003300	4.04819100
H	-3.50395800	1.18404400	3.72918000
C	-4.08108800	-1.49284100	-1.25361100
C	-4.97576000	-0.41355900	-1.38453100
C	-4.45271800	-2.59867500	-0.46688300
C	-6.20133600	-0.43404800	-0.72425400
H	-4.69603400	0.43201200	-2.00502000
C	-5.68016500	-2.61164500	0.19028500
H	-3.77155200	-3.43941600	-0.38136000
C	-6.55441800	-1.52902600	0.06896300
H	-6.88282600	0.40491300	-0.82996300
H	-5.95627500	-3.46892300	0.79714100
H	-7.51041300	-1.54161400	0.58403000
S	2.58367600	-2.59673000	-0.14013800
O	2.05827400	-3.34639200	-1.29650700
O	3.71729000	-3.09778200	0.66085700
C	1.21540400	-2.25668900	0.98049900
C	1.48634800	-1.53434800	2.14308700
C	-0.08081900	-2.60300600	0.60930400
C	0.41925600	-1.14000100	2.94879800
H	2.50661400	-1.26616500	2.39062100
C	-1.13859300	-2.20354300	1.42687200
H	-0.25231800	-3.13837100	-0.31587500
C	-0.89036000	-1.46759800	2.58629500
H	0.60887100	-0.56815800	3.85221100
H	-2.15848800	-2.44099100	1.14300100
H	-1.71990600	-1.13398600	3.20106500
S	2.98500900	-0.27607400	-0.80086900
C	4.56598800	-0.06657600	0.08944100
F	5.46892800	-0.98703900	-0.26134600
F	5.08964600	1.15133100	-0.18239800
F	4.42512800	-0.12977000	1.43521200

Zero-point correction= 0.483435 (Hartree/Particle)
Thermal correction to Energy= 0.520718
Thermal correction to Enthalpy= 0.521662
Thermal correction to Gibbs Free Energy= 0.410670
Sum of electronic and zero-point Energies= -2914.153508
Sum of electronic and thermal Energies= -2914.116225
Sum of electronic and thermal Enthalpies= -2914.115281
Sum of electronic and thermal Free Energies= -2914.226272
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2915.227346

INT14-b

C	-2.75942300	-2.20306100	0.14110400
C	-1.62417000	-2.62516600	0.18545400
C	-0.20651900	-2.98189300	0.19354200
H	-0.04335400	-3.96854500	0.63694100
H	0.15704200	-3.02779400	-0.84457400
O	0.60955100	-2.09941200	0.97284600
C	0.41205600	-0.71618300	0.73259000
H	-0.65510200	-0.49578000	0.78058400
H	0.90561900	-0.19822000	1.55699900
C	1.00529300	-0.26374000	-0.61942900
H	0.84367800	-1.06727400	-1.34478400
C	2.51802300	0.10612100	-0.64114500
C	3.04180900	0.06002800	-2.08410500
H	2.52307900	0.80948400	-2.68577900
H	4.11194600	0.26357700	-2.11303400
H	2.87046700	-0.92735400	-2.52360800
C	2.81142500	1.45809400	0.01509400
H	2.39609900	1.52564700	1.02470200
H	3.88466900	1.63630900	0.07841700
H	2.38435600	2.24700000	-0.60664300
S	-0.14472600	1.01019800	-1.37730200
O	0.60333800	1.92689700	-2.25567100
O	-1.25337400	0.19870000	-1.91180900
C	-0.82423700	2.00664600	-0.03929700
C	-2.01911700	1.60143900	0.55942300
C	-0.19533100	3.19753500	0.32433000
C	-2.57036900	2.38761200	1.56918200
H	-2.51666800	0.69940200	0.22605500
C	-0.75576500	3.97482100	1.33714000
H	0.69864800	3.52111800	-0.19372100
C	-1.93546600	3.56705700	1.96325100
H	-3.49944300	2.07948000	2.03871700
H	-0.27587800	4.90407500	1.62869800
H	-2.36766000	4.17748500	2.75073400
C	-4.07892300	-1.66812400	0.04723500
C	-4.38337700	-0.74627500	-0.97410200
C	-5.07464700	-2.02758000	0.97342000
C	-5.66022200	-0.19718800	-1.05590300
H	-3.60626500	-0.46568600	-1.67756700
C	-6.34908700	-1.47587500	0.87848400
H	-4.83548900	-2.73720900	1.75902200
C	-6.64473300	-0.55977600	-0.13385000
H	-5.88728900	0.51566500	-1.84332000
H	-7.11350500	-1.75958900	1.59617800
H	-7.63996100	-0.13001500	-0.20342200
S	3.32361600	-1.30240500	0.35192200
C	5.03119800	-0.72450300	0.58641100
F	5.73059900	-1.78082600	1.03715200
F	5.64394900	-0.26966400	-0.52726200
F	5.14724700	0.25539200	1.50895200

Zero-point correction= 0.385104 (Hartree/Particle)
Thermal correction to Energy= 0.413243
Thermal correction to Enthalpy= 0.414188
Thermal correction to Gibbs Free Energy= 0.323328
Sum of electronic and zero-point Energies= -2134.037541
Sum of electronic and thermal Energies= -2134.009401

Sum of electronic and thermal Enthalpies= -2134.008457

Sum of electronic and thermal Free Energies= -2134.099316

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2134.874449

TS15-b

P	-2.12049100	0.29065700	-0.20891900
C	-3.38448800	-0.96114300	-0.61602600
C	-2.96876700	-2.25260000	-0.97118200
C	-4.75418300	-0.66077200	-0.56844000
C	-3.91725900	-3.23681000	-1.25361200
H	-1.90740300	-2.47533300	-1.04079100
C	-5.69642900	-1.64744900	-0.85247900
H	-5.08086800	0.34422400	-0.31963800
C	-5.27864400	-2.93737400	-1.19126400
H	-3.58899000	-4.23451200	-1.53001700
H	-6.75557400	-1.40926400	-0.81542800
H	-6.01514200	-3.70392400	-1.41506900
C	-2.65975900	1.84083000	-1.00150300
C	-2.13259600	2.17486300	-2.25589300
C	-3.58551500	2.69466800	-0.38584400
C	-2.54777000	3.33971700	-2.89933300
H	-1.38573600	1.53075800	-2.71101100
C	-3.99679700	3.85928300	-1.03274000
H	-3.96558800	2.45840300	0.60348000
C	-3.48146900	4.18034900	-2.29032100
H	-2.13087500	3.59813600	-3.86819400
H	-4.71093700	4.52076600	-0.55075700
H	-3.79705500	5.09240100	-2.78879300
C	-2.25296700	0.61309600	1.57967500
C	-1.30966800	1.50074000	2.12069500
C	-3.17627500	-0.02302200	2.41641200
C	-1.29170400	1.74658800	3.49010800
H	-0.57950300	1.97849900	1.47658000
C	-3.15509400	0.23184500	3.78987200
H	-3.89884800	-0.71932500	2.00372300
C	-2.21412600	1.11164000	4.32695300
H	-0.54002000	2.41616400	3.89578400
H	-3.87023000	-0.26506400	4.43939300
H	-2.19485900	1.29710300	5.39719100
Au	0.03448600	-0.35666900	-0.73536600
S	1.85157300	2.08726000	-0.41011400
C	2.26809300	1.90708500	1.29603800
F	1.57266900	2.74435100	2.12890800
F	2.01569900	0.64129100	1.79859300
F	3.58048600	2.12561300	1.58309200
C	1.87846300	-1.27528400	-1.24684400
C	2.87326500	-0.50644000	-1.09103700
C	4.19333200	-0.00649800	-0.98756400
C	4.82412600	0.58056500	-2.10607100
C	4.91913800	-0.17913800	0.20945600
C	6.15132400	0.97594100	-2.02556900
H	4.25036500	0.72785500	-3.01464400
C	6.24771000	0.22244400	0.27871600
H	4.42054000	-0.61136200	1.06773100
C	6.86479000	0.79982500	-0.83365200
H	6.63418400	1.42879800	-2.88628000
H	6.80197100	0.09406700	1.20349000
H	7.90144200	1.11846200	-0.77274600
C	1.84420700	-2.70338100	-1.77303600
H	2.80498400	-3.19924600	-1.56371400
H	1.71847400	-2.63940100	-2.85821300
O	0.78273600	-3.50716800	-1.31859700
C	0.92827100	-3.99757000	0.02346500
H	1.98744000	-4.20552100	0.22177000
H	0.40222900	-4.95983000	0.01883800
C	0.32428300	-3.10847600	1.07154600
H	-0.75752300	-3.00274300	1.00380600
C	0.95235000	-2.48802800	2.08334800
C	2.44084900	-2.50842200	2.31434200
H	2.79813200	-1.48024800	2.43187300
H	2.68387500	-3.04087100	3.24422300
H	3.00222500	-2.97267900	1.50043200
C	0.17594300	-1.68582600	3.09469800
H	0.49573100	-0.63969100	3.07658800
H	-0.89968600	-1.71558800	2.90439500
H	0.35761800	-2.06158900	4.11147500

Zero-point correction= 0.555628 (Hartree/Particle)

Thermal correction to Energy= 0.595608

Thermal correction to Enthalpy= 0.596552

Thermal correction to Gibbs Free Energy= 0.476472

Sum of electronic and zero-point Energies= -2525.483024

Sum of electronic and thermal Energies= -2525.443043

Sum of electronic and thermal Enthalpies= -2525.442099

Sum of electronic and thermal Free Energies= -2525.562179

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2526.913719

INT15-b

P	-2.30454100	-0.01078500	-0.28254100
C	-3.16165500	-1.62189200	-0.20221900
C	-2.39257700	-2.78663100	-0.05400100
C	-4.55994300	-1.71554500	-0.26510400
C	-3.02387000	-4.02703400	0.05092000
H	-1.30759400	-2.72625200	-0.03905500
C	-5.18332700	-2.95771600	-0.16096500
H	-5.15724800	-0.81950300	-0.40367400
C	-4.41566200	-4.11411300	0.00127000
H	-2.42318900	-4.92493200	0.16262800
H	-6.26635000	-3.02444300	-0.21198100
H	-4.90343200	-5.08167500	0.07923500
C	-3.25202800	0.99375000	-1.47566400
C	-2.84248300	0.98834400	-2.81652400
C	-4.37264000	1.74506600	-1.09511500
C	-3.55944100	1.71106700	-3.76917000
H	-1.95752900	0.42668100	-3.10328600
C	-5.08466100	2.46938900	-2.05103400
H	-4.67679700	1.77267600	-0.05320400
C	-4.68116800	2.45034100	-3.38775600
H	-3.23606200	1.70562000	-4.80592400
H	-5.95057000	3.05273900	-1.75121000
H	-5.23459300	3.01894700	-4.12958300
C	-2.60451100	0.79380400	1.33110000
C	-1.98122100	2.03096100	1.55914500
C	-3.37888800	0.21280900	2.34182100
C	-2.14880500	2.68488300	2.77653100

H	-1.34587200	2.46452700	0.79338800
C	-3.53438500	0.86800400	3.56581400
H	-3.85452900	-0.74808600	2.17743700
C	-2.92455600	2.10349900	3.78335100
H	-1.65984700	3.63960800	2.94608700
H	-4.13180000	0.40918900	4.34847200
H	-3.04486700	2.60908100	4.73709100
Au	-0.00177100	-0.29138000	-0.65617400
S	2.62680100	1.87868100	-1.25273800
C	2.26293900	2.61214100	0.36028400
F	2.04276500	3.92644400	0.16574500
F	1.16057900	2.11202500	0.96910400
F	3.26077500	2.49947100	1.27155600
C	1.99865600	-0.74881400	-0.75415200
C	3.00672200	0.14261500	-0.88656200
C	4.45995400	-0.18852200	-0.91263200
C	4.94309100	-1.17983100	-1.78155900
C	5.38081800	0.46650900	-0.07813000
C	6.29468200	-1.52553400	-1.79977500
H	4.25314000	-1.66964600	-2.46140100
C	6.72954500	0.11935000	-0.09243200
H	5.03234700	1.25158000	0.58151500
C	7.19360100	-0.88042600	-0.95098500
H	6.64414800	-2.29346800	-2.48464600
H	7.42232900	0.63346000	0.56842400
H	8.24681300	-1.14673000	-0.96329600
C	2.29181900	-2.22859000	-0.58454300
H	3.26417300	-2.41014700	-0.10282900
H	2.33475700	-2.67783300	-1.58419300
O	1.28341200	-2.97669700	0.09139200
C	1.38752100	-2.97469000	1.51915000
H	2.44452600	-3.05148000	1.80508900
H	0.89855800	-3.90595200	1.82975200
C	0.71485100	-1.81847100	2.20487300
H	-0.37445500	-1.85557300	2.20457500
C	1.30592000	-0.78823000	2.83010100
C	2.79217800	-0.55157300	2.87710200
H	3.02187700	0.41559000	2.41773500
H	3.14767600	-0.50318600	3.91546900
H	3.37433700	-1.30990900	2.35061300
C	0.48070100	0.25524400	3.53781600
H	0.67366200	1.24870400	3.12069100
H	-0.59052500	0.05398400	3.45713700
H	0.74468200	0.29946500	4.60405900

Zero-point correction= 0.558454 (Hartree/Particle)
Thermal correction to Energy= 0.597942
Thermal correction to Enthalpy= 0.598886
Thermal correction to Gibbs Free Energy= 0.480668
Sum of electronic and zero-point Energies= -2525.531673
Sum of electronic and thermal Energies= -2525.492185
Sum of electronic and thermal Enthalpies= -2525.491241
Sum of electronic and thermal Free Energies= -2525.609459
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2526.954764

TS16-b

P	-2.06075600	0.20359500	0.27481100
C	-2.74244000	1.89251000	0.15995300
C	-2.27780600	2.72883800	-0.86628400
C	-3.72266900	2.35854100	1.04500900
C	-2.79670300	4.01390500	-1.00934300
H	-1.50709300	2.36966200	-1.54312900
C	-4.23470900	3.64925400	0.90132800
H	-4.07871000	1.71809400	1.84571700
C	-3.77442100	4.47613300	-0.12437500
H	-2.43279900	4.65636700	-1.80575900
H	-4.99102400	4.00840900	1.59328400
H	-4.17233900	5.48109200	-0.23150600
C	-2.41456800	-0.35226900	1.97477100
C	-1.51734700	0.00614100	2.99217100
C	-3.54763400	-1.11495800	2.28337600
C	-1.75879300	-0.38680400	4.30650500
H	-0.63044100	0.58331600	2.74634100
C	-3.78264900	-1.50942200	3.60152500
H	-4.23534400	-1.40541500	1.49565100
C	-2.89130100	-1.14620600	4.61221300
H	-1.05872500	-0.11009300	5.08941500
H	-4.65943600	-2.10581400	3.83644300
H	-3.07428200	-1.46004500	5.63581700
C	-3.08544900	-0.81514000	-0.83341300
C	-2.53861700	-2.01290700	-1.31641300
C	-4.37794300	-0.42792500	-1.21517300
C	-3.28139400	-2.81531700	-2.18012000
H	-1.53445700	-2.30873700	-1.02838900
C	-5.11852800	-1.24237200	-2.07175800
H	-4.79637100	0.50678900	-0.85520800
C	-4.57029500	-2.43262800	-2.55663900
H	-2.83606200	-3.72564000	-2.56887300
H	-6.11884800	-0.94136900	-2.36970800
H	-5.14585500	-3.05574700	-3.23537400
Au	0.18732100	0.11961500	-0.23378400
S	1.08208600	-2.67337900	-0.80523000
C	0.87644000	-2.43943500	-2.56052100
F	0.05665200	-3.37608400	-3.11192300
F	0.31761000	-1.23348900	-2.90103800
F	2.04299800	-2.49842200	-3.25430500
C	2.31910000	4.40992400	-0.78738700
C	1.84291800	3.10618800	-0.66354700
C	2.70712500	2.01285300	-0.83480800
C	4.06067700	2.25562400	-1.13946500
C	4.52857300	3.56020200	-1.26724300
C	3.66127500	4.64216700	-1.09249500
H	1.63846100	5.24538300	-0.64853700
H	0.79972900	2.91924300	-0.42802500
H	4.73177600	1.41090100	-1.25666700
H	5.57508600	3.73338200	-1.50236900
H	4.03015500	5.65888000	-1.19440400
C	2.24175300	0.63601900	-0.68976100
C	2.73162600	-0.52935000	-0.64173800
C	3.83429500	-1.48678800	-0.38316100
H	4.08702300	-2.02357200	-1.30122300
H	3.53435600	-2.21738300	0.37098900
O	4.98596700	-0.76009700	0.01635000
C	4.88378200	-0.17627200	1.33495800
H	4.13768900	0.62391400	1.32377300

H	5.86440800	0.28406600	1.48782600
C	4.60457800	-1.19598500	2.39865600
H	5.42123600	-1.89260600	2.58729100
C	3.45899500	-1.37020600	3.07813100
C	2.21486000	-0.53330400	2.91446600
H	2.34028700	0.31436100	2.23995000
H	1.39632000	-1.14906700	2.51801000
H	1.87945200	-0.15371000	3.88941500
C	3.32695900	-2.48238700	4.08841500
H	2.49833600	-3.15155900	3.82012100
H	4.24040200	-3.07976100	4.16216800
H	3.09546200	-2.08178900	5.08499900

Zero-point correction= 0.555658 (Hartree/Particle)
Thermal correction to Energy= 0.595811
Thermal correction to Enthalpy= 0.596755
Thermal correction to Gibbs Free Energy= 0.473408
Sum of electronic and zero-point Energies= -2525.477697
Sum of electronic and thermal Energies= -2525.437544
Sum of electronic and thermal Enthalpies= -2525.436600
Sum of electronic and thermal Free Energies= -2525.559946
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2526.910749

INT16-b

P	-2.21687900	0.23141200	0.10075100
C	-3.30220700	1.67773600	-0.13381500
C	-2.90973700	2.65171000	-1.06361400
C	-4.50908900	1.82865800	0.56261400
C	-3.72577600	3.75580200	-1.30543700
H	-1.96343400	2.54340800	-1.58688100
C	-5.32007000	2.93752300	0.32021600
H	-4.80784200	1.08573500	1.29564500
C	-4.93106300	3.89912700	-0.61458000
H	-3.41614000	4.50763900	-2.02530600
H	-6.25316100	3.05232100	0.86432800
H	-5.56277300	4.76336900	-0.79864000
C	-2.59232500	-0.39551500	1.77466100
C	-1.85867600	0.11926400	2.85392300
C	-3.57601800	-1.36592100	2.00618300
C	-2.11639900	-0.32242500	4.15026500
H	-1.07812600	0.85221400	2.67053400
C	-3.82820900	-1.80808400	3.30554300
H	-4.13341700	-1.78048100	1.17208800
C	-3.10102900	-1.28692400	4.37721700
H	-1.54163400	0.07752800	4.98041200
H	-4.58877700	-2.56387400	3.47922000
H	-3.29545600	-1.63735900	5.38677200
C	-2.83994900	-1.04799200	-1.04324100
C	-1.97382700	-2.10169100	-1.37309300
C	-4.12527700	-1.00538500	-1.59909300
C	-2.39044000	-3.10290700	-2.24712100
H	-0.97397200	-2.12839200	-0.95323300
C	-4.53954700	-2.01382400	-2.47057000
H	-4.79404800	-0.18451600	-1.36015300
C	-3.67417400	-3.06037000	-2.79580700
H	-1.70126200	-3.89873600	-2.51079300
H	-5.53571500	-1.97620300	-2.90215200
H	-3.99697200	-3.83659000	-3.48376900
Au	0.10112200	0.55748300	-0.20603300
S	1.96327400	-2.11824700	-0.56043100
C	1.63736300	-2.21297900	-2.34209600
F	0.98049600	-3.37513500	-2.57368400
F	0.86398800	-1.21794300	-2.81946400
F	2.76090600	-2.21526000	-3.08340800
C	3.16097700	4.13193600	0.55234600
C	2.52748300	2.89111800	0.55169000
C	2.83295500	1.92297200	-0.42008600
C	3.75759800	2.25954100	-1.42206100
C	4.37232500	3.50944900	-1.43823100
C	4.08605000	4.44806300	-0.44486600
H	2.92161500	4.85896100	1.32402000
H	1.78659100	2.65533000	1.31138300
H	3.98052200	1.53513300	-2.19929800
H	5.08059100	3.75022400	-2.22658900
H	4.57043400	5.42050100	-0.45427900
C	2.15026300	0.61002200	-0.40815200
C	2.85027000	-0.54357500	-0.48436900
C	4.36070400	-0.70835400	-0.35281600
H	4.87760400	-0.40391600	-1.26811100
H	4.57474900	-1.77246800	-0.19632200
O	4.95487200	0.07042900	0.67541900
C	4.31610000	-0.01276700	1.95287900
H	3.42685000	0.62550500	1.96466400
H	5.04740400	0.42916800	2.64030400
C	3.98741700	-1.41818500	2.36551600
H	4.83042600	-2.10891600	2.32548000
C	2.79315400	-1.90578900	2.74013200
C	1.52446000	-1.10011900	2.85909400
H	1.64305700	-0.05838700	2.56006400
H	0.73496200	-1.53204300	2.23087600
H	1.15060000	-1.12373300	3.89208200
C	2.63235000	-3.36602900	3.08246300
H	1.90373100	-3.83753400	2.40891800
H	3.57681200	-3.91198200	2.99892200
H	2.24747800	-3.49519000	4.10351600

Zero-point correction= 0.557919 (Hartree/Particle)
Thermal correction to Energy= 0.597705
Thermal correction to Enthalpy= 0.598650
Thermal correction to Gibbs Free Energy= 0.478055
Sum of electronic and zero-point Energies= -2525.527001
Sum of electronic and thermal Energies= -2525.487215
Sum of electronic and thermal Enthalpies= -2525.486271
Sum of electronic and thermal Free Energies= -2525.606865
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2526.953949

TS17-b

P	-2.77159000	-0.17518900	0.02797800
C	-3.36897200	1.46574000	-0.48841400
C	-2.70184200	2.14117100	-1.51715400
C	-4.47859500	2.06041800	0.13244100
C	-3.15242800	3.39306700	-1.93495600
H	-1.81271800	1.70855100	-1.96104700
C	-4.92814800	3.30840000	-0.29381700
H	-4.97671100	1.55321400	0.95321900
C	-4.26662800	3.97395400	-1.32955200

H	-2.61653300	3.92073300	-2.71768900
H	-5.78608800	3.76705100	0.18939000
H	-4.61135300	4.95247700	-1.65148000
C	-3.13882500	-0.24857800	1.81552100
C	-2.31413700	0.49710200	2.67392000
C	-4.19891200	-0.99752500	2.33896100
C	-2.56120100	0.49387700	4.04474200
H	-1.48591100	1.07089400	2.26493400
C	-4.43600100	-0.99885900	3.71532400
H	-4.83459300	-1.57691200	1.67735600
C	-3.62017200	-0.25425500	4.56750000
H	-1.92320200	1.07325700	4.70576800
H	-5.25820200	-1.58296200	4.11899800
H	-3.80674600	-0.25762200	5.63771000
C	-3.88543000	-1.39894600	-0.74443300
C	-3.43473000	-2.72208300	-0.86279100
C	-5.17371500	-1.06586500	-1.18348800
C	-4.26895000	-3.70197400	-1.39762200
H	-2.42686900	-2.97225600	-0.54282400
C	-6.00247400	-2.04853900	-1.72623900
H	-5.52454600	-0.04203800	-1.10834600
C	-5.55374400	-3.36612200	-1.83064300
H	-3.91256700	-4.72408200	-1.48653800
H	-6.99778700	-1.78264800	-2.07049000
H	-6.20045200	-4.12824500	-2.25589300
Au	-0.50804400	-0.55690400	-0.35764400
S	0.91396200	1.87386000	0.90894000
C	0.77871200	2.83491200	-0.58159500
F	0.56063400	2.07274900	-1.71184600
F	-0.24323100	3.72589200	-0.54699200
F	1.89606900	3.55347300	-0.86870200
C	1.58127100	-1.06051100	-0.70812400
H	1.70276900	-0.87979300	-1.78039700
C	2.36218500	-0.12298200	0.07546900
C	2.70056400	-0.45522600	1.50379000
H	1.84077500	-0.86439600	2.04037300
H	3.50072900	-1.20626700	1.50183800
H	3.06566600	0.42404100	2.03667400
C	3.32389000	0.75565300	-0.66698400
H	2.86876300	1.17502400	-1.56531300
H	3.72759300	1.56204000	-0.05411100
H	4.14633900	0.09764000	-0.98603500
C	1.69670600	-2.56019900	-0.42427700
H	0.86066100	-3.07889400	-0.89868700
H	1.66117300	-2.77995200	0.65012300
O	2.86467100	-3.15922100	-1.01463500
C	3.92600200	-3.53266900	-0.15541100
H	4.36060300	-4.44627900	-0.58049300
H	3.54156500	-3.79514600	0.84349000
C	4.98181600	-2.52060600	-0.02514100
C	5.84535300	-1.67358300	0.06271800
C	6.82791300	-0.64533900	0.18325000
C	8.01451500	-0.69390000	-0.57137000
C	6.61226400	0.44229300	1.05092500
C	8.95979800	0.32192700	-0.45817100
H	8.17931700	-1.53057400	-1.24259400
C	7.56089000	1.45546700	1.15576500
H	5.69735200	0.48164900	1.63251200
C	8.73629400	1.39866800	0.40315200
H	9.87223200	0.27528300	-1.04565600
H	7.38205600	2.29199100	1.82501300
H	9.47439600	2.19111400	0.48646500

Zero-point correction= 0.556074 (Hartree/Particle)
Thermal correction to Energy= 0.595738
Thermal correction to Enthalpy= 0.596683
Thermal correction to Gibbs Free Energy= 0.474956
Sum of electronic and zero-point Energies= -2525.464485
Sum of electronic and thermal Energies= -2525.424821
Sum of electronic and thermal Enthalpies= -2525.423877
Sum of electronic and thermal Free Energies= -2525.545603
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2526.897254

INT17-b

P	-2.26132100	-0.94556500	-0.07919800
C	-3.15550800	-0.23335200	1.34479700
C	-3.15499100	1.16174500	1.48941000
C	-3.82134600	-1.02828500	2.28804900
C	-3.81886200	1.75499600	2.56150200
H	-2.62381000	1.77870900	0.77374100
C	-4.48886800	-0.42956000	3.35681500
H	-3.80769200	-2.10965500	2.19258400
C	-4.48781300	0.96040100	3.49454200
H	-3.79261800	2.83427700	2.67160500
H	-5.00173900	-1.04931300	4.08689700
H	-4.99908600	1.42217500	4.33445400
C	-1.84328000	-2.64825100	0.43529300
C	-0.65435800	-2.84012200	1.15557300
C	-2.66669200	-3.74625900	0.15472400
C	-0.30334600	-4.11254900	1.60191100
H	-0.00796400	-1.99006200	1.35700500
C	-2.30813400	-5.02000000	0.59890400
H	-3.58136000	-3.60605000	-0.41247900
C	-1.12963100	-5.20416400	1.32354900
H	0.61873000	-4.25410600	2.15813700
H	-2.94884700	-5.86829700	0.37552900
H	-0.85149600	-6.19701200	1.66526200
C	-3.51108000	-1.14252800	-1.39544000
C	-3.06079000	-1.24656900	-2.71990600
C	-4.88404300	-1.21090600	-1.12345000
C	-3.97297100	-1.43495400	-3.75680900
H	-1.99754700	-1.17009800	-2.93110000
C	-5.79397700	-1.39420200	-2.16528000
H	-5.23852300	-1.11400800	-0.10218400
C	-5.34011200	-1.50936900	-3.48046400
H	-3.61803300	-1.51316100	-4.78028100
H	-6.85747400	-1.44263400	-1.94943100
H	-6.05100700	-1.64838600	-4.28992000
Au	-0.38658600	0.39250200	-0.64973800
S	0.50967200	2.61225800	1.58416600
C	-0.57563900	3.86235100	0.86408700
F	-1.16552200	3.50063700	-0.30083700
F	-1.57390300	4.08192100	1.75388300
F	0.01646200	5.05041300	0.62971200
C	1.23159500	1.70207500	-1.03273600

H	0.81032500	2.53552600	-1.60633900
C	1.84208700	2.27226900	0.27087600
C	2.71004200	1.23711400	1.00392700
H	2.16276900	0.30021900	1.15932000
H	3.59680000	1.02440700	0.40017200
H	3.04931200	1.61577300	1.97397600
C	2.64721200	3.56016300	0.04320800
H	2.03896700	4.32710400	-0.44098200
H	3.02321200	3.96404400	0.98908200
H	3.48600200	3.32811100	-0.61595100
C	2.22328600	0.96162800	-1.91488400
H	1.71089400	0.61886900	-2.82663300
H	2.61695300	0.07375200	-1.40659600
O	3.33101200	1.79772400	-2.30675600
C	4.38808700	1.06864900	-2.90070900
H	5.09040500	1.81174400	-3.29477000
H	4.02155800	0.47657100	-3.75735900
C	5.06974200	0.18220100	-1.94568400
C	5.55260100	-0.52584100	-1.08773900
C	6.10390800	-1.36027300	-0.07019400
C	7.44036900	-1.79518800	-0.13726900
C	5.30982300	-1.75725200	1.02276200
C	7.96549100	-2.60740600	0.86437700
H	8.05408700	-1.48866200	-0.97823500
C	5.84443800	-2.56642500	2.02136100
H	4.27932900	-1.42118300	1.07552200
C	7.17179300	-2.99510100	1.94630600
H	8.99858200	-2.93740500	0.80159400
H	5.22330700	-2.86348700	2.86176000
H	7.58569900	-3.62679800	2.72699100

Zero-point correction= 0.558122 (Hartree/Particle)
Thermal correction to Energy= 0.597826
Thermal correction to Enthalpy= 0.598770
Thermal correction to Gibbs Free Energy= 0.475293
Sum of electronic and zero-point Energies= -2525.491986
Sum of electronic and thermal Energies= -2525.452283
Sum of electronic and thermal Enthalpies= -2525.451339
Sum of electronic and thermal Free Energies= -2525.574815

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2526.919779

TS18-b

P	2.47894400	0.56404300	-0.03091700
C	3.09845400	0.37713400	1.67354900
C	2.69157600	-0.75688500	2.39417500
C	3.93671700	1.32354300	2.27595700
C	3.13056100	-0.94175400	3.70249400
H	2.04055900	-1.49066300	1.93757700
C	4.36756200	1.13341600	3.59024900
H	4.25241800	2.20226200	1.72372500
C	3.96651500	0.00306600	4.30343400
H	2.80841100	-1.82117500	4.25172800
H	5.01652800	1.87046400	4.05468000
H	4.30176900	-0.14044800	5.32672100
C	3.17381100	2.14269200	-0.62962100
C	2.39240400	3.30235300	-0.52918700
C	4.47432100	2.22660600	-1.14579900
C	2.91131300	4.53360400	-0.92807700
H	1.37817800	3.23115100	-0.14575900
C	4.98707300	3.45894600	-1.55013800
H	5.07963700	1.33025500	-1.23582400
C	4.20822500	4.61279800	-1.43945100
H	2.30046400	5.42802600	-0.84772500
H	5.99371500	3.51742500	-1.95398100
H	4.60940200	5.57097500	-1.75705500
C	3.32295700	-0.73647200	-0.99018800
C	2.74550000	-1.16532400	-2.19327400
C	4.53087500	-1.30099800	-0.55958800
C	3.37831100	-2.13780600	-2.96452700
H	1.79486800	-0.74567500	-2.51015300
C	5.15920000	-2.27690900	-1.33355400
H	4.96923500	-0.98678000	0.38225200
C	4.58533900	-2.69447100	-2.53552200
H	2.92307000	-2.47135800	-3.89238500
H	6.09263300	-2.71581200	-0.99326100
H	5.07267000	-3.45981900	-3.13263400
Au	0.14785100	0.44994500	-0.20484900
S	-1.03668300	-1.85313600	1.69446000
C	0.03330200	-3.07614900	0.98272400
F	0.82221500	-2.59906500	-0.04533500
F	0.91467400	-3.58376100	1.88811800
F	-0.61178400	-4.14529600	0.44295900
C	-2.03751600	0.45449500	-0.41417400
C	-2.33738300	-0.95460300	-0.34231400
H	-3.10888000	-1.30156000	0.33415000
C	-2.64017700	1.24835300	0.74543100
H	-2.28467700	2.28422700	0.74421300
H	-3.73725500	1.27202200	0.67514400
H	-2.37246200	0.80298200	1.70954800
C	-2.29330400	1.15630600	-1.76680900
H	-3.37454300	1.22556800	-1.95233200
H	-1.89141900	2.17296400	-1.73699900
H	-1.82931600	0.65237300	-2.61770600
C	-2.07073200	-1.91821800	-1.47973100
H	-1.39284700	-2.70814800	-1.16788200
H	-1.60318100	-1.39495700	-2.32568600
O	-3.24565600	-2.60539900	-1.89888400
C	-4.18963300	-1.81003100	-2.59995800
H	-4.84179700	-2.52296600	-3.11705800
H	-3.68687500	-1.20319600	-3.37037700
C	-4.99107700	-0.93858100	-1.73428600
C	-5.62984000	-0.23102600	-0.98470000
C	-6.35633000	0.60939400	-0.09020400
C	-6.75648000	0.12669200	1.16994100
C	-6.66152800	1.93670800	-0.44546800
C	-7.44392400	0.95638900	2.05130100
H	-6.51630600	-0.89527400	1.44458100
C	-7.35317100	2.75762300	0.44062400
H	-6.34762000	2.30951600	-1.41516200
C	-7.74527600	2.27167300	1.69026600
H	-7.74459900	0.57582100	3.02308100
H	-7.58401700	3.78053400	0.15738600
H	-8.28181500	2.91603100	2.38063500

Zero-point correction= 0.555635 (Hartree/Particle)
Thermal correction to Energy= 0.595692

Thermal correction to Enthalpy= 0.596636

Thermal correction to Gibbs Free Energy= 0.472056

Sum of electronic and zero-point Energies= -2525.451886

Sum of electronic and thermal Energies= -2525.411829

Sum of electronic and thermal Enthalpies= -2525.410884

Sum of electronic and thermal Free Energies= -2525.535465

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2526.883619

INT18-b

P	2.64666800	0.49559900	-0.11452200
C	3.39331600	0.05220700	1.49400200
C	2.77479700	-0.96380700	2.24146200
C	4.53571500	0.68557600	1.99801600
C	3.30467600	-1.34438800	3.47189400
H	1.88950900	-1.45857500	1.85786900
C	5.05732100	0.30406100	3.23598200
H	5.01572800	1.47353800	1.42708200
C	4.44472500	-0.70982200	3.97276100
H	2.82125200	-2.13224300	4.04204400
H	5.94236900	0.80137400	3.62273900
H	4.85153100	-1.00364500	4.93620200
C	3.57516900	1.95982400	-0.68731900
C	3.05276100	3.22634200	-0.38641700
C	4.78506300	1.85925600	-1.38767800
C	3.74197000	4.37725000	-0.76648500
H	2.10388600	3.30228400	0.13793600
C	5.46809900	3.01319800	-1.77192700
H	5.18670200	0.88187500	-1.63568400
C	4.94978200	4.27169700	-1.45938700
H	3.33153200	5.35474900	-0.53052400
H	6.40359100	2.92935200	-2.31770500
H	5.48273500	5.16860800	-1.76189700
C	3.14158800	-0.86410200	-1.22891800
C	2.34582100	-1.12461800	-2.35378300
C	4.27780800	-1.64866400	-0.98868800
C	2.69267300	-2.14662200	-3.23585800
H	1.44971500	-0.53395800	-2.52310600
C	4.62017700	-2.67223500	-1.87247900
H	4.88388400	-1.46535100	-0.10684600
C	3.82987600	-2.92097000	-2.99632500
H	2.06897200	-2.34676000	-4.10218800
H	5.49985200	-3.27960100	-1.67941300
H	4.09444100	-3.72318200	-3.67924400
Au	0.27282000	0.71907600	0.01832200
S	-1.76826600	-1.78073600	1.54103700
C	-0.53827100	-2.91661700	0.85558200
F	0.43221600	-2.33545500	0.09931700
F	0.08590200	-3.48385700	1.91370000
F	-1.04183500	-3.90855900	0.10623400
C	-1.82619000	0.73378800	0.20875200
C	-2.38053500	-0.70782100	0.12630200
H	-3.45395400	-0.67930800	0.35150200
C	-2.21490100	1.33916400	1.56931300
H	-1.87936400	2.37921400	1.63998600
H	-3.31240000	1.33763500	1.69465800
H	-1.77715400	0.79367800	2.41062500
C	-2.48893800	1.60243100	-0.87947500
H	-3.58816600	1.53672200	-0.83028600
H	-2.21477500	2.65190500	-0.72625400
H	-2.17983900	1.34040300	-1.89561400
C	-2.24591600	-1.39309500	-1.23947700
H	-1.20883900	-1.66979500	-1.44082300
H	-2.55266000	-0.67894900	-2.01016100
O	-3.03058100	-2.57849500	-1.33278900
C	-4.25680300	-2.42822700	-2.02985800
H	-4.72818700	-3.41662700	-2.00094100
H	-4.06924800	-2.18470900	-3.08954100
C	-5.15093600	-1.41226700	-1.46098500
C	-5.77654500	-0.50607000	-0.95398100
C	-6.46574300	0.56557700	-0.31315600
C	-6.36726500	0.72764200	1.08234400
C	-7.22009300	1.48999000	-1.05838400
C	-7.00555400	1.79281600	1.71140700
H	-5.78572500	0.01425300	1.65721300
C	-7.86098100	2.54837100	-0.41988800
H	-7.29227000	1.36806500	-2.13434800
C	-7.75474100	2.70468500	0.96406700
H	-6.91862000	1.91100600	2.78758100
H	-8.44176900	3.25619400	-1.00439100
H	-8.25269400	3.53411600	1.45786700

Zero-point correction= 0.557839 (Hartree/Particle)

Thermal correction to Energy= 0.597650

Thermal correction to Enthalpy= 0.598594

Thermal correction to Gibbs Free Energy= 0.475548

Sum of electronic and zero-point Energies= -2525.480846

Sum of electronic and thermal Energies= -2525.441035

Sum of electronic and thermal Enthalpies= -2525.440091

Sum of electronic and thermal Free Energies= -2525.563137

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2526.907677

INT6-b´

C	0.38419700	0.67656000	-0.58892200
C	-0.41724500	1.74763800	-0.47632200
C	0.11156600	3.16527100	-0.37385900
H	-0.47316100	3.83299700	-1.01176500
H	0.02101500	3.53970000	0.65828000
O	1.44966300	3.24220700	-0.82322000
C	2.26583800	2.31540300	-0.13131800
H	3.29867500	2.52747000	-0.41949600
H	2.17411700	2.48050000	0.95065700
C	1.90786900	0.86242500	-0.50933300
H	2.24980000	0.72339600	-1.54224700
C	2.62177500	-0.16172300	0.35179900
C	3.64348600	-1.05190300	-0.32519300
H	3.87792800	-1.87677000	0.35523100
C	2.69208800	0.04810900	1.85693500
H	3.34387200	0.92469400	2.03716200
C	-0.10481700	-0.68224800	-0.94348600
C	0.03350900	-1.78312400	-0.08688000
C	-0.67097400	-0.87848600	-2.21136100
C	-0.40472400	-3.04507600	-0.48014000
H	0.46338400	-1.64771900	0.89577700
C	-1.09429700	-2.14579700	-2.61006600
H	-0.79084400	-0.02904700	-2.87394800

C	-0.96537900	-3.23228700	-1.74494800
H	-0.30970200	-3.88302300	0.20444800
H	-1.52916800	-2.28017100	-3.59626800
H	-1.30110300	-4.21866200	-2.05251900
S	-2.21573000	1.67710100	-0.44447900
O	-2.61302900	2.87230800	0.32384700
O	-2.75208800	1.46477700	-1.80026000
C	-2.61579400	0.23694100	0.54645800
C	-3.25766700	-0.84430300	-0.04945500
C	-2.27615000	0.23780700	1.89946000
C	-3.54304600	-1.96652400	0.72679000
H	-3.49920100	-0.80467600	-1.10445900
C	-2.55760600	-0.89234800	2.66335400
H	-1.80170500	1.10751700	2.34088200
C	-3.18628400	-1.99389400	2.07561400
H	-4.03209200	-2.82312800	0.27340000
H	-2.29426800	-0.91149100	3.71677100
H	-3.40193800	-2.87429000	2.67427600
C	4.95827000	-0.26758600	-0.55655400
H	5.72902700	-0.91758000	-0.98771700
H	4.79708500	0.56418100	-1.25322700
H	5.34814300	0.14793500	0.37937200
C	1.33892400	0.38347400	2.51982100
H	1.50250500	0.68900300	3.55932700
H	0.80431000	1.18856200	2.01337300
H	0.67474500	-0.48657500	2.53400600
C	3.17740900	-1.70080400	-1.63996700
H	2.97767900	-0.96163200	-2.42348100
H	3.96328100	-2.36485700	-2.01785000
H	2.26850100	-2.28957500	-1.49630000
C	3.33298700	-1.12192200	2.62217300
H	2.78245900	-2.05472400	2.44943700
H	4.37675800	-1.28668700	2.34005800
H	3.31159800	-0.91691900	3.69796300

Zero-point correction= 0.482314 (Hartree/Particle)
Thermal correction to Energy= 0.509423
Thermal correction to Enthalpy= 0.510367
Thermal correction to Gibbs Free Energy= 0.424849
Sum of electronic and zero-point Energies= -1555.392044
Sum of electronic and thermal Energies= -1555.364935
Sum of electronic and thermal Enthalpies= -1555.363991
Sum of electronic and thermal Free Energies= -1555.449509
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1556.223976

TS10-b´

C	2.14749100	-0.22303700	-0.86970500
C	2.84471700	-1.36891800	-0.78324400
C	2.22635200	-2.70736000	-1.12021300
H	2.97497700	-3.35699700	-1.57465900
H	1.83379300	-3.22659900	-0.23160500
O	1.20580200	-2.49658300	-2.07380700
C	0.16710600	-1.72667300	-1.51899100
H	-0.60663500	-1.65131300	-2.28101600
H	-0.25643600	-2.24683300	-0.65803300
C	0.61926100	-0.27492000	-1.12148600
H	0.46583000	0.35809200	-2.00321700
C	-0.25306700	0.33122500	-0.00904300
C	-0.86461600	1.70960600	-0.31324700
H	-1.47479300	1.56888100	-1.21775800
C	-0.08762400	-0.05803400	1.45426900
H	-1.05773800	0.13611600	1.91824900
C	2.83282600	1.09365200	-1.06665800
C	3.27872600	1.93914600	-0.04959200
C	3.03387100	1.48010400	-2.40201900
C	3.89236300	3.15438300	-0.35706900
H	3.16500200	1.65608800	0.98622000
C	3.63955600	2.69432900	-2.70916500
H	2.72385100	0.80965600	-3.19817500
C	4.06638000	3.54109800	-1.68365700
H	4.23618100	3.79523600	0.44979300
H	3.78922400	2.97342000	-3.74786000
H	4.54068700	4.48916000	-1.91997600
S	4.64554000	-1.44276500	-0.57856400
O	4.92793000	-2.86784900	-0.32773800
O	5.32665500	-0.73319700	-1.67159100
C	4.97682200	-0.56107800	0.94664800
C	5.86763400	0.50796700	0.92252700
C	4.36003800	-0.97945600	2.12571100
C	6.13373000	1.18714100	2.11129600
H	6.31358100	0.80596100	-0.01930800
C	4.61886600	-0.28262400	3.30439200
H	3.69001000	-1.83312100	2.12010900
C	5.50331000	0.80018900	3.29531500
H	6.82432800	2.02503100	2.10955100
H	4.13811500	-0.58765200	4.22890400
H	5.70461700	1.33907200	4.21657100
C	-3.04875700	-1.97756900	0.55369800
F	-2.91715700	-1.62987100	1.85584900
F	-4.33884000	-2.31835300	0.36515300
F	-2.31751400	-3.10473500	0.38528100
S	-2.55349100	-0.63958000	-0.56337100
S	-4.86050200	0.05198000	-1.52799000
O	-5.67981600	-1.01581300	-2.14346600
O	-4.39532900	1.22316200	-2.30365300
C	-5.72955900	0.65728400	-0.07773500
C	-6.58847700	-0.20245900	0.60562000
C	-5.45160600	1.94636300	0.37599400
C	-7.19956400	0.25662300	1.77124500
H	-6.77645900	-1.19812200	0.22193300
C	-6.06958200	2.38965500	1.54387200
H	-4.77935800	2.58211100	-0.18782300
C	-6.93855200	1.54624100	2.24037200
H	-7.88013500	-0.39329700	2.31291600
H	-5.87529100	3.39416400	1.90784300
H	-7.41470900	1.89547700	3.15188800
C	-1.79418300	2.25933400	0.78081500
H	-2.30105500	3.15060400	0.39697100
H	-2.56090700	1.53997500	1.07336100
H	-1.23862600	2.56256400	1.67403500
C	0.14601800	2.81528800	-0.69849800
H	0.81536900	3.07542800	0.12370200
H	0.76146100	2.55009800	-1.55759700
H	-0.42592200	3.71097400	-0.96335100
C	0.28275600	-1.51404900	1.76953100

H	0.33991800	-1.62930200	2.85752400
H	-0.44813600	-2.23373300	1.40767200
H	1.26255900	-1.77190500	1.36214200
C	0.93822600	0.84136200	2.19180300
H	1.95540600	0.50380500	1.98651200
H	0.86063400	1.89747100	1.93153700
H	0.77282100	0.74534900	3.27055000

Zero-point correction= 0.601089 (Hartree/Particle)
Thermal correction to Energy= 0.642256
Thermal correction to Enthalpy= 0.643200
Thermal correction to Gibbs Free Energy= 0.523091
Sum of electronic and zero-point Energies= -3071.330004
Sum of electronic and thermal Energies= -3071.288837
Sum of electronic and thermal Enthalpies= -3071.287893
Sum of electronic and thermal Free Energies= -3071.408002
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-3072.569755

P_2'

C	0.52693100	-0.13061500	-0.94810900
C	1.23051700	-1.26544100	-1.10928500
C	0.61213100	-2.49895000	-1.72987900
H	1.36468300	-3.04231900	-2.30179800
H	0.21151000	-3.19375000	-0.97456400
O	-0.39588800	-2.09416900	-2.63233000
C	-1.44686800	-1.43823800	-1.95361900
H	-2.17613300	-1.18376100	-2.72288200
H	-1.92725800	-2.13221700	-1.26311100
C	-0.98576900	-0.12904300	-1.23140700
H	-1.10423900	0.66930200	-1.96959600
C	-1.91747400	0.30636100	-0.01363200
C	-1.75522900	1.84094500	0.27936900
H	-0.72536200	1.95794000	0.61993900
C	-1.77262200	-0.53464200	1.30281600
H	-2.65136700	-0.28860100	1.90193700
C	1.21177900	1.20011400	-0.83522300
C	1.65811700	1.78163600	0.35472700
C	1.41903900	1.88974700	-2.03994000
C	2.27971300	3.03097200	0.34328900
H	1.53718000	1.26134000	1.29468500
C	2.03996200	3.13539800	-2.05212200
H	1.10984200	1.42738400	-2.97284200
C	2.46828200	3.71422500	-0.85619600
H	2.62225700	3.46242600	1.27939900
H	2.19822600	3.64793700	-2.99630700
H	2.95303400	4.68615500	-0.86224800
S	3.03352400	-1.37409400	-0.94856500
O	3.32569900	-2.81687400	-1.03579900
O	3.69472300	-0.42830200	-1.86065300
C	3.39889300	-0.86694200	0.73116200
C	4.26710400	0.20192600	0.93479600
C	2.83637800	-1.57150300	1.79537400
C	4.56444800	0.58577500	2.24202200
H	4.67287000	0.72619500	0.07744100
C	3.12596800	-1.16845600	3.09752600
H	2.18456200	-2.41847600	1.60630000
C	3.98748500	-0.09012500	3.31894400
H	5.23814400	1.41886900	2.41847200
H	2.68702200	-1.69837700	3.93738800
H	4.21321000	0.21923600	4.33532900
C	-4.85435200	-0.39963700	0.52128300
F	-4.86701100	0.38563900	1.61772200
F	-6.06632700	-0.31461800	-0.05569500
F	-4.71388500	-1.66457100	0.96832400
S	-3.66924300	0.08282800	-0.77060700
C	-2.66465500	2.37689000	1.39562400
H	-2.35788000	3.40029800	1.63624700
H	-3.70848800	2.41128100	1.07498200
H	-2.61541100	1.79463400	2.31810600
C	-1.75277500	-2.06487900	1.16321000
H	-1.81953500	-2.50434900	2.16456800
H	-2.58552200	-2.45861500	0.58305300
H	-0.81616000	-2.41190700	0.71992700
C	-1.91028300	2.76511900	-0.94045400
H	-2.89114500	2.64944700	-1.41195600
H	-1.82526600	3.80417000	-0.60574900
H	-1.13474400	2.61789200	-1.69406300
C	-0.55350600	-0.15020900	2.16065100
H	0.38039100	-0.42562400	1.66841900
H	-0.51491400	0.90957500	2.41681000
H	-0.59854300	-0.71166400	3.10040500

Zero-point correction= 0.503203 (Hartree/Particle)
Thermal correction to Energy= 0.534840
Thermal correction to Enthalpy= 0.535784
Thermal correction to Gibbs Free Energy= 0.440611
Sum of electronic and zero-point Energies= -2291.225085
Sum of electronic and thermal Energies= -2291.193448
Sum of electronic and thermal Enthalpies= -2291.192504
Sum of electronic and thermal Free Energies= -2291.287677
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2292.218453

INT6-b´´

C	0.07565100	0.71261500	-0.59967300
C	-0.76457900	1.75166900	-0.47755100
C	-0.28667100	3.18940300	-0.43111000
H	-0.95080400	3.82727300	-1.01929000
H	-0.29728300	3.57391900	0.60153500
O	1.00160400	3.30738500	-1.00203700
C	1.92130700	2.45039100	-0.35036500
H	2.90754100	2.68358300	-0.75691800
H	1.93767000	2.68076700	0.72029800
C	1.59099300	0.96114100	-0.61787500
H	1.84290500	0.80717100	-1.67227900
C	2.44567100	-0.01556000	0.18578100
C	3.51421500	-0.73528400	-0.66613200
C	2.43030300	0.02483800	1.72557400
C	-0.37378800	-0.66290500	-0.95081600
C	-0.21529200	-1.76111800	-0.09706100
C	-0.92292500	-0.87154000	-2.22454900
C	-0.61044500	-3.03475900	-0.49852000
H	0.18144600	-1.61737400	0.89701300
C	-1.30309900	-2.14956700	-2.63245400
H	-1.06362400	-0.02293900	-2.88449800
C	-1.14864800	-3.23541000	-1.77058700
H	-0.50058500	-3.87058000	0.18653000

H	-1.72574500	-2.29271200	-3.62272900
H	-1.45018800	-4.23044300	-2.08546100
S	-2.55689600	1.61783700	-0.41455100
O	-2.98226400	2.79605700	0.36510900
O	-3.10679300	1.39315700	-1.76312100
C	-2.89781100	0.16217800	0.57478100
C	-3.50516000	-0.93936400	-0.02010000
C	-2.55222500	0.17293500	1.92638900
C	-3.74775200	-2.07205400	0.75541000
H	-3.75317900	-0.90602800	-1.07387300
C	-2.78935100	-0.96839800	2.68908600
H	-2.10871000	1.05946700	2.36683900
C	-3.38257200	-2.08987200	2.10221800
H	-4.20964300	-2.94410500	0.30297900
H	-2.51968100	-0.98082300	3.74096400
H	-3.56432600	-2.97838900	2.70011500
C	4.44048600	0.32278600	-1.32830100
H	5.19754800	-0.17735100	-1.94374400
H	3.89310000	1.00679700	-1.98328500
H	4.96163700	0.91942200	-0.57168500
C	1.12127300	0.62199800	2.30239200
H	1.22034000	0.69082400	3.39139400
H	0.89213500	1.62243100	1.93745500
H	0.25374500	-0.00822900	2.09472200
C	2.83879000	-1.56702800	-1.78818000
H	2.19561200	-0.97006600	-2.43942000
H	3.61018400	-2.02444800	-2.41894600
H	2.22279300	-2.36472800	-1.36419000
C	2.55728200	-1.37407200	2.39343100
H	1.94394700	-2.12502400	1.88733900
H	3.58237100	-1.73984300	2.42118800
H	2.21400200	-1.30712100	3.43182100
C	4.44244500	-1.72088600	0.07174200
H	5.00794000	-1.25278500	0.88109400
H	3.89640600	-2.57663100	0.47386500
H	5.17234300	-2.11084500	-0.64633200
C	3.60685000	0.89781900	2.24616200
H	3.62725200	0.88211700	3.34315100
H	4.57187100	0.52835500	1.88967900
H	3.51123600	1.94043300	1.92973100

Zero-point correction= 0.539782 (Hartree/Particle)
Thermal correction to Energy= 0.569023
Thermal correction to Enthalpy= 0.569967
Thermal correction to Gibbs Free Energy= 0.481996
Sum of electronic and zero-point Energies= -1633.960692
Sum of electronic and thermal Energies= -1633.931451
Sum of electronic and thermal Enthalpies= -1633.930507
Sum of electronic and thermal Free Energies= -1634.018479
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1634.870878

TS10-b´´

C	2.12984100	-0.06786700	-0.91564300
C	2.86695100	-1.18562100	-1.05424200
C	2.27213900	-2.50234600	-1.49219000
H	2.99247200	-3.05917200	-2.09075100
H	1.99612600	-3.13243200	-0.62921300
O	1.14687400	-2.24339700	-2.30242300
C	0.16418600	-1.56609600	-1.56130400
H	-0.71948400	-1.51159000	-2.19195900
H	-0.08189900	-2.14124000	-0.66470700
C	0.59634200	-0.11593300	-1.16418400
H	0.50739800	0.47031500	-2.08254300
C	-0.41674600	0.53872500	-0.16544100
C	-1.17792400	1.75116800	-0.81180300
C	-0.13515100	0.49972400	1.37175700
C	2.80483100	1.26672800	-0.85999700
C	3.36113500	1.80491700	0.30252600
C	2.95068500	1.96975900	-2.06499800
C	4.01658400	3.03708200	0.27142100
H	3.30255300	1.25845100	1.23520300
C	3.60357000	3.19741900	-2.09857900
H	2.57173100	1.53174300	-2.98396800
C	4.13272300	3.74014600	-0.92534900
H	4.44409500	3.43616400	1.18657800
H	3.71285800	3.72346900	-3.04222500
H	4.64527400	4.69737700	-0.94966100
S	4.68448900	-1.22211500	-0.96816900
O	5.03842000	-2.64136800	-1.15030600
O	5.27993700	-0.19719900	-1.83752700
C	5.06532400	-0.79829200	0.73192900
C	5.98271800	0.21925300	0.97881100
C	4.45396500	-1.50525800	1.76707900
C	6.28120700	0.54779500	2.30080900
H	6.42150200	0.75225900	0.14319200
C	4.74570900	-1.15699400	3.08460700
H	3.75901100	-2.30939300	1.54662200
C	5.65697500	-0.13069600	3.34968200
H	6.99323400	1.34017400	2.51132900
H	4.26901800	-1.68937100	3.90203000
H	5.88359200	0.13664000	4.37767900
C	-2.60995900	-2.47203300	0.59394900
F	-3.37588500	-2.35491600	1.70674100
F	-3.13775900	-3.46110300	-0.13979300
F	-1.39255300	-2.89592600	1.02248600
S	-2.52172400	-0.92354800	-0.35288100
S	-5.18331700	-0.94389500	-0.85200700
O	-5.89135400	-2.09558400	-0.24291500
O	-5.38759800	-0.55823900	-2.26889600
C	-5.52999900	0.51198500	0.15274300
C	-5.37596700	0.40927000	1.53513200
C	-5.83995100	1.71588500	-0.47384500
C	-5.54717200	1.55397500	2.31015400
H	-5.10868700	-0.54103500	1.98291300
C	-6.01898500	2.85174900	0.31734900
H	-5.93327400	1.75149200	-1.55333800
C	-5.86745000	2.77207200	1.70237800
H	-5.42983600	1.49654000	3.38813700
H	-6.27115400	3.79888400	-0.15037200
H	-5.99666700	3.66151300	2.31209900
C	-0.15933400	2.88645600	-1.13176000
H	0.41996700	3.20987000	-0.26891600
H	0.54018800	2.60424900	-1.91766400
H	-0.72945000	3.74892200	-1.49311500
C	-1.84210800	1.40134100	-2.17510700

H	-2.77295200	0.84245800	-2.06563700
H	-2.09345600	2.33952300	-2.67990500
H	-1.19534200	0.83709600	-2.85102500
C	-2.29512400	2.37838000	0.04837900
H	-2.78182000	3.16028400	-0.54343700
H	-3.06208800	1.65481000	0.31825300
H	-1.92313600	2.85131900	0.95781900
C	0.49736700	1.84079100	1.85312400
H	1.32323400	2.17375000	1.23369200
H	-0.23888000	2.64358600	1.90867300
H	0.88507600	1.68093800	2.86520300
C	-1.37421800	0.29485300	2.28414700
H	-1.70270200	-0.74157600	2.28823600
H	-1.07462400	0.54362400	3.30871300
H	-2.22383600	0.91943300	2.02406100
C	0.84351600	-0.63149500	1.75643100
H	0.88502100	-0.69623300	2.84878700
H	0.50849100	-1.60101800	1.38641600
H	1.85873400	-0.45616300	1.40555000

Zero-point correction= 0.657992 (Hartree/Particle)
Thermal correction to Energy= 0.701530
Thermal correction to Enthalpy= 0.702474
Thermal correction to Gibbs Free Energy= 0.579394
Sum of electronic and zero-point Energies= -3149.889118
Sum of electronic and thermal Energies= -3149.845581
Sum of electronic and thermal Enthalpies= -3149.844636
Sum of electronic and thermal Free Energies= -3149.967717
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-3151.199567

P_2''

O	-0.69953400	-3.12991300	0.92665100
C	0.60381400	-2.61571600	1.11984800
H	0.84442600	-2.79763900	2.16983100
H	1.28450600	-3.20214900	0.51002300
C	0.71781100	-1.08128900	0.82600400
H	0.52510800	-0.59291500	1.77685200
C	2.23079700	-0.56242500	0.44998400
C	3.17120000	-1.70031000	-0.19041300
C	2.76355000	0.20941500	1.74989400
S	1.87112500	0.59750500	-1.03855200
C	3.00073800	2.01097400	-1.27832300
F	2.99817000	2.93821600	-0.29948000
F	4.29882600	1.72189100	-1.50912500
F	2.52273100	2.60504100	-2.38971600
C	-0.48086600	-0.58848200	-0.01753800
C	-1.23695800	-1.48302200	-0.68355400
C	-1.07708500	-2.96438900	-0.43293800
H	-2.03213500	-3.46870400	-0.57638700
H	-0.34663100	-3.44263400	-1.10164900
C	-0.99414900	0.79490000	0.26568600
C	-1.03183400	1.84401900	-0.65720100
C	-1.53611200	1.00086200	1.54355900
C	-1.56759600	3.07936400	-0.29593200
H	-0.65567200	1.68908000	-1.65831800
C	-2.07691100	2.23280100	1.90231900
H	-1.56080100	0.17684400	2.25164800
C	-2.08381200	3.28234600	0.98378700
H	-1.58184100	3.88524700	-1.02407300
H	-2.50023900	2.36654900	2.89335100
H	-2.49946700	4.24736000	1.25957900
S	-2.71606200	-1.02960000	-1.62498800
O	-3.29505600	-2.30799600	-2.07706800
O	-2.37918900	0.01232100	-2.60715800
C	-3.82993800	-0.32571300	-0.40728300
C	-4.33066800	0.95665000	-0.60458900
C	-4.17727400	-1.08961400	0.70835900
C	-5.19825600	1.49173600	0.34720100
H	-4.02076000	1.52164300	-1.47524900
C	-5.03792400	-0.54150800	1.65542000
H	-3.76723600	-2.08541600	0.84296000
C	-5.54805700	0.74726300	1.47379500
H	-5.58996200	2.49535200	0.21265700
H	-5.31282500	-1.11901800	2.53302700
H	-6.21833800	1.17152400	2.21584900
C	2.40308400	-2.41669100	-1.35572100
H	2.47381900	-3.50552300	-1.26745200
H	1.34933700	-2.15197700	-1.41685000
H	2.83304800	-2.14099300	-2.32126500
C	3.70639400	-2.73260500	0.83980300
H	4.12671400	-3.58174400	0.29064200
H	4.52149300	-2.30489200	1.42881500
H	2.97121200	-3.12884600	1.53704500
C	4.45827100	-1.17160800	-0.87395600
H	4.98181100	-2.04113700	-1.28745100
H	4.23651400	-0.50648000	-1.70501300
H	5.14879100	-0.66968000	-0.20037400
C	2.71557400	-0.67710500	3.02449700
H	3.40083700	-1.52186800	2.98989400
H	3.01327200	-0.05353100	3.87428600
H	1.71532300	-1.05460100	3.25206200
C	1.87787700	1.43829800	2.08311600
H	1.72440300	2.10502200	1.23951500
H	0.89189700	1.15688400	2.45564800
H	2.36578400	2.00923700	2.87980700
C	4.22548900	0.69504300	1.64644800
H	4.93269900	-0.13522500	1.69407800
H	4.43616500	1.27261000	0.74985500
H	4.43748300	1.34036500	2.50514500

Zero-point correction= 0.559764 (Hartree/Particle)
Thermal correction to Energy= 0.593887
Thermal correction to Enthalpy= 0.594831
Thermal correction to Gibbs Free Energy= 0.495551
Sum of electronic and zero-point Energies= -2369.763206
Sum of electronic and thermal Energies= -2369.729083
Sum of electronic and thermal Enthalpies= -2369.728139
Sum of electronic and thermal Free Energies= -2369.827419
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2370.834015

c

C	1.48813000	2.34408200	0.04445600
H	1.27825600	3.36583700	-0.17566500
C	1.70381100	1.17992200	0.28071200
C	2.02998200	-0.21947400	0.59162000
H	3.10580900	-0.29831000	0.78702200

H	1.50752000	-0.52287200	1.51334800
O	1.76262600	-1.13769300	-0.45651200
C	0.40967100	-1.60882100	-0.48549200
H	0.41884600	-2.38552800	-1.25846000
H	0.17146500	-2.09477700	0.47107800
C	-0.57749700	-0.53455100	-0.83017300
H	-0.38725300	-0.05295600	-1.78834000
C	-1.59762400	-0.08308200	-0.08695700
C	-2.45193900	1.05796100	-0.57704400
H	-3.51428400	0.77958000	-0.60431500
H	-2.36910200	1.91732100	0.10300600
H	-2.15648500	1.38701700	-1.57741800
C	-1.98076000	-0.60471700	1.27428700
H	-1.33611600	-1.40987200	1.63242500
H	-1.94922900	0.20792800	2.01273400
H	-3.01307600	-0.97974600	1.26822300

Zero-point correction= 0.179740 (Hartree/Particle)
Thermal correction to Energy= 0.190752
Thermal correction to Enthalpy= 0.191696
Thermal correction to Gibbs Free Energy= 0.142009
Sum of electronic and zero-point Energies= -387.040449
Sum of electronic and thermal Energies= -387.029437
Sum of electronic and thermal Enthalpies= -387.028493
Sum of electronic and thermal Free Energies= -387.078180
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-387.340861

c´

C	0.73117100	2.65060200	0.24197900
C	1.49416200	1.70423600	-0.04979600
C	2.25231700	0.60608000	-0.33505300
H	2.24326400	0.14998800	-1.31531600
H	2.96176400	0.20460100	0.37730400
O	1.68106200	-1.81904200	-0.13510200
C	0.44278900	-1.94903100	0.40724700
H	0.13220400	-3.03358800	0.45263100
H	0.36370200	-1.61270100	1.47120500
C	-0.61556000	-1.23257400	-0.41740700
H	-0.54562000	-1.48464200	-1.47911200
C	-1.47749100	-0.27133100	-0.05965300
C	-2.29534200	0.47113400	-1.08811800
H	-3.37207100	0.46223100	-0.85041900
H	-1.98418000	1.52600400	-1.12097900
H	-2.16432900	0.04823500	-2.09097200
C	-1.64365800	0.24972500	1.34584900
H	-1.06597200	-0.32701600	2.07157600
H	-1.29459900	1.29105700	1.39073000
H	-2.70153200	0.23235300	1.65609000
H	0.64854900	3.72276700	0.24779400

Zero-point correction= 0.170730 (Hartree/Particle)
Thermal correction to Energy= 0.183300
Thermal correction to Enthalpy= 0.184244
Thermal correction to Gibbs Free Energy= 0.130907
Sum of electronic and zero-point Energies= -386.998360
Sum of electronic and thermal Energies= -386.985790
Sum of electronic and thermal Enthalpies= -386.984846
Sum of electronic and thermal Free Energies= -387.038183
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-387.3534347

c´´

C	0.00975400	-1.01345300	0.59219400
C	-1.08247600	-1.54978600	0.62252600
C	-2.42260900	-2.14969600	0.63988400
H	-2.36380900	-3.22007400	0.42221200
H	-2.87328900	-2.02120200	1.63487000
O	-3.25393800	-1.58237600	-0.37141700
C	-3.30002600	-0.17699100	-0.28053100
H	-4.11178400	0.14176800	-0.95421600
H	-3.56127800	0.16086300	0.73212800
C	-2.03067200	0.43993400	-0.77769000
H	-1.58945800	-0.04372000	-1.64546600
C	-1.48435900	1.65871600	-0.34124200
C	-0.26966500	2.20427700	-0.99623700
H	-0.52982400	3.14897000	-1.50014700
H	0.47946900	2.48109200	-0.24159100
H	0.17110000	1.52694100	-1.73034500
C	-2.09430400	2.42715100	0.78132800
H	-1.96247800	1.87041100	1.72183400
H	-1.63105900	3.40800500	0.90077200
H	-3.17528800	2.55671300	0.64889400
H	0.99732600	-0.60303300	0.56905500

Zero-point correction= 0.178153 (Hartree/Particle)
Thermal correction to Energy= 0.189307
Thermal correction to Enthalpy= 0.190251
Thermal correction to Gibbs Free Energy= 0.140188
Sum of electronic and zero-point Energies= -386.750788
Sum of electronic and thermal Energies= -386.739633
Sum of electronic and thermal Enthalpies= -386.738689
Sum of electronic and thermal Free Energies= -386.788752
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-387.0869741

INT19-c

C	2.58797000	-1.04622900	-2.42043400
H	2.47088200	-0.70150000	-3.42744300
C	2.93258300	-1.50585800	-1.33643600
C	3.44676500	-2.17927000	-0.11288200
H	3.21936600	-3.24639800	-0.20513800
H	4.54153800	-2.06582600	-0.10588500
O	2.86689200	-1.74513900	1.08913700
C	3.42728400	-0.52812700	1.64432600
H	3.21415200	-0.61042700	2.71256700
H	4.51521900	-0.54853100	1.51291000
C	2.80000200	0.71899600	1.09564900
H	1.82182800	0.95097500	1.50856500
C	3.31653400	1.56352000	0.18535700
C	2.53057900	2.77102400	-0.25578000
H	3.08991000	3.69600700	-0.06633800
H	2.34718500	2.73663200	-1.33941500
H	1.56751200	2.84001000	0.25820200
C	4.65467800	1.40450200	-0.48390700
H	5.22655400	0.54702900	-0.12326500
H	4.52209500	1.28942000	-1.56788400
H	5.26658800	2.30298800	-0.33754000
P	-1.19952500	0.04162100	0.04495200

C	-2.42556300	-1.29225400	0.01822300
C	-2.57058200	-2.06282800	-1.14497100
C	-3.25967500	-1.52081900	1.12247200
C	-3.55128900	-3.05033000	-1.20478800
H	-1.91684400	-1.88967800	-1.99569600
C	-4.23729500	-2.51335900	1.05528300
H	-3.14010700	-0.93489100	2.02806700
C	-4.38387500	-3.27550600	-0.10539600
H	-3.66190800	-3.64764400	-2.10432600
H	-4.88097600	-2.69316300	1.91065900
H	-5.14356000	-4.04959800	-0.15196300
C	-0.79009300	0.36071400	1.78583500
C	-1.01239400	1.61093900	2.37480300
C	-0.16340800	-0.66324100	2.51619000
C	-0.61099200	1.83376600	3.69387600
H	-1.49175600	2.40360700	1.81028500
C	0.22552300	-0.43467700	3.83295900
H	0.03745400	-1.62316100	2.04937100
C	0.00546100	0.81531700	4.42137800
H	-0.78260900	2.80329900	4.15090000
H	0.70495500	-1.22795200	4.39825600
H	0.31599700	0.99324000	5.44629000
C	-1.97365600	1.53520500	-0.62758100
C	-1.18662700	2.48683700	-1.29183400
C	-3.34446200	1.76531600	-0.43811100
C	-1.76519700	3.66848900	-1.75174000
H	-0.12850900	2.30051000	-1.44762500
C	-3.91657400	2.94799600	-0.90390800
H	-3.95896700	1.02358000	0.06200300
C	-3.12893300	3.89891900	-1.55743700
H	-1.15509700	4.40400600	-2.26666800
H	-4.97797400	3.12474800	-0.76110000
H	-3.57997200	4.81686900	-1.92134900
Au	0.77688800	-0.55078000	-1.01368000

Zero-point correction= 0.458352 (Hartree/Particle)
Thermal correction to Energy= 0.488692
Thermal correction to Enthalpy= 0.489636
Thermal correction to Gibbs Free Energy= 0.391721
Sum of electronic and zero-point Energies= -1558.487242
Sum of electronic and thermal Energies= -1558.456903
Sum of electronic and thermal Enthalpies= -1558.455959
Sum of electronic and thermal Free Energies= -1558.553874
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1559.633521

INT19′-c

C	2.65400200	-1.13976300	-1.90693100
H	2.81651800	-1.03283900	-2.98027400
C	3.55280100	-1.66379000	-1.11949900
C	3.81800800	-2.05197400	0.28304000
H	3.69658600	-3.13838300	0.37820000
H	4.86447000	-1.82615700	0.54454100
O	2.96483300	-1.49779700	1.30279300
C	3.38998800	-0.23941700	1.84447300
H	3.03267100	-0.24923300	2.88028400
H	4.48776000	-0.21202700	1.87556100
C	2.82585400	0.96349100	1.14249100
H	1.80186400	1.21152800	1.41498500
C	3.42637100	1.71288400	0.20706400
C	2.68363700	2.84416300	-0.45446300
H	3.25656400	3.78052900	-0.41567800
H	2.51837500	2.61440000	-1.51723900
H	1.70945500	3.01612300	0.01308200
C	4.80639400	1.46362200	-0.33778100
H	5.38431000	0.75622200	0.26115900
H	4.72497600	1.04252900	-1.34814000
H	5.37663700	2.39864200	-0.41070700
P	-1.18292000	0.01381400	-0.00278300
C	-2.47483600	-1.27005400	-0.15408600
C	-2.57138300	-1.96811700	-1.36687300
C	-3.36907000	-1.56116700	0.88505600
C	-3.56303800	-2.93176100	-1.54283000
H	-1.86009400	-1.76070000	-2.16175200
C	-4.35737700	-2.52966700	0.70579800
H	-3.28639300	-1.03810100	1.83255600
C	-4.45737700	-3.21292300	-0.50750300
H	-3.63059200	-3.47019000	-2.48365300
H	-5.04565200	-2.75346200	1.51593500
H	-5.22502700	-3.96944700	-0.64308600
C	-0.95033100	0.21800100	1.79897900
C	-1.64627400	1.17350300	2.55125800
C	-0.03394800	-0.63501200	2.43527000
C	-1.43730200	1.26660800	3.92817400
H	-2.34333500	1.84668500	2.06277800
C	0.16419000	-0.54102700	3.81181500
H	0.55120700	-1.34069200	1.85235700
C	-0.53624700	0.40807500	4.56016100
H	-1.97631000	2.01273700	4.50517900
H	0.87655200	-1.20321200	4.29526400
H	-0.37335300	0.48464700	5.63147900
C	-1.99126700	1.55180800	-0.56755700
C	-1.18367100	2.55811900	-1.11648600
C	-3.37301500	1.76034000	-0.45265100
C	-1.74790400	3.76693400	-1.52267500
H	-0.11882900	2.38276000	-1.23314300
C	-3.93408100	2.96938500	-0.86363300
H	-4.00697500	0.97615600	-0.05061000
C	-3.12259900	3.97455700	-1.39467300
H	-1.11534900	4.54131300	-1.94679200
H	-5.00550000	3.12458200	-0.77392500
H	-3.56295000	4.91396100	-1.71656100
Au	0.84871400	-0.53992500	-1.09921600

Zero-point correction= 0.457702 (Hartree/Particle)
Thermal correction to Energy= 0.487468
Thermal correction to Enthalpy= 0.488413
Thermal correction to Gibbs Free Energy= 0.391722
Sum of electronic and zero-point Energies= -1558.648738
Sum of electronic and thermal Energies= -1558.618971
Sum of electronic and thermal Enthalpies= -1558.618027
Sum of electronic and thermal Free Energies= -1558.714718
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1559.767038

INT19′′-c

C	2.54454900	-1.62407800	-2.11817900
H	2.30279100	-1.48168500	-3.15336400

C	2.99632000	-1.91902000	-1.01953300
C	3.57645500	-2.23076900	0.30786100
H	3.18143000	-3.18302300	0.67175700
H	4.66579300	-2.33218500	0.19805300
O	3.22839200	-1.25531500	1.27189700
C	3.74624400	0.05807000	0.99801900
H	4.27602600	0.38388200	1.90236700
H	4.47345800	0.02916000	0.18237200
C	2.62706500	1.03089800	0.73894700
H	1.91617100	1.13306200	1.55610800
C	2.58218200	1.98717900	-0.26144100
C	1.59348200	3.10930600	-0.16748100
H	2.12761000	4.01483800	0.15743500
H	1.15922600	3.35244900	-1.14241200
H	0.80046800	2.91489400	0.55781400
C	3.55238600	2.04587800	-1.40002900
H	4.10849100	1.12006800	-1.55295000
H	3.03756700	2.30849400	-2.33054100
H	4.27867800	2.85148000	-1.21726900
P	-1.17649500	0.06617100	0.17883700
C	-1.88626900	-1.53625700	0.58124700
C	-1.97432500	-2.49135100	-0.46273300
C	-2.32461300	-1.85892200	1.87789800
C	-2.50423900	-3.74868900	-0.20371200
H	-1.64783300	-2.23366100	-1.46642500
C	-2.85688300	-3.12067000	2.12223200
H	-2.27239700	-1.12651800	2.67526400
C	-2.94200600	-4.06576800	1.08804500
H	-2.58178400	-4.48004200	-1.00129100
H	-3.21788700	-3.37018400	3.11460500
H	-3.35824500	-5.04746900	1.29068500
C	-1.08958000	1.12674700	1.62254600
C	-1.77034700	2.35597900	1.64704500
C	-0.31151700	0.71677400	2.72518900
C	-1.67965300	3.16468100	2.77919000
H	-2.37006700	2.66842200	0.79873500
C	-0.23608800	1.53010100	3.85102400
H	0.21997900	-0.23148400	2.69970700
C	-0.91659300	2.75483500	3.87636200
H	-2.21119900	4.11021700	2.80851100
H	0.34974300	1.21487600	4.70843300
H	-0.85251400	3.38790900	4.75559400
C	-2.11804500	0.81193000	-1.15747300
C	-1.49682700	1.73462700	-2.02177300
C	-3.47983200	0.49141800	-1.31824200
C	-2.23777400	2.34324500	-3.02842500
H	-0.44312000	1.96544000	-1.90238700
C	-4.21189500	1.11071500	-2.32750600
H	-3.95981200	-0.22152700	-0.65652500
C	-3.59414100	2.03131900	-3.18135400
H	-1.76491100	3.05508600	-3.69704700
H	-5.26464400	0.87751800	-2.44876900
H	-4.17040700	2.50611300	-3.96901700
Au	0.95581400	-0.50614200	-0.62890500

Zero-point correction= 0.457499 (Hartree/Particle)
Thermal correction to Energy= 0.487982
Thermal correction to Enthalpy= 0.488926
Thermal correction to Gibbs Free Energy= 0.390896
Sum of electronic and zero-point Energies= -1558.110796
Sum of electronic and thermal Energies= -1558.080313
Sum of electronic and thermal Enthalpies= -1558.079369
Sum of electronic and thermal Free Energies= -1558.177400
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1559.349433

INT20-c

C	1.92967200	4.09782100	1.15206100
H	1.40542600	5.02499600	1.08517500
C	2.57111900	3.07625100	1.22011800
C	3.40278600	1.87153500	1.34164900
H	4.45265900	2.17129700	1.42121300
H	3.14506000	1.32802000	2.26405900
O	3.35009400	0.99207300	0.22280700
C	2.24019000	0.11261800	0.19207700
H	2.52324900	-0.67738400	-0.50814100
H	2.07737500	-0.34948000	1.17497600
C	0.99769800	0.82746600	-0.31075700
H	1.11466900	1.25175000	-1.30873800
C	-0.03661800	1.33203100	0.45860500
C	-0.97194000	2.36183800	-0.11624900
H	-2.01526700	2.14916900	0.13767900
H	-0.71593900	3.32982200	0.33508400
H	-0.87299900	2.45431000	-1.20060100
C	-0.19413000	1.07469400	1.93296400
H	0.39172500	0.22837500	2.29384400
H	0.13610100	1.97627300	2.46547000
H	-1.24549200	0.90960000	2.18892500
P	-1.86351000	-2.63047300	-1.39512600
C	-3.63395500	-2.23682500	-1.44151000
C	-4.03963100	-0.99219300	-1.94774900
C	-4.59062200	-3.17071600	-1.02151600
C	-5.39573300	-0.68923600	-2.04018200
H	-3.29589800	-0.26827400	-2.27138200
C	-5.94739500	-2.85771400	-1.11326800
H	-4.27866700	-4.13126100	-0.62493600
C	-6.34953900	-1.62142300	-1.62130600
H	-5.70923100	0.27271700	-2.43355900
H	-6.68876600	-3.57978200	-0.78572500
H	-7.40611900	-1.38142900	-1.68858900
C	-1.64393300	-4.03743800	-0.27218800
C	-1.58287100	-3.80220000	1.10999300
C	-1.58128100	-5.34785600	-0.76551600
C	-1.46865100	-4.87365200	1.99229800
H	-1.62739100	-2.78470100	1.49024700
C	-1.46230200	-6.41566900	0.12468200
H	-1.62192600	-5.53122300	-1.83419700
C	-1.40684800	-6.18018900	1.49943900
H	-1.42190800	-4.69134100	3.06137700
H	-1.41034500	-7.43045600	-0.25711400
H	-1.31127100	-7.01389500	2.18811200
C	-1.38038900	-3.17462500	-3.05588600
C	-0.01813400	-3.19966100	-3.39255600
C	-2.34123500	-3.60798300	-3.97962300
C	0.37912000	-3.66346600	-4.64408100
H	0.72572700	-2.85997400	-2.67616300

C	-1.93527500	-4.06775600	-5.23289600
H	-3.39529100	-3.58365400	-3.72331500
C	-0.57966300	-4.09626600	-5.56452400
H	1.43279000	-3.68191100	-4.90421500
H	-2.67904100	-4.40077100	-5.94996800
H	-0.26882900	-4.45163000	-6.54205000
Au	-0.61148300	-0.78371500	-0.71064600

Zero-point correction= 0.458326 (Hartree/Particle)
Thermal correction to Energy= 0.488772
Thermal correction to Enthalpy= 0.489716
Thermal correction to Gibbs Free Energy= 0.389236
Sum of electronic and zero-point Energies= -1558.480036
Sum of electronic and thermal Energies= -1558.449589
Sum of electronic and thermal Enthalpies= -1558.448645
Sum of electronic and thermal Free Energies= -1558.549126
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1559.631357

INT20´-c

C	6.69812500	1.19730600	-0.48785000
H	7.05359100	2.12987900	-0.86128600
C	6.24752100	0.15470100	-0.07549900
C	5.81942500	-1.15672000	0.43644700
H	6.70943700	-1.79304200	0.53344300
H	5.39664100	-1.03811500	1.44582200
O	4.92269800	-1.85508700	-0.40423900
C	3.52691900	-1.67161400	-0.11790000
H	3.03826000	-2.48162900	-0.66402100
H	3.35549300	-1.84098200	0.95569200
C	2.96495700	-0.33055300	-0.56903400
H	3.16183300	-0.20298800	-1.63821300
C	3.29302400	0.87566600	0.17774700
C	3.35673100	2.19632600	-0.52350200
H	2.50670500	2.84903100	-0.25625800
H	4.26880500	2.74544900	-0.24591800
H	3.35467200	2.07756300	-1.61189800
C	3.28869500	0.93188600	1.67613300
H	3.17173200	-0.05294700	2.13758800
H	4.21762900	1.37977600	2.06072500
H	2.46152400	1.56055700	2.05040300
P	-1.53906300	-0.01968100	-0.01569200
C	-1.80427600	1.17871100	1.33690300
C	-0.90370500	2.25089600	1.44445800
C	-2.84967600	1.05998500	2.26288400
C	-1.06032400	3.19981300	2.45289200
H	-0.07792800	2.33063300	0.74236000
C	-2.99863400	2.00937500	3.27466100
H	-3.54097300	0.22608900	2.19386600
C	-2.10764000	3.08015200	3.36967400
H	-0.35894900	4.02557700	2.52938500
H	-3.81029200	1.91092600	3.98998400
H	-2.22441200	3.81560600	4.16047300
C	-2.47925200	-1.50294000	0.47983800
C	-1.82850600	-2.45218100	1.28263500
C	-3.81309700	-1.71167000	0.10421600
C	-2.51140300	-3.58607200	1.71916600
H	-0.78718900	-2.29989700	1.55379300
C	-4.49073400	-2.85150400	0.53858000
H	-4.31667500	-0.98647700	-0.52712400
C	-3.84286700	-3.78690900	1.34767500
H	-2.00189900	-4.31711100	2.34017100
H	-5.52406600	-3.00939200	0.24298600
H	-4.37215400	-4.67448500	1.68237500
C	-2.44500200	0.66374300	-1.44328500
C	-2.10889500	0.18867900	-2.72053100
C	-3.45343100	1.62762300	-1.30657700
C	-2.78666400	0.66017900	-3.84335300
H	-1.31081700	-0.54119700	-2.82766500
C	-4.12495000	2.10061300	-2.43440200
H	-3.70815300	2.00739000	-0.32221200
C	-3.79529700	1.61623400	-3.70178900
H	-2.52099500	0.28914800	-4.82895100
H	-4.90441500	2.84901200	-2.32277800
H	-4.31824200	1.98805000	-4.57826800
Au	0.81061900	-0.37292200	-0.41197800

Zero-point correction= 0.454869 (Hartree/Particle)
Thermal correction to Energy= 0.485814
Thermal correction to Enthalpy= 0.486758
Thermal correction to Gibbs Free Energy= 0.383447
Sum of electronic and zero-point Energies= -1558.627146
Sum of electronic and thermal Energies= -1558.596200
Sum of electronic and thermal Enthalpies= -1558.595256
Sum of electronic and thermal Free Energies= -1558.698567
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1559.746761

INT20´´-c

C	1.89257400	3.99673700	0.75487500
H	1.38113000	4.92124200	0.59366200
C	2.52512700	2.97843300	0.93383500
C	3.36043100	1.79618200	1.16682800
H	4.41169600	2.10468600	1.17936400
H	3.13496200	1.35357100	2.14872100
O	3.26989900	0.81105100	0.14176400
C	2.15048900	-0.04537200	0.22837300
H	2.38965900	-0.89124200	-0.42041200
H	2.01473600	-0.42591100	1.24936700
C	0.90726700	0.66979100	-0.28300000
H	1.02542400	1.07320200	-1.28996400
C	-0.10684000	1.24338000	0.49496300
C	-1.03943200	2.25579000	-0.10877400
H	-2.08306300	2.04076800	0.14234100
H	-0.80360700	3.23193200	0.33419800
H	-0.92912300	2.33534900	-1.19268000
C	-0.23635800	1.04033200	1.97683000
H	0.32539300	0.18660700	2.35665900
H	0.14102400	1.94780600	2.46768100
H	-1.28645900	0.93776700	2.26712500
P	-1.97641500	-2.78124800	-1.40724200
C	-3.70104500	-2.28788200	-1.40996100
C	-4.05579800	-1.09654200	-2.08890300
C	-4.68118900	-3.05486600	-0.75050000
C	-5.38549500	-0.70091100	-2.12945000
H	-3.29253600	-0.50234100	-2.58371000
C	-6.00843900	-2.64392700	-0.79551300
H	-4.40908000	-3.96854400	-0.23385100

C	-6.36131100	-1.47010800	-1.47965300
H	-5.66779900	0.20375900	-2.65756700
H	-6.77481100	-3.23978100	-0.31080000
H	-7.40014500	-1.15675300	-1.50741900
C	-1.67584000	-4.13322400	-0.26787700
C	-1.85545700	-3.89489300	1.11653900
C	-1.26361600	-5.39905500	-0.72837600
C	-1.65147900	-4.92662100	2.02197800
H	-2.16014700	-2.91221400	1.46565800
C	-1.05858200	-6.42205600	0.19018800
H	-1.13022200	-5.58193800	-1.78881900
C	-1.24831300	-6.18815800	1.56122800
H	-1.79716100	-4.75579400	3.08337300
H	-0.76295700	-7.40708200	-0.15567300
H	-1.08348700	-6.99279600	2.27081200
C	-1.39619500	-3.17014700	-3.05918800
C	-0.00568800	-3.36552500	-3.25008600
C	-2.28740100	-3.26326000	-4.14605900
C	0.47608800	-3.67852600	-4.51312000
H	0.67790700	-3.27932100	-2.41006100
C	-1.79066600	-3.57438800	-5.40625400
H	-3.35170700	-3.11745400	-3.99869500
C	-0.41366700	-3.77817100	-5.59234100
H	1.53812400	-3.83847200	-4.66608500
H	-2.47079000	-3.67173600	-6.24604000
H	-0.03549400	-4.01727100	-6.58124800
Au	-0.70817300	-0.91842200	-0.66845900

Zero-point correction= 0.456683 (Hartree/Particle)
Thermal correction to Energy= 0.487463
Thermal correction to Enthalpy= 0.488407
Thermal correction to Gibbs Free Energy= 0.387014
Sum of electronic and zero-point Energies= -1558.094739
Sum of electronic and thermal Energies= -1558.063959
Sum of electronic and thermal Enthalpies= -1558.063015
Sum of electronic and thermal Free Energies= -1558.164408
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1559.326931

TS1-c

C	-0.33933500	-1.53075200	-1.36407600
H	-0.18254400	-1.29481600	-2.39922300
C	-1.09290800	-1.85302300	-0.43386700
C	-1.46633000	-2.25631400	0.92996500
H	-1.65472600	-3.33491300	0.95022400
H	-0.58439000	-2.07036400	1.57007500
O	-2.61994400	-1.65015700	1.47235300
C	-2.61018700	-0.21452900	1.44642300
H	-3.21137100	0.07932100	2.31538100
H	-1.59192300	0.16328200	1.60355600
C	-3.23422100	0.30428400	0.18392700
H	-4.21812000	-0.12047400	-0.01351800
C	-2.73398400	1.18611400	-0.69293700
C	-3.51670300	1.57088800	-1.92276700
H	-3.69256600	2.65473600	-1.95778500
H	-2.95552300	1.31735900	-2.83319000
H	-4.48549100	1.06487000	-1.96718700
C	-1.38633900	1.84505300	-0.58046100
H	-0.83091300	1.56464000	0.31428700
H	-0.76565700	1.58648800	-1.44831600
H	-1.48804400	2.93846500	-0.58500700
S	1.85678900	-1.37975600	-0.58527700
O	1.97559600	-2.32132000	0.55424600
O	2.79276400	-1.41705300	-1.73745300
C	1.91602400	0.28327700	0.10560900
C	2.21110900	1.35487300	-0.73552000
C	1.58173500	0.46981500	1.44679400
C	2.17536600	2.64744300	-0.21349200
H	2.47940800	1.17075300	-1.77026000
C	1.55091300	1.76758700	1.95663900
H	1.37697200	-0.38998300	2.07496400
C	1.84172900	2.85343800	1.12713700
H	2.41115900	3.49325600	-0.85237900
H	1.30455800	1.93036500	3.00173100
H	1.81200800	3.86242400	1.52766500

Zero-point correction= 0.279538 (Hartree/Particle)
Thermal correction to Energy= 0.298957
Thermal correction to Enthalpy= 0.299901
Thermal correction to Gibbs Free Energy= 0.228865
Sum of electronic and zero-point Energies= -1167.170298
Sum of electronic and thermal Energies= -1167.150879
Sum of electronic and thermal Enthalpies= -1167.149935
Sum of electronic and thermal Free Energies= -1167.220970
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.708333

INT1-c

C	-0.27478100	-1.32600500	-1.18218800
H	-0.17602400	-1.05675400	-2.23059100
C	-1.38398200	-1.35654200	-0.48977900
C	-1.91232300	-1.64179100	0.86211100
H	-1.88512700	-2.72228700	1.03432600
H	-1.25101300	-1.17431200	1.61323800
O	-3.25528200	-1.23836800	1.05927000
C	-3.41259100	0.18409300	1.05083900
H	-4.45432400	0.34375800	1.34843500
H	-2.77065400	0.63232000	1.82227600
C	-3.15748100	0.77489400	-0.30559500
H	-3.83429200	0.41585800	-1.07997100
C	-2.19476200	1.64529600	-0.65827400
C	-2.04761600	2.08039800	-2.09212300
H	-2.06276500	3.17487000	-2.18066800
H	-1.07690800	1.74846800	-2.48761600
H	-2.83600800	1.67071600	-2.72983700
C	-1.15663700	2.21577500	0.26965100
H	-1.21604900	1.82790700	1.28779000
H	-0.15229400	1.99931100	-0.11326400
H	-1.24405100	3.30951100	0.31883900
S	1.31170800	-1.72039300	-0.40126700
O	1.03662800	-2.49832500	0.81941500
O	2.21324200	-2.21493400	-1.45297900
C	1.90288600	-0.10654100	0.12230200
C	2.45937300	0.75337600	-0.82576700
C	1.75077900	0.27252000	1.45520100
C	2.85604100	2.02891200	-0.42735100
H	2.59101700	0.41778600	-1.84916100
C	2.15806700	1.54872900	1.84363500

H	1.33517800	-0.43306600	2.16600800
C	2.70150300	2.42656300	0.90365800
H	3.29249200	2.70957400	-1.15220200
H	2.05281900	1.85657000	2.87967900
H	3.01310400	3.42100400	1.20944500

Zero-point correction= 0.282511 (Hartree/Particle)
Thermal correction to Energy= 0.301317
Thermal correction to Enthalpy= 0.302262
Thermal correction to Gibbs Free Energy= 0.232745
Sum of electronic and zero-point Energies= -1167.184817
Sum of electronic and thermal Energies= -1167.166011
Sum of electronic and thermal Enthalpies= -1167.165066
Sum of electronic and thermal Free Energies= -1167.234583
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.721434

TS2-c

C	0.08565500	-0.87201300	-1.84970600
H	0.83046000	-0.46093400	-2.49607000
C	-0.53872800	-1.18028000	-0.81720600
C	-1.74048000	-1.87838800	-0.24681100
H	-1.47660100	-2.93148300	-0.10015200
H	-1.98214800	-1.45652400	0.73774300
O	-2.84927700	-1.84042100	-1.11262900
C	-3.72372200	-0.71687100	-0.88498600
H	-4.48964500	-0.82484100	-1.65980200
H	-4.21225200	-0.83808800	0.09022500
C	-3.02297500	0.60205200	-0.99515100
H	-2.60699700	0.80960800	-1.97978900
C	-2.79270300	1.48451500	-0.01047500
C	-1.97389700	2.72242200	-0.27143400
H	-2.54373200	3.63379000	-0.04497600
H	-1.09423800	2.72450100	0.38508800
H	-1.63593600	2.77712700	-1.31093900
C	-3.26137200	1.34738600	1.41483900
H	-3.89936900	0.47767200	1.58507300
H	-2.39193200	1.26933800	2.07775000
H	-3.82455500	2.23983600	1.71829000
S	0.60340300	-0.57973800	1.04396500
O	-0.04505700	0.59323800	1.68564700
O	0.88124700	-1.80773300	1.82889600
C	2.15258300	-0.01010900	0.33543900
C	3.19836700	-0.91836900	0.18191100
C	2.23531900	1.30118300	-0.13204200
C	4.36854900	-0.49062900	-0.44477300
H	3.09172400	-1.92958800	0.55866500
C	3.40924700	1.71368500	-0.76104100
H	1.40033100	1.97901500	0.00704800
C	4.47173400	0.81976100	-0.91699700
H	5.19907700	-1.17997500	-0.56383300
H	3.49664700	2.73316500	-1.12480000
H	5.38395500	1.14643300	-1.40768400

Zero-point correction= 0.279742 (Hartree/Particle)
Thermal correction to Energy= 0.299080
Thermal correction to Enthalpy= 0.300024
Thermal correction to Gibbs Free Energy= 0.227986
Sum of electronic and zero-point Energies= -1167.167566
Sum of electronic and thermal Energies= -1167.148227
Sum of electronic and thermal Enthalpies= -1167.147283
Sum of electronic and thermal Free Energies= -1167.219321
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.703809

INT2-c

C	0.03899400	-0.88323100	-1.74635700
H	0.89270300	-0.42133200	-2.21582300
C	-0.42502200	-1.14917100	-0.55767100
C	-1.72814900	-1.85999600	-0.20602700
H	-1.51014500	-2.92694300	-0.08873800
H	-2.09280400	-1.48694600	0.76075100
O	-2.70208200	-1.74091800	-1.21333300
C	-3.59021400	-0.62124000	-1.03433500
H	-4.26912100	-0.68900700	-1.89052300
H	-4.18198600	-0.77831700	-0.12336600
C	-2.88060600	0.69815300	-1.01392200
H	-2.38776100	0.95841300	-1.94968400
C	-2.72571200	1.52221300	0.03339900
C	-1.88791900	2.76849100	-0.09284600
H	-2.47219500	3.66932000	0.13897800
H	-1.06207800	2.72984500	0.62937400
H	-1.46982100	2.87986200	-1.09832800
C	-3.29717400	1.30401500	1.41004200
H	-3.95893600	0.43805300	1.47734600
H	-2.47765400	1.16321200	2.12447500
H	-3.86534600	2.18620200	1.73327700
S	0.55590200	-0.72093300	0.92997300
O	-0.14494600	0.36017200	1.64790500
O	0.86315700	-1.98487600	1.62170500
C	2.07689000	-0.04504000	0.27159600
C	3.16807300	-0.89354000	0.08958700
C	2.12776600	1.30849400	-0.06403500
C	4.34148500	-0.36851800	-0.45073100
H	3.09042100	-1.93606000	0.37794200
C	3.30531700	1.81912700	-0.60743500
H	1.26274100	1.94011700	0.10548800
C	4.40726600	0.98190700	-0.80102900
H	5.20389200	-1.01202800	-0.59561000
H	3.36560500	2.87001900	-0.87381600
H	5.32306100	1.38552400	-1.22295200

Zero-point correction= 0.282634 (Hartree/Particle)
Thermal correction to Energy= 0.301402
Thermal correction to Enthalpy= 0.302346
Thermal correction to Gibbs Free Energy= 0.233501
Sum of electronic and zero-point Energies= -1167.176009
Sum of electronic and thermal Energies= -1167.157241
Sum of electronic and thermal Enthalpies= -1167.156297
Sum of electronic and thermal Free Energies= -1167.225142
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.710665

TS3-c

C	-4.01676700	2.38621600	0.33636500
H	-3.84539100	3.31373100	0.83378800
C	-4.21587000	1.32540800	-0.20736700
C	-4.51773400	0.06646300	-0.90758600
H	-5.60404400	-0.03755000	-1.00308600
H	-4.09974500	0.11286900	-1.92705900

O	-4.08082200	-1.10900300	-0.24929000
C	-2.66142300	-1.30030900	-0.30590100
H	-2.50579100	-2.33957200	0.00477200
H	-2.31117600	-1.21059400	-1.34128800
C	-1.93360800	-0.37864500	0.61911300
H	-2.20553600	-0.46681500	1.66824600
C	-0.87075000	0.46851300	0.28768400
C	-0.44029300	1.47280400	1.33563100
H	0.56783900	1.85231800	1.14090800
H	-1.13015800	2.32670500	1.31085600
H	-0.46359800	1.03684400	2.33774200
C	-0.65212000	0.91083900	-1.14588400
H	-0.72019100	0.08337700	-1.85462500
H	-1.41593000	1.65562600	-1.40306600
H	0.32879300	1.38003400	-1.26465000
S	0.83438400	-1.08349700	0.46844400
O	0.93027400	-1.45480800	1.90135700
O	0.53847700	-2.10483800	-0.56896700
C	2.38650100	-0.28887000	0.01419600
C	2.77841400	-0.27573100	-1.32541900
C	3.11848300	0.37621100	0.99952900
C	3.93932500	0.40996200	-1.67985900
H	2.19068900	-0.81484200	-2.06028000
C	4.27702900	1.05874200	0.63126100
H	2.79067900	0.33093100	2.03239700
C	4.68420100	1.07848800	-0.70501700
H	4.26577000	0.41837500	-2.71568300
H	4.86520800	1.57011900	1.38761200
H	5.58665900	1.61304200	-0.98696900

Zero-point correction= 0.279633 (Hartree/Particle)
Thermal correction to Energy= 0.298866
Thermal correction to Enthalpy= 0.299810
Thermal correction to Gibbs Free Energy= 0.229462
Sum of electronic and zero-point Energies= -1167.169816
Sum of electronic and thermal Energies= -1167.150583
Sum of electronic and thermal Enthalpies= -1167.149639
Sum of electronic and thermal Free Energies= -1167.219987
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.70994

INT3-c

C	-3.87831600	2.44484800	0.28327800
H	-3.69501400	3.38061400	0.76065800
C	-4.09117300	1.37515700	-0.23783200
C	-4.41342200	0.10676000	-0.91226200
H	-5.49848300	0.04240400	-1.04900700
H	-3.95404500	0.10599900	-1.91486700
O	-4.04832900	-1.06061300	-0.20044100
C	-2.63725500	-1.32007000	-0.21624500
H	-2.54445100	-2.34739100	0.15721900
H	-2.26474500	-1.31727900	-1.24814300
C	-1.87715400	-0.38031600	0.65681700
H	-2.19669100	-0.31919900	1.69268200
C	-0.62602900	0.32708300	0.28448300
C	-0.29731900	1.43524300	1.28715600
H	0.65561000	1.91854200	1.05168400
H	-1.08865400	2.19001500	1.23826000
H	-0.25186800	1.03934900	2.30485500
C	-0.59363500	0.84652100	-1.15761000
H	-0.70557400	0.04043800	-1.88515600
H	-1.41421400	1.55882200	-1.28720600
H	0.34834800	1.36428900	-1.36068700
S	0.71215500	-1.01869700	0.44177000
O	0.78477200	-1.39571700	1.86610500
O	0.41388900	-2.02918500	-0.59446300
C	2.27703400	-0.24997900	0.00678700
C	2.69994800	-0.26781800	-1.32316800
C	3.03786900	0.35585200	1.00798200
C	3.90548700	0.34816600	-1.65603400
H	2.09881500	-0.77582100	-2.06898600
C	4.24143800	0.96907300	0.66278100
H	2.69486200	0.32094700	2.03605800
C	4.67097400	0.96920100	-0.66631100
H	4.25097200	0.33690400	-2.68548200
H	4.84738600	1.43917500	1.43158800
H	5.60991900	1.44712300	-0.93033100

Zero-point correction= 0.281486 (Hartree/Particle)
Thermal correction to Energy= 0.300449
Thermal correction to Enthalpy= 0.301394
Thermal correction to Gibbs Free Energy= 0.232909
Sum of electronic and zero-point Energies= -1167.175012
Sum of electronic and thermal Energies= -1167.156048
Sum of electronic and thermal Enthalpies= -1167.155104
Sum of electronic and thermal Free Energies= -1167.223588
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.70994

TS7-c

C	3.57642600	2.42937700	-0.00596400
H	3.29043100	3.42213500	-0.27312900
C	3.66060100	1.21512100	0.18862900
C	4.40432900	0.02731300	0.69925000
H	5.47676300	0.16433500	0.53593700
H	4.22634600	-0.04979700	1.78613800
O	4.03913200	-1.16743500	0.04820500
C	2.61924200	-1.31163000	0.09650500
H	2.39022900	-2.21699000	-0.47507100
H	2.28677400	-1.47714000	1.12975100
C	1.97394200	-0.09941200	-0.51132400
H	2.17673500	0.03334000	-1.57122000
C	0.66194100	0.45008400	-0.04700200
C	0.28294100	1.71630300	-0.81710100
H	-0.70688600	2.07972000	-0.52642500
H	1.01500400	2.49468000	-0.58558300
H	0.29259000	1.53695400	-1.89522400
C	0.55907600	0.65829800	1.46636600
H	0.71679400	-0.27013800	2.01829100
H	1.32138600	1.38276700	1.76762500
H	-0.42258500	1.05763200	1.73768200
S	-0.59569000	-0.89842400	-0.52806900
O	-0.55372100	-1.02017700	-1.99814500
O	-0.32705000	-2.06803100	0.33389600
C	-2.22034600	-0.27152000	-0.08305200
C	-2.72063000	-0.52320900	1.19539000
C	-2.95083400	0.45482700	-1.02468400
C	-3.97469400	-0.02080100	1.53969400

H	-2.14026600	-1.12044900	1.88976100
C	-4.20384900	0.95183200	-0.66868600
H	-2.54484000	0.60229000	-2.01926300
C	-4.71133300	0.71888800	0.61161900
H	-4.38003300	-0.21332100	2.52854800
H	-4.78682200	1.51370400	-1.39231800
H	-5.68834500	1.10735500	0.88411400

Zero-point correction= 0.281480 (Hartree/Particle)
Thermal correction to Energy= 0.299436
Thermal correction to Enthalpy= 0.300381
Thermal correction to Gibbs Free Energy= 0.234819
Sum of electronic and zero-point Energies= -1167.167781
Sum of electronic and thermal Energies= -1167.149825
Sum of electronic and thermal Enthalpies= -1167.148881
Sum of electronic and thermal Free Energies= -1167.214443
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.704567

TS4-c

C	-4.31864200	-1.42559200	-0.85865600
H	-4.64385800	-1.90821800	-1.75212200
C	-3.94533300	-0.86366800	0.14312200
C	-3.56834000	-0.19037000	1.39423400
H	-4.47625100	-0.00490900	1.97977100
H	-2.92312900	-0.85128500	1.99319700
O	-2.95897300	1.07949600	1.22228600
C	-1.54456700	1.06532800	1.05257300
H	-1.23528600	2.10395200	1.18545200
H	-1.07192500	0.46960000	1.84611800
C	-1.12689500	0.58227800	-0.32431700
H	-1.56372600	1.18543000	-1.12129500
C	-0.92304200	-0.76870500	-0.65331000
C	-0.94322400	-1.19170700	-2.08962200
H	-0.02713200	-1.73713900	-2.35383000
H	-1.78359000	-1.87838400	-2.26884000
H	-1.04131900	-0.33949000	-2.76665300
C	-0.60574400	-1.84088500	0.34497700
H	-0.48410700	-1.46714100	1.36309400
H	-1.40758800	-2.59353900	0.34969400
H	0.32067400	-2.36242900	0.07231900
S	0.87810600	1.58637300	-0.55737600
O	1.09919300	1.74884200	-2.01469000
O	1.01457000	2.73700300	0.37519000
C	2.00510700	0.30133000	0.01040100
C	2.25128200	0.17705600	1.37710600
C	2.51240800	-0.61036200	-0.91352100
C	3.02433600	-0.89250600	1.82694900
H	1.85418400	0.91655200	2.06466100
C	3.28562800	-1.67604600	-0.45220900
H	2.30835200	-0.46968200	-1.96930700
C	3.53450400	-1.81992000	0.91476500
H	3.23267400	-1.00040400	2.88733900
H	3.69573200	-2.39158000	-1.15896300
H	4.13341400	-2.65341600	1.27014700

Zero-point correction= 0.279935 (Hartree/Particle)
Thermal correction to Energy= 0.299194
Thermal correction to Enthalpy= 0.300139
Thermal correction to Gibbs Free Energy= 0.230242
Sum of electronic and zero-point Energies= -1167.173310
Sum of electronic and thermal Energies= -1167.154051
Sum of electronic and thermal Enthalpies= -1167.153106
Sum of electronic and thermal Free Energies= -1167.223003
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.713765

INT7-c

C	3.40327300	2.30804500	0.06116400
H	2.92466200	3.19597400	-0.32384000
C	3.22384300	1.01430500	0.13285400
C	4.24614200	0.03071900	0.69780200
H	5.28027500	0.34448500	0.54407100
H	4.07460200	-0.11761000	1.77905300
O	4.01682100	-1.16638100	-0.02054900
C	2.60347600	-1.29080800	-0.12048300
H	2.37822300	-1.99925600	-0.91753900
H	2.18867000	-1.68415000	0.81526900
C	2.07282300	0.14180500	-0.41821500
H	2.02150100	0.28078400	-1.50214000
C	0.67432200	0.49257100	0.15818900
C	0.21345700	1.87460600	-0.31367100
H	-0.81297700	2.07975700	0.00155000
H	0.85508500	2.63327700	0.14020900
H	0.27381600	1.96504700	-1.40151900
C	0.59310600	0.38554900	1.68192900
H	0.79474600	-0.62662000	2.03627500
H	1.33090800	1.06595400	2.11906200
H	-0.39648500	0.68502100	2.03974400
S	-0.48294500	-0.76666900	-0.60094600
O	-0.36643500	-0.62476400	-2.06550200
O	-0.24035400	-2.06823600	0.05157900
C	-2.14338300	-0.25536600	-0.13753400
C	-2.68026500	-0.70839500	1.06824900
C	-2.87395300	0.55731500	-1.00495400
C	-3.97089300	-0.31584800	1.42094300
H	-2.10063300	-1.37346200	1.69847900
C	-4.16444400	0.94087300	-0.64274700
H	-2.43641700	0.86129900	-1.94938000
C	-4.70811900	0.51017900	0.56965300
H	-4.40387400	-0.66252300	2.35440600
H	-4.74747300	1.56932200	-1.30920100
H	-5.71407200	0.81114400	0.84735400

Zero-point correction= 0.285765 (Hartree/Particle)
Thermal correction to Energy= 0.303005
Thermal correction to Enthalpy= 0.303949
Thermal correction to Gibbs Free Energy= 0.239946
Sum of electronic and zero-point Energies= -1167.201560
Sum of electronic and thermal Energies= -1167.184320
Sum of electronic and thermal Enthalpies= -1167.183376
Sum of electronic and thermal Free Energies= -1167.247379
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.73833

INT4-c

C	4.46424600	-0.83814000	0.87776900
H	4.97444500	-0.79994600	1.81320500
C	3.86112100	-0.86749300	-0.16797100
C	3.20212300	-0.91818000	-1.47896300

H	3.96247400	-1.08947100	-2.25013800
H	2.50207800	-1.76602000	-1.51555900
O	2.54536100	0.28732600	-1.84502300
C	1.17419500	0.38557200	-1.49780400
H	0.78985600	1.21246000	-2.09803800
H	0.63855100	-0.53004400	-1.78425100
C	0.95000300	0.71162400	-0.01280400
H	1.60714600	1.55023900	0.24774700
C	1.07270600	-0.37326400	0.98117100
C	1.51186300	-0.04152600	2.37034200
H	0.64981900	0.16772900	3.02296200
H	2.06643500	-0.87757000	2.81413500
H	2.14979800	0.84751100	2.39279100
C	0.61911500	-1.77617100	0.71910300
H	0.11270800	-1.90155800	-0.24106800
H	1.47591000	-2.46792400	0.74733700
H	-0.07827200	-2.11679700	1.49690200
S	-0.73229800	1.58325900	0.16681400
O	-0.81845700	2.04621000	1.56416500
O	-0.90137300	2.52521300	-0.95808500
C	-1.93223900	0.26198400	-0.03607100
C	-2.31177200	-0.12092000	-1.32270400
C	-2.42929600	-0.38034600	1.09667000
C	-3.19371300	-1.19039300	-1.47440300
H	-1.93583300	0.42474400	-2.18152200
C	-3.31409800	-1.44554100	0.93334300
H	-2.12840400	-0.03569500	2.07977200
C	-3.68821300	-1.85381400	-0.34882900
H	-3.50184900	-1.49947900	-2.46873400
H	-3.71331000	-1.95466800	1.80552700
H	-4.37529000	-2.68599600	-0.47163500

Zero-point correction= 0.281433 (Hartree/Particle)
Thermal correction to Energy= 0.300704
Thermal correction to Enthalpy= 0.301649
Thermal correction to Gibbs Free Energy= 0.232138
Sum of electronic and zero-point Energies= -1167.176313
Sum of electronic and thermal Energies= -1167.157042
Sum of electronic and thermal Enthalpies= -1167.156097
Sum of electronic and thermal Free Energies= -1167.225609
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.716473

TS8-c

C	4.30364000	-0.17792800	1.17999800
H	4.79424600	0.48045700	1.86388400
C	3.39913900	-0.69192700	0.51054700
C	3.00210900	-1.75605800	-0.44883200
H	3.89940400	-2.28466300	-0.78209700
H	2.34151000	-2.48324700	0.04877000
O	2.38705500	-1.26320100	-1.62673100
C	1.06155300	-0.81081500	-1.43568700
H	0.67660900	-0.58496300	-2.43117800
H	0.44598400	-1.60639700	-0.99090700
C	1.01641700	0.46060600	-0.57501900
H	1.65667200	1.20950400	-1.05762300
C	1.42010100	0.30727100	0.85744300
C	1.82981400	1.56181200	1.57751100
H	0.94916500	2.16709800	1.82657100
H	2.35380700	1.31696100	2.50737100
H	2.48842800	2.18188600	0.96158600
C	0.75100400	-0.72768300	1.72734600
H	0.39323800	-1.60007900	1.17451700
H	1.44640300	-1.07285000	2.50060900
H	-0.11838700	-0.30067800	2.24599700
S	-0.65351900	1.29955000	-0.83596700
O	-0.66842000	2.52993300	-0.02375700
O	-0.87113400	1.35268600	-2.29466900
C	-1.89323100	0.19394800	-0.14715000
C	-2.32527800	-0.90176900	-0.89526100
C	-2.41344800	0.46665700	1.11722000
C	-3.27493700	-1.76175500	-0.34483700
H	-1.94161800	-1.05937700	-1.89721600
C	-3.36859300	-0.39512900	1.65451600
H	-2.07700500	1.34778700	1.65238600
C	-3.79041500	-1.51143600	0.92889200
H	-3.62082600	-2.61891400	-0.91462900
H	-3.78612500	-0.19332300	2.63637900
H	-4.53245500	-2.18209800	1.35218900

Zero-point correction= 0.282254 (Hartree/Particle)
Thermal correction to Energy= 0.300032
Thermal correction to Enthalpy= 0.300976
Thermal correction to Gibbs Free Energy= 0.235681
Sum of electronic and zero-point Energies= -1167.164485
Sum of electronic and thermal Energies= -1167.146707
Sum of electronic and thermal Enthalpies= -1167.145763
Sum of electronic and thermal Free Energies= -1167.211058
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.70234

INT8-c

C	4.24152500	-0.19831400	0.88780400
H	4.79270400	0.67916900	1.19460900
C	3.01080000	-0.54789800	0.59630900
C	2.70262600	-1.97195200	0.17403400
H	3.62011900	-2.55248700	0.07226700
H	2.05607800	-2.46673600	0.91901500
O	2.06324000	-1.99086300	-1.09661100
C	0.83363900	-1.29930200	-1.05487800
H	0.39397400	-1.38446500	-2.05000100
H	0.15749100	-1.77217300	-0.32682500
C	1.04741000	0.18701400	-0.70859200
H	1.65201400	0.62282700	-1.51305700
C	1.79593100	0.41722900	0.63763800
C	2.27880900	1.86986400	0.76074900
H	1.43517100	2.55923500	0.76536700
H	2.84190400	1.99694900	1.69124900
H	2.93588800	2.13449200	-0.07445200
C	0.93799700	0.06341100	1.86963700
H	0.46349900	-0.91902400	1.79427600
H	1.56948900	0.06573500	2.76313700
H	0.15103900	0.80690400	2.01222200
S	-0.54440500	1.09129300	-0.99814100
O	-0.47505200	2.43318600	-0.39336800
O	-0.79132900	0.92808200	-2.44221100
C	-1.85781100	0.20384200	-0.14252200
C	-2.42270500	-0.92565400	-0.73765200

C	-2.34273800	0.70873500	1.06345500
C	-3.45997400	-1.58802100	-0.08292500
H	-2.07114200	-1.26097100	-1.70662100
C	-3.38451600	0.04246300	1.70695700
H	-1.92092300	1.62133000	1.46860500
C	-3.93418200	-1.10919800	1.14027400
H	-3.90570400	-2.46919400	-0.53427200
H	-3.77200800	0.42747600	2.64533000
H	-4.74485700	-1.62631100	1.64520000

Zero-point correction= 0.286723 (Hartree/Particle)
Thermal correction to Energy= 0.303590
Thermal correction to Enthalpy= 0.304534
Thermal correction to Gibbs Free Energy= 0.241209
Sum of electronic and zero-point Energies= -1167.197831
Sum of electronic and thermal Energies= -1167.180964
Sum of electronic and thermal Enthalpies= -1167.180020
Sum of electronic and thermal Free Energies= -1167.243344
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.735632

TS5-c

C	-0.36518600	1.13364400	1.10041500
H	-0.30780400	0.71637500	2.10242900
C	-1.42574200	1.11816100	0.32615200
C	-1.82000000	1.52880300	-1.04005500
H	-1.73018700	2.61151600	-1.15878900
H	-1.15268500	1.05344200	-1.78132400
O	-3.17381400	1.18654400	-1.30107800
C	-3.38134500	-0.19689300	-1.04384700
H	-4.45279700	-0.36197900	-1.19725300
H	-2.83662100	-0.80332800	-1.78185500
C	-2.99896600	-0.57715400	0.36743900
H	-3.61013700	-0.11003100	1.13772200
C	-2.18823400	-1.60929300	0.74245000
C	-2.01988300	-1.94334400	2.19752900
H	-2.19550100	-3.01165900	2.38281400
H	-0.98665200	-1.74044100	2.51645500
H	-2.69518900	-1.36635200	2.83554700
C	-1.27984900	-2.36654200	-0.18448700
H	-1.39594500	-2.09411700	-1.23451200
H	-0.23211400	-2.18262400	0.09208500
H	-1.44305900	-3.44853600	-0.09248000
S	1.23242500	1.70356100	0.49368600
O	1.00756400	2.57567700	-0.67263500
O	2.03997600	2.13808500	1.64408600
C	1.91904100	0.15675000	-0.11646300
C	2.50826600	-0.72688700	0.78864100
C	1.76472000	-0.17100900	-1.46333300
C	2.93722600	-1.97291100	0.33299700
H	2.63583900	-0.43052300	1.82459300
C	2.20011500	-1.41879100	-1.90848900
H	1.32581000	0.55241800	-2.14166200
C	2.77694500	-2.32036800	-1.01111000
H	3.40151400	-2.67013500	1.02419600
H	2.09293200	-1.68586000	-2.95569700
H	3.11134300	-3.29259200	-1.36126300

Zero-point correction= 0.281974 (Hartree/Particle)
Thermal correction to Energy= 0.300063
Thermal correction to Enthalpy= 0.301007
Thermal correction to Gibbs Free Energy= 0.233319
Sum of electronic and zero-point Energies= -1167.183270
Sum of electronic and thermal Energies= -1167.165181
Sum of electronic and thermal Enthalpies= -1167.164236
Sum of electronic and thermal Free Energies= -1167.231925
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.719489

INT5-c

C	0.48868000	-0.41618000	0.85822900
H	0.41051500	0.40035500	1.56995300
C	1.58693500	-0.62800500	0.13153700
C	1.86628400	-1.69205700	-0.91270500
H	1.73590700	-2.70994900	-0.54419100
H	1.19543700	-1.56269400	-1.77628300
O	3.22968500	-1.50820000	-1.28620300
C	3.52145800	-0.13079700	-1.12610300
H	4.60601400	-0.01064600	-1.08858900
H	3.12587500	0.46188700	-1.96700900
C	2.81884600	0.27516500	0.19680000
H	3.44773000	-0.08686200	1.02140600
C	2.54698900	1.73674000	0.36419000
C	3.06784200	2.47542700	1.55422300
H	3.34098600	3.50845400	1.29890400
H	2.31355900	2.55139700	2.35888400
H	3.94694300	1.98678900	1.98892300
C	1.53764400	2.41224800	-0.51159500
H	1.34843400	1.85607100	-1.43574300
H	0.56128900	2.52221500	-0.00921900
H	1.86135000	3.42622900	-0.78234100
S	-0.98829200	-1.39054200	0.75875900
O	-0.77965200	-2.46461900	-0.22883900
O	-1.43176800	-1.68725700	2.12964400
C	-2.14819600	-0.21575200	0.05343500
C	-2.91650800	0.57670200	0.90593600
C	-2.22957100	-0.09280600	-1.33428900
C	-3.78116100	1.52013500	0.35131400
H	-2.84403300	0.43553200	1.97898600
C	-3.09745100	0.85286000	-1.87675900
H	-1.63440900	-0.74249700	-1.96699500
C	-3.86793800	1.65970100	-1.03536600
H	-4.39087700	2.14106500	1.00088400
H	-3.17789700	0.95660200	-2.95473500
H	-4.54339300	2.39504800	-1.46288000

Zero-point correction= 0.284059 (Hartree/Particle)
Thermal correction to Energy= 0.302292
Thermal correction to Enthalpy= 0.303236
Thermal correction to Gibbs Free Energy= 0.233595
Sum of electronic and zero-point Energies= -1167.227990
Sum of electronic and thermal Energies= -1167.209756
Sum of electronic and thermal Enthalpies= -1167.208812
Sum of electronic and thermal Free Energies= -1167.278454
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.763581

TS6-c

C	-1.36804600	-1.26474300	-0.89786500
H	-1.45556600	-1.03335400	-1.95002800

C	-0.34804400	-1.48036100	-0.10636300
C	-0.39048100	-1.73232500	1.38821900
H	-0.09647100	-2.76628000	1.59202200
H	0.34501300	-1.07819400	1.88594800
O	-1.66825300	-1.55492800	1.95259600
C	-2.18388800	-0.23125400	1.82037600
H	-2.81324000	-0.07815100	2.70643900
H	-1.36711300	0.50059200	1.86789300
C	-3.02793400	-0.06069200	0.58488200
H	-3.76439500	-0.84993000	0.44677600
C	-3.07876300	1.01690300	-0.22984600
C	-4.07827200	1.07874300	-1.35355000
H	-4.70268100	1.97941100	-1.27678000
H	-3.56843300	1.13759800	-2.32573300
H	-4.73675600	0.20560800	-1.36450800
C	-2.14257900	2.19269100	-0.14465600
H	-1.72989900	2.41947800	-1.13657800
H	-2.67723100	3.09518500	0.18285200
H	-1.30293900	2.03298800	0.53441500
S	1.32441300	-1.39809500	-0.81456700
O	2.15005700	-2.41120800	-0.13318200
O	1.21125800	-1.35260500	-2.27998600
C	1.87476400	0.21867700	-0.25367000
C	1.43629600	1.35434000	-0.93611800
C	2.68383700	0.31060300	0.87771500
C	1.81337700	2.61034500	-0.46611300
H	0.82127100	1.24557400	-1.82286500
C	3.05797900	1.57409600	1.33759200
H	3.01906200	-0.59633300	1.36914700
C	2.61958000	2.71932300	0.67087600
H	1.48360800	3.50375900	-0.98801200
H	3.69306900	1.66267100	2.21392700
H	2.91062800	3.70074900	1.03385200

Zero-point correction= 0.282077 (Hartree/Particle)
Thermal correction to Energy= 0.300187
Thermal correction to Enthalpy= 0.301132
Thermal correction to Gibbs Free Energy= 0.233590
Sum of electronic and zero-point Energies= -1167.176081
Sum of electronic and thermal Energies= -1167.157971
Sum of electronic and thermal Enthalpies= -1167.157027
Sum of electronic and thermal Free Energies= -1167.224568
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.71193

INT6-c

C	0.95299000	0.04272400	0.51935600
H	0.22200900	0.81066000	0.75374000
C	0.56840600	-1.17445100	0.13209300
C	1.54975700	-2.28566700	-0.16835300
H	1.24628800	-3.20376600	0.34427400
H	1.55862200	-2.49050700	-1.25045800
O	2.84510500	-1.96597800	0.30157100
C	3.25194700	-0.66811100	-0.10447400
H	4.30660300	-0.57442100	0.16343800
H	3.16069500	-0.56449400	-1.19716400
C	2.41504100	0.42983800	0.59081100
H	2.71011500	0.45978700	1.64928800
C	2.66013800	1.78252600	-0.02692300
C	3.29942100	2.86948700	0.77405600
H	3.85499200	3.56816200	0.13509700
H	2.55397700	3.47748300	1.31967900
H	3.99011300	2.47038700	1.52628000
C	2.00508600	2.12465200	-1.32901400
H	1.76912300	1.23177600	-1.91876600
H	1.05143400	2.66372300	-1.18365500
H	2.64016100	2.78096900	-1.93822400
S	-1.14591400	-1.62271500	-0.10180200
O	-1.24684300	-2.13683800	-1.47977000
O	-1.57767400	-2.45641000	1.03250900
C	-2.02986500	-0.06582900	-0.01981400
C	-2.61756900	0.31959200	1.18392400
C	-2.08707800	0.73798600	-1.15920800
C	-3.27511000	1.54847500	1.24677900
H	-2.56215700	-0.34200800	2.04152100
C	-2.74416800	1.96436800	-1.08313300
H	-1.63281100	0.39492900	-2.08242200
C	-3.33364900	2.36850100	0.11813200
H	-3.74315600	1.86347900	2.17452200
H	-2.80267900	2.60157500	-1.96042200
H	-3.84548100	3.32497900	0.17225600

Zero-point correction= 0.284913 (Hartree/Particle)
Thermal correction to Energy= 0.303019
Thermal correction to Enthalpy= 0.303963
Thermal correction to Gibbs Free Energy= 0.235220
Sum of electronic and zero-point Energies= -1167.229469
Sum of electronic and thermal Energies= -1167.211362
Sum of electronic and thermal Enthalpies= -1167.210418
Sum of electronic and thermal Free Energies= -1167.279162
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1167.766368

TS9-c

C	0.14561800	2.37241300	0.43528600
H	0.59714600	1.51808600	0.92391300
C	-1.03578700	2.88730200	0.76742300
C	-1.74758600	4.10403000	0.18825300
H	-1.10735600	4.98501400	0.14681600
H	-2.10131900	3.88177800	-0.82808500
O	-2.82975800	4.35560800	1.07435500
C	-3.29780600	3.09689400	1.50689700
H	-3.93644400	3.24637500	2.38013300
H	-3.85713400	2.58328100	0.71607600
C	-1.99178300	2.33481700	1.83971500
H	-1.60120700	2.74042900	2.79291900
C	-2.07318500	0.86818900	2.08822200
C	-3.38924400	0.18897400	2.15191400
H	-3.29777700	-0.89166200	2.03105100
H	-3.75476100	0.36397900	3.18235400
H	-4.13377900	0.58099700	1.46633400
C	-0.97507100	0.23217500	2.85987400
H	0.01979900	0.61741700	2.63900500
H	-1.17880800	0.48543800	3.91663800
H	-0.98424100	-0.85432800	2.78692000
S	-2.84801400	0.92431200	-1.34533500
C	-4.25491700	-0.20729600	-1.16737300
F	-3.94742600	-1.35216500	-0.49349600

F	-5.25879100	0.37988100	-0.46560900
F	-4.75657500	-0.56483900	-2.35089100
S	1.02607700	2.86581400	-1.03751500
O	0.76592000	1.81623600	-2.04062000
O	0.70511500	4.27030500	-1.32166100
C	2.73034900	2.70616700	-0.52269700
C	3.19982600	3.50270900	0.52477400
C	3.54123700	1.76835700	-1.16183700
C	4.51525100	3.33591700	0.95419900
H	2.55189900	4.24142500	0.98614000
C	4.85859000	1.61846500	-0.72603000
H	3.14176900	1.16982600	-1.97159000
C	5.34045500	2.39290500	0.33111300
H	4.90109000	3.94825800	1.76328500
H	5.50156100	0.89252700	-1.21215400
H	6.36547800	2.27005800	0.66735400
P	0.77259600	-1.71084300	0.07805900
C	2.02029500	-1.56474300	-1.23639800
C	1.61831000	-1.15700000	-2.51658200
C	3.36670700	-1.88048700	-0.99412000
C	2.55530300	-1.06909400	-3.54539200
H	0.58547300	-0.88423100	-2.70662700
C	4.29739100	-1.79420700	-2.02774500
H	3.69016300	-2.17477200	-0.00096100
C	3.89326400	-1.38740400	-3.30244800
H	2.24021700	-0.74096200	-4.53054600
H	5.33714600	-2.04332100	-1.83821900
H	4.62140600	-1.31578400	-4.10460600
C	0.24178400	-3.44582400	0.17761000
C	-1.12520500	-3.75781300	0.20389300
C	1.19500700	-4.47541600	0.23308900
C	-1.53417300	-5.08894200	0.29366100
H	-1.86693200	-2.96717900	0.13384200
C	0.77996800	-5.80121800	0.32403300
H	2.25449700	-4.24228000	0.19708600
C	-0.58384000	-6.10836700	0.35586800
H	-2.59311900	-5.32736000	0.30576900
H	1.51840700	-6.59587200	0.36359100
H	-0.90322200	-7.14388200	0.42115700
C	1.65402200	-1.34909900	1.63023700
C	1.44851500	-2.12601400	2.77804100
C	2.45984900	-0.20037900	1.70379600
C	2.03031500	-1.74658600	3.98950800
H	0.84227600	-3.02464400	2.72499400
C	3.03771900	0.17333400	2.91581000
H	2.65650100	0.38753700	0.81487300
C	2.81766800	-0.59560100	4.06257400
H	1.87368500	-2.35599000	4.87437000
H	3.66414500	1.05890700	2.95520300
H	3.26912600	-0.30595100	5.00647600
Au	-1.07154200	-0.32593100	-0.41324600

Zero-point correction= 0.580659 (Hartree/Particle)
Thermal correction to Energy= 0.622424
Thermal correction to Enthalpy= 0.623368
Thermal correction to Gibbs Free Energy= 0.502724
Sum of electronic and zero-point Energies= -3074.479729
Sum of electronic and thermal Energies= -3074.437963
Sum of electronic and thermal Enthalpies= -3074.437019
Sum of electronic and thermal Free Energies= -3074.557663
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-3076.042769

INT9-c

C	-1.81478300	-1.46955300	0.55736700
H	-1.73963000	-0.51235600	1.06001200
C	-1.14333500	-2.56335700	0.92726200
C	-1.21225100	-3.97477200	0.36522000
H	-2.23274100	-4.32458200	0.21227800
H	-0.68499600	-4.03702300	-0.59736400
O	-0.59023000	-4.77611700	1.35999700
C	0.49768100	-4.02381000	1.85719800
H	0.82449400	-4.46986300	2.79854400
H	1.32918000	-4.01845200	1.14283800
C	-0.08731900	-2.59987900	2.03748000
H	-0.62996800	-2.57974600	2.99650800
C	0.90182800	-1.43937800	2.13005000
C	2.33866600	-1.78584700	2.41192300
H	2.96965200	-0.89516200	2.41111500
H	2.36284900	-2.20248500	3.43336600
H	2.75663000	-2.52374200	1.73352900
C	0.41398000	-0.26352800	2.92804400
H	-0.59123700	0.06584300	2.66675200
H	0.37961000	-0.59285900	3.97930600
H	1.10462600	0.57956500	2.87765100
S	1.78184400	-2.61211500	-1.16987300
C	3.48626900	-2.00903800	-1.32337200
F	3.56713300	-0.81734100	-1.97000900
F	4.08236000	-1.80684500	-0.11604000
F	4.22561200	-2.88901900	-1.99855800
S	-2.64782200	-1.34209600	-1.00947400
O	-1.86847100	-0.33670700	-1.76779200
O	-2.84272100	-2.69144000	-1.55414200
C	-4.21873900	-0.59281200	-0.60429200
C	-4.97432800	-1.10571800	0.45123600
C	-4.66542200	0.47620600	-1.38178100
C	-6.20192100	-0.51502600	0.74661700
H	-4.60974700	-1.94715800	1.03252000
C	-5.90146200	1.05033200	-1.08322100
H	-4.04983600	0.84626300	-2.19443500
C	-6.66374200	0.55932900	-0.01963200
H	-6.80091200	-0.89705200	1.56709700
H	-6.26877300	1.87883300	-1.68059800
H	-7.62373400	1.01125400	0.21007200
P	0.59372000	1.70873700	0.15512500
C	0.36322400	2.28199800	-1.55169800
C	1.10213600	1.65042700	-2.56619300
C	-0.50545600	3.33588200	-1.86833900
C	0.95709000	2.06181800	-3.88870000
H	1.79475300	0.84618800	-2.33279500
C	-0.63874000	3.74462800	-3.19401300
H	-1.07544700	3.83128700	-1.09009100
C	0.08504300	3.10580200	-4.20354100
H	1.52218100	1.56467000	-4.67042800
H	-1.30909900	4.56279600	-3.43857400
H	-0.02857300	3.42380300	-5.23520500

C	2.09322600	2.49654300	0.80975000
C	3.26478100	1.74177900	0.97307600
C	2.11242500	3.87840700	1.06248500
C	4.43630200	2.35962500	1.41118000
H	3.27568000	0.68467900	0.72544000
C	3.28442400	4.48682000	1.50513400
H	1.21843600	4.47511300	0.90947100
C	4.44453800	3.72789100	1.68474400
H	5.34169200	1.77277800	1.53023700
H	3.29540800	5.55415800	1.70237100
H	5.35664300	4.20701100	2.02658500
C	-0.83568100	2.26281300	1.12317100
C	-0.69501100	2.83973100	2.39466200
C	-2.12139900	1.99492500	0.61873500
C	-1.82793200	3.14488300	3.14911000
H	0.29036600	3.05073500	2.79489900
C	-3.24753600	2.29600800	1.38188000
H	-2.23233800	1.55239900	-0.36467200
C	-3.10179600	2.87034400	2.64763000
H	-1.71308900	3.59762700	4.12906000
H	-4.23409800	2.08064200	0.98513900
H	-3.97987400	3.10592000	3.24102000
Au	0.97365300	-0.63471700	-0.10755700

Zero-point correction= 0.582264 (Hartree/Particle)
Thermal correction to Energy= 0.624419
Thermal correction to Enthalpy= 0.625363
Thermal correction to Gibbs Free Energy= 0.503019
Sum of electronic and zero-point Energies= -3074.480450
Sum of electronic and thermal Energies= -3074.438295
Sum of electronic and thermal Enthalpies= -3074.437351
Sum of electronic and thermal Free Energies= -3074.559695
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-3076.042717

INT10-c

C	1.34740900	-2.15836000	0.13420100
H	0.77595400	-1.58606400	0.85526800
C	2.68319200	-2.18971400	0.08384300
C	3.55859900	-3.03720400	-0.82800900
H	3.22024000	-4.06759900	-0.92039600
H	3.59865700	-2.60033000	-1.83890500
O	4.83348500	-3.01950100	-0.20381600
C	5.00353600	-1.71850200	0.30869500
H	5.82633400	-1.73441300	1.02462700
H	5.24549200	-1.00969600	-0.49986300
C	3.63470800	-1.36082500	0.94957000
H	3.61750300	-1.75622100	1.97401000
C	3.36226800	0.16443800	1.08443000
C	4.64480400	0.88577300	1.52696600
H	4.45208800	1.93816800	1.74192100
H	4.98933800	0.41586400	2.45464000
H	5.45021600	0.82271300	0.79384500
C	2.24097300	0.49489500	2.07560400
H	1.30077900	-0.01372000	1.86609700
H	2.56872600	0.19194500	3.07680300
H	2.04328000	1.56792300	2.09361400
S	2.90582300	0.71737500	-0.69713900
C	3.23676400	2.53445500	-0.70483500
F	2.69993300	3.16243700	0.35695500
F	4.54415400	2.78987500	-0.72496400
F	2.67982700	3.02379300	-1.81511700
S	0.31048500	-2.89056400	-1.11727300
O	-0.27556100	-1.75946300	-1.87259300
O	1.06765000	-3.92465900	-1.83429400
C	-1.00950300	-3.62901000	-0.16528600
C	-0.69470000	-4.44756100	0.92173900
C	-2.32868700	-3.37046800	-0.53836400
C	-1.73436900	-5.00241200	1.66651100
H	0.34087500	-4.64488400	1.18133800
C	-3.35843800	-3.94031300	0.21061700
H	-2.53730500	-2.72556900	-1.38337400
C	-3.06292600	-4.74649800	1.31185300
H	-1.50938800	-5.64019900	2.51559600
H	-4.38916200	-3.74488000	-0.06530500
H	-3.86864200	-5.18254200	1.89436700
P	-1.73280000	1.15930100	0.01921600
C	-3.00901500	0.21600200	-0.84822700
C	-2.83823300	-0.07004000	-2.20988200
C	-4.16922900	-0.20454300	-0.17930400
C	-3.82902800	-0.76651400	-2.90026000
H	-1.92576500	0.22471700	-2.71653800
C	-5.15578300	-0.89996100	-0.87689800
H	-4.29392800	-0.00167100	0.87971300
C	-4.98604700	-1.18095600	-2.23537500
H	-3.69194600	-0.99481500	-3.95231800
H	-6.05493400	-1.22224800	-0.36063500
H	-5.75424300	-1.72611700	-2.77532600
C	-2.21044200	2.90892600	0.06312600
C	-1.21204100	3.88927600	0.17631500
C	-3.56116800	3.28392400	0.03164700
C	-1.56702800	5.23361900	0.27334500
H	-0.16451900	3.60006200	0.18480400
C	-3.90704200	4.63132100	0.12045800
H	-4.33558100	2.53130400	-0.07299100
C	-2.91316700	5.60460400	0.24415700
H	-0.79390500	5.99074300	0.35973300
H	-4.95263300	4.92117900	0.08878900
H	-3.18734000	6.65295300	0.30985300
C	-1.68179300	0.55966800	1.74169100
C	-1.46907400	1.44906700	2.80220500
C	-1.68746500	-0.82433200	1.97904100
C	-1.26255700	0.95382600	4.09099600
H	-1.46468900	2.51953600	2.62438800
C	-1.48009700	-1.31112200	3.26824400
H	-1.86387800	-1.51721900	1.16521000
C	-1.26276000	-0.42278400	4.32538700
H	-1.10628600	1.64595900	4.91278500
H	-1.49491900	-2.38283700	3.44064800
H	-1.10226600	-0.80194700	5.33001200
Au	0.44738100	0.85295500	-0.68267700

Zero-point correction= 0.584163 (Hartree/Particle)
Thermal correction to Energy= 0.625793
Thermal correction to Enthalpy= 0.626737
Thermal correction to Gibbs Free Energy= 0.505877
Sum of electronic and zero-point Energies= -3074.529544

Sum of electronic and thermal Energies= -3074.487914
Sum of electronic and thermal Enthalpies= -3074.486970
Sum of electronic and thermal Free Energies= -3074.607830
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-3076.084335

TS10-c

C	3.33909900	-0.57115800	-1.03094200
H	3.01310500	0.24815600	-1.66203800
C	2.49879700	-1.42723400	-0.44770800
C	2.82090100	-2.62071800	0.43668400
H	3.56396800	-3.29301300	0.00928100
H	3.20272300	-2.27360100	1.41051000
O	1.59233100	-3.31809100	0.57815000
C	0.56719600	-2.34280700	0.57956200
H	-0.38235200	-2.83708100	0.37897100
H	0.50612100	-1.83638100	1.55358000
C	0.96867600	-1.34430200	-0.53566000
H	0.65746600	-1.77624600	-1.49490600
C	0.42293800	0.06164000	-0.42613400
C	0.20749800	0.80091100	-1.71883900
H	-0.37323600	1.71500700	-1.56337600
H	1.17306700	1.10211300	-2.15307600
H	-0.30210500	0.18093600	-2.46376300
C	0.85283800	0.90590000	0.74072300
H	0.96240500	0.33222400	1.66213700
H	1.83053900	1.36249200	0.52036400
H	0.14453100	1.72012600	0.91885000
S	5.10588100	-0.60166100	-0.84541700
O	5.46667900	-1.68473400	0.08540000
O	5.70931300	-0.50886700	-2.18312200
C	5.38348900	0.96331700	-0.01072700
C	5.74793700	2.08014200	-0.76137800
C	5.19090200	1.03678900	1.37024300
C	5.91869600	3.30195800	-0.10988700
H	5.90718000	1.97775100	-1.82938600
C	5.36144800	2.26313900	2.00901300
H	4.93025600	0.14288500	1.92703900
C	5.72176400	3.39306700	1.26924800
H	6.20944100	4.18034400	-0.67822500
H	5.22136300	2.33690000	3.08326900
H	5.85535600	4.34650200	1.77197200
S	-4.26157700	-0.80017000	-0.94092400
O	-4.05247200	-0.82139900	-2.39825300
O	-4.81388200	-1.95194900	-0.20651600
C	-5.23531700	0.64886900	-0.53910900
C	-6.01936200	0.64368400	0.61360800
C	-5.14740200	1.76142600	-1.37576300
C	-6.74871600	1.78964200	0.92541200
H	-6.05759900	-0.24133100	1.23731300
C	-5.88039000	2.90012300	-1.04786300
H	-4.53242400	1.72123700	-2.26779600
C	-6.67701200	2.91402900	0.09987000
H	-7.37410800	1.80348800	1.81284500
H	-5.83396700	3.77402500	-1.69058500
H	-7.24561400	3.80462500	0.35086200
S	-2.03207900	-0.32136600	-0.20799600
C	-2.33367400	-0.75145200	1.54297800
F	-2.43696000	-2.07327100	1.74066800
F	-1.32425600	-0.30499400	2.32015600
F	-3.46648300	-0.18634400	2.00254300

Zero-point correction= 0.402880 (Hartree/Particle)
Thermal correction to Energy= 0.434944
Thermal correction to Enthalpy= 0.435889
Thermal correction to Gibbs Free Energy= 0.332233
Sum of electronic and zero-point Energies= -2683.187366
Sum of electronic and thermal Energies= -2683.155301
Sum of electronic and thermal Enthalpies= -2683.154357
Sum of electronic and thermal Free Energies= -2683.258013
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2684.124335

P_3

C	-1.39957900	1.15955100	-0.85563600
H	-1.36865300	0.72085100	-1.84678100
C	-0.30608100	1.52172700	-0.18330000
C	-0.20148200	2.25835400	1.13676000
H	-1.01816800	2.95145000	1.32132100
H	-0.15876200	1.53790800	1.97339600
O	1.00863800	2.99004800	1.01541800
C	1.94096400	2.15724600	0.33923500
H	2.67401100	2.80123900	-0.14876200
H	2.47173400	1.51497000	1.05151400
C	1.12282500	1.30942900	-0.67330100
H	1.22817000	1.72761900	-1.68037100
C	1.54371900	-0.19373400	-0.73953300
C	0.88800700	-0.92248000	-1.92183100
H	1.29929100	-1.93058600	-2.01672200
H	-0.18946800	-1.01299500	-1.75863400
H	1.05363300	-0.39541600	-2.86780100
C	1.22537100	-0.95224000	0.55319300
H	1.67943500	-0.50117900	1.43630600
H	0.13835400	-0.95709600	0.68807700
H	1.56062300	-1.98870600	0.48817500
S	-3.06566800	1.22792900	-0.22999400
O	-3.08780200	1.95403800	1.05071300
O	-3.94409600	1.60879000	-1.34541100
C	-3.34137300	-0.51075200	0.12410400
C	-3.90289800	-1.32551200	-0.85817400
C	-2.93477300	-1.02136200	1.35842500
C	-4.05440500	-2.68750400	-0.59661300
H	-4.22599300	-0.88837300	-1.79692200
C	-3.08974300	-2.38372100	1.60709100
H	-2.52523700	-0.35277500	2.10830500
C	-3.64470100	-3.21455600	0.62968500
H	-4.49601200	-3.33525900	-1.34792200
H	-2.78528800	-2.79622900	2.56429500
H	-3.76380800	-4.27565900	0.82815800
S	3.38808400	-0.18028300	-1.18222700
C	4.27359800	-0.85740000	0.25092800
F	4.07870500	-0.17869500	1.40266100
F	3.97755400	-2.14583100	0.51098900
F	5.58117300	-0.78962900	-0.04610000

Zero-point correction= 0.305389 (Hartree/Particle)
Thermal correction to Energy= 0.327817
Thermal correction to Enthalpy= 0.328761

Thermal correction to Gibbs Free Energy= 0.250455
Sum of electronic and zero-point Energies= -1903.083029
Sum of electronic and thermal Energies= -1903.060600
Sum of electronic and thermal Enthalpies= -1903.059656
Sum of electronic and thermal Free Energies= -1903.137963
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1903.780868

TS1´-c

C	5.68768100	-0.56736400	-0.34098600
H	6.22782200	-0.12847000	-1.15996500
C	5.38979900	-1.58545400	0.30279200
C	4.78840300	-2.45913000	1.31544900
H	5.43208200	-3.32155000	1.51607400
H	4.67772500	-1.88978400	2.25255800
O	3.54282200	-2.99095000	0.87930100
C	2.48366000	-2.03828200	0.88577800
H	2.08094900	-1.92862400	1.90240400
H	2.83384600	-1.05517800	0.56046900
C	1.44088400	-2.59637300	-0.05347500
H	0.93473400	-3.49294200	0.30649600
C	1.41834500	-2.37229200	-1.42068600
C	0.63012900	-3.28028200	-2.32790600
H	0.03046500	-2.71004800	-3.04507400
H	1.33885000	-3.88158500	-2.91361400
H	-0.02077900	-3.96105000	-1.77386600
C	2.28682300	-1.35562500	-2.10731000
H	2.66184900	-0.58245200	-1.43982600
H	3.15194100	-1.87863600	-2.53743800
H	1.74900300	-0.87675400	-2.93069600
S	4.85508100	1.31097300	0.70551300
O	4.35252800	0.85197900	2.02317600
O	5.84032700	2.40678300	0.57153200
C	3.39508600	1.75853100	-0.25859900
C	3.54351600	2.12636400	-1.59661000
C	2.14277200	1.70658400	0.35288300
C	2.40376000	2.42926000	-2.34329400
H	4.53178700	2.19239700	-2.04072900
C	1.01643300	2.04566800	-0.39638700
H	2.07478600	1.43747000	1.40122300
C	1.14109800	2.38944500	-1.74494200
H	2.50455600	2.71614300	-3.38552100
H	0.04516600	2.07578300	0.07996300
H	0.25613700	2.64450600	-2.31835300
P	-2.24376600	0.15818700	0.20833200
C	-2.21899500	1.01807300	1.80411600
C	-1.01795600	1.14471600	2.51722200
C	-3.39976800	1.57874500	2.31644500
C	-0.99230600	1.84570600	3.72200200
H	-0.10963700	0.68791400	2.13550400
C	-3.36736400	2.27804000	3.52124000
H	-4.33697200	1.46046300	1.78107200
C	-2.16529500	2.41506100	4.22109700
H	-0.06105400	1.94110200	4.27142000
H	-4.28070700	2.71032500	3.91763000
H	-2.14572300	2.95819700	5.16075600
C	-3.76477400	-0.82794700	0.13923500
C	-3.78133100	-2.08650200	0.75974400
C	-4.92375000	-0.33024600	-0.47268200
C	-4.95414800	-2.83753500	0.77404900
H	-2.88066700	-2.47270100	1.23022900
C	-6.09363100	-1.09032400	-0.45659200
H	-4.91091900	0.63796100	-0.96245500
C	-6.10975800	-2.33986600	0.16540700
H	-4.96637500	-3.81092800	1.25426000
H	-6.99066700	-0.70654100	-0.93239700
H	-7.02149000	-2.92904300	0.17299600
C	-2.37008600	1.40808700	-1.10776700
C	-2.29457700	0.97129200	-2.44033300
C	-2.51132000	2.77210800	-0.82652600
C	-2.37298100	1.89281300	-3.48101000
H	-2.17941800	-0.08735400	-2.65896800
C	-2.57716400	3.69283600	-1.87490200
H	-2.56432200	3.11608200	0.20080900
C	-2.51068900	3.25609300	-3.19851500
H	-2.32217300	1.55155800	-4.51032700
H	-2.68203900	4.75036900	-1.65402200
H	-2.56541100	3.97471900	-4.01033400
Au	-0.33491800	-1.14437200	-0.12872400

Zero-point correction= 0.558573 (Hartree/Particle)
Thermal correction to Energy= 0.597419
Thermal correction to Enthalpy= 0.598363
Thermal correction to Gibbs Free Energy= 0.480535
Sum of electronic and zero-point Energies= -2338.608319
Sum of electronic and thermal Energies= -2338.569474
Sum of electronic and thermal Enthalpies= -2338.568530
Sum of electronic and thermal Free Energies= -2338.686357
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2340.0069524

INT1´-c

C	-2.58252500	1.30742000	-0.51137900
H	-2.27661900	1.10719300	-1.53515000
C	-1.81849600	1.13379700	0.55349100
C	-2.09904000	1.36415700	2.01665800
H	-1.58797800	2.27266500	2.34702900
H	-3.18071500	1.51794100	2.14553000
O	-1.64103400	0.32570500	2.86381900
C	-2.05595900	-0.97270400	2.44807200
H	-2.14819500	-1.56744600	3.36408200
H	-3.04179800	-0.93527900	1.97201400
C	-1.00996300	-1.61023100	1.57128300
H	-0.04010400	-1.73093400	2.05166100
C	-1.19094500	-2.22436200	0.35438500
C	-0.07374500	-3.01978800	-0.25819400
H	-0.37428600	-4.07335600	-0.33609300
H	0.13540600	-2.68406800	-1.28132000
H	0.84744300	-2.96380100	0.32350600
C	-2.47732200	-2.21031900	-0.41248400
H	-3.27293200	-1.63815400	0.05958300
H	-2.30620300	-1.79369300	-1.41347400
H	-2.83238000	-3.23764100	-0.56461400
P	2.46730500	0.07760200	-0.19428900
C	3.48848500	1.48534600	0.32470000
C	3.01532700	2.78439700	0.08606200
C	4.74598200	1.29374800	0.91511000

C	3.80089300	3.88358200	0.42638600
H	2.03672700	2.93272300	-0.36397000
C	5.52542400	2.39915600	1.25581500
H	5.10820500	0.29035400	1.11530900
C	5.05527500	3.69089900	1.01095800
H	3.43261200	4.88798100	0.24262400
H	6.49744200	2.25097600	1.71592300
H	5.66334200	4.54853400	1.28155400
C	3.00005800	-1.34157100	0.81303100
C	3.61741200	-2.46632400	0.25359200
C	2.71495400	-1.31048500	2.18923200
C	3.94682300	-3.55330400	1.06701500
H	3.83658700	-2.49645900	-0.80832900
C	3.05068700	-2.39555100	2.99491000
H	2.23707300	-0.43663000	2.62596500
C	3.66316000	-3.52072900	2.43265300
H	4.42668700	-4.42395700	0.63079400
H	2.83608500	-2.36524100	4.05873100
H	3.91995100	-4.36806800	3.06076400
C	2.88010600	-0.29283900	-1.92211900
C	1.86878500	-0.69346900	-2.80652200
C	4.20606900	-0.20267900	-2.37298500
C	2.18183400	-1.02014400	-4.12537700
H	0.83785900	-0.73311200	-2.46466200
C	4.51347000	-0.53019000	-3.69219100
H	4.98897600	0.13033500	-1.69865600
C	3.50396800	-0.94123600	-4.56674500
H	1.39584300	-1.32514400	-4.80926400
H	5.53917700	-0.45792400	-4.04005800
H	3.74730300	-1.18998800	-5.59503300
Au	0.13931300	0.46636800	0.19985400
S	-4.31351400	1.89121900	-0.49057100
O	-4.58618800	2.53531500	0.80329600
O	-4.50945400	2.57784400	-1.77084600
C	-5.18365000	0.32673200	-0.52744700
C	-5.34786800	-0.32399100	-1.75133900
C	-5.61812400	-0.23570700	0.67510100
C	-5.95362900	-1.58036200	-1.76465200
H	-5.02846100	0.15744800	-2.66954400
C	-6.22470000	-1.49164700	0.64540100
H	-5.51029000	0.31799400	1.60134700
C	-6.38369400	-2.16423400	-0.56965300
H	-6.10182800	-2.09712500	-2.70767700
H	-6.58544900	-1.93794300	1.56689700
H	-6.85949700	-3.13994600	-0.58718400

Zero-point correction= 0.561422 (Hartree/Particle)
Thermal correction to Energy= 0.599575
Thermal correction to Enthalpy= 0.600520
Thermal correction to Gibbs Free Energy= 0.483572
Sum of electronic and zero-point Energies= -2338.629723
Sum of electronic and thermal Energies= -2338.591570
Sum of electronic and thermal Enthalpies= -2338.590626
Sum of electronic and thermal Free Energies= -2338.707573
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2340.02536

TS5´-c

C	-4.53347700	0.45305100	-0.83691400
H	-4.29506900	-0.43638400	-1.41215100
C	-3.69815000	1.19908300	-0.16958300
C	-3.59800600	2.42178600	0.65548800
H	-4.26497800	3.19814400	0.27076600
H	-3.89627800	2.19171400	1.69154400
O	-2.27486900	2.94251400	0.61658900
C	-1.32920400	1.94776600	0.94525300
H	-0.35740700	2.44745300	0.90166700
H	-1.47946400	1.57900800	1.96965800
C	-1.38804700	0.80441100	-0.06011100
H	-1.34699900	1.12265700	-1.10134100
C	-1.31201200	-0.56718200	0.20507000
C	-1.54891400	-1.55006800	-0.92360300
H	-0.90390700	-2.43029900	-0.83702300
H	-2.58453500	-1.91283600	-0.86424700
H	-1.39816700	-1.09746700	-1.90766300
C	-1.52970900	-1.13732300	1.58975100
H	-1.19087400	-0.47954300	2.39179000
H	-2.60515200	-1.31989200	1.72886100
H	-1.02001500	-2.09940900	1.69800500
S	-6.29644900	0.93456100	-0.96434700
O	-6.46698700	2.14240700	-0.14335000
O	-6.62498000	0.90679200	-2.39410400
C	-7.12466800	-0.42751200	-0.16031700
C	-7.51045400	-1.52899900	-0.92662700
C	-7.35003400	-0.36479200	1.21639100
C	-8.13602100	-2.59938300	-0.28832200
H	-7.34649900	-1.52772700	-1.99877700
C	-7.97785800	-1.44190400	1.83927900
H	-7.06187100	0.52076800	1.77216000
C	-8.36526100	-2.55608400	1.08928200
H	-8.45479500	-3.46043500	-0.86733400
H	-8.17520200	-1.40798700	2.90620000
H	-8.85776300	-3.39029300	1.57966200
P	3.31219100	-0.10863500	-0.04126600
C	4.01935100	0.48718300	1.51830500
C	3.44781900	0.06353300	2.72826900
C	5.14379600	1.32362600	1.52640500
C	4.00527500	0.46863700	3.93827000
H	2.57341400	-0.58239200	2.71942600
C	5.69336500	1.72906900	2.74330600
H	5.58378400	1.65609300	0.59203600
C	5.12697400	1.30299100	3.94568700
H	3.56372400	0.14017800	4.87394600
H	6.56241100	2.37942900	2.75024100
H	5.55623000	1.62335100	4.88992300
C	3.93949200	0.95072900	-1.37191600
C	3.32348100	2.19076200	-1.60154900
C	5.05052500	0.56500200	-2.13455900
C	3.82327400	3.04271400	-2.58316000
H	2.45866600	2.48582400	-1.01280200
C	5.54268000	1.42278800	-3.11876100
H	5.52432900	-0.39576900	-1.96224600
C	4.93197200	2.65795700	-3.34251200
H	3.34609500	4.00134100	-2.76075400
H	6.40144500	1.12387700	-3.71159900
H	5.31636700	3.32042700	-4.11181700

C	3.94636200	-1.78331900	-0.32663500
C	3.29991500	-2.60449700	-1.26345300
C	5.09119200	-2.24201100	0.33900000
C	3.80264600	-3.87400400	-1.53706100
H	2.41075500	-2.24760600	-1.77713100
C	5.58604200	-3.51704500	0.06233100
H	5.58925500	-1.61036600	1.06716700
C	4.94479000	-4.33079000	-0.87299200
H	3.30325500	-4.50839000	-2.26268100
H	6.47123600	-3.87381200	0.57947200
H	5.33202000	-5.32291800	-1.08329700
Au	0.98194800	-0.09312800	0.02831200

Zero-point correction= 0.560079 (Hartree/Particle)
Thermal correction to Energy= 0.598101
Thermal correction to Enthalpy= 0.599045
Thermal correction to Gibbs Free Energy= 0.477889
Sum of electronic and zero-point Energies= -2338.601907
Sum of electronic and thermal Energies= -2338.563884
Sum of electronic and thermal Enthalpies= -2338.562940
Sum of electronic and thermal Free Energies= -2338.684097
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2339.99795

INT5′-c

C	4.28672900	-0.81592200	-0.77944900
H	4.17837200	-0.08523700	-1.57434900
C	3.25740600	-1.40087700	-0.17045800
C	3.27047600	-2.45612000	0.92690900
H	3.92384400	-3.30018400	0.71144200
H	3.59557900	-2.00798600	1.87802500
O	1.92878700	-2.92327400	1.00553900
C	1.09373300	-1.82889100	0.72342200
H	0.09930000	-2.20997700	0.48099300
H	1.01319000	-1.14987800	1.58916800
C	1.77738300	-1.09978100	-0.47317000
H	1.50129700	-1.62897700	-1.39304900
C	1.47390800	0.37438500	-0.63627300
C	1.54177400	0.92815900	-2.03961700
H	1.08811900	1.92131600	-2.12067600
H	2.60087900	1.05113800	-2.32803600
H	1.08714600	0.25946200	-2.77662200
C	1.92374700	1.31210100	0.45920900
H	1.71008300	0.92877200	1.46060000
H	3.01645800	1.44338300	0.39359500
H	1.47406900	2.30422500	0.35567800
S	5.99970300	-1.14971700	-0.39559000
O	6.03198600	-2.00486300	0.80176100
O	6.66391300	-1.53857900	-1.64485900
C	6.55943400	0.48795000	0.05747200
C	7.18053100	1.28294100	-0.90645900
C	6.33732900	0.94241900	1.36017800
C	7.58492600	2.57055100	-0.55299100
H	7.35943000	0.88426200	-1.89919700
C	6.74412400	2.23183000	1.69833700
H	5.88232100	0.28412800	2.09273300
C	7.36332000	3.04328000	0.74270900
H	8.08111700	3.19984900	-1.28521900
H	6.59248100	2.59900100	2.70871100
H	7.68420000	4.04473200	1.01316600
P	-3.12893100	0.13571000	0.04495200
C	-3.36761000	-1.46675900	0.85382800
C	-2.53260400	-1.81117000	1.92991000
C	-4.37267200	-2.34778400	0.43196300
C	-2.70716400	-3.02904400	2.58064600
H	-1.75242700	-1.12712400	2.25357300
C	-4.53918200	-3.56756400	1.08916500
H	-5.01668400	-2.08448000	-0.40022800
C	-3.70903000	-3.90867500	2.15793400
H	-2.05991600	-3.29658500	3.40979400
H	-5.31640900	-4.25133700	0.76281300
H	-3.83845200	-4.86166200	2.66127600
C	-4.08222800	0.14120100	-1.49255100
C	-3.59359500	-0.57593300	-2.59671000
C	-5.31025200	0.81279900	-1.57403200
C	-4.33851100	-0.62993100	-3.77125400
H	-2.63755100	-1.08910600	-2.53181100
C	-6.04728500	0.75721600	-2.75732300
H	-5.68652900	1.36991900	-0.72266200
C	-5.56433200	0.03835100	-3.85199100
H	-3.96256700	-1.18519200	-4.62474800
H	-6.99801100	1.27680600	-2.82264700
H	-6.14027300	0.00089800	-4.77138600
C	-3.78509300	1.42516600	1.13000700
C	-3.42068800	2.76102100	0.89834000
C	-4.68266400	1.10564600	2.15893600
C	-3.96236800	3.77221500	1.68718000
H	-2.71859600	3.00346600	0.10481700
C	-5.21726500	2.12538200	2.94653000
H	-4.96055100	0.07283000	2.34078800
C	-4.85914600	3.45410600	2.71176600
H	-3.68198500	4.80553500	1.50902000
H	-5.91184900	1.88040300	3.74382700
H	-5.27522200	4.24363700	3.32979400
Au	-0.84567600	0.41807500	-0.36514600

Zero-point correction= 0.563065 (Hartree/Particle)
Thermal correction to Energy= 0.600618
Thermal correction to Enthalpy= 0.601562
Thermal correction to Gibbs Free Energy= 0.482092
Sum of electronic and zero-point Energies= -2338.641214
Sum of electronic and thermal Energies= -2338.603661
Sum of electronic and thermal Enthalpies= -2338.602717
Sum of electronic and thermal Free Energies= -2338.722186
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2340.038354

TS2′-c

C	2.03394000	-0.41830800	0.62011300
H	2.48651900	-1.37573500	0.42185600
C	2.32488000	0.76817900	0.91504400
C	2.03122300	2.20693500	1.22588700
H	1.87188800	2.29470500	2.30532900
H	2.90064200	2.81904000	0.95632600
O	0.86420700	2.66883100	0.59676800
C	1.01179200	3.03906000	-0.80132500
H	0.40280200	3.94095600	-0.90605200
H	2.05500200	3.31023100	-0.99165700

C	0.50839500	1.97867600	-1.73557600
H	-0.57386500	1.92560900	-1.81715900
C	1.23950300	1.12831200	-2.47698700
C	0.55528300	0.12903600	-3.37420000
H	0.85769700	0.26662000	-4.42039100
H	0.84253900	-0.89599800	-3.09994200
H	-0.53402000	0.21100100	-3.31804900
C	2.74264300	1.06299200	-2.49295600
H	3.22590500	1.76851100	-1.81455900
H	3.07469100	0.05410000	-2.21465100
H	3.12293000	1.24898400	-3.50571900
P	-2.44864400	-0.29949700	0.14984000
C	-3.32832900	-0.40783100	1.73160600
C	-2.82925200	-1.25663300	2.73071600
C	-4.51755600	0.30496000	1.94436000
C	-3.52269000	-1.39894100	3.93057900
H	-1.90107900	-1.79786700	2.56759100
C	-5.20436800	0.15910600	3.14946600
H	-4.89784900	0.97294800	1.17829700
C	-4.70931100	-0.69147600	4.13995800
H	-3.13475000	-2.05441900	4.70399000
H	-6.12332300	0.71269100	3.31539700
H	-5.24478800	-0.79876200	5.07823700
C	-2.90280000	1.29227300	-0.60077600
C	-3.54239600	1.36486800	-1.84402300
C	-2.51463100	2.46888800	0.06246000
C	-3.79647700	2.61202300	-2.41888800
H	-3.83845700	0.45749500	-2.35955400
C	-2.78001000	3.70782500	-0.51359000
H	-1.98672200	2.41191900	1.00966800
C	-3.41733600	3.78032200	-1.75684600
H	-4.29247500	2.66811800	-3.38289600
H	-2.48384600	4.61607800	0.00229800
H	-3.61616600	4.74764600	-2.20783000
C	-3.08096600	-1.61050900	-0.93147200
C	-2.24697500	-2.14847500	-1.92214700
C	-4.40902100	-2.04744800	-0.81903100
C	-2.74305400	-3.10710600	-2.80393700
H	-1.21556100	-1.81764800	-1.99784100
C	-4.89703400	-3.00999100	-1.70152400
H	-5.05277000	-1.64319700	-0.04441700
C	-4.06721800	-3.53745100	-2.69376200
H	-2.09604600	-3.52274500	-3.57021800
H	-5.92366000	-3.35105500	-1.61167000
H	-4.45106200	-4.28885600	-3.37691200
Au	-0.13104400	-0.30850300	0.40022800
S	4.78641100	0.85826100	1.10480100
O	5.16340100	1.97248200	0.20375800
O	5.09152700	0.86162400	2.55214600
C	5.30107700	-0.69127100	0.38260700
C	5.26927700	-1.83523000	1.18377400
C	5.61806300	-0.72791600	-0.97688300
C	5.58836000	-3.05855600	0.59564300
H	5.02781800	-1.76089600	2.23849200
C	5.93940200	-1.96084800	-1.54300700
H	5.63483200	0.18596000	-1.55889300
C	5.91914600	-3.11975200	-0.76166700
H	5.58883300	-3.96060100	1.19902100
H	6.21121500	-2.01476100	-2.59232000
H	6.16827200	-4.07583400	-1.21129300

Zero-point correction= 0.558565 (Hartree/Particle)
Thermal correction to Energy= 0.597457
Thermal correction to Enthalpy= 0.598401
Thermal correction to Gibbs Free Energy= 0.478456
Sum of electronic and zero-point Energies= -2338.608806
Sum of electronic and thermal Energies= -2338.569915
Sum of electronic and thermal Enthalpies= -2338.568971
Sum of electronic and thermal Free Energies= -2338.688915
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2339.998873

INT2´-c

C	-1.18447600	-0.19496000	0.54789900
H	-1.13438000	-1.00658700	1.26597700
C	-2.09323400	-0.10972100	-0.40355000
C	-2.25771600	0.92538200	-1.49620100
H	-1.94997100	0.49133900	-2.45027900
H	-3.31754200	1.20326800	-1.58483200
O	-1.45750800	2.07856400	-1.30354800
C	-1.84683800	2.89683600	-0.19497900
H	-2.17117000	3.86815400	-0.59017700
H	-2.69306100	2.44758900	0.33254400
C	-0.70532800	3.09100900	0.79078300
H	-0.98350700	3.05122900	1.84390400
C	0.51360600	3.67676400	0.48154500
C	1.44525700	4.12961000	1.57654500
H	2.48214100	3.84484100	1.36851800
H	1.42568200	5.22760400	1.62599100
H	1.15852300	3.73945400	2.55663000
C	0.89999800	4.06331600	-0.92193800
H	0.83954600	5.15753400	-1.01311200
H	1.93942000	3.78782300	-1.13132800
H	0.25513600	3.61041200	-1.67484100
S	-3.30088300	-1.47537100	-0.49843700
O	-3.46574300	-1.76637300	-1.93328300
O	-2.88624700	-2.51091800	0.45802100
C	-4.80669200	-0.71320500	0.09173200
C	-5.00972600	-0.59716600	1.46878400
C	-5.73128400	-0.23149800	-0.83614700
C	-6.17052300	0.02526000	1.92303500
H	-4.28347700	-1.00835200	2.16173700
C	-6.88973500	0.38837000	-0.36604200
H	-5.55112700	-0.36704800	-1.89696000
C	-7.10510700	0.51936800	1.00746500
H	-6.35258900	0.11568400	2.98935600
H	-7.62618300	0.75974300	-1.07168200
H	-8.00939700	1.00017700	1.36781400
P	2.04180200	-0.63656500	-0.00878000
C	1.10355700	-1.73116200	-1.09935000
C	0.66728800	-1.22413700	-2.33607700
C	0.64587500	-2.97411300	-0.64792400
C	-0.21682100	-1.96551300	-3.11170100
H	1.00543500	-0.24848200	-2.67548700
C	-0.25155700	-3.70466300	-1.42838000
H	0.96870700	-3.36055300	0.31290900

C	-0.68653300	-3.20094200	-2.65259600
H	-0.55966300	-1.57524300	-4.06488700
H	-0.62652000	-4.65581100	-1.06608700
H	-1.40767000	-3.75622400	-3.24210300
C	2.60478400	-1.58682100	1.42467200
C	1.85353800	-1.57271700	2.60887000
C	3.76203400	-2.37521200	1.33445200
C	2.25094900	-2.35432300	3.69246800
H	0.96657300	-0.95016500	2.68181400
C	4.15452900	-3.15114500	2.42320600
H	4.35137000	-2.37754000	0.42287100
C	3.39968500	-3.14293100	3.59904600
H	1.66892200	-2.34374300	4.60861600
H	5.05043700	-3.76019000	2.35507400
H	3.71050500	-3.74800200	4.44507000
C	3.49583800	-0.03331900	-0.90837300
C	4.12138800	1.14291500	-0.46512300
C	4.01362700	-0.73085700	-2.00923100
C	5.26089100	1.61234600	-1.11306400
H	3.71621400	1.68155100	0.38840600
C	5.15394600	-0.25238900	-2.65549600
H	3.52579800	-1.63410600	-2.36037900
C	5.77600300	0.91535900	-2.21008500
H	5.74608500	2.51986500	-0.76733000
H	5.55457400	-0.79213100	-3.50786400
H	6.66113700	1.28490800	-2.71843800
Au	0.54809900	1.13036400	0.54101600

Zero-point correction= 0.561946 (Hartree/Particle)
Thermal correction to Energy= 0.599852
Thermal correction to Enthalpy= 0.600796
Thermal correction to Gibbs Free Energy= 0.485039
Sum of electronic and zero-point Energies= -2338.633371
Sum of electronic and thermal Energies= -2338.595465
Sum of electronic and thermal Enthalpies= -2338.594521
Sum of electronic and thermal Free Energies= -2338.710279
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2340.027055

TS6´-c

C	3.70086000	-1.33359200	-0.77453000
H	3.86403800	-1.72476100	-1.76781700
C	4.43605100	-1.07620600	0.26944800
C	4.00454300	-0.55832300	1.62299200
H	4.35917800	-1.24509300	2.39550700
H	4.47873600	0.42068800	1.79875400
O	2.60302500	-0.46814600	1.78163600
C	1.94151600	0.31573900	0.80993200
H	1.10221900	0.79779300	1.32353900
H	2.59268600	1.11036300	0.42349400
C	1.44444800	-0.57237400	-0.32515300
H	1.31448400	-1.61740200	-0.04989700
C	1.06708800	-0.15925800	-1.59908000
C	0.83965800	-1.19096200	-2.68471900
H	0.02525700	-0.90229700	-3.35630900
H	1.74862700	-1.26466200	-3.29857800
H	0.62667400	-2.18233600	-2.27508800
C	1.34644200	1.24514300	-2.08631200
H	2.34967900	1.27533500	-2.53568000
H	0.63421900	1.53835300	-2.86338100
H	1.31009300	1.99105300	-1.28917300
S	6.24863000	-1.40798800	0.11227200
O	6.64374600	-2.04860200	1.37502100
O	6.45869100	-2.04275500	-1.19283200
C	6.94101700	0.23894700	0.07188300
C	7.01827400	0.90845900	-1.15110300
C	7.37418100	0.82067900	1.26490000
C	7.54039300	2.20026100	-1.17297100
H	6.69967700	0.41221200	-2.06135100
C	7.89385200	2.11462100	1.22663200
H	7.32807700	0.25639000	2.18993400
C	7.97249400	2.80163400	0.01293800
H	7.62176300	2.73354200	-2.11500700
H	8.24727200	2.58033900	2.14117300
H	8.38239400	3.80674900	-0.01141900
P	-3.24774700	0.09448900	0.14339600
C	-3.67029200	-1.10583800	1.43472500
C	-2.74149400	-1.36431500	2.45473100
C	-4.92123000	-1.73848200	1.44498400
C	-3.06803500	-2.24435500	3.48352600
H	-1.76888600	-0.87902300	2.44145100
C	-5.23910900	-2.62112900	2.47757700
H	-5.63737600	-1.54550700	0.65297000
C	-4.31617600	-2.87329200	3.49422500
H	-2.34854700	-2.44523500	4.27103200
H	-6.20643900	-3.11359100	2.48495400
H	-4.56652300	-3.56417700	4.29327900
C	-4.35698300	-0.19634600	-1.26139700
C	-4.06695600	-1.24360300	-2.14972400
C	-5.51181900	0.57740400	-1.43947100
C	-4.93313700	-1.51824000	-3.20492800
H	-3.16949200	-1.84122500	-2.01120900
C	-6.37239400	0.29840900	-2.50191100
H	-5.73507800	1.39056200	-0.75669500
C	-6.08499900	-0.74617800	-3.38189900
H	-4.70904900	-2.32893600	-3.89114600
H	-7.26566400	0.89906600	-2.64186900
H	-6.75610400	-0.95796400	-4.20849500
C	-3.60592700	1.75055800	0.78933100
C	-3.06239700	2.86680200	0.13478000
C	-4.44648600	1.92518300	1.89696300
C	-3.36680900	4.14986500	0.58225000
H	-2.40773600	2.72869200	-0.72209900
C	-4.74261900	3.21410500	2.34220700
H	-4.86328400	1.06306800	2.40710600
C	-4.20559500	4.32337900	1.68708300
H	-2.94747500	5.01312500	0.07497300
H	-5.39124700	3.34981800	3.20194300
H	-4.43690800	5.32415400	2.03844400
Au	-1.01558200	-0.11069300	-0.48795800

Zero-point correction= 0.559863 (Hartree/Particle)
Thermal correction to Energy= 0.597875
Thermal correction to Enthalpy= 0.598819
Thermal correction to Gibbs Free Energy= 0.477416
Sum of electronic and zero-point Energies= -2338.595899
Sum of electronic and thermal Energies= -2338.557887

Sum of electronic and thermal Enthalpies= -2338.556943

Sum of electronic and thermal Free Energies= -2338.678346

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2339.99097

INT6´-c

C	3.29022000	-1.38761100	-0.45763400
H	3.61452500	-1.81025700	-1.40487800
C	4.19559400	-1.04366200	0.45463600
C	3.84109100	-0.53223800	1.82544800
H	4.39181100	-1.09498700	2.58357000
H	4.11734600	0.53096600	1.91998900
O	2.46194200	-0.71933200	2.09883800
C	1.63133400	-0.29088200	1.04333400
H	0.60880100	-0.34322100	1.42576900
H	1.85026400	0.75522000	0.77773800
C	1.80148100	-1.20367800	-0.19616000
H	1.37258000	-2.18617900	0.04367900
C	1.15024300	-0.70096000	-1.47589800
C	0.88496800	-1.76196200	-2.51766000
H	0.29303300	-1.38704700	-3.35806000
H	1.85272100	-2.09299100	-2.93686300
H	0.40221900	-2.65061700	-2.09954100
C	1.60531400	0.63548600	-2.01347000
H	2.64733500	0.53806900	-2.36392700
H	1.00525500	0.95506100	-2.87033400
H	1.59868200	1.42812600	-1.26100400
S	5.93789800	-1.28207800	0.06735700
O	6.54497800	-1.91533100	1.24615100
O	6.00755500	-1.88392400	-1.27192600
C	6.53213800	0.40153200	-0.03733500
C	6.43704000	1.07916500	-1.25477300
C	7.06106400	1.00489700	1.10489100
C	6.87750700	2.39953800	-1.32248800
H	6.05231600	0.56558900	-2.12936300
C	7.49690900	2.32752200	1.02269900
H	7.15097200	0.43562700	2.02370700
C	7.40137900	3.02202800	-0.18551400
H	6.82462700	2.93934800	-2.26294600
H	7.92140800	2.81048900	1.89724700
H	7.74730000	4.04952500	-0.24516800
P	-3.11702900	0.18058800	0.13451400
C	-4.23587300	-1.22541600	-0.07362300
C	-3.74671200	-2.52036800	0.16430600
C	-5.57837100	-1.03132400	-0.42786200
C	-4.60260000	-3.61286600	0.06003800
H	-2.70337900	-2.66697200	0.43189700
C	-6.42733700	-2.13332300	-0.53512400
H	-5.95568000	-0.03162300	-0.61475800
C	-5.94231600	-3.41932000	-0.29189400
H	-4.22626200	-4.61393500	0.24525600
H	-7.46702600	-1.98546700	-0.80954000
H	-6.60627100	-4.27360800	-0.37991000
C	-3.90533500	1.64940000	-0.56608100
C	-3.89561700	1.82807300	-1.95866300
C	-4.55832400	2.57471600	0.26088100
C	-4.54794300	2.92251000	-2.51973000
H	-3.38085000	1.11311400	-2.59525600
C	-5.20581200	3.67029800	-0.31035700
H	-4.56167900	2.43888300	1.33725100
C	-5.20149300	3.84386600	-1.69557800
H	-4.54196000	3.06167900	-3.59615100
H	-5.71197200	4.38788800	0.32763000
H	-5.70396200	4.69999400	-2.13490700
C	-2.87264900	0.45085000	1.90803500
C	-1.82823300	1.29159400	2.32709900
C	-3.71686100	-0.14853700	2.85287800
C	-1.63528300	1.53334700	3.68414600
H	-1.17327800	1.75233000	1.59203000
C	-3.51447600	0.09781400	4.21139400
H	-4.52145900	-0.80105300	2.53107600
C	-2.47695700	0.93391300	4.62651000
H	-0.82674600	2.18073900	4.00843300
H	-4.16645200	-0.36696000	4.94421700
H	-2.31975200	1.11685100	5.68486900
Au	-1.03589500	-0.24592200	-0.84342300

Zero-point correction= 0.563707 (Hartree/Particle)

Thermal correction to Energy= 0.601189

Thermal correction to Enthalpy= 0.602133

Thermal correction to Gibbs Free Energy= 0.481987

Sum of electronic and zero-point Energies= -2338.646979

Sum of electronic and thermal Energies= -2338.609497

Sum of electronic and thermal Enthalpies= -2338.608553

Sum of electronic and thermal Free Energies= -2338.728699

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2340.044642

TS3´-c

C	0.04110700	-2.23442300	-2.74151700
H	-0.00733300	-1.91510300	-3.76246300
C	0.25370300	-2.75344300	-1.64957400
C	0.52441300	-3.53016400	-0.40886900
H	-0.15483000	-4.38859900	-0.40006600
H	1.55494100	-3.90995800	-0.46797300
O	0.29556300	-2.82079800	0.78340900
C	1.38934900	-1.95622500	1.20029200
H	1.12353100	-1.68029800	2.22280600
H	2.31094000	-2.54463600	1.23637700
C	1.52329500	-0.73146800	0.35510400
H	0.82947600	0.07259800	0.57726900
C	2.58786700	-0.43059400	-0.51405800
C	2.38546400	0.73588700	-1.46038100
H	3.33810000	1.11244100	-1.84516500
H	1.79203900	0.39857800	-2.32151300
H	1.85317300	1.55483200	-0.97248600
C	3.49416300	-1.52375700	-1.04738100
H	3.78363600	-2.24560500	-0.28021300
H	2.97786900	-2.06041600	-1.85320000
H	4.40792100	-1.10184300	-1.47294700
S	3.96364700	0.53287200	1.03813800
O	3.44985600	1.90615100	1.25715300
O	4.01411000	-0.45268500	2.14218700
C	5.59795100	0.66564900	0.31620900
C	6.49994600	-0.38792800	0.48145500
C	5.90228400	1.78883600	-0.45731700
C	7.74722400	-0.30085800	-0.13480100

H	6.23213300	-1.23615500	1.10153700
C	7.15299500	1.85887600	-1.06893500
H	5.18414600	2.59653600	-0.54510000
C	8.07006900	0.81606700	-0.91072800
H	8.46949100	-1.10066100	-0.00422000
H	7.41537900	2.73012000	-1.66095800
H	9.04277400	0.87678600	-1.38908200
P	-2.49829000	0.45239200	0.12083000
C	-1.33337800	1.37281300	1.16352600
C	-0.54745800	2.37532900	0.56766800
C	-1.08832300	0.98301500	2.48563700
C	0.48048100	2.96988900	1.29175100
H	-0.73291400	2.67302400	-0.46090800
C	-0.05088700	1.58419100	3.20246400
H	-1.69246000	0.21098900	2.94931800
C	0.73895900	2.56518900	2.60560400
H	1.10346000	3.72741600	0.82881700
H	0.14409600	1.27505200	4.22456200
H	1.56938400	3.00250600	3.14777100
C	-3.53713400	-0.56811700	1.20153700
C	-3.01631700	-1.77449900	1.69996700
C	-4.82343600	-0.14937700	1.56605700
C	-3.78252200	-2.54709500	2.57027300
H	-2.01855300	-2.10174400	1.41706900
C	-5.58482700	-0.93562100	2.43090300
H	-5.22879700	0.77774200	1.17463100
C	-5.06605800	-2.13013800	2.93340900
H	-3.38036500	-3.47715900	2.95988900
H	-6.58359200	-0.61476200	2.70981700
H	-5.66291000	-2.73894400	3.60551300
C	-3.54429700	1.64162200	-0.75066700
C	-4.09170400	1.29690400	-1.99507300
C	-3.85758900	2.87560900	-0.16022100
C	-4.95301700	2.18050300	-2.64229900
H	-3.84419900	0.34166200	-2.45037700
C	-4.71809400	3.75509500	-0.81603600
H	-3.42662200	3.14710700	0.79817000
C	-5.26517500	3.40836000	-2.05351400
H	-5.37558300	1.91442500	-3.60603700
H	-4.95875300	4.71118500	-0.36191900
H	-5.93232100	4.09763000	-2.56181500
Au	-1.22693400	-0.93669200	-1.24031200

Zero-point correction= 0.558549 (Hartree/Particle)
Thermal correction to Energy= 0.597043
Thermal correction to Enthalpy= 0.597987
Thermal correction to Gibbs Free Energy= 0.480715
Sum of electronic and zero-point Energies= -2338.607745
Sum of electronic and thermal Energies= -2338.569251
Sum of electronic and thermal Enthalpies= -2338.568307
Sum of electronic and thermal Free Energies= -2338.685579
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2340.000544

INT3′-c

C	0.63521900	3.49302300	-1.86202500
H	0.92792600	3.44289000	-2.89118300
C	0.19466900	3.80575800	-0.76033900
C	-0.32304400	4.27286800	0.54818500
H	0.52911500	4.42604100	1.21848100
H	-0.80240100	5.25129300	0.38437300
O	-1.18277100	3.36292700	1.18233900
C	-2.57405600	3.42971100	0.78614900
H	-3.11338000	3.01597000	1.63685800
H	-2.84992900	4.49103500	0.67907900
C	-2.86024600	2.67637700	-0.46891000
H	-2.31060700	2.95854500	-1.36135400
C	-3.68043700	1.43528700	-0.54732100
C	-3.87167200	0.99059300	-2.00008900
H	-4.43240100	0.05435500	-2.06142300
H	-4.43789300	1.76026400	-2.53457200
H	-2.90752700	0.85841900	-2.49912100
C	-5.01448800	1.51264400	0.20665700
H	-4.87734900	1.75513200	1.26212700
H	-5.63851600	2.28473500	-0.25413000
H	-5.55016500	0.56097600	0.13909100
S	-2.61872700	0.12283300	0.32140500
O	-1.33681100	0.07238100	-0.42332100
O	-2.61888500	0.44554100	1.76260900
C	-3.41506400	-1.46029100	0.10309900
C	-4.36242000	-1.87748000	1.04192100
C	-3.06518200	-2.24689000	-0.99604700
C	-4.98555200	-3.11092500	0.85995700
H	-4.58160200	-1.25659800	1.90335800
C	-3.69635900	-3.47834900	-1.16263000
H	-2.29609000	-1.91089600	-1.68128000
C	-4.65716600	-3.90510300	-0.24257000
H	-5.72056500	-3.45524300	1.58053300
H	-3.43040500	-4.10735700	-2.00617600
H	-5.14668500	-4.86452500	-0.37951700
P	1.83907000	-0.50948200	0.08621300
C	3.61423700	-0.76701500	-0.20466600
C	4.49476000	0.31034300	-0.02644600
C	4.11520500	-2.03088800	-0.54678400
C	5.86606000	0.12166200	-0.18117600
H	4.10430100	1.29129700	0.23163200
C	5.48978400	-2.21174200	-0.70396300
H	3.43700200	-2.86500800	-0.69321400
C	6.36390200	-1.13914200	-0.52090000
H	6.54512800	0.95735000	-0.04333400
H	5.87605400	-3.19027100	-0.97206400
H	7.43253000	-1.28325700	-0.64721800
C	0.98816800	-1.88239800	-0.74738600
C	0.88357500	-1.85999600	-2.14512700
C	0.47909400	-2.96638100	-0.02406800
C	0.29236700	-2.92820300	-2.81600700
H	1.26667600	-1.01047300	-2.70457000
C	-0.11549100	-4.03225800	-0.70117600
H	0.54329700	-2.97748700	1.05852400
C	-0.20279200	-4.01821100	-2.09355700
H	0.22013200	-2.91275200	-3.89929700
H	-0.51355900	-4.87057800	-0.13819900
H	-0.65890700	-4.85299300	-2.61747300
C	1.55882000	-0.67833400	1.86956300
C	0.48071900	-0.00663400	2.46301700
C	2.38172500	-1.51456500	2.64008200

C	0.21474800	-0.19059100	3.81856800
H	-0.15782400	0.64269500	1.87762000
C	2.11240400	-1.68486000	3.99703600
H	3.22635500	-2.02192500	2.18477400
C	1.02860400	-1.02675000	4.58506300
H	-0.63207700	0.31964800	4.26575500
H	2.75001300	-2.32840800	4.59537800
H	0.82266900	-1.16459100	5.64230400
Au	1.10857500	1.56258600	-0.66953300

Zero-point correction= 0.559696 (Hartree/Particle)
Thermal correction to Energy= 0.598240
Thermal correction to Enthalpy= 0.599185
Thermal correction to Gibbs Free Energy= 0.482462
Sum of electronic and zero-point Energies= -2338.622403
Sum of electronic and thermal Energies= -2338.583859
Sum of electronic and thermal Enthalpies= -2338.582915
Sum of electronic and thermal Free Energies= -2338.699637
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2340.008896

TS7′-c

C	0.79957700	-0.73598100	0.81202200
H	1.09798800	-1.76884600	0.78851400
C	1.16056700	0.45546500	0.84013400
C	1.26643700	1.92380400	0.97472300
H	0.25867200	2.33189300	1.10876300
H	1.83841100	2.14098100	1.89271300
O	1.82232600	2.54372500	-0.15070200
C	3.22500900	2.24089900	-0.26193100
H	3.56358200	2.77006900	-1.15910600
H	3.76253800	2.66225100	0.59457700
C	3.44116100	0.76941600	-0.40431100
H	2.95562900	0.30534400	-1.25901300
C	4.56928100	0.02040400	0.20699400
C	4.40867700	-1.49191600	0.03372200
H	5.30331400	-2.02305900	0.36989600
H	3.56895200	-1.83875000	0.64550900
H	4.21852700	-1.75104000	-1.01079800
C	4.87908600	0.39707900	1.65956100
H	5.12064400	1.45584700	1.76856400
H	4.01066900	0.16510400	2.28670600
H	5.72533700	-0.18593000	2.03262300
S	6.05444100	0.57274300	-0.86987500
O	5.77030700	0.08126100	-2.22849000
O	6.22534500	2.01222200	-0.59631500
C	7.48404700	-0.29287000	-0.23771100
C	8.24327700	0.29782000	0.77563900
C	7.81497700	-1.53761300	-0.77935500
C	9.35366700	-0.38767200	1.26581100
H	7.97914800	1.28226000	1.14513300
C	8.92840700	-2.21064300	-0.27868300
H	7.22519500	-1.94701400	-1.59185900
C	9.69068100	-1.63941500	0.74376100
H	9.96140600	0.05905800	2.04637700
H	9.20707600	-3.17436100	-0.69316700
H	10.55833100	-2.16714000	1.12782900
P	-3.60239700	-0.14778200	-0.04663300
C	-4.64765000	-0.81448600	1.27550300
C	-4.25821300	-0.63410500	2.61127100
C	-5.85645600	-1.45834800	0.97589400
C	-5.07901100	-1.08843400	3.64078800
H	-3.31732800	-0.14065300	2.84069000
C	-6.67112300	-1.91350500	2.01265600
H	-6.15526700	-1.60563300	-0.05677500
C	-6.28453600	-1.72882700	3.34142500
H	-4.77668700	-0.94973400	4.67405100
H	-7.60563300	-2.41504800	1.78142900
H	-6.92007400	-2.08806800	4.14491200
C	-4.04638300	-1.00571200	-1.58070400
C	-3.51752400	-2.28311100	-1.82067400
C	-4.93732000	-0.42947700	-2.49630400
C	-3.88476900	-2.98157700	-2.96804700
H	-2.82392300	-2.72657800	-1.11075800
C	-5.29751200	-1.13445900	-3.64517500
H	-5.34176200	0.56094300	-2.31550800
C	-4.77353900	-2.40658200	-3.88087700
H	-3.47487200	-3.96935000	-3.15391000
H	-5.98499800	-0.68760800	-4.35652100
H	-5.05372800	-2.94977200	-4.77807100
C	-4.03090200	1.60323200	-0.25844800
C	-3.17037400	2.42304300	-1.00583000
C	-5.21233900	2.12962800	0.28003100
C	-3.49622000	3.76020200	-1.21758600
H	-2.25386100	2.01308700	-1.42304600
C	-5.52948400	3.47180400	0.06652600
H	-5.87600800	1.49889500	0.86204000
C	-4.67502600	4.28508000	-0.67948100
H	-2.83090100	4.39290200	-1.79669400
H	-6.44356200	3.88089000	0.48544100
H	-4.92477900	5.32924800	-0.84034900
Au	-1.33328800	-0.35599800	0.42232000

Zero-point correction= 0.559243 (Hartree/Particle)
Thermal correction to Energy= 0.597144
Thermal correction to Enthalpy= 0.598088
Thermal correction to Gibbs Free Energy= 0.478137
Sum of electronic and zero-point Energies= -2338.595456
Sum of electronic and thermal Energies= -2338.557555
Sum of electronic and thermal Enthalpies= -2338.556611
Sum of electronic and thermal Free Energies= -2338.676562
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2339.991141

INT7′-c

C	-0.94490200	-0.52704200	-0.26190600
H	-1.36567000	-1.52814200	-0.18882700
C	-1.69276400	0.59345200	-0.32140100
C	-1.24026900	1.94353200	-0.86067200
H	-0.15713500	2.06040300	-0.91578100
H	-1.67697500	2.09955800	-1.86225400
O	-1.76669100	2.83657400	0.09252600
C	-3.10559400	2.40826800	0.33029900
H	-3.43652600	2.82892600	1.27778900
H	-3.76603500	2.76731800	-0.46467700
C	-3.03967200	0.84459400	0.35304100
H	-2.98713700	0.51336800	1.39555900
C	-4.22468900	0.07267900	-0.30010900

C	-4.09794200	-1.44170500	-0.11525500
H	-5.02781200	-1.94367500	-0.39315100
H	-3.32070900	-1.83298100	-0.77754900
H	-3.85932500	-1.70336800	0.91908800
C	-4.47130500	0.42826100	-1.76688300
H	-4.67473200	1.49074000	-1.91006500
H	-3.59676300	0.15107300	-2.36629900
H	-5.32486700	-0.13494500	-2.15441300
S	-5.69929700	0.63820600	0.73416300
O	-5.36279500	0.27345500	2.12237500
O	-5.97386600	2.03698400	0.35881300
C	-7.08629000	-0.35529100	0.20030800
C	-7.85869700	0.08884100	-0.87575200
C	-7.38631300	-1.53074000	0.89268200
C	-8.94726600	-0.68286200	-1.27990300
H	-7.62520300	1.03025200	-1.36003900
C	-8.47991400	-2.28937600	0.47816300
H	-6.78717700	-1.82233400	1.74802600
C	-9.25239200	-1.86938900	-0.60806800
H	-9.56359200	-0.35173100	-2.10964300
H	-8.73490800	-3.20129300	1.00863900
H	-10.10408500	-2.46356400	-0.92470000
P	3.45635000	-0.17011300	0.00448200
C	4.28419500	-1.23213300	-1.20826300
C	3.68095700	-1.43577200	-2.45866000
C	5.53156500	-1.80749000	-0.92709800
C	4.32791200	-2.20285000	-3.42457300
H	2.71027300	-0.99514400	-2.67071100
C	6.17119800	-2.57747100	-1.89841300
H	5.99575400	-1.65665100	0.04203700
C	5.57204900	-2.77447000	-3.14404300
H	3.86058200	-2.36091000	-4.39150300
H	7.13584300	-3.02510000	-1.68056300
H	6.07190000	-3.37758800	-3.89570300
C	4.15355800	-0.55652800	1.63352900
C	3.72815900	-1.72589500	2.28447700
C	5.11780300	0.26934700	2.22779000
C	4.27636600	-2.07184100	3.51647900
H	2.97382600	-2.35960800	1.82513800
C	5.65935900	-0.08314800	3.46407200
H	5.44193600	1.17649800	1.72889200
C	5.24068800	-1.24963700	4.10705000
H	3.94840900	-2.97617800	4.01930800
H	6.40724500	0.55470900	3.92471600
H	5.66203000	-1.51714600	5.07113400
C	3.88978400	1.54947500	-0.38079700
C	3.14271700	2.57973800	0.21320600
C	4.95833600	1.85855100	-1.23263600
C	3.46995000	3.90956100	-0.03892900
H	2.31342500	2.33904900	0.87402500
C	5.27738600	3.19368700	-1.48373100
H	5.53346600	1.06425500	-1.69680300
C	4.53626900	4.21645400	-0.88963300
H	2.89266800	4.70473600	0.42239200
H	6.10424500	3.43328400	-2.14503400
H	4.78649500	5.25357500	-1.09049100
Au	1.10379000	-0.40898600	-0.01276300

Zero-point correction= 0.563791 (Hartree/Particle)
Thermal correction to Energy= 0.600765
Thermal correction to Enthalpy= 0.601710
Thermal correction to Gibbs Free Energy= 0.484588
Sum of electronic and zero-point Energies= -2338.639248
Sum of electronic and thermal Energies= -2338.602274
Sum of electronic and thermal Enthalpies= -2338.601330
Sum of electronic and thermal Free Energies= -2338.718451
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2340.032539

TS4´-c

C	0.25098400	-3.56273700	1.34314700
H	0.62050000	-3.77638600	2.32539100
C	-0.32760300	-3.49423900	0.26332100
C	-1.02904900	-3.60479200	-1.04284700
H	-0.53420200	-4.39633700	-1.61577100
H	-2.06260800	-3.92278100	-0.84633700
O	-0.97600000	-2.43911800	-1.83016300
C	-2.05758000	-1.50627400	-1.65625600
H	-1.95518400	-0.81528700	-2.49305800
H	-3.01481300	-2.03034600	-1.75733800
C	-1.94618800	-0.76253900	-0.34375100
H	-0.98210500	-0.26559300	-0.24798500
C	-2.50527700	-1.21601800	0.86180500
C	-1.96173500	-0.72533500	2.16963700
H	-2.73291600	-0.19296700	2.74255700
H	-1.64445700	-1.57342800	2.79422200
H	-1.10728600	-0.05529200	2.04515700
C	-3.72541400	-2.08397400	0.94309500
H	-4.11736800	-2.38403400	-0.03059600
H	-3.51510000	-2.99214800	1.52635700
H	-4.53206600	-1.55758500	1.47085700
S	-2.87439900	1.23003700	-0.84204300
O	-2.11139800	2.20218300	-0.01766900
O	-2.99590900	1.39798200	-2.31181200
C	-4.51976200	1.09007100	-0.14844600
C	-5.52377500	0.50657200	-0.92207900
C	-4.72238200	1.44437500	1.18546800
C	-6.76842200	0.27604900	-0.33736200
H	-5.33459600	0.26053200	-1.96158900
C	-5.97249600	1.20737100	1.75747400
H	-3.92057000	1.91085700	1.74675200
C	-6.98891900	0.61883300	0.99978000
H	-7.56735400	-0.16484200	-0.92531100
H	-6.15567800	1.48798900	2.79013200
H	-7.95948400	0.43499900	1.45019800
P	2.13076100	0.45680600	-0.01997100
C	1.25751400	1.20484900	-1.42044600
C	0.82258800	0.37333800	-2.46637400
C	1.03068400	2.58730000	-1.48354300
C	0.16111800	0.92508900	-3.55992300
H	0.98080800	-0.69991000	-2.41457500
C	0.36229000	3.12842000	-2.58072900
H	1.35023100	3.23291300	-0.67310900
C	-0.07653300	2.30050700	-3.61375700
H	-0.18387500	0.28039200	-4.36211800
H	0.16979000	4.19566500	-2.61778100

H	-0.61701600	2.72313100	-4.45422300
C	3.89561700	0.35661100	-0.41445600
C	4.66829700	-0.69918600	0.08891500
C	4.49603600	1.36582700	-1.18182400
C	6.03859100	-0.73907300	-0.16527600
H	4.19794300	-1.48526500	0.67386100
C	5.86508100	1.31614700	-1.43597800
H	3.89594600	2.17616800	-1.58359800
C	6.63554000	0.26736100	-0.92727900
H	6.63662300	-1.55728700	0.22350100
H	6.32996900	2.09349600	-2.03417000
H	7.70135000	0.23150000	-1.13058200
C	1.93853000	1.55057800	1.41594800
C	3.02490400	1.79626400	2.26606300
C	0.67322800	2.08695900	1.70922500
C	2.84486600	2.57576400	3.40905000
H	4.00396000	1.38935700	2.03528100
C	0.50820000	2.86773000	2.85134900
H	-0.17097200	1.93451900	1.04347700
C	1.58917200	3.10957400	3.70344000
H	3.68821400	2.77039600	4.06429400
H	-0.46646900	3.29454000	3.06701300
H	1.45457600	3.71944100	4.59155000
Au	1.17229100	-1.61336700	0.43041300

Zero-point correction= 0.558448 (Hartree/Particle)
Thermal correction to Energy= 0.597147
Thermal correction to Enthalpy= 0.598091
Thermal correction to Gibbs Free Energy= 0.481479
Sum of electronic and zero-point Energies= -2338.616379
Sum of electronic and thermal Energies= -2338.577679
Sum of electronic and thermal Enthalpies= -2338.576735
Sum of electronic and thermal Free Energies= -2338.693348
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2340.008878

INT4´-c

C	0.13354200	3.57643000	-1.21234200
H	0.53611600	3.87005300	-2.16031200
C	-0.49886800	3.39983000	-0.17592200
C	-1.26401200	3.37135700	1.09647200
H	-0.85930100	4.15737700	1.74369300
H	-2.31030600	3.61909500	0.87407000
O	-1.14452400	2.15662800	1.80171000
C	-2.17522700	1.18322500	1.60451700
H	-2.04481700	0.47658400	2.42372000
H	-3.15930500	1.65659300	1.70040800
C	-2.02575600	0.43903300	0.27493700
H	-0.98183500	0.11473100	0.20236700
C	-2.45142700	1.12170400	-0.96534300
C	-1.79552000	0.77613400	-2.26393300
H	-2.39813600	0.05235000	-2.83446200
H	-1.69063900	1.66649600	-2.89848400
H	-0.80716900	0.32570500	-2.13277600
C	-3.68029500	1.97628600	-1.03660300
H	-4.21738600	2.05494900	-0.08863400
H	-3.43222000	2.99391700	-1.37706000
H	-4.39176100	1.57621300	-1.77184100
S	-2.81285800	-1.28466100	0.42123200
O	-2.25158700	-2.05287900	-0.70926200
O	-2.64895300	-1.75252500	1.80980900
C	-4.54958200	-1.01609600	0.10222500
C	-5.36454100	-0.57894100	1.14819300
C	-5.03873600	-1.19722100	-1.19142600
C	-6.70345900	-0.29694800	0.87992400
H	-4.96148200	-0.48747000	2.15131900
C	-6.38126300	-0.91640400	-1.44431700
H	-4.37896600	-1.56458100	-1.96947800
C	-7.20708300	-0.46002000	-0.41365400
H	-7.35569500	0.03761900	1.68045900
H	-6.78390500	-1.05947200	-2.44219400
H	-8.25108300	-0.24176700	-0.61631600
P	2.16235200	-0.41348800	0.02953900
C	1.28554500	-1.23311800	1.38862900
C	0.87627800	-0.45602900	2.48530700
C	1.04962900	-2.61565300	1.38094000
C	0.24017800	-1.06264900	3.56464300
H	1.03972700	0.61757700	2.48563200
C	0.40350700	-3.21113500	2.46342200
H	1.35282200	-3.21847600	0.53220200
C	-0.00093400	-2.43831400	3.55168400
H	-0.07806900	-0.45996400	4.40968400
H	0.20591600	-4.27799700	2.44881400
H	-0.51631300	-2.90539100	4.38464900
C	3.90598000	-0.24764500	0.48896100
C	4.65196200	0.84563900	0.02708200
C	4.51992500	-1.24373000	1.26272100
C	6.00972900	0.93677500	0.33000700
H	4.17083500	1.62033800	-0.56426400
C	5.87636600	-1.14301100	1.56535900
H	3.93972800	-2.08425100	1.63034900
C	6.62043900	-0.05635200	1.09874400
H	6.58720200	1.78392600	-0.02651500
H	6.35176600	-1.91037300	2.16817200
H	7.67629400	0.01919000	1.33965700
C	2.06546800	-1.47810800	-1.43575300
C	3.20986300	-1.74153500	-2.20021900
C	0.81685100	-1.98714000	-1.83057500
C	3.10307000	-2.51246900	-3.35831200
H	4.17546600	-1.35415800	-1.89275900
C	0.72431200	-2.75971400	-2.98564200
H	-0.07761800	-1.81743400	-1.23990600
C	1.86380300	-3.01998100	-3.75202300
H	3.99043400	-2.71999200	-3.94820300
H	-0.24080300	-3.16152700	-3.27785100
H	1.78661900	-3.62238400	-4.65200400
Au	1.12324500	1.62613200	-0.37176200

Zero-point correction= 0.559932 (Hartree/Particle)
Thermal correction to Energy= 0.598622
Thermal correction to Enthalpy= 0.599566
Thermal correction to Gibbs Free Energy= 0.483144
Sum of electronic and zero-point Energies= -2338.619689
Sum of electronic and thermal Energies= -2338.580999
Sum of electronic and thermal Enthalpies= -2338.580055
Sum of electronic and thermal Free Energies= -2338.696477

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2340.011368

TS8´-c

C	-0.18306300	-3.49750900	0.37853000
H	0.01799100	-3.99844800	1.30637300
C	-0.88344400	-2.78820500	-0.39254800
C	-1.32933300	-2.51304000	-1.79482300
H	-0.66444000	-3.04399200	-2.48120100
H	-2.34612200	-2.91307900	-1.91600600
O	-1.26248600	-1.15212900	-2.15014100
C	-2.29265500	-0.33295600	-1.60723900
H	-2.17465500	0.63718000	-2.09019100
H	-3.27423400	-0.74437600	-1.87281100
C	-2.14752300	-0.16281100	-0.09124300
H	-1.15376200	0.25636400	0.11101800
C	-2.36384800	-1.38315500	0.74284100
C	-1.76119200	-1.37969100	2.11611200
H	-2.39779600	-0.79955700	2.79677000
H	-1.67761500	-2.39623700	2.51467500
H	-0.77483000	-0.90545200	2.13066300
C	-3.61177300	-2.20968100	0.58682700
H	-4.04597300	-2.17002500	-0.41489100
H	-3.41680300	-3.25733400	0.84248100
H	-4.38773500	-1.85836400	1.28052400
S	-3.18547800	1.32385900	0.44551800
O	-3.01458700	1.45622300	1.90172000
O	-2.80453300	2.40953500	-0.47597300
C	-4.89344200	0.89466300	0.12844400
C	-5.39980400	1.01820100	-1.16743900
C	-5.68773000	0.46396700	1.19236500
C	-6.72774300	0.66463800	-1.40459200
H	-4.77673900	1.41294800	-1.96240100
C	-7.01579000	0.12083700	0.94212200
H	-5.27080200	0.42325500	2.19258400
C	-7.52997000	0.21163400	-0.35395300
H	-7.14002000	0.75816800	-2.40427900
H	-7.65067400	-0.20813800	1.75872500
H	-8.56471000	-0.05668000	-0.54338700
P	2.39232200	0.32602800	-0.00382400
C	1.36722200	1.54680900	0.86554400
C	1.10733700	1.34595000	2.23285900
C	0.75174300	2.60144900	0.18087900
C	0.24156800	2.20267800	2.90452000
H	1.58175300	0.52369400	2.76263700
C	-0.12139500	3.45109500	0.86283800
H	0.94027300	2.75185900	-0.87646400
C	-0.37797800	3.25154900	2.21792900
H	0.03531400	2.04524500	3.95837400
H	-0.62057900	4.24927100	0.32532600
H	-1.07766800	3.89754600	2.73700400
C	2.65234300	0.91787400	-1.69654100
C	1.67361600	0.65818800	-2.66942200
C	3.78854900	1.67228400	-2.02012600
C	1.83263800	1.16498200	-3.95784100
H	0.79546700	0.06666800	-2.42433100
C	3.94036500	2.16900800	-3.31420400
H	4.54899500	1.86492900	-1.27043500
C	2.96433200	1.91802500	-4.28069700
H	1.07669000	0.96533800	-4.71099900
H	4.82212600	2.74925400	-3.56737900
H	3.08794000	2.30531400	-5.28737700
C	3.99299500	0.23241200	0.83375300
C	4.75295900	-0.94192200	0.72808900
C	4.49709800	1.33815900	1.53439700
C	6.01491800	-1.00551100	1.31497700
H	4.35730700	-1.79831900	0.18825000
C	5.76028800	1.26506100	2.12082600
H	3.90409700	2.24248700	1.62606700
C	6.51769100	0.09694200	2.01080100
H	6.60262900	-1.91455000	1.23482800
H	6.15069300	2.11886600	2.66571800
H	7.49902600	0.04339300	2.47198000
Au	1.14628700	-1.63265800	0.03517100

Zero-point correction= 0.560387 (Hartree/Particle)
Thermal correction to Energy= 0.597749
Thermal correction to Enthalpy= 0.598693
Thermal correction to Gibbs Free Energy= 0.484803
Sum of electronic and zero-point Energies= -2338.610060
Sum of electronic and thermal Energies= -2338.572699
Sum of electronic and thermal Enthalpies= -2338.571754
Sum of electronic and thermal Free Energies= -2338.685644

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2339.999995

INT8´-c

C	0.41792900	-3.12089900	-0.60723300
H	0.41210400	-3.54486700	-1.60575300
C	1.32877400	-2.38658400	0.07138500
C	1.33217300	-2.36816700	1.59493100
H	0.51251900	-2.96385300	1.99606500
H	2.28413700	-2.79425900	1.94746400
O	1.16283700	-1.04759800	2.07260600
C	2.19260000	-0.17223800	1.62574600
H	1.96322500	0.80769900	2.04105300
H	3.16140200	-0.50945500	2.01775600
C	2.20864900	-0.09106800	0.09252100
H	1.24185000	0.32207700	-0.22350600
C	2.37964700	-1.47872200	-0.60805500
C	2.12947000	-1.38600000	-2.11952800
H	2.86135500	-0.72863200	-2.58688800
H	2.20603300	-2.37540400	-2.58108700
H	1.13681400	-0.97509100	-2.33321100
C	3.75247800	-2.15570400	-0.35637200
H	4.08363200	-2.08650100	0.68184900
H	3.70343300	-3.21385100	-0.63215500
H	4.51422800	-1.68599900	-0.97934400
S	3.30225700	1.31028600	-0.43548000
O	3.15437500	1.46304400	-1.89206100
O	2.93720800	2.40429600	0.47932300
C	4.99902400	0.85869300	-0.09748600
C	5.47401200	0.91836400	1.21462400
C	5.82341300	0.49486400	-1.16364800
C	6.79784000	0.55894400	1.46531600
H	4.83204800	1.27113100	2.01415500
C	7.14755700	0.14685100	-0.89958700

H	5.43162700	0.50501400	-2.17478700
C	7.62866700	0.16770500	0.41214100
H	7.18482900	0.60073100	2.47848900
H	7.80489100	-0.13157300	-1.71715800
H	8.66010000	-0.10522800	0.61248900
P	-2.48849300	0.27906900	-0.00277400
C	-1.40803800	1.69596100	-0.35872100
C	-0.72680900	1.71796600	-1.58889600
C	-1.18378100	2.70663100	0.58418000
C	0.17321600	2.74184200	-1.86794000
H	-0.89729700	0.92969800	-2.31837600
C	-0.27749300	3.72860700	0.29659200
H	-1.70176300	2.68926800	1.53686500
C	0.40391900	3.74304800	-0.91967200
H	0.72127500	2.74190800	-2.80328700
H	-0.09248900	4.50459800	1.03241400
H	1.13245500	4.52017400	-1.12341500
C	-3.03554500	0.42443100	1.71877900
C	-2.11806300	0.12685500	2.74075500
C	-4.33084100	0.85421400	2.03362800
C	-2.50138500	0.27126800	4.07184100
H	-1.11210500	-0.20589900	2.49641700
C	-4.70604300	0.98855800	3.37101100
H	-5.03930800	1.07953900	1.24344100
C	-3.79455600	0.69904100	4.38734500
H	-1.79367800	0.04464700	4.86332600
H	-5.71070000	1.31808200	3.61677300
H	-4.09145300	0.80370200	5.42637800
C	-3.93463900	0.37610400	-1.08352500
C	-4.63783700	-0.79666000	-1.39573800
C	-4.37908200	1.61578300	-1.56570000
C	-5.78724300	-0.72648800	-2.17996900
H	-4.28604600	-1.75640300	-1.02591000
C	-5.52859800	1.67669400	-2.35274300
H	-3.82751600	2.52100500	-1.33213900
C	-6.23149900	0.50911800	-2.65805800
H	-6.33157700	-1.63350200	-2.42331200
H	-5.87263100	2.63464800	-2.72992000
H	-7.12387200	0.56087600	-3.27416500
Au	-1.10327900	-1.58084700	-0.29819900

Zero-point correction= 0.565158 (Hartree/Particle)
Thermal correction to Energy= 0.601524
Thermal correction to Enthalpy= 0.602468
Thermal correction to Gibbs Free Energy= 0.490951
Sum of electronic and zero-point Energies= -2338.643744
Sum of electronic and thermal Energies= -2338.607378
Sum of electronic and thermal Enthalpies= -2338.606434
Sum of electronic and thermal Free Energies= -2338.717951
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2340.034243

TS11-c

C	0.92053800	1.65386000	-1.35553900
H	0.09655600	2.34660800	-1.21663600
C	0.83822000	0.35296800	-1.45194800
C	1.71862800	-0.81973100	-1.59798500
H	2.28032900	-0.73735900	-2.54200000
H	2.44582500	-0.78996400	-0.76969500
O	0.96135400	-2.01316500	-1.55183600
C	1.75311800	-3.15926200	-1.20375400
H	1.07785100	-4.00470700	-1.36298200
H	2.59131300	-3.26205300	-1.90562600
C	2.20261000	-3.10676300	0.22719500
H	1.38943500	-3.16815400	0.94680400
C	3.44901200	-2.93172200	0.69315900
C	3.70674400	-2.85323800	2.17694100
H	4.43600600	-3.61155500	2.49257300
H	4.12972200	-1.87576900	2.44402800
H	2.79010600	-2.99583600	2.75630000
C	4.68245200	-2.80128600	-0.16409400
H	4.47167000	-2.79672500	-1.23536900
H	5.21732800	-1.87350200	0.07759600
H	5.38162300	-3.62354100	0.03827800
S	2.54309400	2.47423500	-1.42096500
O	3.37600100	1.78549200	-2.42042700
O	2.27918000	3.91866000	-1.49065300
C	3.24199800	2.10027300	0.19051900
C	2.76597100	2.78004800	1.31255300
C	4.23660300	1.12796100	0.28878600
C	3.29060200	2.46337500	2.56356700
H	2.00979700	3.54981700	1.19979800
C	4.76168500	0.82811800	1.54641100
H	4.59903900	0.64204800	-0.61007300
C	4.28459600	1.48767600	2.68013800
H	2.93121800	2.98293700	3.44659300
H	5.54922400	0.08632500	1.63861500
H	4.69420200	1.24839400	3.65708500
S	-3.81633000	-0.85676700	-0.93410100
O	-4.19782300	-0.52084100	-2.30893700
O	-4.00548200	-2.19446600	-0.36427600
C	-4.57311200	0.33831600	0.16083800
C	-4.89381100	-0.03939800	1.46335900
C	-4.82187600	1.62120000	-0.32713000
C	-5.48597300	0.90464500	2.30078100
H	-4.68744100	-1.04784800	1.80045400
C	-5.41053500	2.55362300	0.52405700
H	-4.57102600	1.87140900	-1.35192200
C	-5.73958300	2.19605700	1.83415900
H	-5.75046400	0.62991400	3.31726200
H	-5.61734300	3.55640000	0.16315600
H	-6.19884200	2.92710000	2.49299000
S	-1.65502300	-0.35704800	-0.94212300
C	-1.17700700	-1.22727800	0.60348700
F	-1.13349100	-2.55467000	0.46279100
F	0.03605500	-0.80428300	0.99545200
F	-2.03868600	-0.95690800	1.60551500

Zero-point correction= 0.400153 (Hartree/Particle)
Thermal correction to Energy= 0.433305
Thermal correction to Enthalpy= 0.434250
Thermal correction to Gibbs Free Energy= 0.328882
Sum of electronic and zero-point Energies= -2683.144445
Sum of electronic and thermal Energies= -2683.111293
Sum of electronic and thermal Enthalpies= -2683.110349
Sum of electronic and thermal Free Energies= -2683.215717

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2684.076834

INT11-c

C	-0.48506100	-2.24477900	-0.37570000
H	-0.48590600	-3.19155600	0.15222200
C	0.62419000	-1.51814300	-0.57422700
C	0.64905600	-0.16368800	-1.24354600
H	0.07517800	-0.21705500	-2.17836600
H	0.13908200	0.55052700	-0.58026200
O	1.97806600	0.23089800	-1.47681100
C	2.12041600	1.63790600	-1.71164100
H	3.18271000	1.76021900	-1.94401700
H	1.54714100	1.92547200	-2.60263100
C	1.74537300	2.44427600	-0.50293000
H	2.34432000	2.22054600	0.37787900
C	0.74593800	3.33175000	-0.38570000
C	0.47839900	4.01759800	0.93030600
H	0.51273600	5.11011200	0.82254200
H	-0.52644600	3.76695900	1.29630500
H	1.20199900	3.72478900	1.69636900
C	-0.18194900	3.73844900	-1.50235900
H	-0.04283100	3.16186700	-2.41893000
H	-1.22751800	3.62727900	-1.18898200
H	-0.04411200	4.79964100	-1.74933900
S	-2.13150600	-1.76271500	-0.89440400
O	-2.09430200	-1.19305500	-2.25164700
O	-2.98992800	-2.90942100	-0.56812700
C	-2.52674600	-0.42622400	0.23810000
C	-2.79609900	-0.73416200	1.57331400
C	-2.55860100	0.88607600	-0.23167900
C	-3.08425300	0.30138700	2.45879500
H	-2.79170100	-1.76779400	1.90276300
C	-2.86158300	1.91335700	0.66302100
H	-2.36688200	1.08361200	-1.28036400
C	-3.11492000	1.62280700	2.00427400
H	-3.29393300	0.07824200	3.50039600
H	-2.90783100	2.93924700	0.31090800
H	-3.34648500	2.42662700	2.69689800
S	2.15252300	-2.29402000	-0.06354800
C	2.87228700	-1.01133400	1.04019600
F	3.84661800	-0.28912800	0.47577300
F	1.93500300	-0.16218300	1.49793900
F	3.41669400	-1.64757800	2.09352800

Zero-point correction= 0.302143 (Hartree/Particle)
Thermal correction to Energy= 0.326046
Thermal correction to Enthalpy= 0.326990
Thermal correction to Gibbs Free Energy= 0.245702
Sum of electronic and zero-point Energies= -1903.061385
Sum of electronic and thermal Energies= -1903.037482
Sum of electronic and thermal Enthalpies= -1903.036537
Sum of electronic and thermal Free Energies= -1903.117826

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1903.754744

TS12-c

C	0.94902700	0.47460900	-0.08414700
H	0.85785200	1.38039500	0.49240200
C	1.82758200	-0.13237800	-0.83302500
C	1.66138600	-1.46233000	-1.56349200
H	1.16942500	-1.26089700	-2.52049400
H	2.65215300	-1.88668000	-1.77074300
O	0.84257800	-2.36390400	-0.86223700
C	1.54924800	-3.25961900	0.01645200
H	0.74799000	-3.85032900	0.47001500
H	2.16719300	-3.93451100	-0.58856300
C	2.35462900	-2.55763500	1.06646600
H	1.76542500	-1.97333900	1.76906900
C	3.69034600	-2.54159200	1.18982100
C	4.34592000	-1.73238700	2.27920700
H	4.94218400	-2.36987000	2.94623100
H	5.03611700	-1.00382500	1.83496600
H	3.61037900	-1.19594000	2.88749000
C	4.66186800	-3.26032200	0.29114100
H	4.18020300	-3.89017700	-0.45946100
H	5.28424200	-2.52468000	-0.23144000
H	5.33367500	-3.89655200	0.88238600
S	3.42300100	0.69407400	-1.20181300
O	4.51649400	-0.15393600	-0.69609300
O	3.38428700	1.07393600	-2.62385600
C	3.37558500	2.18364300	-0.21106900
C	2.93513600	3.36883300	-0.79837500
C	3.75622900	2.11769700	1.12992400
C	2.87032300	4.52017300	-0.01392000
H	2.66128300	3.37712300	-1.84763700
C	3.68217400	3.27474000	1.90302200
H	4.10363800	1.17990100	1.54872400
C	3.23933900	4.47107000	1.33210600
H	2.53476400	5.45438700	-0.45378400
H	3.97482600	3.24497500	2.94819600
H	3.18565600	5.37013400	1.93907200
S	-3.64332300	-0.47523500	-1.25580200
O	-3.54803700	0.18172400	-2.56319600
O	-4.06748100	-1.86983400	-1.09953400
C	-4.66081600	0.54493700	-0.19511600
C	-5.38948600	-0.05533300	0.82995600
C	-4.69833000	1.91902400	-0.43132200
C	-6.18173400	0.75391200	1.64269300
H	-5.33559400	-1.12723300	0.97590500
C	-5.49259400	2.71392100	0.39204100
H	-4.12885400	2.34519900	-1.24968900
C	-6.23014700	2.13257400	1.42663300
H	-6.76235200	0.30622300	2.44337500
H	-5.54067500	3.78516400	0.22223300
H	-6.84816100	2.75713100	2.06493600
S	-1.57782400	-0.24097100	-0.49871700
C	-1.66139500	-1.44509400	0.88594400
F	-1.68382000	-2.71306400	0.47914400
F	-0.59336700	-1.27076600	1.68227300
F	-2.76164900	-1.24361900	1.64167400

Zero-point correction= 0.400405 (Hartree/Particle)
Thermal correction to Energy= 0.433443
Thermal correction to Enthalpy= 0.434387
Thermal correction to Gibbs Free Energy= 0.329943
Sum of electronic and zero-point Energies= -2683.140555
Sum of electronic and thermal Energies= -2683.107517

Sum of electronic and thermal Enthalpies= -2683.106573
Sum of electronic and thermal Free Energies= -2683.211017
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2684.072336

INT12-c

C	-0.32500200	-0.78240000	-0.42861200
H	-1.19023200	-0.36495100	0.07086200
C	0.58796700	0.00395700	-1.00259600
C	1.81943500	-0.46505800	-1.74991900
H	1.56744100	-0.58135400	-2.81002700
H	2.61371700	0.28794900	-1.67489000
O	2.25729100	-1.72908200	-1.29355700
C	3.24830200	-1.67160600	-0.24087000
H	3.44689400	-2.72525100	-0.02293700
H	4.16328100	-1.23131800	-0.65426900
C	2.77738900	-0.94771400	0.98146800
H	1.97060900	-1.44390000	1.51854400
C	3.19688400	0.24574000	1.42916200
C	2.55043900	0.87598300	2.63526700
H	3.28582100	1.06615900	3.42858800
H	2.12260200	1.84683500	2.35517800
H	1.75497100	0.24721100	3.04745600
C	4.27697900	1.08566800	0.80015100
H	4.79219300	0.59161000	-0.02639400
H	3.83588200	2.01486700	0.42118300
H	5.03132100	1.36242800	1.54814300
S	0.37685900	1.78324300	-1.01406000
O	1.42813100	2.38123500	-0.17077600
O	0.26801700	2.17898700	-2.42853000
C	-1.19771700	2.07333700	-0.21492900
C	-2.34981300	2.13092200	-0.99907300
C	-1.24043900	2.21182300	1.17318300
C	-3.57856900	2.32744000	-0.37051300
H	-2.27080300	2.03168000	-2.07609200
C	-2.47590000	2.40434900	1.78891600
H	-0.32170000	2.17211100	1.74782600
C	-3.64025100	2.45951000	1.01862000
H	-4.48620200	2.37847600	-0.96398300
H	-2.53007000	2.51430800	2.86766300
H	-4.60038900	2.60875900	1.50369400
S	-0.22545400	-2.54725200	-0.36310800
C	-1.91441500	-2.80620900	0.28117200
F	-2.13308900	-2.15664500	1.44312800
F	-2.86917600	-2.39844300	-0.57396800
F	-2.06963100	-4.11991600	0.49622800

Zero-point correction= 0.302791 (Hartree/Particle)
Thermal correction to Energy= 0.326587
Thermal correction to Enthalpy= 0.327531
Thermal correction to Gibbs Free Energy= 0.246301
Sum of electronic and zero-point Energies= -1903.072552
Sum of electronic and thermal Energies= -1903.048756
Sum of electronic and thermal Enthalpies= -1903.047812
Sum of electronic and thermal Free Energies= -1903.129042
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1903.767156

TS13-c

C	-3.00185400	1.92038700	1.83445700
H	-3.54137500	1.37966600	2.57721900
C	-2.40709700	2.49976100	0.95882900
C	-1.65080900	3.17149200	-0.10625900
H	-2.33292000	3.50720100	-0.89424600
H	-1.14908400	4.06505700	0.29887500
O	-0.71987600	2.31864800	-0.75278200
C	0.35285800	1.90218100	0.08087400
H	1.15987900	2.65677300	0.06171300
H	0.02296200	1.79398500	1.12012300
C	0.88815300	0.61043400	-0.45169800
H	0.79360900	0.51061000	-1.53066400
C	2.12523900	-0.02324900	0.11002200
C	2.25468900	-1.49388100	-0.30133000
H	3.22921800	-1.89592000	-0.01110700
H	1.48092000	-2.07300600	0.20791900
H	2.12330200	-1.61612400	-1.37909500
C	2.34575500	0.17016200	1.61072700
H	2.33342100	1.22592900	1.89063500
H	1.56068000	-0.34828000	2.16255100
H	3.30691200	-0.25561200	1.91181800
S	3.53158300	0.92886700	-0.78766300
O	3.35745800	0.68892600	-2.23188300
O	3.54239600	2.30168000	-0.24088000
C	5.07034700	0.14788200	-0.28805000
C	5.73323900	0.61569300	0.84758200
C	5.57878700	-0.90135700	-1.05526600
C	6.92558900	0.00297100	1.23032000
H	5.32719900	1.45662900	1.39843500
C	6.77230900	-1.50476200	-0.66206100
H	5.05282900	-1.21626100	-1.94958700
C	7.43993200	-1.05716500	0.48036700
H	7.45650900	0.35803500	2.10839300
H	7.18398700	-2.31895400	-1.25067700
H	8.36945700	-1.53074300	0.78241300
S	-3.17403400	-1.77325900	-1.02773600
O	-2.97574600	-1.76797100	-2.48478600
O	-3.52010000	-2.99877800	-0.28931700
C	-4.36180000	-0.49777300	-0.61944100
C	-5.18847200	-0.66239300	0.48920200
C	-4.38786400	0.65388400	-1.40541000
C	-6.08466200	0.35841600	0.80575700
H	-5.13241500	-1.57284300	1.07423700
C	-5.28675100	1.66442300	-1.07402800
H	-3.72193200	0.74589900	-2.25601600
C	-6.13184400	1.51709900	0.02833400
H	-6.74869100	0.24579200	1.65770400
H	-5.32884500	2.56652900	-1.67691500
H	-6.82839300	2.31013900	0.28373100
S	-1.13838000	-0.83382700	-0.34538300
C	-1.24106900	-1.20009900	1.44064500
F	-0.56530000	-2.31735500	1.77243700
F	-0.70986100	-0.19862600	2.17621000
F	-2.50984200	-1.35598200	1.85810900

Zero-point correction= 0.399785 (Hartree/Particle)
Thermal correction to Energy= 0.432789
Thermal correction to Enthalpy= 0.433733
Thermal correction to Gibbs Free Energy= 0.331387

Sum of electronic and zero-point Energies= -2683.137377
Sum of electronic and thermal Energies= -2683.104373
Sum of electronic and thermal Enthalpies= -2683.103428
Sum of electronic and thermal Free Energies= -2683.205774
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2684.072887

INT13-c

C	5.06323100	-1.40295900	1.48195700
H	5.69985100	-0.84547900	2.13070900
C	4.35596200	-2.03635000	0.73664800
C	3.45920100	-2.76547600	-0.17041700
H	4.03681000	-3.25013700	-0.96399700
H	2.93178600	-3.55688400	0.38678600
O	2.53492000	-1.91959000	-0.83470900
C	1.58705700	-1.33005700	0.04007200
H	0.84404400	-2.07540500	0.34944000
H	2.07843800	-0.93332600	0.93272200
C	0.88843400	-0.21451500	-0.74117400
H	0.61187000	-0.63371900	-1.71617200
C	-0.42159300	0.31944100	-0.08865600
C	-0.94584300	1.57841400	-0.78525400
H	-1.92658100	1.85627000	-0.39236800
H	-0.26114500	2.40580100	-0.59848800
H	-1.02337200	1.43166400	-1.86561900
C	-0.33995100	0.50568100	1.42779600
H	-0.08914600	-0.42536400	1.93931400
H	0.41432700	1.25584900	1.66799600
H	-1.29813700	0.86352100	1.81626600
S	-1.68774400	-1.04696200	-0.42719000
O	-1.69592600	-1.26332300	-1.88730600
O	-1.43021200	-2.16732300	0.50064000
C	-3.28618300	-0.36396900	0.02799600
C	-3.72613600	-0.48998600	1.34626300
C	-4.07131500	0.24282200	-0.95286500
C	-4.97298300	0.02987100	1.69186400
H	-3.10966300	-1.00727000	2.07265000
C	-5.31741100	0.75502100	-0.59544100
H	-3.70972600	0.29245000	-1.97380600
C	-5.76317100	0.65446300	0.72459500
H	-5.33087600	-0.06173700	2.71283800
H	-5.94226700	1.22659200	-1.34779400
H	-6.73473000	1.05546300	0.99809400
S	2.09518200	1.06369900	-1.33785900
C	2.64823200	1.96267200	0.13685700
F	1.73899300	2.85118400	0.61675700
F	2.98192800	1.17486700	1.17804500
F	3.73175300	2.67010000	-0.21905100

Zero-point correction= 0.302341 (Hartree/Particle)
Thermal correction to Energy= 0.326049
Thermal correction to Enthalpy= 0.326993
Thermal correction to Gibbs Free Energy= 0.247351
Sum of electronic and zero-point Energies= -1903.035175
Sum of electronic and thermal Energies= -1903.011467
Sum of electronic and thermal Enthalpies= -1903.010523
Sum of electronic and thermal Free Energies= -1903.090165
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1903.733092

TS14-c

C	-1.61042800	4.25226100	-0.89040200
H	-2.13130000	4.69355700	-1.70964000
C	-0.98991200	3.77388300	0.02868700
C	-0.25698700	3.15954300	1.14206100
H	0.80084600	3.42929600	1.10803500
H	-0.67524000	3.50460300	2.10079000
O	-0.26867200	1.73702900	1.08720000
C	-1.55308800	1.16344600	1.24009100
H	-1.88737000	1.25876000	2.27935200
H	-2.28117300	1.66703800	0.59255400
C	-1.44238100	-0.31790900	0.87100700
H	-0.67757600	-0.78722600	1.50180900
C	-1.17186300	-0.64450800	-0.57859000
C	-0.98065500	-2.09861600	-0.91035400
H	-1.95000900	-2.61365100	-0.89492700
H	-0.55920700	-2.22288400	-1.90742300
H	-0.34527500	-2.60684300	-0.18132400
C	-1.78100400	0.22127600	-1.64814100
H	-1.63999400	1.28649800	-1.45235700
H	-1.32979200	-0.00993200	-2.61566300
H	-2.86123300	0.02948000	-1.72949100
S	-2.97809500	-1.17971100	1.56325600
O	-2.77220700	-2.63163500	1.44441700
O	-3.24652200	-0.56629300	2.87587700
C	-4.31469000	-0.72112900	0.45811800
C	-4.89823800	0.54041100	0.58381400
C	-4.72676300	-1.62576400	-0.51956900
C	-5.89357800	0.91374100	-0.31748700
H	-4.58875700	1.20500000	1.38265700
C	-5.72832700	-1.24332600	-1.41134600
H	-4.27487000	-2.61017000	-0.56341400
C	-6.30145400	0.02668100	-1.31670500
H	-6.35559000	1.89269800	-0.23494900
H	-6.06215100	-1.93696700	-2.17698600
H	-7.07694600	0.32250500	-2.01700800
S	3.21979100	1.38166300	-0.10034900
O	3.94716700	1.94409200	-1.25199300
O	2.76319400	2.24700400	1.00535800
C	4.19668500	0.05637100	0.60601200
C	3.89333500	-0.37159400	1.89853400
C	5.17441800	-0.55870100	-0.17369700
C	4.61016700	-1.44155400	2.42923300
H	3.12075000	0.13316300	2.46769600
C	5.88389600	-1.62692900	0.37378300
H	5.37319200	-0.19852800	-1.17584300
C	5.60115300	-2.06755600	1.66820200
H	4.39636400	-1.78640600	3.43636300
H	6.65687400	-2.11503700	-0.21203000
H	6.15407000	-2.90363900	2.08624400
S	1.16564900	0.25067700	-0.70126400
C	1.85579800	-0.87094000	-1.97294600
F	2.04410200	-2.12292500	-1.50907800
F	1.01626400	-0.96696400	-3.03183200
F	3.03926300	-0.44671800	-2.45014200

Zero-point correction= 0.400265 (Hartree/Particle)
Thermal correction to Energy= 0.433379

Thermal correction to Enthalpy= 0.434323
Thermal correction to Gibbs Free Energy= 0.330124
Sum of electronic and zero-point Energies= -2683.139260
Sum of electronic and thermal Energies= -2683.106147
Sum of electronic and thermal Enthalpies= -2683.105203
Sum of electronic and thermal Free Energies= -2683.209401
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2684.076227

INT14-c

C	0.27957000	4.10099900	1.78758400
H	0.69700400	4.26022100	2.75605700
C	-0.21333800	3.93673800	0.69774100
C	-0.79458100	3.70411100	-0.63047900
H	-1.80876000	4.11158500	-0.67700800
H	-0.18902100	4.21620600	-1.39519300
O	-0.92632400	2.32698000	-0.95014300
C	0.30970800	1.64205900	-1.05071600
H	0.85781900	1.97208000	-1.93897000
H	0.92541700	1.84207200	-0.16557700
C	0.00500400	0.14399100	-1.15739100
H	-0.54817100	-0.04323200	-2.08519800
C	-0.81543000	-0.45437500	0.03383000
C	-0.83705100	-1.98767000	0.00389700
H	0.16201900	-2.37014200	0.20985800
H	-1.49495000	-2.37277500	0.78114300
H	-1.15381100	-2.37886000	-0.96376200
C	-0.34713300	0.04726200	1.40589600
H	-0.40564700	1.13440300	1.48347400
H	-0.98883600	-0.37997200	2.17974400
H	0.68245700	-0.26800700	1.60258100
S	1.61669100	-0.69479000	-1.60418600
O	1.32939800	-2.08312000	-1.99072700
O	2.26992100	0.22031900	-2.55667800
C	2.63411200	-0.72995200	-0.12481300
C	3.28222300	0.43725300	0.28386100
C	2.77530000	-1.92704900	0.57601000
C	4.04616600	0.41128600	1.44895200
H	3.20542100	1.33919200	-0.31239800
C	3.54856200	-1.94280700	1.73637300
H	2.30095800	-2.82658100	0.20084900
C	4.17103800	-0.77378200	2.17812500
H	4.55220400	1.31253800	1.78119800
H	3.66845600	-2.86834500	2.29104900
H	4.76770600	-0.78912200	3.08537000
S	-2.57081100	0.23011700	-0.26529500
C	-3.65737300	-1.01200500	0.49319000
F	-3.74756900	-2.17880800	-0.17559300
F	-3.32668400	-1.32371000	1.76977600
F	-4.88896700	-0.46929100	0.51320500

Zero-point correction= 0.302636 (Hartree/Particle)
Thermal correction to Energy= 0.326212
Thermal correction to Enthalpy= 0.327156
Thermal correction to Gibbs Free Energy= 0.248342
Sum of electronic and zero-point Energies= -1903.025821
Sum of electronic and thermal Energies= -1903.002245
Sum of electronic and thermal Enthalpies= -1903.001301
Sum of electronic and thermal Free Energies= -1903.080115
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1903.725674

TS15-c

P	1.94124600	0.49965700	-0.07323800
C	2.40361300	2.14506700	-0.71691600
C	1.57755600	3.23755400	-0.41371900
C	3.56892500	2.34580300	-1.46785700
C	1.92116300	4.51675000	-0.84548700
H	0.66566900	3.07453200	0.15434500
C	3.90485500	3.62810700	-1.90497400
H	4.20688700	1.50368000	-1.71404600
C	3.08497400	4.71336100	-1.59321700
H	1.27711800	5.35809900	-0.60686700
H	4.80653500	3.77673100	-2.49201400
H	3.34794400	5.70958000	-1.93702500
C	2.92223900	-0.70565400	-1.01758900
C	2.33667200	-1.34383200	-2.11837900
C	4.24784300	-0.99476400	-0.66200600
C	3.08217800	-2.25036800	-2.87078200
H	1.29343900	-1.16675400	-2.35562400
C	4.98754500	-1.90050300	-1.42028900
H	4.69320100	-0.52134600	0.20754600
C	4.40585700	-2.52638900	-2.52575400
H	2.61900000	-2.75474400	-3.71320200
H	6.01338900	-2.12503800	-1.14271600
H	4.98148500	-3.23968600	-3.10877900
C	2.60242400	0.44384100	1.62676700
C	2.15121600	-0.57203300	2.48422400
C	3.55436900	1.36740300	2.07733700
C	2.65989600	-0.66049900	3.77838300
H	1.41320300	-1.28856100	2.14039100
C	4.05576300	1.27303900	3.37651900
H	3.89898600	2.15829900	1.41918100
C	3.61013000	0.26051100	4.22682700
H	2.30876200	-1.44803600	4.43850900
H	4.79160500	1.99309400	3.72295700
H	3.99924800	0.19059800	5.23859300
Au	-0.33953300	0.14104400	-0.10183700
S	-0.97077000	-2.61970000	-1.12303700
C	-0.16098600	-3.20829700	0.34955500
F	1.19236800	-2.99135500	0.34813000
F	-0.60212400	-2.59402400	1.50065000
F	-0.31490200	-4.53428300	0.56837700
C	-2.49616500	0.25662300	0.16809300
C	-2.82168300	-0.92740300	-0.08550300
C	-3.10343900	1.55957200	0.61513800
H	-2.86797200	2.32500100	-0.14205700
H	-2.62587500	1.85970300	1.55194700
O	-4.48502400	1.50863900	0.86643900
C	-5.27295300	1.33024200	-0.31057200
H	-5.00280000	2.11419700	-1.04140600
H	-5.04053300	0.36497000	-0.77674000
C	-6.71499400	1.44421000	0.06878000
H	-6.96238300	2.36460000	0.59639800
C	-7.69466600	0.56087700	-0.16970900
C	-7.52002700	-0.75917300	-0.87710000
H	-6.48073300	-0.99093300	-1.11914600

H	-7.91442900	-1.57640200	-0.25884300
H	-8.09300600	-0.77352100	-1.81427200
C	-9.10916700	0.84875100	0.26879600
H	-9.79469100	0.85251600	-0.58995700
H	-9.47122400	0.06943000	0.95325100
H	-9.19109400	1.81481500	0.77562900
H	-3.33169800	-1.85587600	-0.20305700

Zero-point correction= 0.472189 (Hartree/Particle)
Thermal correction to Energy= 0.508341
Thermal correction to Enthalpy= 0.509286
Thermal correction to Gibbs Free Energy= 0.394252
Sum of electronic and zero-point Energies= -2294.462661
Sum of electronic and thermal Energies= -2294.426509
Sum of electronic and thermal Enthalpies= -2294.425565
Sum of electronic and thermal Free Energies= -2294.540599
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2295.753329

INT15-c

P	2.15990900	0.25325400	-0.09559000
C	3.30924700	0.94355400	1.14363000
C	2.90854100	0.93155300	2.48811500
C	4.56861800	1.45241800	0.80050800
C	3.76546500	1.40907600	3.47789300
H	1.92499000	0.55158800	2.75144600
C	5.42093800	1.93475900	1.79472200
H	4.87851800	1.47594400	-0.23933700
C	5.02227900	1.91147300	3.13218100
H	3.44930300	1.39682100	4.51680400
H	6.39507400	2.33122800	1.52305300
H	5.68675000	2.28993800	3.90358500
C	2.72725300	0.91581300	-1.69877600
C	2.17630900	2.12469900	-2.14829700
C	3.69836600	0.26644000	-2.47271900
C	2.60531300	2.68526400	-3.35025600
H	1.40701500	2.61555400	-1.55831100
C	4.12153800	0.82904200	-3.67722600
H	4.11412000	-0.67848500	-2.13755100
C	3.57829500	2.03825400	-4.11534100
H	2.17337100	3.62050600	-3.69406000
H	4.87163700	0.31988500	-4.27552300
H	3.90648700	2.47171000	-5.05567800
C	2.52869400	-1.53420400	-0.14242700
C	1.52315100	-2.40152400	-0.59427200
C	3.76417900	-2.05536900	0.26642500
C	1.75258700	-3.77530300	-0.63964000
H	0.56012800	-2.00233300	-0.89533500
C	3.99141000	-3.43064100	0.21171400
H	4.53848900	-1.39046700	0.63642900
C	2.98695400	-4.29025000	-0.23911600
H	0.95640200	-4.43639800	-0.96549500
H	4.94917500	-3.83142800	0.53125800
H	3.16334200	-5.36175600	-0.26743500
Au	-0.14571900	0.59762200	0.34592400
S	-2.44705000	-1.57212200	-0.87617100
C	-2.05545300	-2.87399200	0.32764200
F	-1.57327500	-3.93668500	-0.36105600
F	-1.11301600	-2.51497100	1.22240800
F	-3.12042900	-3.28952200	1.03407500
C	-2.16814500	0.68295200	0.68729500
C	-2.99627700	-0.26215500	0.21407500
C	-2.73446500	1.78400700	1.55730200
H	-2.34495900	2.75675500	1.21288500
H	-2.36268300	1.64474800	2.58081800
O	-4.14823500	1.81850700	1.64898600
C	-4.76952400	2.39537300	0.49406200
H	-4.86839700	3.48237400	0.65328600
H	-4.13865900	2.24905000	-0.38787800
C	-6.11601900	1.76534300	0.31130900
H	-6.80044600	1.91636700	1.14566700
C	-6.53188600	1.02089400	-0.72422900
C	-5.70795300	0.68837100	-1.94329000
H	-4.69399500	1.09000200	-1.90772700
H	-5.62728400	-0.40057000	-2.05998500
H	-6.19476100	1.06658500	-2.85272900
C	-7.92180100	0.43349400	-0.73691800
H	-8.49133300	0.78568000	-1.60833400
H	-7.88095300	-0.66173600	-0.81336900
H	-8.48291000	0.69269100	0.16593400
H	-4.06177200	-0.26478100	0.42524100

Zero-point correction= 0.476471 (Hartree/Particle)
Thermal correction to Energy= 0.511734
Thermal correction to Enthalpy= 0.512678
Thermal correction to Gibbs Free Energy= 0.400339
Sum of electronic and zero-point Energies= -2294.524519
Sum of electronic and thermal Energies= -2294.489257
Sum of electronic and thermal Enthalpies= -2294.488313
Sum of electronic and thermal Free Energies= -2294.600652
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2295.809932

TS16-c

P	-1.79021900	-0.33089500	0.01453400
C	-3.03323200	-1.23911100	0.98970600
C	-3.01057500	-1.13520300	2.38675100
C	-4.03059100	-2.00093600	0.36451700
C	-3.98444300	-1.77741500	3.15093900
H	-2.22436700	-0.55745700	2.86509600
C	-4.99877900	-2.64588200	1.13300400
H	-4.04401800	-2.09236800	-0.71711800
C	-4.97788500	-2.53300200	2.52513600
H	-3.96243200	-1.69431400	4.23354700
H	-5.76724500	-3.23883800	0.64560100
H	-5.73186100	-3.03878200	3.12142000
C	-1.53224600	-1.31729500	-1.49710300
C	-0.61162400	-2.37396000	-1.45334500
C	-2.22536900	-1.04772900	-2.68333600
C	-0.39335900	-3.15816600	-2.58331700
H	-0.06080400	-2.56795100	-0.53763600
C	-2.00183700	-1.83530000	-3.81373400
H	-2.92303200	-0.21776200	-2.72608500
C	-1.08796400	-2.88883700	-3.76536900
H	0.32742100	-3.96970500	-2.54551000
H	-2.53605400	-1.61886000	-4.73423300
H	-0.91009600	-3.49409500	-4.64953400
C	-2.59741200	1.21000800	-0.52483100

C	-1.81940900	2.12560100	-1.25058400
C	-3.92721100	1.51374100	-0.20787600
C	-2.37020100	3.34014100	-1.64897900
H	-0.78853600	1.88774900	-1.49175700
C	-4.47372100	2.73107700	-0.61826500
H	-4.52953500	0.81060700	0.35761000
C	-3.69722100	3.64414300	-1.33404600
H	-1.74907800	4.04910000	-2.18699800
H	-5.50488800	2.96712500	-0.37126900
H	-4.12456700	4.59466100	-1.64087800
Au	0.23027000	0.08489300	1.06544400
S	1.81087000	1.36520200	-1.19117700
C	1.54419000	3.00420100	-0.55629100
F	1.00203900	3.84966900	-1.48009000
F	0.68342100	3.05663200	0.51262200
F	2.68272900	3.61395600	-0.11841600
C	2.02631000	0.38117000	2.20911500
C	2.90360600	0.65069700	1.35378600
C	4.22317400	0.75457500	0.68922800
H	4.50790700	1.80668200	0.60727300
H	4.17229400	0.33849900	-0.31762700
O	5.18565300	0.09694900	1.49287100
C	5.09688500	-1.34294300	1.42422700
H	4.13637700	-1.66872500	1.83969200
H	5.88729600	-1.68485600	2.09822900
C	5.31630400	-1.86947900	0.03616000
H	6.34435500	-1.80734900	-0.31923500
C	4.38204800	-2.32792500	-0.81391800
C	2.90842300	-2.43251100	-0.51021000
H	2.64992200	-2.16602500	0.51560100
H	2.33894600	-1.76862100	-1.17306700
H	2.55122800	-3.45393600	-0.70125000
C	4.75866700	-2.76953500	-2.20582500
H	4.21574800	-2.18011700	-2.95669000
H	5.83089100	-2.66209800	-2.39400800
H	4.48280300	-3.82007000	-2.37191500
H	1.98130700	0.24244800	3.27823600

Zero-point correction= 0.473039 (Hartree/Particle)
Thermal correction to Energy= 0.508643
Thermal correction to Enthalpy= 0.509587
Thermal correction to Gibbs Free Energy= 0.397955
Sum of electronic and zero-point Energies= -2294.472465
Sum of electronic and thermal Energies= -2294.436861
Sum of electronic and thermal Enthalpies= -2294.435917
Sum of electronic and thermal Free Energies= -2294.547550
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2295.762233

INT16-c

P	1.93256500	-0.16970700	-0.05064600
C	3.42295700	-0.31684800	-1.09158400
C	3.41858500	0.32693500	-2.33772600
C	4.56208400	-1.02063300	-0.67828900
C	4.54832900	0.28055000	-3.15289200
H	2.52748800	0.85629900	-2.66460700
C	5.68855100	-1.06864200	-1.49997000
H	4.56446200	-1.53368600	0.27823000
C	5.68390300	-0.41681200	-2.73467800
H	4.53893000	0.78063400	-4.11686400
H	6.56810800	-1.61815500	-1.17701000
H	6.56137700	-0.45839700	-3.37353800
C	1.99041600	-1.58502500	1.10304300
C	1.31843700	-2.76313100	0.74535500
C	2.67360600	-1.52164600	2.32507800
C	1.34181200	-3.86841500	1.59440300
H	0.76670000	-2.80302200	-0.18942900
C	2.69317300	-2.62972100	3.17256100
H	3.17634100	-0.60465300	2.61639500
C	2.02920300	-3.80282600	2.80831200
H	0.81494500	-4.77538900	1.31289300
H	3.22081900	-2.57398100	4.12036800
H	2.04022200	-4.66155800	3.47337000
C	2.20783700	1.30314600	0.99424100
C	1.08699900	1.87705400	1.61359600
C	3.47384500	1.87184900	1.18468500
C	1.23143900	3.00672900	2.41526600
H	0.10464600	1.44395800	1.45801900
C	3.61410800	3.00059200	1.99379800
H	4.34243200	1.44135600	0.69636100
C	2.49563700	3.56899200	2.60681400
H	0.35137800	3.45268400	2.86741900
H	4.59680500	3.44082300	2.13724700
H	2.60830100	4.45462200	3.22567800
Au	-0.17792000	-0.02625500	-1.11329900
S	-2.76732500	0.99278700	0.80845300
C	-2.40008800	2.74835900	0.54489100
F	-2.11443200	3.29025800	1.75358700
F	-1.33894700	2.97506300	-0.25260200
F	-3.43284300	3.43105500	0.01727500
C	-2.12178600	0.10188000	-1.71082600
C	-3.11610800	0.48123800	-0.89363400
C	-4.59537600	0.38954000	-1.23479700
H	-4.89942600	1.22976700	-1.86940200
H	-5.17958400	0.44560600	-0.30797700
O	-4.94349300	-0.77184800	-1.97669400
C	-4.50364900	-2.01261300	-1.40639500
H	-3.45044900	-2.18258900	-1.65367300
H	-5.09637800	-2.76930800	-1.93409600
C	-4.73089400	-2.10398700	0.07444500
H	-5.76112700	-1.92666500	0.38507800
C	-3.81831000	-2.33967300	1.03161500
C	-2.35332000	-2.60684900	0.79262400
H	-2.06689500	-2.55078600	-0.25766300
H	-1.73699300	-1.88034900	1.33758900
H	-2.07926700	-3.59986600	1.17526600
C	-4.21862100	-2.35081400	2.48609800
H	-3.66955400	-1.57653200	3.03907900
H	-5.28951800	-2.16889900	2.61714000
H	-3.97095400	-3.31114100	2.95913400
H	-2.45108500	-0.20356100	-2.70697200

Zero-point correction= 0.476843 (Hartree/Particle)
Thermal correction to Energy= 0.511812
Thermal correction to Enthalpy= 0.512756
Thermal correction to Gibbs Free Energy= 0.402805
Sum of electronic and zero-point Energies= -2294.526305

Sum of electronic and thermal Energies= -2294.491336
Sum of electronic and thermal Enthalpies= -2294.490392
Sum of electronic and thermal Free Energies= -2294.600343
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2295.809685

TS17-c

P	-1.80730700	-0.33056600	-0.02793600
C	-2.57440500	1.26081500	-0.47013400
C	-1.96000200	2.06899500	-1.43402100
C	-3.76315200	1.68649000	0.14295200
C	-2.53996700	3.28448600	-1.79583100
H	-1.01425600	1.76818700	-1.86975100
C	-4.34118300	2.89901300	-0.22725600
H	-4.22335500	1.07683700	0.91464200
C	-3.73101700	3.69719900	-1.19870900
H	-2.04617800	3.91620500	-2.52754400
H	-5.26017700	3.22688900	0.25007100
H	-4.17689600	4.64798600	-1.47648100
C	-2.23189700	-0.56453400	1.73280800
C	-1.53675900	0.21447000	2.67252100
C	-3.21383600	-1.46572200	2.15979100
C	-1.83467900	0.09163200	4.02763600
H	-0.76810300	0.90727000	2.33838500
C	-3.50230500	-1.58588700	3.52101700
H	-3.74922800	-2.07058200	1.43524800
C	-2.81560800	-0.80859900	4.45400000
H	-1.29711400	0.69696200	4.75169100
H	-4.26342600	-2.28789200	3.84967000
H	-3.04188700	-0.90455000	5.51218100
C	-2.73742300	-1.62016000	-0.92589900
C	-2.12454900	-2.86703500	-1.11883200
C	-4.04363400	-1.41294600	-1.38903700
C	-2.81638200	-3.89801200	-1.75193600
H	-1.10329000	-3.01672800	-0.77913000
C	-4.72955100	-2.44543400	-2.02958600
H	-4.51927600	-0.44696700	-1.25621900
C	-4.11957200	-3.68815600	-2.20857300
H	-2.33487100	-4.86045900	-1.89841900
H	-5.73959800	-2.27662900	-2.39173100
H	-4.65529400	-4.48908700	-2.70997500
Au	0.49846200	-0.42228300	-0.32611600
S	1.57344300	2.06766500	1.12893200
C	1.38057800	3.09287100	-0.31163800
F	1.29244500	2.37872100	-1.49016600
F	0.26194900	3.85830200	-0.27163300
F	2.41679600	3.94934300	-0.51238400
C	2.64658500	-0.67214300	-0.60134600
H	2.78681500	-0.42943700	-1.65899800
C	3.28332500	0.30910600	0.25440400
C	3.62774400	-0.05346300	1.67351800
H	2.82374800	-0.61303900	2.15818400
H	4.53093800	-0.67729000	1.65700600
H	3.85065900	0.83555900	2.26461800
C	4.15434500	1.33441100	-0.40809900
H	3.69024600	1.73058000	-1.31243800
H	4.42036600	2.15840100	0.25483800
H	5.06858500	0.79759200	-0.70680900
C	2.91167600	-2.16033000	-0.37246600
H	2.17054300	-2.74455500	-0.92209600
H	2.83609700	-2.43469800	0.68721200
O	4.17396000	-2.60271200	-0.90701800
C	5.22324300	-2.86746300	0.00080100
H	5.74223800	-3.76305400	-0.36541300
H	4.82653800	-3.11293800	0.99856700
C	6.20541100	-1.77879000	0.11898300
C	7.03451400	-0.90503100	0.21042400
H	7.76075000	-0.12865900	0.29284500

Zero-point correction= 0.473564 (Hartree/Particle)
Thermal correction to Energy= 0.508688
Thermal correction to Enthalpy= 0.509632
Thermal correction to Gibbs Free Energy= 0.400480
Sum of electronic and zero-point Energies= -2294.459059
Sum of electronic and thermal Energies= -2294.423935
Sum of electronic and thermal Enthalpies= -2294.422991
Sum of electronic and thermal Free Energies= -2294.532143
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2295.747235

INT17-c

P	-1.88156300	-0.31192000	-0.01189400
C	-2.42493100	1.27765300	0.70434000
C	-1.70920300	2.43281900	0.35705900
C	-3.51090400	1.37306500	1.58547400
C	-2.07995700	3.67014300	0.88003200
H	-0.85618900	2.36004500	-0.30779800
C	-3.88140400	2.61475800	2.10256100
H	-4.05583200	0.47943400	1.87371500
C	-3.16710500	3.76247200	1.75129200
H	-1.50418900	4.55201200	0.61841900
H	-4.72214100	2.68410000	2.78703400
H	-3.45161700	4.72575800	2.16508700
C	-2.49627700	-1.58072600	1.15002800
C	-1.69132900	-1.90024900	2.25411000
C	-3.73342100	-2.21764400	0.98841100
C	-2.12776200	-2.83366500	3.19211100
H	-0.72417000	-1.41809500	2.36883500
C	-4.16364400	-3.15663400	1.92727300
H	-4.35500000	-1.98304600	0.13021300
C	-3.36426300	-3.46337000	3.02945100
H	-1.49981500	-3.07604400	4.04448600
H	-5.12252300	-3.64972900	1.79519600
H	-3.70055400	-4.19618700	3.75731800
C	-2.87794900	-0.53294900	-1.52581300
C	-2.39346900	-1.40531700	-2.51166400
C	-4.10274300	0.11969500	-1.72002800
C	-3.13514100	-1.63493200	-3.66928000
H	-1.43235300	-1.89216100	-2.36964100
C	-4.83927000	-0.10912700	-2.88280000
H	-4.47353600	0.80873400	-0.96782700
C	-4.35864700	-0.98751400	-3.85569800
H	-2.75364800	-2.31019800	-4.42959500
H	-5.78616900	0.40236500	-3.03018200
H	-4.93234100	-1.16087000	-4.76164700
Au	0.46832800	-0.32539800	-0.34282300
S	2.13959700	2.06560300	1.14995900

C	1.94987400	3.16835600	-0.26657600
F	1.39036500	2.59747700	-1.36082400
F	1.12062900	4.16913000	0.11710700
F	3.09489000	3.74099700	-0.68855200
C	2.56134500	-0.15432800	-0.60587200
H	2.69259900	0.41289800	-1.53453200
C	3.23578000	0.63590000	0.54192800
C	3.35636000	-0.20044600	1.82551000
H	2.38984100	-0.62841000	2.11354800
H	4.05856400	-1.02160800	1.65299600
H	3.74173400	0.40011600	2.65647500
C	4.61078900	1.20143900	0.15617800
H	4.54636800	1.82767500	-0.73618100
H	5.03333100	1.80129400	0.96906800
H	5.27632400	0.36512400	-0.06645500
C	3.12299900	-1.55027100	-0.81634900
H	2.59884800	-2.02787100	-1.65823000
H	2.96725400	-2.18077000	0.06732700
O	4.53173700	-1.52023100	-1.12286400
C	5.11588700	-2.80557100	-1.15666400
H	6.11948500	-2.67649100	-1.57712300
H	4.55711000	-3.47242300	-1.83560100
C	5.21224800	-3.43517600	0.17093400
C	5.27960600	-3.92660600	1.27236900
H	5.34891300	-4.36729200	2.24058900

Zero-point correction= 0.475703 (Hartree/Particle)
Thermal correction to Energy= 0.510824
Thermal correction to Enthalpy= 0.511768
Thermal correction to Gibbs Free Energy= 0.402225
Sum of electronic and zero-point Energies= -2294.487735
Sum of electronic and thermal Energies= -2294.452614
Sum of electronic and thermal Enthalpies= -2294.451670
Sum of electronic and thermal Free Energies= -2294.561213
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2295.77081

TS18-c

P	1.77890200	-0.24091600	0.08965500
C	2.54394900	0.69695900	-1.27358000
C	1.91573700	1.88449700	-1.68076500
C	3.70850600	0.26534000	-1.92078700
C	2.45827500	2.63460400	-2.72084100
H	1.01297500	2.22305100	-1.18917700
C	4.24247100	1.02040900	-2.96663800
H	4.19645700	-0.65251100	-1.61059400
C	3.61997200	2.20344300	-3.36673900
H	1.96409000	3.55069000	-3.02968500
H	5.14506800	0.68174800	-3.46731700
H	4.03696400	2.78731500	-4.18238700
C	2.82622100	-1.71992200	0.30983700
C	2.45486200	-2.90877500	-0.33378800
C	4.00420900	-1.68192500	1.06858400
C	3.25993700	-4.04251000	-0.23031000
H	1.53183000	-2.94008800	-0.90630700
C	4.80301200	-2.82020800	1.17526600
H	4.29095800	-0.76732200	1.57775800
C	4.43375900	-3.99945900	0.52475000
H	2.96627400	-4.96029100	-0.73130200
H	5.71220800	-2.78670700	1.76860100
H	5.05672900	-4.88505900	0.61137300
C	2.04896000	0.77654400	1.57801900
C	1.20932800	0.58633500	2.68418800
C	3.07813400	1.72523200	1.64217500
C	1.40745400	1.32712300	3.84735000
H	0.39537900	-0.13039500	2.62158300
C	3.27058000	2.46704500	2.80788500
H	3.71638300	1.88973000	0.77991400
C	2.43784000	2.26797700	3.91030700
H	0.74986200	1.18054000	4.69909800
H	4.06616500	3.20518400	2.85142100
H	2.58508200	2.85197600	4.81420500
Au	-0.47562800	-0.75079700	-0.26224400
S	-2.02819000	1.71739800	-1.56795200
C	-1.51196800	2.80337600	-0.26211800
F	-0.81427800	2.17313600	0.74627300
F	-0.67645400	3.78321300	-0.70516300
F	-2.53100000	3.43901600	0.37785400
C	-2.56269700	-1.37136400	-0.57156100
C	-3.27713000	-0.14397100	-0.32180700
H	-3.99934600	0.20240300	-1.05158800
C	-2.71837800	-1.85918700	-2.01154300
H	-2.06211600	-2.71086800	-2.21892600
H	-3.75528900	-2.18113600	-2.19727800
H	-2.47676300	-1.06579900	-2.72692900
C	-2.75766700	-2.52579600	0.43689000
H	-3.77135900	-2.94010900	0.34161700
H	-2.04827700	-3.32927300	0.21987900
H	-2.59838900	-2.23121700	1.47668100
C	-3.54761800	0.39489000	1.06686100
H	-3.19463200	1.41754300	1.16559300
H	-3.03543300	-0.21185300	1.82626200
O	-4.94378800	0.48017400	1.34482700
C	-5.61020600	-0.76101500	1.50457300
H	-6.51979800	-0.53484300	2.07211100
H	-5.00534900	-1.45285200	2.11096400
C	-5.98036800	-1.40960200	0.23900600
C	-6.30387400	-1.93746100	-0.79831600
H	-6.59145000	-2.39666800	-1.71654800

Zero-point correction= 0.473323 (Hartree/Particle)
Thermal correction to Energy= 0.508684
Thermal correction to Enthalpy= 0.509628
Thermal correction to Gibbs Free Energy= 0.399614
Sum of electronic and zero-point Energies= -2294.446201
Sum of electronic and thermal Energies= -2294.410840
Sum of electronic and thermal Enthalpies= -2294.409896
Sum of electronic and thermal Free Energies= -2294.519909
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2295.333732

INT18-c

P	-1.94202500	0.02976700	0.08953000
C	-2.41057600	-0.96342500	-1.37092300
C	-1.41301400	-1.75201500	-1.96691600
C	-3.70551400	-0.96366100	-1.90361900
C	-1.71618600	-2.53915000	-3.07514000
H	-0.40786200	-1.75530400	-1.56121000

C	-4.00084000	-1.74939500	-3.01955200
H	-4.47917800	-0.35266800	-1.45022900
C	-3.00932900	-2.53744000	-3.60495400
H	-0.93851800	-3.14740400	-3.52752500
H	-5.00649700	-1.74338100	-3.43042200
H	-3.24171500	-3.14644100	-4.47395300
C	-3.38191200	1.10179800	0.42270400
C	-3.39386700	2.38130300	-0.15209400
C	-4.46853500	0.68376900	1.20291000
C	-4.48763000	3.22473200	0.03770200
H	-2.54143800	2.71149000	-0.73983100
C	-5.55806900	1.53336700	1.39578800
H	-4.45846800	-0.30009100	1.66118300
C	-5.57033600	2.80164900	0.81170500
H	-4.49024300	4.21422200	-0.41010600
H	-6.39604500	1.20556400	2.00436600
H	-6.41909400	3.46190800	0.96545000
C	-1.90103100	-1.17533900	1.46102300
C	-1.10421600	-0.88426100	2.57767300
C	-2.63079300	-2.37124400	1.42461100
C	-1.05155100	-1.77150300	3.65135000
H	-0.51803900	0.03048000	2.59232900
C	-2.57348600	-3.25781200	2.50015100
H	-3.23143900	-2.61103500	0.55269600
C	-1.78608900	-2.95864300	3.61368500
H	-0.42798200	-1.54268300	4.51060900
H	-3.13813800	-4.18512600	2.46513700
H	-1.73740300	-3.65400200	4.44674400
Au	0.15943300	1.12553600	-0.18994300
S	3.06689600	-0.59008100	-1.36590100
C	2.33525200	-1.98989000	-0.47855500
F	1.27383400	-1.68583400	0.31258800
F	1.87933900	-2.84196100	-1.43025900
F	3.18839000	-2.68113500	0.28856200
C	2.09049700	1.92739300	-0.46964100
C	3.16902500	0.85552500	-0.17713900
H	4.14793500	1.26863200	-0.45987600
C	2.23866100	2.40303500	-1.92521900
H	1.52355700	3.20300600	-2.14460900
H	3.25181000	2.80575600	-2.10390500
H	2.06574300	1.59866600	-2.64600000
C	2.32578000	3.14975300	0.43913000
H	3.36742400	3.51031900	0.36342100
H	1.67312000	3.97200500	0.12648700
H	2.11105800	2.95753700	1.49427200
C	3.26092300	0.43041700	1.29389900
H	2.33559500	-0.05513500	1.60826900
H	3.38689900	1.33875000	1.89777600
O	4.30272400	-0.48269200	1.60027200
C	5.59668800	0.08247200	1.70903500
H	6.16989400	-0.61072300	2.33539000
H	5.54848600	1.04530700	2.24454400
C	6.30354700	0.26863500	0.43364600
C	6.90827900	0.41435700	-0.60102800
H	7.42544700	0.53317200	-1.52563900

Zero-point correction= 0.475278 (Hartree/Particle)
Thermal correction to Energy= 0.510518
Thermal correction to Enthalpy= 0.511462
Thermal correction to Gibbs Free Energy= 0.401074
Sum of electronic and zero-point Energies= -2294.475478
Sum of electronic and thermal Energies= -2294.440238
Sum of electronic and thermal Enthalpies= -2294.439294
Sum of electronic and thermal Free Energies= -2294.549681
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2295.356666

INT6-c´

C	0.07770100	-0.84937800	-0.85332200
H	-0.08881800	-0.00104800	-1.50958700
C	-0.86046500	-1.29126400	-0.01498500
C	-0.82819600	-2.46219200	0.94614500
H	-0.44419300	-3.38040900	0.50384400
H	-0.20088900	-2.22078000	1.81969000
O	-2.18656100	-2.66706300	1.32549000
C	-2.81128600	-1.39440200	1.34534700
H	-3.89142700	-1.54278400	1.28103100
H	-2.58408100	-0.85495000	2.27405500
C	-2.23782600	-0.64683800	0.10520900
H	-2.81694000	-1.01142900	-0.75336600
C	-2.29532800	0.85285900	0.11534100
C	-3.29747100	1.52163900	-0.79912300
H	-3.24776300	2.60216200	-0.60916800
C	-1.42252700	1.75976300	0.95881700
H	-2.10445100	2.51072700	1.39307300
S	1.73132800	-1.47544200	-0.94393800
O	1.86346900	-2.62056900	-0.02529500
O	2.11031300	-1.58225400	-2.36111100
C	2.63527300	-0.09494700	-0.23574100
C	3.05274000	0.94227800	-1.06994600
C	2.82442400	-0.04541600	1.14578800
C	3.66364000	2.05967200	-0.50151200
H	2.90766400	0.85980900	-2.14186100
C	3.43694800	1.07604400	1.70240200
H	2.50535200	-0.87985400	1.76092600
C	3.84920600	2.12819700	0.88106400
H	3.99712400	2.87440500	-1.13724200
H	3.59482300	1.12801500	2.77550000
H	4.32283800	3.00172300	1.31956200
C	-2.96772000	1.30581100	-2.29081000
H	-3.69318300	1.82533800	-2.92791200
H	-1.96897600	1.68293600	-2.53535900
H	-2.99795900	0.24270700	-2.55728200
C	-4.74187200	1.07377600	-0.49682900
H	-4.87685200	0.00341000	-0.69295400
H	-5.00173400	1.25931000	0.55111900
H	-5.45640200	1.61546000	-1.12754500
C	-0.67066200	1.11463100	2.13184600
H	0.02539600	0.34268800	1.79325100
H	-0.07706000	1.87725500	2.64808500
H	-1.34866700	0.67232700	2.86704000
C	-0.41866700	2.56014100	0.09019600
H	0.37171800	1.91058700	-0.29589000
H	-0.91240100	3.04388000	-0.75869000
H	0.06039400	3.34243600	0.69069300

Zero-point correction= 0.399802 (Hartree/Particle)

Thermal correction to Energy= 0.422715
Thermal correction to Enthalpy= 0.423660
Thermal correction to Gibbs Free Energy= 0.345996
Sum of electronic and zero-point Energies= -1324.388573
Sum of electronic and thermal Energies= -1324.365660
Sum of electronic and thermal Enthalpies= -1324.364716
Sum of electronic and thermal Free Energies= -1324.442380
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1325.081816

TS10-c´

C	-3.10174700	-1.28073400	0.68707600
H	-2.90052400	-0.81609100	1.64541600
C	-2.16550100	-1.47927600	-0.24237200
C	-2.30684200	-2.14986800	-1.59654100
H	-2.92650300	-3.04404900	-1.57457100
H	-2.75218400	-1.44306500	-2.31916600
O	-0.98643400	-2.50677800	-1.96119300
C	-0.12526900	-1.47729000	-1.50053800
H	0.88251800	-1.88884500	-1.45645200
H	-0.12867800	-0.62508800	-2.18356700
C	-0.68409500	-1.11503700	-0.08602000
H	-0.26353000	-1.87818700	0.57251500
C	-0.41371300	0.24841900	0.54357700
C	-0.27106800	0.24734500	2.07058600
H	-1.31055000	0.21836500	2.44414900
C	-0.98458200	1.53595000	-0.05671900
H	-0.28539000	2.32796100	0.21883100
S	-4.83197900	-1.65229000	0.49823600
O	-5.03428100	-2.48010200	-0.70247200
O	-5.32900700	-2.07323200	1.81651800
C	-5.49502900	-0.02152200	0.15184100
C	-5.86708800	0.79991100	1.21559900
C	-5.53384500	0.42563200	-1.16979600
C	-6.27822600	2.10498000	0.94623600
H	-5.84008500	0.41134200	2.22799700
C	-5.94624400	1.73177000	-1.42635600
H	-5.25634500	-0.24820400	-1.97328800
C	-6.31098600	2.57062400	-0.37001400
H	-6.57480700	2.75687300	1.76242500
H	-5.98634100	2.09432100	-2.44909700
H	-6.62827600	3.58896700	-0.57460400
C	2.49252100	2.00073700	-0.52991800
F	2.14310300	2.34553400	-1.77951500
F	1.89036400	2.87369500	0.30699900
F	3.81956600	2.19942600	-0.41425500
S	2.04788100	0.27724300	-0.12482600
S	3.95599900	-0.75725300	-1.18598400
O	4.33203300	-0.04704300	-2.42198700
O	3.47455800	-2.15224100	-1.19906300
C	5.31567600	-0.65069800	-0.02571500
C	6.26178300	0.36215100	-0.17840100
C	5.35332000	-1.55173800	1.03874300
C	7.28802700	0.45860000	0.75956900
H	6.19348700	1.04362600	-1.01802700
C	6.38444500	-1.43948600	1.96901400
H	4.60094400	-2.32848100	1.11778000
C	7.34739500	-0.43660500	1.83022400
H	8.04211200	1.23252400	0.65333700
H	6.43893400	-2.13726800	2.79911300
H	8.14788800	-0.35310700	2.55938300
C	0.42970800	-0.98285600	2.67473700
H	0.53395900	-0.84124400	3.75507200
H	-0.13316700	-1.90918000	2.52931700
H	1.43351900	-1.11361500	2.25878800
C	0.35319100	1.52298700	2.66247500
H	1.41002400	1.59584600	2.39417200
H	-0.14477400	2.43632200	2.33052100
H	0.28227100	1.48593200	3.75421500
C	-1.11916000	1.58574900	-1.58373900
H	-1.83862100	0.84928800	-1.95574000
H	-1.49169300	2.57460100	-1.87235900
H	-0.16370900	1.43422700	-2.08848600
C	-2.34728000	1.95271600	0.56028500
H	-3.15636900	1.31592000	0.20314800
H	-2.34731600	1.93062600	1.65305900
H	-2.57180700	2.97900500	0.25083900

Zero-point correction= 0.518722 (Hartree/Particle)
Thermal correction to Energy= 0.555671
Thermal correction to Enthalpy= 0.556615
Thermal correction to Gibbs Free Energy= 0.443848
Sum of electronic and zero-point Energies= -2840.339966
Sum of electronic and thermal Energies= -2840.303017
Sum of electronic and thermal Enthalpies= -2840.302073
Sum of electronic and thermal Free Energies= -2840.414840
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2841.434528

P_3´

C	-1.63702300	-1.12974300	1.05699100
H	-1.35584400	-0.70297500	2.01063000
C	-0.76528800	-1.57947500	0.15092600
C	-1.10179000	-2.28848600	-1.15030200
H	-1.63456100	-3.22387500	-0.93340100
H	-1.73307200	-1.69948000	-1.82062000
O	0.13764600	-2.53372100	-1.79383100
C	1.13902600	-2.61195100	-0.78761500
H	1.14282500	-3.61612700	-0.33651000
H	2.10583400	-2.43657800	-1.25305400
C	0.75515300	-1.57872000	0.29757300
H	1.00430700	-2.00417500	1.27250300
C	1.46210400	-0.15770100	0.26143300
C	0.94663700	0.69734400	1.47368500
H	-0.12076600	0.83002100	1.27677700
C	1.35701900	0.64791100	-1.07407200
H	2.01949100	1.50606200	-0.93350900
S	-3.39755200	-1.04550000	0.80154200
O	-3.80827000	-2.06049500	-0.18364900
O	-4.01209400	-0.97055600	2.13454700
C	-3.54344100	0.56313800	0.01928000
C	-3.40091700	1.70867900	0.80508600
C	-3.71110500	0.63939900	-1.36248600
C	-3.40960800	2.95619600	0.18491000
H	-3.29944600	1.61694100	1.88151100
C	-3.72381100	1.89461100	-1.97157400
H	-3.84353500	-0.27145500	-1.93581800

C	-3.56451500	3.04773300	-1.20138700
H	-3.30199000	3.85690400	0.78176700
H	-3.85819900	1.97085300	-3.04631100
H	-3.56900000	4.02232200	-1.68049600
C	4.43525800	0.51716700	-0.05674400
F	4.63998900	0.41289100	-1.38380400
F	4.13043400	1.80875700	0.17710700
F	5.60950600	0.25427200	0.54505700
S	3.25653500	-0.69558600	0.62380000
C	1.07939400	0.02675400	2.85255800
H	0.61165700	0.66768000	3.60770300
H	0.59721500	-0.95203200	2.92232600
H	2.13014200	-0.09939200	3.12861600
C	1.54181100	2.10862100	1.58661100
H	2.59739900	2.07567700	1.86250200
H	1.44747600	2.69221900	0.66857800
H	1.00923500	2.65083800	2.37539800
C	1.82299100	-0.05469000	-2.36144500
H	1.09283900	-0.79023200	-2.70011600
H	1.93439300	0.70262800	-3.14518800
H	2.78838800	-0.54662400	-2.25006800
C	-0.05293800	1.21666700	-1.32572000
H	-0.78462300	0.42536500	-1.49955100
H	-0.42866600	1.84510900	-0.51572300
H	-0.02659100	1.83186000	-2.23143200

Zero-point correction= 0.420980 (Hartree/Particle)
Thermal correction to Energy= 0.448248
Thermal correction to Enthalpy= 0.449192
Thermal correction to Gibbs Free Energy= 0.362849
Sum of electronic and zero-point Energies= -2060.234796
Sum of electronic and thermal Energies= -2060.207527
Sum of electronic and thermal Enthalpies= -2060.206583
Sum of electronic and thermal Free Energies= -2060.292927
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2061.088505

INT6-c´´

C	0.48540800	1.06900700	0.78572100
H	0.18796300	0.31560000	1.50704600
C	-0.36297600	1.56347900	-0.11745100
C	-0.14126000	2.63565400	-1.16580200
H	0.38823300	3.50955900	-0.78919900
H	0.43724900	2.23006800	-2.01147800
O	-1.44798600	3.03180600	-1.57449400
C	-2.28385300	1.88799300	-1.49753700
H	-3.31973400	2.22852700	-1.42956700
H	-2.18148000	1.25854000	-2.38965700
C	-1.82653900	1.14495000	-0.21091600
H	-2.30620600	1.69000000	0.60726700
C	-2.18382700	-0.32088100	-0.08255600
C	-3.19331000	-0.60311100	1.04896800
C	-1.45595600	-1.40534400	-0.89807300
S	2.21665200	1.43106300	0.85419100
O	2.53684800	2.45956500	-0.15196000
O	2.60344800	1.59193000	2.26415400
C	2.88435600	-0.13238400	0.27518900
C	3.12753900	-1.14995600	1.19794800
C	3.05646100	-0.32971900	-1.09532800
C	3.54237000	-2.39709700	0.73190800
H	3.00160400	-0.95411800	2.25751100
C	3.47216100	-1.58018800	-1.54933900
H	2.87587800	0.49024200	-1.78193600
C	3.70782800	-2.61254900	-0.63814300
H	3.73893600	-3.19892000	1.43732800
H	3.61448800	-1.74843000	-2.61265400
H	4.02804200	-3.58650300	-0.99667400
C	-2.51206900	-0.30641600	2.41269700
H	-1.69236300	-1.00889500	2.59929600
H	-2.10361600	0.70790500	2.46220200
H	-3.23583300	-0.41046200	3.23007300
C	-4.43111000	0.32180300	0.89673800
H	-4.91958800	0.15409300	-0.06961600
H	-5.15878100	0.10016300	1.68582000
H	-4.19013300	1.38565000	0.97368200
C	-3.77081600	-2.03128100	1.13763300
H	-4.39499400	-2.09666500	2.03587900
H	-4.41022500	-2.26491500	0.28295200
H	-3.00594500	-2.80524800	1.22151500
C	-0.54310800	-0.84479000	-2.01521400
H	0.00317400	-1.68029700	-2.46591900
H	-1.11310100	-0.36482700	-2.81512600
H	0.20460200	-0.14427000	-1.64504300
C	-0.53439100	-2.26346500	0.01195400
H	-0.12707400	-3.10507500	-0.56167800
H	0.31293500	-1.67736500	0.37599700
H	-1.05929900	-2.67457000	0.87672700
C	-2.45328300	-2.34162600	-1.63488300
H	-2.95270800	-3.04601500	-0.97220100
H	-3.21915200	-1.76025500	-2.16029600
H	-1.90953600	-2.93141500	-2.38198400

Zero-point correction= 0.457307 (Hartree/Particle)
Thermal correction to Energy= 0.482350
Thermal correction to Enthalpy= 0.483294
Thermal correction to Gibbs Free Energy= 0.402638
Sum of electronic and zero-point Energies= -1402.955975
Sum of electronic and thermal Energies= -1402.930932
Sum of electronic and thermal Enthalpies= -1402.929987
Sum of electronic and thermal Free Energies= -1403.010644
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-1403.728234

TS10-c´´

C	-3.26835700	-0.36185300	1.32838600
H	-2.97644800	0.61207000	1.69459700
C	-2.39596100	-1.31158600	0.98671300
C	-2.70893100	-2.74545000	0.58731900
H	-3.55182800	-3.17040900	1.12680900
H	-2.92295500	-2.80880600	-0.49241600
O	-1.53360300	-3.46296500	0.92594200
C	-0.44231800	-2.62860800	0.59535500
H	0.43939500	-2.99160100	1.12088100
H	-0.24555600	-2.64173700	-0.47972500
C	-0.86461600	-1.20358700	1.07835800
H	-0.65806500	-1.20478900	2.14960400
C	-0.13081500	0.01101800	0.47233700
C	0.47858200	0.93345100	1.58552000

C	-0.61595900	0.60120000	-0.89189200
S	-5.03169400	-0.45404900	1.11489700
O	-5.41619000	-1.80436700	0.67098200
O	-5.65760200	0.17831600	2.28534300
C	-5.21491400	0.65850300	-0.28235200
C	-5.37187400	2.02427700	-0.04597300
C	-5.09434200	0.14651600	-1.57482000
C	-5.39668800	2.89706500	-1.13328200
H	-5.48201700	2.38333200	0.97183500
C	-5.12063000	1.02851100	-2.65366000
H	-4.99360900	-0.92337000	-1.72173800
C	-5.26443700	2.40061400	-2.43227400
H	-5.52273800	3.96275200	-0.96744900
H	-5.03255700	0.64568400	-3.66594500
H	-5.28187900	3.08445300	-3.27587100
S	4.72356600	-0.84828400	0.38519000
O	4.95036400	-1.18310400	1.80857600
O	5.54340900	-1.43187400	-0.69970700
C	4.79559500	0.94460800	0.23543300
C	4.58511900	1.51072000	-1.02185100
C	4.96959000	1.71762800	1.38022400
C	4.55576000	2.89915900	-1.12898200
H	4.42961100	0.87451700	-1.88560500
C	4.94746400	3.10763700	1.25469300
H	5.11697900	1.23346500	2.33894500
C	4.73626300	3.69518700	0.00669500
H	4.39159600	3.36071300	-2.09800900
H	5.09098000	3.72932200	2.13343100
H	4.70984700	4.77713300	-0.08351500
S	2.14920100	-1.03138000	-0.06019000
C	2.39349900	-1.87728100	-1.65668400
F	3.14346200	-2.97585300	-1.50885600
F	1.22423400	-2.26123800	-2.22375500
F	3.01286000	-1.08994200	-2.56869800
C	-0.68565400	1.50916600	2.44642000
H	-1.39678300	2.09280400	1.86086900
H	-1.22776200	0.72647400	2.98375400
H	-0.25455800	2.17803200	3.19853500
C	1.39501100	0.17318800	2.58791000
H	2.39297600	-0.01600300	2.19034600
H	1.52640700	0.80202200	3.47431600
H	0.99119600	-0.78274700	2.92803200
C	1.31654500	2.12729800	1.08721300
H	1.71600100	2.65596500	1.95884900
H	2.16745700	1.80091500	0.49013300
H	0.73738800	2.84975300	0.51018800
C	-1.39129400	-0.42429000	-1.74910400
H	-1.63766700	0.04704500	-2.70616200
H	-0.79724900	-1.30932700	-1.96830600
H	-2.33538600	-0.72373700	-1.29531300
C	-1.59044000	1.80060300	-0.67944700
H	-1.95805800	2.11119700	-1.66263400
H	-2.46337000	1.53235700	-0.08962200
H	-1.10517500	2.66469800	-0.22380300
C	0.51761000	1.12826600	-1.81071800
H	1.22157600	1.78922100	-1.31333300
H	1.08244400	0.31245600	-2.25680900
H	0.05378100	1.68902300	-2.62975400

Zero-point correction= 0.576405 (Hartree/Particle)
Thermal correction to Energy= 0.615359
Thermal correction to Enthalpy= 0.616304
Thermal correction to Gibbs Free Energy= 0.503595
Sum of electronic and zero-point Energies= -2918.900096
Sum of electronic and thermal Energies= -2918.861142
Sum of electronic and thermal Enthalpies= -2918.860198
Sum of electronic and thermal Free Energies= -2918.972907
(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2920.072052

P_3''

C	-1.40401000	-1.16582700	1.08540200
H	-1.22543500	-0.71833800	2.05110500
C	-0.49760100	-1.28868300	0.11283700
C	-0.75601500	-2.02956100	-1.19302300
H	-0.95111300	-3.08901000	-0.97782200
H	-1.60518600	-1.64511800	-1.76073100
O	0.41896900	-1.86828700	-1.96121800
C	1.48421800	-1.80575900	-1.02710100
H	1.69144200	-2.80987400	-0.62943200
H	2.35897400	-1.45824500	-1.55710400
C	0.99982200	-0.91134000	0.15009700
H	1.42086200	-1.32654100	1.06313300
C	1.42916600	0.62345600	0.16165600
C	1.00505000	1.32406600	1.57471400
C	1.06580800	1.43349500	-1.17762900
S	-3.12929800	-1.59643100	0.91245900
O	-3.28129400	-2.75537000	0.01676000
O	-3.68455900	-1.59737800	2.27361700
C	-3.75697800	-0.15291200	0.04807900
C	-3.93011900	1.03407800	0.76304700
C	-3.98146800	-0.21741100	-1.32652500
C	-4.31075000	2.18522900	0.07676000
H	-3.77669900	1.04520100	1.83688900
C	-4.36579200	0.94107400	-2.00252800
H	-3.87476600	-1.16523600	-1.84207400
C	-4.51979000	2.13998200	-1.30452900
H	-4.44959600	3.11563900	0.61905300
H	-4.54685900	0.90549200	-3.07248400
H	-4.81332800	3.04056700	-1.83572900
S	3.35699700	0.73469800	0.36720000
C	4.28281500	-0.76680900	-0.05460300
F	5.51883200	-0.55517400	0.43238100
F	3.81182200	-1.89998900	0.51016600
F	4.42830300	-1.01744600	-1.37591700
C	-0.44438900	1.86767500	1.57309500
H	-0.51719300	2.81562100	1.03565600
H	-1.17486000	1.19025200	1.14643400
H	-0.73871100	2.06496100	2.61047800
C	1.17441600	0.33248500	2.75306800
H	2.19178200	-0.06893500	2.78117000
H	1.01023500	0.87564700	3.68930400
H	0.48161100	-0.50802800	2.74857300
C	1.88333400	2.53980900	2.01241000
H	1.35135700	3.04701200	2.82475100
H	2.85051500	2.23031600	2.41044000

H	2.05612600	3.27682800	1.23274500
C	1.82280600	0.90124700	-2.42156700
H	1.67666600	1.61451600	-3.23949200
H	2.89802900	0.81720800	-2.25335300
H	1.42744900	-0.05390600	-2.76249500
C	-0.43519000	1.35340300	-1.54927500
H	-0.58446000	1.93863600	-2.46366200
H	-0.74160500	0.33695700	-1.78236400
H	-1.10787700	1.76008300	-0.79788700
C	1.42867000	2.93284300	-1.08732800
H	0.82974900	3.47680400	-0.35613400
H	2.48849100	3.08708500	-0.86684900
H	1.23164500	3.39066900	-2.06195900

Zero-point correction= 0.478560 (Hartree/Particle)
Thermal correction to Energy= 0.507848
Thermal correction to Enthalpy= 0.508792
Thermal correction to Gibbs Free Energy= 0.420346
Sum of electronic and zero-point Energies= -2138.779983
Sum of electronic and thermal Energies= -2138.750696
Sum of electronic and thermal Enthalpies= -2138.749752
Sum of electronic and thermal Free Energies= -2138.838197

(U)B3LYP-D3/6-311++G(d,p)-SDD/SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ energy =-2139.711476