

Supplementary Information

Table of Contents

Computational details	2
-----------------------------	---

Computational Details

B3LYP geometries and energies for all optimized minima and transition state structures

Species A

HF energy= -2015.19127372

No imaginary frequency

Zero-point correction= 0.178592 (Hartree/Particle)

Thermal correction to Energy= 0.210897

Thermal correction to Enthalpy= 0.211842

Thermal correction to Gibbs Free Energy= 0.111213

Sum of electronic and zero-point Energies= -2015.012682

Sum of electronic and thermal Energies= -2014.980376

Sum of electronic and thermal Enthalpies= -2014.979432

Sum of electronic and thermal Free Energies= -2015.080060

Coordinates: A

Os	-1.07660000	1.52240000	0.59750000
Os	0.70550000	-0.65760000	1.15800000
Os	1.39160000	1.33210000	-0.79400000
O	-2.66540000	3.99080000	-0.41520000
O	-1.06230000	2.42900000	3.52180000
O	-3.45680000	-0.35690000	1.07760000
O	-0.98380000	-2.23410000	3.21300000
O	2.06550000	1.01540000	3.32510000
O	3.13660000	-2.54560000	0.86400000
O	1.63400000	3.66930000	-2.82370000
O	3.98300000	2.03170000	0.68210000
O	2.79490000	-0.83140000	-2.46030000
N	-0.32970000	-1.60200000	-0.54600000
C	-2.04590000	-0.82230000	-3.67150000
C	-1.94470000	0.56980000	-3.69640000
C	-1.29650000	1.26730000	-2.66390000
C	-0.71030000	0.62760000	-1.54590000
C	-1.48170000	-1.49740000	-2.58480000
C	-0.83590000	-0.78600000	-1.55610000
C	-2.05060000	3.07950000	-0.07380000
C	-1.07350000	2.07930000	2.42490000
C	-2.56580000	0.35650000	0.91600000
C	-0.36850000	-1.64450000	2.43440000
C	1.55000000	0.39180000	2.50320000
C	2.22700000	-1.84110000	0.95690000
C	1.50280000	2.81080000	-2.06820000
C	3.01290000	1.76010000	0.12470000
C	2.28670000	-0.01290000	-1.82730000
H	0.48000000	2.47170000	0.33210000
S	-1.43030000	-3.22080000	-2.24300000

C	-0.56660000	-2.86510000	-0.77790000
H	-0.25040000	-3.65510000	-0.10550000
H	-1.24530000	2.35130000	-2.73450000
H	-2.37530000	1.11990000	-4.52990000
H	-2.54750000	-1.36070000	-4.47180000

Species TSAA_alt

HF energy= -2015.16190052

Imaginary frequency= 23i

Zero-point correction= 0.178526 (Hartree/Particle)

Thermal correction to Energy= 0.210104

Thermal correction to Enthalpy= 0.211048

Thermal correction to Gibbs Free Energy= 0.111888

Sum of electronic and zero-point Energies= -2014.983374

Sum of electronic and thermal Energies= -2014.951797

Sum of electronic and thermal Enthalpies= -2014.950852

Sum of electronic and thermal Free Energies= -2015.050012

Coordinates: TSAA_alt

Os	-0.94310000	1.54460000	0.50780000
Os	0.66390000	-0.84670000	0.95910000
Os	1.89940000	1.28210000	-0.38340000
O	-2.35820000	4.15940000	-0.32270000
O	0.01690000	2.88280000	3.14730000
O	-3.45550000	0.27070000	1.74320000
O	-1.64380000	-2.25730000	2.46030000
O	1.88430000	0.30350000	3.52330000
O	2.63700000	-3.22650000	1.00640000
O	2.35270000	1.97640000	-3.31070000
O	3.35380000	3.80960000	0.50110000
O	4.31310000	-0.62740000	-0.17020000
N	-0.18750000	-1.50500000	-0.97090000
C	-2.37740000	-0.77820000	-3.81280000
C	-2.83920000	0.48830000	-3.47200000
C	-2.43100000	1.12310000	-2.28350000
C	-1.53910000	0.55320000	-1.35790000
C	-1.49280000	-1.37820000	-2.91570000
C	-1.08390000	-0.73190000	-1.72480000
C	-1.83320000	3.17300000	-0.04320000
C	-0.31550000	2.37080000	2.17250000
C	-2.49470000	0.73180000	1.30940000
C	-0.80480000	-1.71960000	1.88580000
C	1.41500000	-0.10900000	2.55380000
C	1.91230000	-2.32890000	0.95130000
C	2.22660000	1.77770000	-2.18320000

C	2.8040000	2.8853000	0.0893000
C	3.3576000	0.0140000	-0.2111000
H	0.3813000	2.2842000	-0.4772000
S	-0.7325000	-2.9552000	-3.0405000
C	0.0629000	-2.6594000	-1.5345000
H	0.7271000	-3.3985000	-1.1031000
H	-2.8450000	2.1095000	-2.0894000
H	-3.5340000	1.0003000	-4.1351000
H	-2.6893000	-1.2757000	-4.7270000

Species A_alt

HF energy= -2015.16390934

No imaginary frequency

Zero-point correction= 0.178052 (Hartree/Particle)

Thermal correction to Energy= 0.210656

Thermal correction to Enthalpy= 0.211600

Thermal correction to Gibbs Free Energy= 0.108667

Sum of electronic and zero-point Energies= -2014.985857

Sum of electronic and thermal Energies= -2014.953253

Sum of electronic and thermal Enthalpies= -2014.952309

Sum of electronic and thermal Free Energies= -2015.055243

Coordinates: A_alt

Os	-0.8130000	1.5821000	0.4079000
Os	0.6116000	-0.9013000	0.8070000
Os	2.0177000	1.3136000	-0.1192000
O	-2.1634000	4.1773000	-0.6139000
O	0.4584000	3.1989000	2.7469000
O	-3.0962000	0.5294000	2.1834000
O	-1.8092000	-2.6183000	1.7091000
O	1.3117000	-0.1010000	3.6757000
O	2.7545000	-3.1242000	0.7122000
O	3.1806000	0.6234000	-2.8190000
O	2.9940000	4.2688000	-0.2170000
O	4.4262000	0.0514000	1.3183000
N	-0.0490000	-1.2982000	-1.2698000
C	-2.7884000	-0.7699000	-3.6375000
C	-3.4489000	0.2964000	-3.0363000
C	-2.9524000	0.9026000	-1.8655000
C	-1.7828000	0.4806000	-1.2142000
C	-1.6377000	-1.2345000	-2.9961000
C	-1.1724000	-0.6495000	-1.7971000
C	-1.6705000	3.2034000	-0.2531000
C	0.0456000	2.5801000	1.8668000
C	-2.2282000	0.9311000	1.5452000

C	-0.91530000	-1.97470000	1.37670000
C	1.05570000	-0.39330000	2.58880000
C	1.95060000	-2.29480000	0.72230000
C	2.78330000	0.91540000	-1.77550000
C	2.60170000	3.19020000	-0.23440000
C	3.51350000	0.49710000	0.77790000
H	0.43000000	1.86620000	-0.88810000
S	-0.58440000	-2.56030000	-3.46190000
C	0.35240000	-2.28190000	-2.03150000
H	1.19980000	-2.91210000	-1.78820000
H	-3.50830000	1.75040000	-1.47060000
H	-4.35970000	0.68330000	-3.48910000
H	-3.15440000	-1.22520000	-4.55360000

Species B

HF energy= -611.696894688

No imaginary frequency

Zero-point correction= 0.172339 (Hartree/Particle)

Thermal correction to Energy= 0.185794

Thermal correction to Enthalpy= 0.186738

Thermal correction to Gibbs Free Energy= 0.129640

Sum of electronic and zero-point Energies= -611.524555

Sum of electronic and thermal Energies= -611.511101

Sum of electronic and thermal Enthalpies= -611.510157

Sum of electronic and thermal Free Energies= -611.567255

Coordinates: B

C	0.90410000	1.99940000	-0.31260000
C	1.76040000	1.18370000	-0.04160000
C	2.71870000	0.13700000	0.26880000
O	2.42480000	-1.03440000	0.34220000
O	3.94490000	0.65320000	0.45030000
C	5.00150000	-0.29180000	0.76940000
H	5.91170000	0.21180000	0.43130000
H	4.84740000	-1.20100000	0.18040000
C	5.04320000	-0.59330000	2.26100000
H	4.13100000	-1.10920000	2.57870000
H	5.89970000	-1.24290000	2.48130000
H	5.15150000	0.32940000	2.84290000
C	-0.11510000	3.00750000	-0.54870000
O	-0.70350000	3.58390000	0.33700000
O	-0.30340000	3.20140000	-1.86300000
C	-1.30520000	4.19090000	-2.21370000
H	-2.26220000	3.88800000	-1.77310000
H	-1.02000000	5.14920000	-1.76420000

C	-1.36330000	4.25870000	-3.72850000
H	-1.64110000	3.28760000	-4.15400000
H	-2.11260000	4.99820000	-4.03590000
H	-0.39390000	4.55480000	-4.14530000

Species TSABC

HF energy= -2626.86493549

Imaginary frequency= 54i

Zero-point correction= 0.351297 (Hartree/Particle)

Thermal correction to Energy= 0.398339

Thermal correction to Enthalpy= 0.399284

Thermal correction to Gibbs Free Energy= 0.262997

Sum of electronic and zero-point Energies= -2626.513639

Sum of electronic and thermal Energies= -2626.466596

Sum of electronic and thermal Enthalpies= -2626.465652

Sum of electronic and thermal Free Energies= -2626.601938

Coordinates: TSABC

Os	-1.43480000	1.37880000	1.04890000
Os	0.34240000	-0.91020000	1.22730000
Os	1.63080000	1.66820000	1.35130000
O	-2.84040000	4.09580000	0.61700000
O	-1.78660000	1.64190000	4.12630000
O	-3.96250000	-0.34280000	0.83220000
O	-1.96370000	-2.93200000	0.93210000
O	0.17770000	-0.94540000	4.28010000
O	2.62880000	-2.99040000	1.26850000
O	4.08690000	-0.09130000	1.96770000
O	3.03000000	4.42540000	1.02990000
O	1.36390000	2.24780000	4.28700000
N	0.40380000	-0.73930000	-0.98030000
C	-1.20750000	0.58330000	-3.99020000
C	-2.07350000	1.51990000	-3.43320000
C	-2.10800000	1.75140000	-2.04480000
C	-1.30280000	1.06510000	-1.11580000
C	-0.39590000	-0.12000000	-3.09920000
C	-0.45650000	0.10190000	-1.70320000
C	-2.30350000	3.08620000	0.75620000
C	-1.59590000	1.54200000	2.99620000
C	-3.00250000	0.28560000	0.93590000
C	-1.11150000	-2.16210000	1.03050000
C	0.23160000	-0.91000000	3.12790000
C	1.80480000	-2.18180000	1.22290000
C	3.14450000	0.51760000	1.69860000
C	2.45880000	3.43280000	1.11370000

C	1.45460000	2.02020000	3.16000000
H	0.06190000	2.44590000	0.88770000
S	0.78790000	-1.36480000	-3.45990000
C	1.09420000	-1.52540000	-1.76370000
H	1.82230000	-2.23740000	-1.39910000
H	-2.81200000	2.49970000	-1.68740000
H	-2.74240000	2.08220000	-4.08300000
H	-1.17280000	0.39920000	-5.06070000
C	2.10030000	2.34010000	-1.80660000
C	2.99080000	1.54980000	-1.54710000
C	4.10820000	0.60760000	-1.47810000
O	3.97390000	-0.59510000	-1.45940000
O	5.26330000	1.27560000	-1.47680000
C	6.49190000	0.48370000	-1.49240000
H	7.19160000	1.11080000	-2.05160000
H	6.29910000	-0.43760000	-2.04880000
C	6.98190000	0.20300000	-0.08100000
H	6.27050000	-0.42050000	0.46940000
H	7.94020000	-0.32930000	-0.13150000
H	7.13650000	1.13630000	0.47260000
C	1.18190000	3.42850000	-2.14960000
O	0.73150000	4.20450000	-1.34050000
O	0.97730000	3.45330000	-3.46660000
C	0.11720000	4.52440000	-3.95280000
H	-0.86180000	4.41260000	-3.47550000
H	0.54760000	5.48040000	-3.63440000
C	0.04520000	4.39260000	-5.46160000
H	-0.37730000	3.42260000	-5.74650000
H	-0.59620000	5.18400000	-5.86780000
H	1.03870000	4.48730000	-5.91430000

Species C

HF energy= -2626.87681841

No imaginary frequency

Zero-point correction= 0.351697 (Hartree/Particle)

Thermal correction to Energy= 0.398849

Thermal correction to Enthalpy= 0.399794

Thermal correction to Gibbs Free Energy= 0.264630

Sum of electronic and zero-point Energies= -2626.525121

Sum of electronic and thermal Energies= -2626.477969

Sum of electronic and thermal Enthalpies= -2626.477025

Sum of electronic and thermal Free Energies= -2626.612188

Coordinates: C

Os -1.40210000 1.26260000 1.04890000

Os	0.66070000	-0.74230000	1.10340000
Os	1.70970000	2.11080000	1.21330000
O	-3.12660000	3.82750000	0.90180000
O	-1.81240000	1.11500000	4.12650000
O	-3.69750000	-0.72400000	0.69210000
O	-1.27990000	-3.11460000	1.19430000
O	0.88900000	-0.76390000	4.15050000
O	3.31450000	-2.32320000	0.87370000
O	4.42820000	0.96760000	2.12210000
O	2.56460000	5.09020000	1.34810000
O	0.96950000	2.42180000	4.17460000
N	0.35940000	-0.73110000	-1.10060000
C	-1.39820000	0.65410000	-3.99840000
C	-2.15330000	1.65490000	-3.39340000
C	-2.10500000	1.86800000	-2.00220000
C	-1.30020000	1.11630000	-1.12590000
C	-0.57980000	-0.10460000	-3.15930000
C	-0.52390000	0.13040000	-1.76660000
C	-2.47430000	2.87900000	0.92130000
C	-1.57820000	1.19620000	3.00280000
C	-2.82680000	0.01260000	0.85670000
C	-0.56390000	-2.21170000	1.14090000
C	0.79680000	-0.71590000	3.00100000
C	2.33700000	-1.70980000	0.92850000
C	3.42440000	1.38450000	1.74680000
C	2.20020000	4.00820000	1.24140000
C	1.20880000	2.24670000	3.06640000
H	-0.01420000	2.49390000	0.82910000
S	0.46810000	-1.44660000	-3.58360000
C	0.91500000	-1.58520000	-1.91930000
H	1.62870000	-2.33410000	-1.60200000
H	-2.74540000	2.64950000	-1.59980000
H	-2.81230000	2.27060000	-4.00340000
H	-1.45200000	0.46330000	-5.06710000
C	1.69940000	2.47860000	-1.05240000
C	2.50280000	1.53110000	-0.90380000
C	3.62430000	0.68710000	-1.36260000
O	3.49960000	-0.33530000	-1.99560000
O	4.78570000	1.24650000	-1.00690000
C	6.00660000	0.56940000	-1.43840000
H	6.73300000	1.38270000	-1.51520000
H	5.82850000	0.14280000	-2.42950000
C	6.44070000	-0.48820000	-0.43550000
H	5.69900000	-1.29010000	-0.35910000
H	7.39010000	-0.92840000	-0.76600000
H	6.58940000	-0.05040000	0.55730000

C	1.05480000	3.57910000	-1.78560000
O	0.54690000	4.54680000	-1.26930000
O	1.15010000	3.35600000	-3.10300000
C	0.54250000	4.36300000	-3.95740000
H	-0.52000000	4.42970000	-3.69950000
H	1.00870000	5.33030000	-3.73830000
C	0.76030000	3.92550000	-5.39310000
H	0.29270000	2.95140000	-5.57460000
H	0.31190000	4.65980000	-6.07330000
H	1.82890000	3.84860000	-5.62420000

Species TSCD

HF energy= -2626.85804983

Imaginary frequency= 809i

Zero-point correction= 0.349202 (Hartree/Particle)

Thermal correction to Energy= 0.396245

Thermal correction to Enthalpy= 0.397190

Thermal correction to Gibbs Free Energy= 0.260741

Sum of electronic and zero-point Energies= -2626.508847

Sum of electronic and thermal Energies= -2626.461804

Sum of electronic and thermal Enthalpies= -2626.460860

Sum of electronic and thermal Free Energies= -2626.597308

Coordinates: TSCD

Os	-1.37240000	1.26550000	1.06240000
Os	0.40550000	-0.92930000	1.22380000
Os	1.79910000	1.82310000	1.37010000
O	-2.55090000	4.12310000	0.79570000
O	-1.84760000	1.27970000	4.13380000
O	-4.05170000	-0.13360000	0.77280000
O	-1.90730000	-2.93320000	1.12910000
O	0.43440000	-0.91770000	4.28120000
O	2.74060000	-2.97190000	1.14160000
O	3.86500000	-0.14110000	2.52290000
O	3.67990000	4.28460000	1.53290000
O	0.87010000	2.74460000	4.16180000
N	0.34590000	-0.86630000	-0.99130000
C	-1.32790000	0.46370000	-3.96290000
C	-2.13580000	1.44250000	-3.39100000
C	-2.12560000	1.68140000	-2.00310000
C	-1.31920000	0.96650000	-1.09940000
C	-0.51700000	-0.26730000	-3.09160000
C	-0.52330000	-0.02740000	-1.69980000
C	-2.09380000	3.07060000	0.85380000
C	-1.57450000	1.29490000	3.01690000

C	-3.03730000	0.39970000	0.90030000
C	-1.04190000	-2.17120000	1.14950000
C	0.41040000	-0.89770000	3.12820000
C	1.90270000	-2.17880000	1.15230000
C	3.01810000	0.52720000	2.11510000
C	2.96430000	3.39320000	1.43430000
C	1.15150000	2.36240000	3.11520000
H	0.39730000	2.28950000	0.29090000
S	0.61010000	-1.55750000	-3.46880000
C	0.98360000	-1.68580000	-1.78640000
H	1.70980000	-2.40830000	-1.43750000
H	-2.78280000	2.46270000	-1.62680000
H	-2.79330000	2.03210000	-4.02760000
H	-1.33400000	0.27090000	-5.03250000
C	1.42890000	2.37640000	-0.83860000
C	2.40810000	1.55340000	-0.73320000
C	3.54880000	0.94510000	-1.42920000
O	3.51620000	-0.12190000	-2.00200000
O	4.63590000	1.72220000	-1.29860000
C	5.87520000	1.22600000	-1.88050000
H	6.43840000	2.13600000	-2.10530000
H	5.63720000	0.70450000	-2.81200000
C	6.61790000	0.32630000	-0.90410000
H	6.04020000	-0.57890000	-0.68810000
H	7.57780000	0.02340000	-1.34130000
H	6.81940000	0.85140000	0.03680000
C	0.83270000	3.44360000	-1.66660000
O	0.14300000	4.33870000	-1.23530000
O	1.19540000	3.28280000	-2.94740000
C	0.67600000	4.26900000	-3.87840000
H	-0.41490000	4.29050000	-3.78180000
H	1.06230000	5.25400000	-3.59150000
C	1.12190000	3.85500000	-5.26800000
H	0.72780000	2.86420000	-5.52090000
H	0.74890000	4.57640000	-6.00510000
H	2.21520000	3.82360000	-5.33860000

Species D

HF energy= -2626.92105742

No imaginary frequency

Zero-point correction= 0.355861 (Hartree/Particle)

Thermal correction to Energy= 0.402660

Thermal correction to Enthalpy= 0.403604

Thermal correction to Gibbs Free Energy= 0.269799

Sum of electronic and zero-point Energies= -2626.565196

Sum of electronic and thermal Energies= -2626.518398
Sum of electronic and thermal Enthalpies= -2626.517454
Sum of electronic and thermal Free Energies= -2626.651258

Coordinates: **D**

Os	-1.48440000	0.53180000	2.07990000
Os	0.53360000	-1.06310000	0.83840000
Os	0.76680000	1.84390000	0.92190000
O	-3.59470000	2.52990000	3.16840000
O	-1.20440000	-0.89400000	4.81030000
O	-3.47980000	-1.56180000	1.09800000
O	-0.80450000	-3.84260000	0.98340000
O	1.86090000	-1.35050000	3.57910000
O	3.14230000	-2.10030000	-0.44790000
O	3.56900000	1.23180000	1.95970000
O	0.92870000	4.95020000	0.93060000
O	0.34290000	2.53660000	3.90840000
N	-0.49920000	-0.54650000	-1.02970000
C	-2.38810000	2.14150000	-2.61310000
C	-2.62510000	2.98970000	-1.52900000
C	-2.17820000	2.65610000	-0.24210000
C	-1.46900000	1.46270000	0.04960000
C	-1.69490000	0.95230000	-2.37240000
C	-1.24170000	0.63080000	-1.08090000
C	-2.77290000	1.83440000	2.76070000
C	-1.29830000	-0.36610000	3.79410000
C	-2.70650000	-0.79470000	1.47560000
C	-0.32140000	-2.79800000	0.92140000
C	1.35460000	-1.23760000	2.54950000
C	2.16140000	-1.65510000	-0.03900000
C	2.51780000	1.43790000	1.53330000
C	0.81170000	3.80880000	0.88260000
C	0.22360000	2.08320000	2.84570000
H	0.14690000	3.51560000	-1.68580000
S	-1.18210000	-0.28090000	-3.51110000
C	-0.39660000	-1.10550000	-2.20640000
H	0.16820000	-2.01470000	-2.37690000
H	-2.39040000	3.34940000	0.56860000
H	-3.15570000	3.92510000	-1.69080000
H	-2.71350000	2.40960000	-3.61410000
C	1.00670000	2.91610000	-1.97420000
C	1.58000000	2.06630000	-1.09540000
C	2.69250000	1.19030000	-1.58120000
O	2.53960000	0.23430000	-2.31740000
O	3.87920000	1.56700000	-1.07960000
C	5.03880000	0.79880000	-1.48870000

H	5.11320000	0.84540000	-2.58140000
H	4.88630000	-0.24750000	-1.20470000
C	6.24930000	1.40880000	-0.80560000
H	6.14620000	1.36130000	0.28430000
H	7.15360000	0.85800000	-1.09290000
H	6.37610000	2.45810000	-1.09660000
C	1.28300000	3.03960000	-3.43180000
O	0.40550000	3.26980000	-4.24220000
O	2.57910000	2.88910000	-3.76360000
C	2.87620000	2.91990000	-5.17820000
H	2.30100000	2.12900000	-5.67400000
H	2.53970000	3.88060000	-5.58520000
C	4.37270000	2.72340000	-5.33890000
H	4.68400000	1.75240000	-4.93640000
H	4.63970000	2.75640000	-6.40230000
H	4.92980000	3.51140000	-4.81880000

Species TSDE

HF energy= -2626.91009662

Imaginary frequency= 60i

Zero-point correction= 0.355713 (Hartree/Particle)

Thermal correction to Energy= 0.401559

Thermal correction to Enthalpy= 0.402503

Thermal correction to Gibbs Free Energy= 0.271868

Sum of electronic and zero-point Energies= -2626.554384

Sum of electronic and thermal Energies= -2626.508538

Sum of electronic and thermal Enthalpies= -2626.507594

Sum of electronic and thermal Free Energies= -2626.638229

Coordinates: TSDE

Os	-1.29840000	0.26880000	1.99340000
Os	0.41710000	-0.88490000	-0.16630000
Os	0.81750000	1.78420000	0.94950000
O	-3.27230000	1.69830000	3.88240000
O	-0.24830000	-1.68060000	4.13610000
O	-3.54130000	-1.56710000	0.94390000
O	-0.96020000	-3.54210000	0.45300000
O	2.69400000	-1.64840000	1.73460000
O	1.74800000	-2.13480000	-2.66660000
O	3.58930000	1.60540000	2.18120000
O	1.25160000	4.73390000	0.24740000
O	0.16010000	2.48910000	3.85910000
N	-1.21990000	-0.05820000	-1.38990000
C	-3.27980000	2.93860000	-1.73290000
C	-3.01960000	3.58290000	-0.52660000

C	-2.19890000	2.98930000	0.45390000
C	-1.57170000	1.73810000	0.27480000
C	-2.66520000	1.69740000	-1.95240000
C	-1.80810000	1.14070000	-0.98890000
C	-2.52450000	1.17860000	3.17980000
C	-0.66070000	-0.95830000	3.34120000
C	-2.65160000	-0.92150000	1.29140000
C	-0.47950000	-2.51890000	0.22960000
C	1.84900000	-1.34410000	1.01990000
C	1.30700000	-1.62090000	-1.74050000
C	2.55660000	1.67510000	1.67240000
C	1.11750000	3.62430000	0.52180000
C	0.09360000	1.99040000	2.79710000
H	0.06700000	2.01970000	-2.27930000
S	-2.75300000	0.64110000	-3.35090000
C	-1.62990000	-0.42380000	-2.57750000
H	-1.28030000	-1.32330000	-3.07220000
H	-2.06450000	3.51690000	1.39560000
H	-3.47100000	4.55310000	-0.33210000
H	-3.92610000	3.38830000	-2.48200000
C	1.11320000	1.73360000	-2.26400000
C	1.66070000	1.21910000	-1.12300000
C	3.14250000	0.92970000	-1.10760000
O	3.64940000	-0.17340000	-1.15140000
O	3.85600000	2.06030000	-0.94620000
C	5.29370000	1.90570000	-0.87170000
H	5.63790000	1.43180000	-1.79760000
H	5.53130000	1.23320000	-0.03960000
C	5.88980000	3.28800000	-0.67610000
H	5.53100000	3.74090000	0.25550000
H	6.98330000	3.21590000	-0.62400000
H	5.62510000	3.95120000	-1.50790000
C	1.71570000	1.97050000	-3.59000000
O	1.07980000	2.43480000	-4.52060000
O	3.01030000	1.59210000	-3.70560000
C	3.59740000	1.75810000	-5.01330000
H	2.99560000	1.20160000	-5.74200000
H	3.55030000	2.81800000	-5.29080000
C	5.02540000	1.24610000	-4.95000000
H	5.05060000	0.19560000	-4.63810000
H	5.49330000	1.32640000	-5.93910000
H	5.62310000	1.83180000	-4.24150000

Species E

HF energy= -2626.91965442

No imaginary frequency
 Zero-point correction= 0.356498 (Hartree/Particle)
 Thermal correction to Energy= 0.402637
 Thermal correction to Enthalpy= 0.403582
 Thermal correction to Gibbs Free Energy= 0.272179
 Sum of electronic and zero-point Energies= -2626.563157
 Sum of electronic and thermal Energies= -2626.517017
 Sum of electronic and thermal Enthalpies= -2626.516073
 Sum of electronic and thermal Free Energies= -2626.647475

Coordinates: E

Os	-9.74900000	10.20540000	8.53870000
Os	-12.74940000	10.40100000	7.61500000
Os	-11.90470000	8.18470000	9.36280000
S	-10.94620000	13.13290000	12.07280000
O	-9.08140000	8.23780000	6.27720000
O	-6.80850000	10.84840000	9.19660000
O	-12.62910000	13.52730000	7.78260000
O	-15.78140000	10.53940000	7.20910000
O	-9.73070000	12.49660000	6.43920000
O	-12.18860000	10.24050000	4.60200000
O	-13.57480000	7.48180000	6.96070000
O	-13.95460000	6.75590000	11.09840000
O	-11.09910000	5.36250000	8.51300000
O	-8.59900000	6.79890000	9.02010000
O	-7.56940000	7.95890000	10.66550000
O	-10.77880000	7.93950000	13.50110000
O	-9.67420000	6.50850000	12.14160000
N	-10.61510000	11.48130000	10.11410000
C	-9.32380000	8.94120000	7.14850000
C	-7.91240000	10.59560000	8.99780000
C	-12.54930000	12.37890000	7.77600000
C	-14.64150000	10.48670000	7.35560000
C	-9.81770000	11.63920000	7.20100000
C	-12.41320000	10.31380000	5.72750000
C	-13.01670000	8.26400000	7.66540000
C	-13.17460000	7.27850000	10.42490000
C	-11.29160000	6.43990000	8.85860000
C	-10.01070000	12.41110000	10.81020000
H	-8.98460000	12.71110000	10.63070000
C	-11.92990000	11.27440000	10.55040000
C	-12.28820000	12.09020000	11.63560000
C	-13.56480000	12.01160000	12.21620000
H	-13.84050000	12.63710000	13.06090000
C	-14.45950000	11.10100000	11.66710000
H	-15.45710000	11.00980000	12.09100000

C	-14.10090000	10.30220000	10.56060000
H	-14.85290000	9.62800000	10.15740000
C	-12.82950000	10.34640000	9.95010000
C	-6.46380000	5.89300000	11.40670000
H	-5.52730000	5.32630000	11.32340000
H	-6.61260000	6.16990000	12.45620000
H	-7.29300000	5.24900000	11.09950000
C	-6.38430000	7.13020000	10.52440000
H	-6.27050000	6.86210000	9.46950000
H	-5.56420000	7.79070000	10.82210000
C	-8.62120000	7.65580000	9.87640000
C	-9.72440000	8.66710000	10.09970000
C	-10.37020000	8.66930000	11.32500000
H	-10.93600000	9.51570000	11.68610000
C	-10.20840000	7.58300000	12.32670000
C	-10.73500000	6.94800000	14.55270000
H	-11.22940000	6.03670000	14.19630000
H	-9.68680000	6.69910000	14.75700000
C	-11.42930000	7.53720000	15.76750000
H	-12.47450000	7.77920000	15.54190000
H	-11.41360000	6.81350000	16.59160000
H	-10.92560000	8.45160000	16.10250000

Species TSEF

HF energy= -2626.91657397

Imaginary frequency= 26i

Zero-point correction= 0.356731 (Hartree/Particle)

Thermal correction to Energy= 0.401866

Thermal correction to Enthalpy= 0.402810

Thermal correction to Gibbs Free Energy= 0.275047

Sum of electronic and zero-point Energies= -2626.559843

Sum of electronic and thermal Energies= -2626.514708

Sum of electronic and thermal Enthalpies= -2626.513764

Sum of electronic and thermal Free Energies= -2626.641527

Coordinates: TSEF

Os	-9.64550000	10.47680000	8.66470000
Os	-12.51700000	10.21810000	7.62130000
Os	-12.10950000	8.11890000	9.60090000
S	-11.18950000	13.09740000	12.28780000
O	-8.70570000	8.69740000	6.34720000
O	-6.81420000	11.02420000	9.74660000
O	-12.39960000	13.29920000	7.41640000
O	-15.48060000	10.34730000	6.80250000
O	-9.35560000	12.92370000	6.77260000

O	-11.54840000	9.57820000	4.76020000
O	-13.78740000	7.31230000	7.22450000
O	-14.10920000	7.01140000	11.60910000
O	-11.32740000	5.20360000	9.22080000
O	-8.92470000	6.86430000	8.85330000
O	-7.66570000	7.92540000	10.40390000
O	-10.70170000	7.98660000	13.48700000
O	-9.70830000	6.55390000	12.04740000
N	-10.70360000	11.62100000	10.22200000
C	-9.06080000	9.33310000	7.23290000
C	-7.88190000	10.78950000	9.38670000
C	-12.34290000	12.15050000	7.49920000
C	-14.38020000	10.25940000	7.12660000
C	-9.52220000	12.01740000	7.45910000
C	-11.91480000	9.82470000	5.82190000
C	-13.14370000	8.02720000	7.91310000
C	-13.33520000	7.41560000	10.85150000
C	-11.53790000	6.32140000	9.37890000
C	-10.16340000	12.49440000	11.03480000
H	-9.13230000	12.81790000	10.95040000
C	-12.04330000	11.36470000	10.54700000
C	-12.47850000	12.07570000	11.68010000
C	-13.77860000	11.92580000	12.18820000
H	-14.10610000	12.47350000	13.06790000
C	-14.62740000	11.05240000	11.52250000
H	-15.64110000	10.90450000	11.88760000
C	-14.20030000	10.36960000	10.36350000
H	-14.92260000	9.73550000	9.85560000
C	-12.90290000	10.49040000	9.81740000
C	-6.62470000	5.78180000	11.00880000
H	-5.73620000	5.16240000	10.82880000
H	-6.65500000	6.04910000	12.07080000
H	-7.51680000	5.19320000	10.77590000
C	-6.55490000	7.02710000	10.13730000
H	-6.56220000	6.77130000	9.07320000
H	-5.66950000	7.63030000	10.36050000
C	-8.80600000	7.70950000	9.71540000
C	-9.81400000	8.78410000	10.04980000
C	-10.42670000	8.73480000	11.29460000
H	-10.92720000	9.59670000	11.71790000
C	-10.21940000	7.63120000	12.27390000
C	-10.59190000	6.98950000	14.52930000
H	-11.12360000	6.08640000	14.20770000
H	-9.53450000	6.72710000	14.65310000
C	-11.18560000	7.58190000	15.79470000
H	-12.24160000	7.83790000	15.64910000

H	-11.11740000	6.85400000	16.61240000
H	-10.64630000	8.48820000	16.09460000

Species F

HF energy= -2626.92888614

No imaginary frequency

Zero-point correction= 0.357285 (Hartree/Particle)

Thermal correction to Energy= 0.403030

Thermal correction to Enthalpy= 0.403974

Thermal correction to Gibbs Free Energy= 0.273591

Sum of electronic and zero-point Energies= -2626.571601

Sum of electronic and thermal Energies= -2626.525856

Sum of electronic and thermal Enthalpies= -2626.524912

Sum of electronic and thermal Free Energies= -2626.655295

Coordinates: F

Os	-9.35400000	10.95300000	9.22020000
Os	-11.67460000	9.71840000	7.97740000
Os	-12.80950000	8.10890000	10.11920000
S	-11.88470000	13.07580000	12.60770000
O	-7.47100000	9.96610000	7.02330000
O	-7.16270000	10.73940000	11.36770000
O	-11.50260000	12.41930000	6.51490000
O	-14.20920000	9.01560000	6.38760000
O	-8.99760000	13.89990000	8.24200000
O	-10.15030000	8.14740000	5.76860000
O	-15.40460000	7.17130000	8.68030000
O	-13.95090000	7.67670000	12.94410000
O	-11.95070000	5.20510000	9.83240000
O	-9.73920000	6.85710000	8.50300000
O	-8.03790000	7.91750000	9.53190000
O	-10.50470000	8.09420000	13.17990000
O	-9.76190000	6.64810000	11.61730000
N	-10.84040000	11.74840000	10.65510000
C	-8.18150000	10.31520000	7.85830000
C	-7.98470000	10.83050000	10.56570000
C	-11.45960000	11.42320000	7.10010000
C	-13.27510000	9.24090000	7.02890000
C	-9.14430000	12.80730000	8.57320000
C	-10.67440000	8.70480000	6.62300000
C	-14.43690000	7.57550000	9.15110000
C	-13.50430000	7.83070000	11.89440000
C	-12.21370000	6.31560000	9.94080000
C	-10.55060000	12.56640000	11.63570000
H	-9.54290000	12.91180000	11.83540000

C	-12.20650000	11.45670000	10.60180000
C	-12.94140000	12.09910000	11.61240000
C	-14.33410000	11.94020000	11.74010000
H	-14.88990000	12.44000000	12.52870000
C	-14.95840000	11.13690000	10.80870000
H	-16.03710000	11.00110000	10.84360000
C	-14.21810000	10.50510000	9.77060000
H	-14.80040000	10.02350000	8.99270000
C	-12.81190000	10.60980000	9.61650000
C	-6.98250000	5.79840000	10.20700000
H	-6.23190000	5.06160000	9.89140000
H	-6.65560000	6.24230000	11.15440000
H	-7.93380000	5.28760000	10.37710000
C	-7.12270000	6.86300000	9.12960000
H	-7.47970000	6.43630000	8.18820000
H	-6.17670000	7.38620000	8.95560000
C	-9.33480000	7.78970000	9.16540000
C	-10.15810000	8.98850000	9.63730000
C	-10.83680000	8.72960000	10.94900000
H	-11.01660000	9.62570000	11.53250000
C	-10.29060000	7.70670000	11.89250000
C	-10.11360000	7.14760000	14.19910000
H	-10.63190000	6.19810000	14.01840000
H	-9.03730000	6.95890000	14.11070000
C	-10.47900000	7.74550000	15.54620000
H	-11.55830000	7.92580000	15.61440000
H	-10.19330000	7.05500000	16.34930000
H	-9.95730000	8.69620000	15.70870000

Species TSFG

HF energy= -2626.92472741

Imaginary frequency= 73i

Zero-point correction= 0.356604 (Hartree/Particle)

Thermal correction to Energy= 0.401714

Thermal correction to Enthalpy= 0.402658

Thermal correction to Gibbs Free Energy= 0.274383

Sum of electronic and zero-point Energies= -2626.568123

Sum of electronic and thermal Energies= -2626.523013

Sum of electronic and thermal Enthalpies= -2626.522069

Sum of electronic and thermal Free Energies= -2626.650345

Coordinates: TSFG

Os	-9.27530000	10.84280000	9.44740000
Os	-11.55510000	9.68930000	8.07700000
Os	-12.67490000	7.94040000	10.18110000

S	-11.95310000	13.16300000	12.59160000
O	-7.31350000	9.89570000	7.30260000
O	-7.18760000	10.53620000	11.68660000
O	-11.23130000	12.39740000	6.65440000
O	-14.00310000	9.10510000	6.31850000
O	-8.76770000	13.78030000	8.51130000
O	-9.90870000	8.03730000	6.03000000
O	-14.98620000	6.96100000	8.32440000
O	-14.38290000	8.14080000	12.69690000
O	-12.09870000	5.02830000	10.78640000
O	-10.17410000	6.59580000	9.17120000
O	-8.19840000	7.65770000	9.25360000
O	-10.84740000	7.93320000	13.36750000
O	-9.30600000	7.01810000	11.99760000
N	-10.83440000	11.69360000	10.78340000
C	-8.05490000	10.20540000	8.12620000
C	-7.97370000	10.66340000	10.85370000
C	-11.25470000	11.40180000	7.24110000
C	-13.10560000	9.27060000	7.02790000
C	-8.97160000	12.69320000	8.82990000
C	-10.49210000	8.65750000	6.80210000
C	-14.11890000	7.37770000	8.95010000
C	-13.71630000	8.01200000	11.76540000
C	-12.28430000	6.13610000	10.54570000
C	-10.57800000	12.52660000	11.75990000
H	-9.57040000	12.81610000	12.03530000
C	-12.21170000	11.48370000	10.61920000
C	-12.98770000	12.22060000	11.53680000
C	-14.38850000	12.16830000	11.53390000
H	-14.97850000	12.74080000	12.24430000
C	-14.98330000	11.36170000	10.57580000
H	-16.06800000	11.29820000	10.52260000
C	-14.20420000	10.62360000	9.65730000
H	-14.74260000	10.05340000	8.90550000
C	-12.79030000	10.63030000	9.63440000
C	-6.04900000	6.67300000	8.87380000
H	-5.51650000	5.74230000	8.64210000
H	-5.81530000	7.40670000	8.09370000
H	-5.67810000	7.05200000	9.83330000
C	-7.54080000	6.40190000	8.93980000
H	-7.79970000	5.68550000	9.72610000
H	-7.93730000	6.02920000	7.98880000
C	-9.52670000	7.60710000	9.39930000
C	-10.15920000	8.91150000	9.84410000
C	-10.85780000	8.68660000	11.14410000
H	-11.14060000	9.59740000	11.66380000

C	-10.23440000	7.78380000	12.16290000
C	-10.35680000	7.09650000	14.43840000
H	-10.47590000	6.04560000	14.14770000
H	-9.28470000	7.28360000	14.57140000
C	-11.15450000	7.43340000	15.68590000
H	-12.22350000	7.24590000	15.53110000
H	-10.81320000	6.81340000	16.52410000
H	-11.02530000	8.48670000	15.96180000

Species G

HF energy= -2626.96316339

No imaginary frequency

Zero-point correction= 0.358017 (Hartree/Particle)

Thermal correction to Energy= 0.403370

Thermal correction to Enthalpy= 0.404315

Thermal correction to Gibbs Free Energy= 0.275351

Sum of electronic and zero-point Energies= -2626.605146

Sum of electronic and thermal Energies= -2626.559793

Sum of electronic and thermal Enthalpies= -2626.558849

Sum of electronic and thermal Free Energies= -2626.687812

Coordinates: G

Os	-8.78210000	9.73070000	10.21180000
Os	-10.56450000	10.48560000	8.15380000
Os	-12.76650000	8.55150000	8.22470000
S	-11.18880000	11.74960000	13.64880000
O	-6.81760000	8.70360000	8.14030000
O	-7.94790000	7.52450000	12.12020000
O	-6.79880000	12.01780000	10.79700000
O	-8.42740000	12.64410000	8.09290000
O	-12.21520000	11.96000000	6.06260000
O	-9.36120000	8.86480000	5.82570000
O	-13.24620000	9.02530000	5.21340000
O	-14.87300000	10.49950000	9.15610000
O	-14.82030000	6.35540000	8.67450000
O	-11.21630000	7.09010000	7.87900000
O	-9.09490000	6.90100000	8.54640000
O	-13.10810000	6.95890000	11.43360000
O	-11.12320000	6.19890000	10.73800000
N	-10.14280000	10.70780000	11.56550000
C	-7.58390000	9.04450000	8.91780000
C	-8.27100000	8.38650000	11.45020000
C	-7.50790000	11.15730000	10.58300000
C	-9.19540000	11.81140000	8.19540000
C	-11.64720000	11.40820000	6.87600000

C	-9.78840000	9.46930000	6.70050000
C	-13.09770000	8.83200000	6.31880000
C	-14.05660000	9.80170000	8.77310000
C	-14.03060000	7.15940000	8.50280000
C	-10.02640000	10.75960000	12.85410000
H	-9.36460000	10.29620000	13.31530000
C	-11.20490000	11.48050000	11.07620000
C	-11.88830000	12.16190000	12.10610000
C	-12.95470000	13.02520000	11.83710000
H	-13.42550000	13.45670000	12.51470000
C	-13.26030000	13.19450000	10.52280000
H	-13.93480000	13.79320000	10.29350000
C	-12.59870000	12.50430000	9.49940000
H	-12.86790000	12.66060000	8.62320000
C	-11.55640000	11.59290000	9.71330000
C	-9.13120000	4.46880000	8.37980000
H	-9.06720000	3.73150000	7.76880000
H	-8.45690000	4.38340000	9.05750000
H	-9.99890000	4.46960000	8.79100000
C	-8.93140000	5.75130000	7.63560000
H	-9.57790000	5.81250000	6.91450000
H	-8.04320000	5.76660000	7.24750000
C	-10.26190000	7.46860000	8.59120000
C	-10.44680000	8.65430000	9.47630000
C	-11.78680000	8.40030000	10.16030000
H	-12.04030000	9.12960000	10.76370000
C	-11.93300000	7.08500000	10.78800000
C	-13.38090000	5.67370000	12.04590000
H	-13.53040000	5.00510000	11.35930000
H	-12.62200000	5.39460000	12.58260000
C	-14.56140000	5.79750000	12.88360000
H	-15.31860000	6.02460000	12.33790000
H	-14.72770000	4.96320000	13.32810000
H	-14.41980000	6.48640000	13.53690000

Species TSDH

HF energy= -2626.90191667

Imaginary frequency= $62i$

Zero-point correction= 0.355826 (Hartree/Particle)

Thermal correction to Energy= 0.401833

Thermal correction to Enthalpy= 0.402777

Thermal correction to Gibbs Free Energy= 0.270289

Sum of electronic and zero-point Energies= -2626.546090

Sum of electronic and thermal Energies= -2626.500084

Sum of electronic and thermal Enthalpies= -2626.499140

Sum of electronic and thermal Free Energies= -2626.631628

Coordinates: **TSDH**

Os	-1.62430000	0.65200000	1.96440000
Os	0.37810000	-1.35390000	1.22520000
Os	0.79020000	1.58250000	0.97130000
O	-2.84090000	3.36990000	2.68650000
O	-1.27740000	-0.03110000	4.97380000
O	-4.35110000	-0.72550000	1.63110000
O	-2.06190000	-3.13660000	1.81110000
O	1.41280000	-1.65030000	4.09770000
O	2.25470000	-3.62340000	0.27980000
O	3.32040000	-0.16600000	0.81500000
O	0.19820000	4.58510000	1.35000000
O	1.97610000	1.90400000	3.74410000
N	-0.29230000	-0.98840000	-0.83230000
C	-1.84610000	1.46130000	-3.05040000
C	-2.36130000	2.37770000	-2.13250000
C	-2.21790000	2.17960000	-0.75370000
C	-1.55280000	1.06580000	-0.18110000
C	-1.17920000	0.35110000	-2.53600000
C	-1.01910000	0.16660000	-1.14340000
C	-2.38260000	2.35230000	2.39520000
C	-1.39640000	0.22290000	3.85840000
C	-3.32180000	-0.23330000	1.78940000
C	-1.21290000	-2.38630000	1.60000000
C	1.00920000	-1.52840000	3.02990000
C	1.58550000	-2.74880000	0.61220000
C	2.17880000	0.07870000	0.83080000
C	0.37170000	3.46550000	1.17540000
C	1.48980000	1.74920000	2.70550000
H	0.21860000	3.80590000	-1.31480000
S	-0.42700000	-0.96870000	-3.41000000
C	0.06460000	-1.64810000	-1.90420000
H	0.65480000	-2.55580000	-1.87030000
H	-2.65860000	2.92480000	-0.09590000
H	-2.88160000	3.26060000	-2.49660000
H	-1.95850000	1.61190000	-4.12060000
C	1.07140000	3.24970000	-1.69370000
C	1.64320000	2.26030000	-0.96820000
C	2.76540000	1.46220000	-1.54900000
O	2.60960000	0.39680000	-2.11960000
O	3.96330000	1.99690000	-1.27750000
C	5.11990000	1.24950000	-1.72140000
H	5.07860000	1.16310000	-2.81350000
H	5.06880000	0.24070000	-1.29810000

C	6.35220000	2.00340000	-1.25450000
H	6.36970000	2.08160000	-0.16140000
H	7.25720000	1.47420000	-1.57790000
H	6.37480000	3.01630000	-1.67350000
C	1.38710000	3.70330000	-3.07490000
O	0.69340000	4.50530000	-3.66910000
O	2.49420000	3.14780000	-3.61110000
C	2.80780000	3.54850000	-4.96200000
H	1.95320000	3.31200000	-5.60760000
H	2.94430000	4.63630000	-4.98410000
C	4.06280000	2.80600000	-5.38450000
H	3.90910000	1.72150000	-5.33770000
H	4.32560000	3.07490000	-6.41500000
H	4.90800000	3.06540000	-4.73610000

Species H

HF energy= -2626.92540907

No imaginary frequency

Zero-point correction= 0.356193 (Hartree/Particle)

Thermal correction to Energy= 0.402974

Thermal correction to Enthalpy= 0.403918

Thermal correction to Gibbs Free Energy= 0.268459

Sum of electronic and zero-point Energies= -2626.569216

Sum of electronic and thermal Energies= -2626.522435

Sum of electronic and thermal Enthalpies= -2626.521491

Sum of electronic and thermal Free Energies= -2626.656950

Coordinates: H

Os	-1.66750000	0.48680000	1.79420000
Os	0.65980000	-0.96190000	0.97080000
Os	0.64870000	1.97750000	1.30590000
O	-4.12580000	2.26910000	2.41000000
O	-1.68830000	-0.82300000	4.58720000
O	-3.40060000	-1.66260000	0.48070000
O	-0.74820000	-3.66920000	1.28510000
O	1.65050000	-0.97360000	3.86790000
O	3.30310000	-2.18240000	-0.09530000
O	2.86620000	1.08470000	-0.69400000
O	-1.01610000	3.35970000	3.53200000
O	2.91840000	2.43600000	3.27900000
N	-0.11290000	-0.53040000	-1.04950000
C	-1.82410000	2.06320000	-2.96660000
C	-2.20170000	2.94260000	-1.95500000
C	-1.92370000	2.66080000	-0.60630000
C	-1.24360000	1.49740000	-0.18690000

C	-1.13610000	0.90270000	-2.59460000
C	-0.83770000	0.64530000	-1.24650000
C	-3.18840000	1.64390000	2.17960000
C	-1.68060000	-0.34350000	3.54160000
C	-2.73930000	-0.87070000	0.99540000
C	-0.24270000	-2.64250000	1.15320000
C	1.26790000	-0.95880000	2.78250000
C	2.32540000	-1.70400000	0.27830000
C	1.98680000	1.23550000	0.04490000
C	-0.57010000	2.71420000	2.67880000
C	2.06600000	2.26590000	2.52330000
H	-0.18670000	5.08060000	1.91710000
S	-0.50750000	-0.39220000	-3.60100000
C	0.11500000	-1.15500000	-2.17730000
H	0.66830000	-2.08600000	-2.23340000
H	-2.25120000	3.37960000	0.14060000
H	-2.72070000	3.86220000	-2.21400000
H	-2.04380000	2.27950000	-4.00870000
C	0.38720000	5.09280000	0.99480000
C	0.91800000	3.96160000	0.48340000
C	1.70260000	3.98490000	-0.79300000
O	1.25080000	3.71230000	-1.88680000
O	3.00650000	4.23450000	-0.56320000
C	3.87470000	4.22180000	-1.71920000
H	3.52580000	4.98670000	-2.42270000
H	3.79320000	3.24640000	-2.21130000
C	5.28560000	4.49710000	-1.22990000
H	5.61260000	3.72280000	-0.52600000
H	5.97990000	4.50650000	-2.07940000
H	5.34280000	5.46820000	-0.72460000
C	0.44060000	6.47070000	0.44330000
O	-0.13540000	7.40510000	0.96360000
O	1.16930000	6.59700000	-0.68970000
C	1.20590000	7.91910000	-1.26540000
H	0.17980000	8.23260000	-1.49360000
H	1.60380000	8.61910000	-0.52110000
C	2.07100000	7.85740000	-2.51180000
H	1.67060000	7.13240000	-3.23000000
H	2.10170000	8.84270000	-2.99330000
H	3.09830000	7.56660000	-2.26190000

Species TSHI

HF energy= -2626.91734540

Imaginary frequency= 57i

Zero-point correction= 0.355610 (Hartree/Particle)

Thermal correction to Energy=	0.401655
Thermal correction to Enthalpy=	0.402599
Thermal correction to Gibbs Free Energy=	0.270261
Sum of electronic and zero-point Energies=	-2626.561736
Sum of electronic and thermal Energies=	-2626.515691
Sum of electronic and thermal Enthalpies=	-2626.514747
Sum of electronic and thermal Free Energies=	-2626.647085

Coordinates: **TSHI**

Os	-1.53800000	0.60100000	1.88200000
Os	0.77120000	-0.86570000	1.03410000
Os	0.67550000	2.08860000	1.03900000
O	-4.00850000	2.36710000	2.49280000
O	-1.28280000	-0.37370000	4.79750000
O	-3.28330000	-1.73810000	0.96940000
O	-0.50180000	-3.56150000	1.75770000
O	1.98640000	-0.52350000	3.82360000
O	3.36840000	-2.11820000	-0.10520000
O	2.76580000	1.04720000	-1.02510000
O	-0.87350000	3.68860000	3.20050000
O	3.06360000	2.82940000	2.77180000
N	-0.17320000	-0.68860000	-0.95100000
C	-2.13800000	1.61280000	-2.99360000
C	-2.46680000	2.59100000	-2.05880000
C	-2.06740000	2.47590000	-0.71630000
C	-1.30920000	1.38990000	-0.22850000
C	-1.37500000	0.52510000	-2.55410000
C	-0.95760000	0.43400000	-1.21630000
C	-3.06830000	1.74740000	2.25820000
C	-1.37810000	-0.01970000	3.70700000
C	-2.61430000	-0.87260000	1.33370000
C	-0.04840000	-2.54140000	1.47280000
C	1.51920000	-0.64160000	2.77840000
C	2.40490000	-1.63060000	0.29260000
C	1.94200000	1.25220000	-0.23760000
C	-0.46650000	2.95190000	2.40300000
C	2.16630000	2.55030000	2.10550000
H	-0.23720000	5.23660000	1.33180000
S	-0.77730000	-0.85630000	-3.45920000
C	-0.01170000	-1.43110000	-2.01720000
H	0.57260000	-2.34470000	-2.01530000
H	-2.36040000	3.26590000	-0.02950000
H	-3.04090000	3.45850000	-2.37460000
H	-2.45010000	1.70090000	-4.03080000
C	0.32490000	5.14850000	0.40640000
C	0.81540000	3.96550000	-0.02160000

C	1.40950000	3.84300000	-1.39360000
O	0.81680000	3.27880000	-2.29100000
O	2.73480000	4.07550000	-1.35440000
C	3.51830000	3.48350000	-2.41540000
H	3.21280000	3.94530000	-3.36120000
H	3.29660000	2.41170000	-2.46890000
C	4.97800000	3.61120000	-2.01750000
H	5.16950000	3.10500000	-1.06390000
H	5.61510000	3.15370000	-2.78480000
H	5.26340000	4.66430000	-1.91310000
C	0.35800000	6.42510000	-0.34960000
O	-0.49680000	6.78530000	-1.13470000
O	1.45920000	7.16260000	-0.07180000
C	1.57430000	8.41170000	-0.78320000
H	1.66500000	8.25260000	-1.86470000
H	0.64550000	8.98190000	-0.65920000
C	2.64310000	9.26270000	-0.12010000
H	3.63400000	8.79530000	-0.15820000
H	2.69430000	10.22390000	-0.64660000
H	2.36470000	9.51560000	0.90980000

Species I

HF energy= -2626.92900211

No imaginary frequency

Zero-point correction= 0.356175 (Hartree/Particle)

Thermal correction to Energy= 0.402899

Thermal correction to Enthalpy= 0.403843

Thermal correction to Gibbs Free Energy= 0.269436

Sum of electronic and zero-point Energies= -2626.572827

Sum of electronic and thermal Energies= -2626.526103

Sum of electronic and thermal Enthalpies= -2626.525159

Sum of electronic and thermal Free Energies= -2626.659566

Coordinates: I

Os	-1.74500000	0.41610000	1.76330000
Os	0.64450000	-0.98970000	1.03800000
Os	0.56420000	1.94380000	1.37020000
O	-4.26520000	2.14540000	2.26390000
O	-1.84960000	-0.88050000	4.56010000
O	-3.37420000	-1.77610000	0.38770000
O	-0.71860000	-3.72730000	1.28090000
O	1.50830000	-0.99510000	3.97550000
O	3.35760000	-2.14910000	0.08610000
O	2.89230000	1.11300000	-0.52840000
O	-1.24080000	3.34160000	3.47100000

O	2.71140000	2.43050000	3.46940000
N	-0.04670000	-0.56900000	-1.01350000
C	-1.74480000	1.98020000	-3.00000000
C	-2.18020000	2.85240000	-2.00600000
C	-1.94380000	2.58100000	-0.64770000
C	-1.25330000	1.43430000	-0.19970000
C	-1.04260000	0.83790000	-2.59960000
C	-0.78920000	0.58970000	-1.24090000
C	-3.30560000	1.53880000	2.07720000
C	-1.81040000	-0.40620000	3.51250000
C	-2.75080000	-0.96880000	0.92530000
C	-0.22960000	-2.68950000	1.17440000
C	1.17280000	-0.98270000	2.87450000
C	2.35400000	-1.69340000	0.41720000
C	1.97870000	1.23930000	0.17080000
C	-0.73870000	2.68000000	2.66150000
C	1.90750000	2.24730000	2.66480000
H	-0.11500000	5.10280000	2.04610000
S	-0.34340000	-0.44170000	-3.57840000
C	0.24070000	-1.18870000	-2.13050000
H	0.81790000	-2.10620000	-2.16270000
H	-2.31360000	3.29380000	0.08510000
H	-2.70840000	3.75990000	-2.28750000
H	-1.92950000	2.18990000	-4.05020000
C	0.40010000	5.07220000	1.09020000
C	0.85490000	3.91870000	0.55550000
C	1.57840000	3.95670000	-0.76000000
O	1.09810000	3.60410000	-1.81840000
O	2.86440000	4.31660000	-0.60040000
C	3.64690000	4.43280000	-1.81040000
H	3.16040000	5.17000000	-2.45900000
H	3.64660000	3.46630000	-2.32760000
C	5.04570000	4.86290000	-1.40610000
H	5.51060000	4.11840000	-0.74900000
H	5.67370000	4.97510000	-2.29890000
H	5.01960000	5.82300000	-0.87830000
C	0.56270000	6.39180000	0.43320000
O	1.02520000	6.60250000	-0.67120000
O	0.10360000	7.37850000	1.24080000
C	0.20570000	8.71880000	0.71960000
H	1.25700000	8.93040000	0.48870000
H	-0.35420000	8.77700000	-0.22220000
C	-0.34840000	9.66320000	1.77220000
H	0.22160000	9.58630000	2.70540000
H	-0.28790000	10.69850000	1.41440000
H	-1.39800000	9.43410000	1.99060000

Species TSIJ

HF energy= -2626.92331858

Imaginary frequency= $8i$

Zero-point correction= 0.355904 (Hartree/Particle)

Thermal correction to Energy= 0.401933

Thermal correction to Enthalpy= 0.402877

Thermal correction to Gibbs Free Energy= 0.270767

Sum of electronic and zero-point Energies= -2626.567414

Sum of electronic and thermal Energies= -2626.521386

Sum of electronic and thermal Enthalpies= -2626.520442

Sum of electronic and thermal Free Energies= -2626.652552

Coordinates: TSIJ

Os	-2.16200000	0.36310000	1.24880000
Os	0.41810000	-0.77520000	1.60340000
Os	0.02180000	2.15530000	1.20540000
O	-4.83380000	1.80580000	0.64310000
O	-3.04130000	-0.31370000	4.13000000
O	-3.11210000	-2.28400000	0.05630000
O	-0.56080000	-3.66610000	1.90650000
O	0.20430000	-0.26240000	4.61280000
O	3.43870000	-1.45020000	1.81840000
O	2.78830000	1.35970000	-0.00650000
O	-2.46070000	3.77790000	2.13550000
O	1.26820000	2.80340000	3.88920000
N	0.43530000	-0.83430000	-0.59980000
C	-0.73060000	0.97930000	-3.54680000
C	-1.60290000	1.89900000	-2.96870000
C	-1.84070000	1.90180000	-1.58180000
C	-1.21840000	1.00590000	-0.68510000
C	-0.08390000	0.07700000	-2.69430000
C	-0.30840000	0.11070000	-1.30630000
C	-3.81700000	1.31190000	0.86540000
C	-2.70330000	-0.07200000	3.05690000
C	-2.75560000	-1.29460000	0.53070000
C	-0.20370000	-2.57790000	1.77530000
C	0.27160000	-0.44020000	3.47750000
C	2.32540000	-1.17550000	1.71350000
C	1.77000000	1.54300000	0.49500000
C	-1.64630000	3.03980000	1.78600000
C	0.80330000	2.57650000	2.85870000
H	-0.93110000	4.24050000	-1.19550000
S	1.05980000	-1.19730000	-3.08400000
C	1.17060000	-1.56780000	-1.39540000

H	1.82580000	-2.35280000	-1.03400000
H	-2.56170000	2.61860000	-1.19540000
H	-2.11610000	2.61870000	-3.60220000
H	-0.55770000	0.96680000	-4.61980000
C	-0.08780000	4.69130000	-0.68480000
C	0.53200000	4.08100000	0.34380000
C	1.71340000	4.74190000	0.99380000
O	2.86750000	4.45670000	0.75680000
O	1.32670000	5.59700000	1.95940000
C	2.38730000	6.32270000	2.62490000
H	2.93800000	6.88910000	1.86540000
H	3.07770000	5.60420000	3.08220000
C	1.73920000	7.22860000	3.65640000
H	1.18360000	6.64350000	4.39880000
H	2.51030000	7.80720000	4.18030000
H	1.04590000	7.92950000	3.17740000
C	0.31800000	6.01920000	-1.20630000
O	1.23240000	6.70910000	-0.80460000
O	-0.49090000	6.38720000	-2.23250000
C	-0.20560000	7.67080000	-2.82530000
H	-0.28200000	8.44360000	-2.05060000
H	0.82950000	7.67210000	-3.18810000
C	-1.20460000	7.89030000	-3.94810000
H	-2.23220000	7.88160000	-3.56580000
H	-1.02290000	8.86100000	-4.42560000
H	-1.11380000	7.10900000	-4.71200000

Species J

HF energy= -2626.92832706

No imaginary frequency

Zero-point correction= 0.356147 (Hartree/Particle)

Thermal correction to Energy= 0.402899

Thermal correction to Enthalpy= 0.403843

Thermal correction to Gibbs Free Energy= 0.269104

Sum of electronic and zero-point Energies= -2626.572180

Sum of electronic and thermal Energies= -2626.525428

Sum of electronic and thermal Enthalpies= -2626.524484

Sum of electronic and thermal Free Energies= -2626.659223

Coordinates: J

Os	-1.74200000	0.47550000	1.76960000
Os	0.62140000	-0.95440000	1.04070000
Os	0.58150000	1.98180000	1.35850000
O	-4.21950000	2.26570000	2.27850000
O	-1.86660000	-0.82850000	4.56170000

O	-3.40870000	-1.69140000	0.39950000
O	-0.73860000	-3.69130000	1.30520000
O	1.49920000	-0.94700000	3.97350000
O	3.33670000	-2.09850000	0.07250000
O	2.82370000	1.16970000	-0.63620000
O	-1.15340000	3.32290000	3.56710000
O	2.80060000	2.40330000	3.40130000
N	-0.08810000	-0.54660000	-1.00950000
C	-1.72740000	2.03720000	-3.00310000
C	-2.13530000	2.92510000	-2.00950000
C	-1.91040000	2.64940000	-0.64840000
C	-1.25400000	1.48290000	-0.20060000
C	-1.05870000	0.87410000	-2.60050000
C	-0.81030000	0.62520000	-1.24030000
C	-3.27500000	1.63640000	2.09030000
C	-1.81940000	-0.35100000	3.51630000
C	-2.77500000	-0.89130000	0.93620000
C	-0.24830000	-2.65500000	1.18980000
C	1.15940000	-0.93760000	2.87390000
C	2.33290000	-1.64840000	0.41100000
C	1.94980000	1.29580000	0.11200000
C	-0.67870000	2.70460000	2.71110000
C	1.96720000	2.26690000	2.62090000
H	1.74480000	3.42300000	-1.36170000
S	-0.39860000	-0.43070000	-3.57510000
C	0.17790000	-1.18000000	-2.12310000
H	0.73530000	-2.10980000	-2.15290000
H	-2.24940000	3.38030000	0.08090000
H	-2.64010000	3.84580000	-2.29190000
H	-1.91330000	2.24650000	-4.05340000
C	1.39820000	4.20660000	-0.69380000
C	0.88430000	3.93760000	0.52470000
C	0.51160000	5.07020000	1.43510000
O	1.22390000	5.48690000	2.32060000
O	-0.75840000	5.48480000	1.22720000
C	-1.18730000	6.60740000	2.03470000
H	-0.51220000	7.44630000	1.83280000
H	-1.09350000	6.33840000	3.09280000
C	-2.62140000	6.92550000	1.65170000
H	-3.28310000	6.07450000	1.85570000
H	-2.98000000	7.78290000	2.23460000
H	-2.69460000	7.17840000	0.58740000
C	1.54900000	5.58180000	-1.22540000
O	1.24590000	6.61580000	-0.66450000
O	2.09020000	5.54850000	-2.46980000
C	2.32080000	6.82980000	-3.08890000

H	1.36230000	7.35480000	-3.18910000
H	2.95620000	7.43320000	-2.42950000
C	2.97510000	6.57690000	-4.43620000
H	2.32700000	5.97050000	-5.08010000
H	3.16930000	7.53040000	-4.94250000
H	3.92890000	6.05030000	-4.31450000

Species TSJK

HF energy= -2626.89735623

Imaginary frequency= 53i

Zero-point correction= 0.355375 (Hartree/Particle)

Thermal correction to Energy= 0.401630

Thermal correction to Enthalpy= 0.402574

Thermal correction to Gibbs Free Energy= 0.267551

Sum of electronic and zero-point Energies= -2626.541982

Sum of electronic and thermal Energies= -2626.495726

Sum of electronic and thermal Enthalpies= -2626.494782

Sum of electronic and thermal Free Energies= -2626.629805

Coordinates: TSJK

Os	-1.14220000	-1.26970000	1.80200000
Os	0.40060000	-1.47770000	-0.63600000
Os	1.04720000	0.60370000	1.50200000
O	-2.28440000	-0.66040000	4.60960000
O	-0.32910000	-4.13130000	2.70220000
O	-3.80530000	-2.17600000	0.63350000
O	-1.87280000	-3.14970000	-1.86000000
O	1.80540000	-4.01320000	0.36230000
O	2.22560000	-1.34760000	-3.14670000
O	3.42190000	-0.83110000	0.29710000
O	2.74480000	2.82580000	0.13530000
O	1.72360000	-1.21360000	3.86760000
N	-0.65160000	0.35680000	-1.24400000
C	-2.58090000	3.23320000	-0.07310000
C	-2.77700000	2.89900000	1.26780000
C	-2.27930000	1.70300000	1.80280000
C	-1.55280000	0.74470000	1.05370000
C	-1.84940000	2.33410000	-0.84710000
C	-1.33990000	1.13200000	-0.29960000
C	-1.85270000	-0.85630000	3.56250000
C	-0.60480000	-3.07010000	2.36060000
C	-2.78590000	-1.86780000	1.07500000
C	-1.04240000	-2.51650000	-1.37630000
C	1.27120000	-3.05980000	0.01010000
C	1.57170000	-1.35510000	-2.20090000

C	2.31780000	-0.50430000	0.51110000
C	2.07690000	2.03140000	0.62540000
C	1.31180000	-0.59240000	2.98120000
H	-0.07280000	3.61700000	1.84880000
S	-1.44710000	2.43900000	-2.55430000
C	-0.64590000	0.90990000	-2.42780000
H	-0.15340000	0.46560000	-3.28510000
H	-2.47380000	1.51100000	2.85410000
H	-3.33100000	3.57960000	1.91030000
H	-2.97910000	4.15310000	-0.49240000
C	0.49890000	3.42360000	2.75270000
C	1.11300000	2.24120000	2.95800000
C	1.99060000	2.03120000	4.15480000
O	3.19230000	2.16980000	4.13410000
O	1.28990000	1.57920000	5.21120000
C	2.05250000	1.35880000	6.42220000
H	2.53670000	2.30290000	6.69570000
H	2.83560000	0.62040000	6.21470000
C	1.08510000	0.88150000	7.48990000
H	0.60410000	-0.05790000	7.19240000
H	1.62490000	0.70940000	8.42940000
H	0.30460000	1.62950000	7.67160000
C	0.52720000	4.53870000	3.73050000
O	1.13170000	4.56320000	4.78200000
O	-0.23920000	5.56940000	3.29040000
C	-0.28430000	6.72620000	4.15170000
H	-0.65270000	6.42010000	5.13840000
H	0.73560000	7.10650000	4.28660000
C	-1.19280000	7.75190000	3.49670000
H	-2.20740000	7.35480000	3.37160000
H	-1.25080000	8.65200000	4.12090000
H	-0.81100000	8.04090000	2.51040000

Species K

HF energy= -2626.92262191

No imaginary frequency

Zero-point correction= 0.355818 (Hartree/Particle)

Thermal correction to Energy= 0.402565

Thermal correction to Enthalpy= 0.403510

Thermal correction to Gibbs Free Energy= 0.269897

Sum of electronic and zero-point Energies= -2626.566804

Sum of electronic and thermal Energies= -2626.520057

Sum of electronic and thermal Enthalpies= -2626.519112

Sum of electronic and thermal Free Energies= -2626.652725

Coordinates: **K**

Os	-1.36780000	0.64540000	2.22060000
Os	0.94910000	-0.64530000	1.05260000
Os	0.64100000	2.20790000	0.77840000
O	-4.02350000	1.97910000	3.10090000
O	-0.94990000	-0.95520000	4.80150000
O	-2.82690000	-1.83310000	1.16020000
O	0.28380000	-3.61600000	1.59910000
O	2.53200000	-0.51270000	3.66320000
O	3.52820000	-1.03210000	-0.60400000
O	1.73480000	1.75270000	-2.01930000
O	3.58070000	2.64240000	1.56090000
O	0.09410000	5.19940000	0.17210000
N	-0.33300000	-0.62000000	-0.75830000
C	-2.99240000	1.24250000	-2.43550000
C	-3.19370000	2.29320000	-1.53850000
C	-2.43840000	2.39630000	-0.35920000
C	-1.43930000	1.46450000	0.00610000
C	-2.01360000	0.29560000	-2.11580000
C	-1.26570000	0.40630000	-0.92910000
C	-3.01160000	1.54950000	2.76010000
C	-1.07690000	-0.31140000	3.85650000
C	-2.25480000	-0.91420000	1.55710000
C	0.50470000	-2.50070000	1.39810000
C	1.92910000	-0.51780000	2.68120000
C	2.55500000	-0.86350000	-0.00660000
C	1.34030000	1.90840000	-0.94490000
C	2.46090000	2.48430000	1.36820000
C	0.23720000	4.09370000	0.46000000
H	-1.67050000	3.97320000	2.47430000
S	-1.50780000	-1.13040000	-3.00970000
C	-0.35820000	-1.46790000	-1.75180000
H	0.29330000	-2.33320000	-1.80280000
H	-2.63540000	3.23820000	0.30030000
H	-3.94750000	3.04520000	-1.76060000
H	-3.57590000	1.16600000	-3.34930000
C	-0.91030000	3.69900000	3.20200000
C	-0.24950000	2.51160000	3.10280000
C	0.80790000	2.26830000	4.15220000
O	1.99230000	2.45740000	3.97290000
O	0.28880000	1.78130000	5.28670000
C	1.21300000	1.62600000	6.39640000
H	1.65340000	2.60790000	6.59950000
H	2.01260000	0.94330000	6.08960000
C	0.42210000	1.09450000	7.57750000
H	-0.02500000	0.12110000	7.34620000

H	1.08810000	0.97270000	8.44080000
H	-0.37870000	1.78960000	7.85580000
C	-0.69230000	4.72920000	4.25140000
O	0.12870000	4.69220000	5.14460000
O	-1.55580000	5.75470000	4.07130000
C	-1.45810000	6.83820000	5.02240000
H	-1.61980000	6.43620000	6.03000000
H	-0.43960000	7.24350000	4.98840000
C	-2.50120000	7.87460000	4.64510000
H	-3.50980000	7.44650000	4.68040000
H	-2.45900000	8.71670000	5.34660000
H	-2.32360000	8.25900000	3.63390000

Species TSKL

HF energy= -2626.91496039

Imaginary frequency= 69i

Zero-point correction= 0.355654 (Hartree/Particle)

Thermal correction to Energy= 0.401672

Thermal correction to Enthalpy= 0.402616

Thermal correction to Gibbs Free Energy= 0.271052

Sum of electronic and zero-point Energies= -2626.559306

Sum of electronic and thermal Energies= -2626.513288

Sum of electronic and thermal Enthalpies= -2626.512344

Sum of electronic and thermal Free Energies= -2626.643908

Coordinates: TSKL

Os	-1.50550000	0.50470000	2.27180000
Os	0.86330000	-0.86240000	1.06760000
Os	0.95070000	1.93410000	0.89300000
O	-4.39420000	1.45720000	2.79500000
O	-1.13480000	-1.05760000	4.89580000
O	-2.73990000	-2.02410000	0.97110000
O	0.10250000	-3.84390000	1.45240000
O	2.32460000	-0.80940000	3.75190000
O	3.44010000	-1.34970000	-0.54490000
O	1.58130000	1.86340000	-2.05100000
O	3.93940000	1.95830000	1.50290000
O	0.60130000	5.04050000	0.95730000
N	-0.39060000	-0.62900000	-0.75700000
C	-2.64320000	1.71880000	-2.42360000
C	-2.77990000	2.70060000	-1.44180000
C	-2.16340000	2.56660000	-0.18490000
C	-1.37080000	1.45420000	0.17250000
C	-1.84250000	0.61070000	-2.12210000
C	-1.20930000	0.50070000	-0.87160000

C	-3.29670000	1.16680000	2.60450000
C	-1.26420000	-0.46190000	3.91870000
C	-2.21190000	-1.10290000	1.41960000
C	0.35200000	-2.72740000	1.30940000
C	1.76820000	-0.80100000	2.74210000
C	2.45970000	-1.16400000	0.03560000
C	1.34510000	1.88800000	-0.91810000
C	2.81050000	1.94700000	1.28600000
C	0.67550000	3.89600000	0.97770000
H	-2.47160000	3.66090000	2.84870000
S	-1.41760000	-0.76560000	-3.12960000
C	-0.41970000	-1.36080000	-1.83830000
H	0.15160000	-2.27630000	-1.94550000
H	-2.32530000	3.35040000	0.55180000
H	-3.38640000	3.57950000	-1.65030000
H	-3.12960000	1.81930000	-3.39020000
C	-1.54290000	3.50940000	3.39360000
C	-0.87370000	2.33200000	3.33960000
C	0.38700000	2.20830000	4.11630000
O	1.48150000	2.18430000	3.55670000
O	0.22650000	2.00140000	5.41530000
C	1.43370000	1.88610000	6.21960000
H	1.95770000	2.84650000	6.16330000
H	2.07190000	1.11200000	5.78170000
C	1.00130000	1.54740000	7.63370000
H	0.46270000	0.59310000	7.66050000
H	1.88550000	1.46310000	8.27750000
H	0.34960000	2.32830000	8.04170000
C	-1.06620000	4.69040000	4.14910000
O	0.01290000	4.79950000	4.70160000
O	-1.99200000	5.67640000	4.13320000
C	-1.63320000	6.89140000	4.82590000
H	-1.43270000	6.65150000	5.87720000
H	-0.70390000	7.28270000	4.39460000
C	-2.78910000	7.86420000	4.67340000
H	-3.70830000	7.45170000	5.10540000
H	-2.55590000	8.80340000	5.18980000
H	-2.97510000	8.08900000	3.61660000

Species L

HF energy= -2626.92422452

No imaginary frequency

Zero-point correction= 0.356680 (Hartree/Particle)

Thermal correction to Energy= 0.402962

Thermal correction to Enthalpy= 0.403907

Thermal correction to Gibbs Free Energy=	0.271616
Sum of electronic and zero-point Energies=	-2626.567545
Sum of electronic and thermal Energies=	-2626.521262
Sum of electronic and thermal Enthalpies=	-2626.520318
Sum of electronic and thermal Free Energies=	-2626.652608

Coordinates: **L**

Os	-1.57810000	0.42170000	2.29070000
Os	0.88200000	-0.77530000	1.06640000
Os	1.21840000	2.01930000	1.26190000
O	-4.40470000	1.25900000	3.18970000
O	-0.86620000	-1.13590000	4.88530000
O	-2.76310000	-2.15290000	1.04880000
O	0.07800000	-3.76120000	1.23910000
O	2.33540000	-0.94110000	3.74940000
O	3.46020000	-1.27520000	-0.53840000
O	1.22270000	2.07790000	-1.77780000
O	4.24100000	1.94340000	1.16740000
O	0.96350000	5.13640000	1.19360000
N	-0.34440000	-0.42410000	-0.77060000
C	-2.77810000	1.73680000	-2.45570000
C	-3.24880000	2.49090000	-1.38530000
C	-2.83100000	2.23250000	-0.06460000
C	-1.89940000	1.23730000	0.27340000
C	-1.83070000	0.75260000	-2.16020000
C	-1.36970000	0.54040000	-0.84220000
C	-3.34250000	0.97870000	2.84610000
C	-1.10680000	-0.52500000	3.93920000
C	-2.25890000	-1.21970000	1.49600000
C	0.31690000	-2.63730000	1.14950000
C	1.78070000	-0.85530000	2.74100000
C	2.48590000	-1.08770000	0.05250000
C	1.17180000	2.01760000	-0.62730000
C	3.08860000	1.97800000	1.17810000
C	1.02040000	4.00040000	1.33710000
H	-2.47170000	3.68420000	2.70270000
S	-1.01880000	-0.34120000	-3.26700000
C	-0.09340000	-0.95450000	-1.93890000
H	0.66580000	-1.71340000	-2.09030000
H	-3.28810000	2.82380000	0.72600000
H	-3.97910000	3.27720000	-1.56760000
H	-3.12310000	1.90930000	-3.47130000
C	-1.55440000	3.51170000	3.25910000
C	-0.92450000	2.31120000	3.23140000
C	0.30650000	2.13850000	4.03240000
O	1.40940000	1.97910000	3.46410000

O	0.17160000	1.99700000	5.32820000
C	1.37960000	1.79350000	6.12560000
H	2.00250000	2.68580000	6.00290000
H	1.91490000	0.92800000	5.72400000
C	0.93610000	1.58870000	7.56080000
H	0.29830000	0.70200000	7.65090000
H	1.81820000	1.44550000	8.19660000
H	0.38210000	2.45980000	7.92800000
C	-1.00580000	4.68220000	3.97520000
O	0.10810000	4.74410000	4.47080000
O	-1.87990000	5.70800000	3.99030000
C	-1.42850000	6.92090000	4.63450000
H	-1.21650000	6.70050000	5.68780000
H	-0.48900000	7.23880000	4.16720000
C	-2.52630000	7.95790000	4.47780000
H	-3.45780000	7.61730000	4.94450000
H	-2.22220000	8.89600000	4.95800000
H	-2.72430000	8.16100000	3.41900000

Species TSLM

HF energy= -2626.92386235

Imaginary frequency= 21i

Zero-point correction= 0.356676 (Hartree/Particle)

Thermal correction to Energy= 0.402077

Thermal correction to Enthalpy= 0.403021

Thermal correction to Gibbs Free Energy= 0.273567

Sum of electronic and zero-point Energies= -2626.567186

Sum of electronic and thermal Energies= -2626.521786

Sum of electronic and thermal Enthalpies= -2626.520842

Sum of electronic and thermal Free Energies= -2626.650295

Coordinates: TSLM

Os	-1.59050000	0.32680000	2.36150000
Os	0.91860000	-0.65990000	1.06020000
Os	1.29800000	2.17510000	1.36110000
O	-4.33780000	1.17690000	3.46550000
O	-0.74570000	-1.22260000	4.92180000
O	-2.81430000	-2.22040000	1.11450000
O	0.07360000	-3.62800000	1.14090000
O	2.36670000	-0.94040000	3.73840000
O	3.46510000	-1.22690000	-0.58880000
O	1.09500000	2.40990000	-1.66660000
O	4.26210000	1.68410000	1.08000000
O	1.54980000	5.28900000	1.46420000
N	-0.30350000	-0.25560000	-0.75730000

C	-2.92580000	1.77230000	-2.31990000
C	-3.48980000	2.38290000	-1.20470000
C	-3.05690000	2.07040000	0.09910000
C	-2.01760000	1.16740000	0.38150000
C	-1.88100000	0.87640000	-2.08050000
C	-1.41130000	0.61420000	-0.77300000
C	-3.30900000	0.88580000	3.03640000
C	-1.03520000	-0.61450000	3.98710000
C	-2.30800000	-1.29670000	1.57870000
C	0.33130000	-2.50540000	1.09310000
C	1.81310000	-0.81320000	2.73330000
C	2.51060000	-0.98740000	0.01520000
C	1.13580000	2.28770000	-0.52120000
C	3.12280000	1.84710000	1.16280000
C	1.37440000	4.15810000	1.54200000
H	-2.31400000	3.62720000	2.47300000
S	-0.96270000	-0.05350000	-3.25130000
C	0.00300000	-0.67530000	-1.95740000
H	0.82790000	-1.35040000	-2.15330000
H	-3.59310000	2.53860000	0.92190000
H	-4.30380000	3.09300000	-1.33930000
H	-3.27820000	1.98160000	-3.32610000
C	-1.44980000	3.46520000	3.11110000
C	-0.85320000	2.24640000	3.19040000
C	0.33400000	2.09920000	4.06100000
O	1.47150000	2.00560000	3.54390000
O	0.13810000	1.91710000	5.34180000
C	1.30980000	1.71810000	6.19490000
H	1.90580000	2.63540000	6.14510000
H	1.89520000	0.89030000	5.78380000
C	0.79850000	1.43050000	7.59260000
H	0.18960000	0.51950000	7.60560000
H	1.65060000	1.28640000	8.26790000
H	0.19510000	2.26390000	7.96950000
C	-0.95170000	4.64940000	3.84330000
O	0.10200000	4.69980000	4.45710000
O	-1.79640000	5.69180000	3.73090000
C	-1.39720000	6.91260000	4.39690000
H	-1.28530000	6.70570000	5.46810000
H	-0.41620000	7.21670000	4.01320000
C	-2.46800000	7.95340000	4.12380000
H	-3.44090000	7.62590000	4.50810000
H	-2.20190000	8.89680000	4.61580000
H	-2.56620000	8.14120000	3.04830000

Species M

HF energy= -2626.96347900

No imaginary frequency

Zero-point correction= 0.357832 (Hartree/Particle)

Thermal correction to Energy= 0.403236

Thermal correction to Enthalpy= 0.404180

Thermal correction to Gibbs Free Energy= 0.275342

Sum of electronic and zero-point Energies= -2626.605647

Sum of electronic and thermal Energies= -2626.560243

Sum of electronic and thermal Enthalpies= -2626.559299

Sum of electronic and thermal Free Energies= -2626.688137

Coordinates: **M**

Os	1.97890000	6.22230000	7.44600000
Os	4.66090000	6.85480000	8.47930000
Os	5.78580000	4.26820000	9.49000000
C	0.70530000	4.85410000	7.10010000
C	0.80950000	7.77960000	7.16450000
C	2.58610000	6.29530000	5.57620000
C	5.63750000	6.62080000	6.86420000
C	3.75220000	8.48310000	7.87260000
C	6.21570000	7.64470000	9.29890000
C	6.12440000	2.44560000	10.03790000
C	5.89050000	4.89020000	11.26840000
C	7.64850000	4.76090000	9.05530000
O	-0.04590000	4.00770000	6.88410000
O	0.09480000	8.67070000	7.03570000
O	2.87500000	6.42980000	4.47080000
O	6.23900000	6.49630000	5.88930000
O	3.45610000	9.55620000	7.56340000
O	7.14020000	8.14450000	9.77730000
O	6.34440000	1.36920000	10.37460000
O	5.94050000	5.25910000	12.36150000
O	8.73280000	5.02350000	8.78620000
N	3.53050000	7.12220000	10.39740000
S	2.98340000	7.72270000	12.85370000
O	5.41040000	3.57840000	7.43640000
O	3.81390000	3.84440000	5.90970000
O	2.98300000	2.03650000	8.26830000
O	2.83000000	2.15600000	10.51890000
C	4.05210000	7.58720000	11.50380000
H	5.09380000	7.86430000	11.60210000
C	2.15650000	6.85110000	10.54140000
C	1.31180000	6.38630000	9.50870000
C	-0.01670000	6.16510000	9.91130000
H	-0.74010000	5.81050000	9.17970000

C	-0.48550000	6.39040000	11.21860000
H	-1.53050000	6.19350000	11.45100000
C	0.35610000	6.87400000	12.21450000
H	-0.00100000	7.06880000	13.22200000
C	1.68460000	7.10140000	11.85200000
C	3.77760000	2.85710000	3.72600000
H	4.31600000	2.20680000	3.02590000
H	3.64460000	3.83750000	3.25560000
H	2.79070000	2.41990000	3.91450000
C	4.57070000	2.97300000	5.01300000
H	4.69420000	2.01090000	5.51980000
H	5.55820000	3.42080000	4.85990000
C	4.28700000	4.04650000	7.11120000
C	3.51560000	4.87530000	8.09740000
C	3.58300000	4.08710000	9.39300000
H	3.10100000	4.57930000	10.23310000
C	3.10610000	2.67550000	9.30020000
C	2.39240000	0.77840000	10.54470000
H	3.19740000	0.14520000	10.15180000
H	1.52830000	0.66960000	9.87930000
C	2.05260000	0.43390000	11.98390000
H	1.71650000	-0.60840000	12.04750000
H	1.25060000	1.07900000	12.36150000
H	2.92770000	0.55410000	12.63350000

Species N

HF energy= -344.509527570

No imaginary frequency

Zero-point correction= 0.099855 (Hartree/Particle)

Thermal correction to Energy= 0.107491

Thermal correction to Enthalpy= 0.108435

Thermal correction to Gibbs Free Energy= 0.067785

Sum of electronic and zero-point Energies= -344.409673

Sum of electronic and thermal Energies= -344.402037

Sum of electronic and thermal Enthalpies= -344.401093

Sum of electronic and thermal Free Energies= -344.441742

Coordinates: N

C	-0.86830000	-0.36070000	0.66930000
H	-1.75150000	-0.37030000	1.27030000
C	0.13030000	-0.35020000	-0.01300000
C	1.31670000	-0.40500000	-0.84890000
O	1.65370000	-1.38060000	-1.48110000
O	1.97370000	0.76960000	-0.82210000
C	3.18190000	0.84780000	-1.62140000

H	3.28940000	1.91630000	-1.82980000
H	3.01830000	0.30850000	-2.55950000
C	4.38450000	0.29750000	-0.86670000
H	4.26730000	-0.77520000	-0.68080000
H	5.29400000	0.44580000	-1.46270000
H	4.51270000	0.81320000	0.09210000

Species TSANO

HF energy= -2359.67996412

Imaginary frequency= 24i

Zero-point correction= 0.279226 (Hartree/Particle)

Thermal correction to Energy= 0.320525

Thermal correction to Enthalpy= 0.321470

Thermal correction to Gibbs Free Energy= 0.197845

Sum of electronic and zero-point Energies= -2359.400738

Sum of electronic and thermal Energies= -2359.359439

Sum of electronic and thermal Enthalpies= -2359.358495

Sum of electronic and thermal Free Energies= -2359.482119

Coordinates: TSANO

Os	-1.57160000	1.34380000	1.15560000
Os	0.25420000	-0.91720000	1.37360000
Os	1.41380000	1.69680000	1.39720000
O	-3.16750000	3.95980000	0.78150000
O	-1.95080000	1.51410000	4.23670000
O	-3.98410000	-0.51010000	0.73590000
O	-2.01820000	-3.00020000	1.28410000
O	0.25730000	-0.78500000	4.43050000
O	2.56710000	-2.96740000	1.41270000
O	3.96150000	-0.00780000	1.76060000
O	2.70120000	4.36750000	0.50330000
O	1.51940000	2.61760000	4.25700000
N	0.25970000	-0.82590000	-0.83770000
C	-0.97060000	0.78480000	-3.88590000
C	-1.71640000	1.83020000	-3.34950000
C	-1.84570000	1.99850000	-1.95700000
C	-1.24680000	1.15000000	-1.00610000
C	-0.35180000	-0.07150000	-2.97350000
C	-0.47850000	0.11190000	-1.57620000
C	-2.55620000	2.98860000	0.89300000
C	-1.78210000	1.43850000	3.10170000
C	-3.06590000	0.16050000	0.91740000
C	-1.18370000	-2.20640000	1.29590000
C	0.24150000	-0.81640000	3.27760000
C	1.72940000	-2.17420000	1.36990000

C	2.96800000	0.55030000	1.58750000
C	2.19560000	3.39550000	0.85290000
C	1.49610000	2.28350000	3.15320000
H	-0.17890000	2.52980000	1.14380000
S	0.69550000	-1.43660000	-3.31150000
C	0.90410000	-1.66120000	-1.60990000
H	1.54290000	-2.44860000	-1.23060000
H	-2.45890000	2.83040000	-1.61860000
H	-2.21900000	2.52700000	-4.01800000
H	-0.87000000	0.64480000	-4.95880000
C	1.98220000	2.18990000	-2.14740000
H	1.09830000	2.77370000	-2.30370000
C	2.97460000	1.50980000	-1.99730000
C	4.10680000	0.61100000	-1.83060000
O	3.98310000	-0.56510000	-1.55870000
O	5.26490000	1.25130000	-2.02290000
C	6.48290000	0.46280000	-1.89000000
H	7.18910000	0.96350000	-2.55800000
H	6.28390000	-0.54780000	-2.25790000
C	6.97380000	0.45190000	-0.44990000
H	6.25380000	-0.04600000	0.20770000
H	7.92490000	-0.09260000	-0.39300000
H	7.14040000	1.47280000	-0.08680000

Species O

HF energy= -2359.69126103

No imaginary frequency

Zero-point correction= 0.279866 (Hartree/Particle)

Thermal correction to Energy= 0.321042

Thermal correction to Enthalpy= 0.321986

Thermal correction to Gibbs Free Energy= 0.201353

Sum of electronic and zero-point Energies= -2359.411395

Sum of electronic and thermal Energies= -2359.370219

Sum of electronic and thermal Enthalpies= -2359.369275

Sum of electronic and thermal Free Energies= -2359.489908

Coordinates: O

Os	-1.39150000	1.41190000	0.99020000
Os	0.44260000	-0.81500000	1.20500000
Os	1.76810000	1.87760000	1.12590000
O	-2.87620000	4.09280000	0.59060000
O	-1.73970000	1.64890000	4.07120000
O	-3.87750000	-0.35930000	0.81420000
O	-1.81210000	-2.89790000	1.23970000
O	0.50190000	-0.67000000	4.25870000

O	2.77940000	-2.84360000	1.21430000
O	4.14110000	0.08090000	1.94580000
O	3.16630000	4.64180000	0.92700000
O	1.27650000	2.53760000	4.06460000
N	0.32210000	-0.82320000	-1.00170000
C	-1.19460000	0.56090000	-4.03350000
C	-1.96820000	1.58530000	-3.49760000
C	-2.00670000	1.82360000	-2.10970000
C	-1.28060000	1.07330000	-1.16530000
C	-0.46310000	-0.20820000	-3.12620000
C	-0.50680000	0.03910000	-1.73450000
C	-2.31260000	3.09450000	0.71060000
C	-1.53830000	1.56780000	2.94160000
C	-2.93130000	0.29180000	0.90550000
C	-0.97830000	-2.10210000	1.21230000
C	0.47170000	-0.69720000	3.10560000
C	1.93460000	-2.05810000	1.17810000
C	3.22020000	0.69120000	1.61210000
C	2.60610000	3.63850000	0.96850000
C	1.42640000	2.24930000	2.96290000
H	0.11310000	2.52550000	0.78360000
S	0.62430000	-1.54250000	-3.46720000
C	0.94860000	-1.67230000	-1.77290000
H	1.64250000	-2.41410000	-1.39990000
H	-2.64460000	2.63580000	-1.76790000
H	-2.56000000	2.21270000	-4.16180000
H	-1.16070000	0.36840000	-5.10240000
C	1.64120000	2.11530000	-1.25260000
H	0.81300000	2.66750000	-1.64920000
C	2.65170000	1.42360000	-1.10360000
C	3.85070000	0.61800000	-1.38910000
O	3.81530000	-0.56230000	-1.65180000
O	4.94540000	1.37930000	-1.33770000
C	6.21790000	0.72990000	-1.64240000
H	6.83440000	1.54800000	-2.02400000
H	6.04730000	-0.00180000	-2.43730000
C	6.82530000	0.08940000	-0.40430000
H	6.19690000	-0.72570000	-0.03130000
H	7.80970000	-0.32350000	-0.65880000
H	6.95800000	0.82740000	0.39470000

Species TSOP

HF energy= -2359.66695751

Imaginary frequency= 833i

Zero-point correction= 0.277927 (Hartree/Particle)

Thermal correction to Energy=	0.318873
Thermal correction to Enthalpy=	0.319817
Thermal correction to Gibbs Free Energy=	0.198775
Sum of electronic and zero-point Energies=	-2359.389030
Sum of electronic and thermal Energies=	-2359.348084
Sum of electronic and thermal Enthalpies=	-2359.347140
Sum of electronic and thermal Free Energies=	-2359.468182

Coordinates: **TSOP**

Os	-1.28830000	1.39810000	0.94610000
Os	0.37230000	-0.89660000	1.28560000
Os	1.86220000	1.78460000	1.31440000
O	-2.30110000	4.27880000	0.43460000
O	-1.81650000	1.64710000	4.00050000
O	-4.00110000	0.05320000	0.67310000
O	-2.05960000	-2.75970000	1.20370000
O	0.30220000	-0.73480000	4.33870000
O	2.55380000	-3.09540000	1.39740000
O	3.91990000	-0.25740000	2.33660000
O	3.68550000	4.29050000	1.43360000
O	1.08830000	2.63110000	4.16640000
N	0.40030000	-0.92840000	-0.92680000
C	-1.07360000	0.33910000	-4.03000000
C	-1.86900000	1.37020000	-3.54130000
C	-1.92040000	1.66450000	-2.16440000
C	-1.18950000	0.95900000	-1.19170000
C	-0.34100000	-0.38800000	-3.08830000
C	-0.40790000	-0.09300000	-1.70860000
C	-1.92360000	3.20300000	0.60050000
C	-1.52470000	1.56910000	2.89150000
C	-2.97280000	0.55860000	0.79780000
C	-1.15230000	-2.04840000	1.21840000
C	0.31800000	-0.77090000	3.18620000
C	1.77380000	-2.24790000	1.33540000
C	3.06210000	0.42570000	1.97350000
C	2.98330000	3.38540000	1.34660000
C	1.30620000	2.27940000	3.09330000
H	0.49760000	2.27540000	0.20460000
S	0.76130000	-1.72470000	-3.36050000
C	1.05090000	-1.79560000	-1.65840000
H	1.73840000	-2.52360000	-1.24740000
H	-2.56750000	2.48360000	-1.85570000
H	-2.46370000	1.96190000	-4.23470000
H	-1.02550000	0.10870000	-5.09080000
C	1.50770000	2.26110000	-0.94270000
H	0.88150000	2.85930000	-1.58650000

C	2.52590000	1.51640000	-0.80760000
C	3.68490000	0.84480000	-1.40550000
O	3.66580000	-0.27650000	-1.86530000
O	4.76800000	1.63450000	-1.33680000
C	6.02070000	1.08030000	-1.83010000
H	6.58950000	1.96120000	-2.14020000
H	5.80610000	0.45820000	-2.70370000
C	6.73910000	0.29640000	-0.74190000
H	6.15410000	-0.57810000	-0.43750000
H	7.70770000	-0.05410000	-1.12050000
H	6.92070000	0.92460000	0.13780000

Species P

HF energy= -2359.73045641

No imaginary frequency

Zero-point correction= 0.284173 (Hartree/Particle)

Thermal correction to Energy= 0.325039

Thermal correction to Enthalpy= 0.325983

Thermal correction to Gibbs Free Energy= 0.206549

Sum of electronic and zero-point Energies= -2359.446284

Sum of electronic and thermal Energies= -2359.405418

Sum of electronic and thermal Enthalpies= -2359.404474

Sum of electronic and thermal Free Energies= -2359.523908

Coordinates: P

Os	-1.32940000	0.95040000	1.41450000
Os	0.71090000	-1.00930000	1.00040000
Os	1.22650000	1.81290000	0.52750000
O	-3.38470000	3.27030000	1.56860000
O	-1.75080000	0.15380000	4.37080000
O	-3.30320000	-1.18940000	0.48140000
O	-0.92160000	-3.59200000	1.47040000
O	1.46600000	-0.72610000	3.95120000
O	3.37980000	-2.46680000	0.47890000
O	3.69220000	1.33600000	2.25660000
O	1.67830000	4.82830000	-0.08240000
O	0.30290000	3.19310000	3.13850000
N	0.10600000	-0.88360000	-1.10620000
C	-1.18490000	1.44510000	-3.59800000
C	-1.50180000	2.55040000	-2.80590000
C	-1.32310000	2.51500000	-1.41450000
C	-0.81470000	1.38580000	-0.72650000
C	-0.66760000	0.31240000	-2.96350000
C	-0.47890000	0.29260000	-1.57010000
C	-2.57930000	2.44990000	1.50730000

C	-1.58530000	0.44840000	3.27260000
C	-2.54340000	-0.40400000	0.84840000
C	-0.32870000	-2.62200000	1.28040000
C	1.17750000	-0.82720000	2.83950000
C	2.39560000	-1.87950000	0.60810000
C	2.77670000	1.48140000	1.57220000
C	1.46860000	3.71170000	0.08760000
C	0.33990000	2.51430000	2.19580000
H	1.56000000	3.05930000	-2.47010000
S	-0.11700000	-1.19990000	-3.66440000
C	0.34400000	-1.72330000	-2.07800000
H	0.82100000	-2.68390000	-1.92150000
H	-1.60020000	3.39790000	-0.84270000
H	-1.89830000	3.44750000	-3.27610000
H	-1.33040000	1.47000000	-4.67510000
C	2.26360000	2.23340000	-2.38830000
H	2.81940000	1.99250000	-3.29690000
C	2.43840000	1.52590000	-1.25700000
C	3.48160000	0.45650000	-1.36320000
O	3.40270000	-0.51580000	-2.09110000
O	4.55340000	0.71410000	-0.58960000
C	5.67600000	-0.19840000	-0.69610000
H	5.97940000	-0.25070000	-1.74840000
H	5.34880000	-1.19660000	-0.38990000
C	6.78310000	0.33870000	0.19330000
H	6.45390000	0.39470000	1.23700000
H	7.65490000	-0.32510000	0.13970000
H	7.09200000	1.34110000	-0.12580000

Species TSPQ

HF energy= -2359.72562112

Imaginary frequency= 13i

Zero-point correction= 0.284095 (Hartree/Particle)

Thermal correction to Energy= 0.324038

Thermal correction to Enthalpy= 0.324983

Thermal correction to Gibbs Free Energy= 0.208273

Sum of electronic and zero-point Energies= -2359.441526

Sum of electronic and thermal Energies= -2359.401583

Sum of electronic and thermal Enthalpies= -2359.400638

Sum of electronic and thermal Free Energies= -2359.517348

Coordinates: TSPQ

Os -1.56300000 0.93210000 1.26830000

Os 0.78040000 -0.74540000 1.40650000

Os 0.98450000 2.06100000 0.77080000

O	-3.98860000	2.78240000	0.71800000
O	-2.37920000	0.34190000	4.18080000
O	-2.90160000	-1.66720000	0.31930000
O	-0.35920000	-3.57220000	1.95970000
O	1.04230000	-0.12130000	4.38970000
O	3.75080000	-1.52710000	1.16340000
O	2.99590000	2.26830000	3.05560000
O	0.89890000	4.96670000	-0.33390000
O	-0.68950000	3.55970000	2.86430000
N	0.40170000	-0.95580000	-0.75260000
C	-0.85840000	0.85660000	-3.65360000
C	-1.28270000	2.05160000	-3.06720000
C	-1.19200000	2.24440000	-1.68090000
C	-0.65290000	1.27560000	-0.79760000
C	-0.31120000	-0.12160000	-2.82180000
C	-0.19080000	0.09890000	-1.43770000
C	-3.05580000	2.13950000	0.92090000
C	-2.07480000	0.55970000	3.09430000
C	-2.37060000	-0.71280000	0.68670000
C	0.03910000	-2.51350000	1.73380000
C	0.94710000	-0.34610000	3.26300000
C	2.64220000	-1.21440000	1.23400000
C	2.23860000	2.17350000	2.19280000
C	0.91780000	3.88600000	0.05420000
C	-0.42990000	2.75010000	2.06360000
H	3.62500000	3.98610000	0.38620000
S	0.32660000	-1.70400000	-3.22850000
C	0.71500000	-1.93650000	-1.55620000
H	1.19470000	-2.84620000	-1.21190000
H	-1.57370000	3.17630000	-1.26890000
H	-1.70390000	2.83390000	-3.69430000
H	-0.94770000	0.69930000	-4.72570000
C	3.79590000	3.09620000	-0.21730000
H	4.74560000	3.06000000	-0.74930000
C	2.90270000	2.09420000	-0.31180000
C	3.29460000	0.97370000	-1.22490000
O	2.58400000	0.44410000	-2.05830000
O	4.58570000	0.61420000	-1.04850000
C	5.09600000	-0.41620000	-1.92280000
H	4.98460000	-0.08610000	-2.96300000
H	4.49060000	-1.32100000	-1.79280000
C	6.54820000	-0.65030000	-1.54600000
H	6.62980000	-0.97410000	-0.50230000
H	6.97890000	-1.42950000	-2.18700000
H	7.13810000	0.26510000	-1.67190000

Species Q

HF energy= -2359.73178912

No imaginary frequency

Zero-point correction= 0.284230 (Hartree/Particle)

Thermal correction to Energy= 0.324991

Thermal correction to Enthalpy= 0.325936

Thermal correction to Gibbs Free Energy= 0.207088

Sum of electronic and zero-point Energies= -2359.447559

Sum of electronic and thermal Energies= -2359.406798

Sum of electronic and thermal Enthalpies= -2359.405854

Sum of electronic and thermal Free Energies= -2359.524701

Coordinates: Q

Os	-1.59180000	0.94960000	1.11380000
Os	0.61620000	-0.58750000	2.09110000
Os	1.00190000	2.06720000	1.03120000
O	-3.79580000	2.64340000	-0.26320000
O	-3.09220000	0.88510000	3.80660000
O	-2.71610000	-1.78400000	0.32310000
O	-0.66850000	-3.31370000	2.80180000
O	0.12110000	0.56860000	4.87840000
O	3.52660000	-1.33040000	2.78650000
O	2.52200000	2.73190000	3.58170000
O	1.38570000	4.83490000	-0.36210000
O	-1.09600000	3.92720000	2.33720000
N	0.86840000	-1.13370000	-0.02820000
C	0.33140000	0.10510000	-3.41960000
C	-0.30400000	1.32130000	-3.16850000
C	-0.58130000	1.73380000	-1.85630000
C	-0.24930000	0.96380000	-0.71710000
C	0.70730000	-0.67500000	-2.32140000
C	0.42670000	-0.24900000	-1.01010000
C	-2.93980000	2.06610000	0.24630000
C	-2.52980000	0.90390000	2.80430000
C	-2.27480000	-0.76950000	0.64970000
C	-0.20450000	-2.29920000	2.50920000
C	0.30510000	0.13890000	3.82420000
C	2.44600000	-1.04100000	2.50440000
C	1.94680000	2.46850000	2.61710000
C	1.27030000	3.77380000	0.05370000
C	-0.59810000	3.01830000	1.80870000
H	4.16910000	1.30230000	1.96840000
S	1.53170000	-2.22630000	-2.28050000
C	1.45150000	-2.18120000	-0.54640000
H	1.87060000	-2.97950000	0.05620000

H	-1.08670000	2.68660000	-1.71660000
H	-0.58820000	1.95670000	-4.00380000
H	0.53150000	-0.22050000	-4.43750000
C	4.10560000	1.31650000	0.88400000
H	5.03710000	1.11950000	0.35450000
C	2.96180000	1.56620000	0.21610000
C	3.10790000	1.67430000	-1.27410000
O	2.53970000	2.48880000	-1.97760000
O	3.97810000	0.76870000	-1.78600000
C	4.28610000	0.90510000	-3.19110000
H	4.67400000	1.91480000	-3.37180000
H	3.35980000	0.80060000	-3.76870000
C	5.30260000	-0.16730000	-3.54190000
H	4.89910000	-1.16900000	-3.35150000
H	5.56710000	-0.09750000	-4.60430000
H	6.21790000	-0.04760000	-2.95090000

Species TSQR

HF energy= -2359.71339888

Imaginary frequency= 102i

Zero-point correction= 0.283599 (Hartree/Particle)

Thermal correction to Energy= 0.323690

Thermal correction to Enthalpy= 0.324634

Thermal correction to Gibbs Free Energy= 0.207853

Sum of electronic and zero-point Energies= -2359.429800

Sum of electronic and thermal Energies= -2359.389709

Sum of electronic and thermal Enthalpies= -2359.388765

Sum of electronic and thermal Free Energies= -2359.505546

Coordinates: TSQR

Os	-1.54120000	0.79790000	1.21480000
Os	1.15740000	-0.46640000	1.46480000
Os	0.75800000	2.39960000	0.88370000
O	-4.23230000	2.12820000	0.51990000
O	-2.21810000	0.43610000	4.19790000
O	-2.59270000	-1.93940000	0.26770000
O	-0.37060000	-2.91840000	2.45940000
O	1.45250000	0.57190000	4.33090000
O	3.82870000	-2.01730000	1.57090000
O	2.15920000	3.82720000	3.16740000
O	1.52000000	4.68440000	-1.00750000
O	-1.63380000	3.97780000	1.94010000
N	0.81440000	-0.81860000	-0.68160000
C	-0.57160000	0.75330000	-3.67120000
C	-1.18490000	1.87780000	-3.12540000

C	-1.20160000	2.09180000	-1.73370000
C	-0.59000000	1.21450000	-0.81290000
C	0.06110000	-0.13130000	-2.78960000
C	0.08100000	0.11950000	-1.40890000
C	-3.21610000	1.65460000	0.77940000
C	-1.98290000	0.56140000	3.07780000
C	-2.12980000	-0.95360000	0.64830000
C	0.16660000	-1.98220000	2.05610000
C	1.33400000	0.19490000	3.25090000
C	2.85170000	-1.41860000	1.48010000
C	1.64310000	3.28030000	2.29160000
C	1.26790000	3.81600000	-0.29470000
C	-0.98420000	3.09490000	1.51510000
H	3.82840000	1.74040000	2.36820000
S	0.95040000	-1.60350000	-3.14010000
C	1.30710000	-1.75410000	-1.45320000
H	1.90860000	-2.57380000	-1.07620000
H	-1.72880000	2.96630000	-1.35840000
H	-1.67230000	2.59250000	-3.78440000
H	-0.57370000	0.57730000	-4.74370000
C	3.91030000	1.53300000	1.30300000
H	4.92290000	1.51970000	0.90140000
C	2.82850000	1.31300000	0.51300000
C	3.17010000	1.09790000	-0.93360000
O	2.59950000	1.60730000	-1.87920000
O	4.22700000	0.26110000	-1.10180000
C	4.72920000	0.12220000	-2.45080000
H	4.95440000	1.11930000	-2.84700000
H	3.94360000	-0.31250000	-3.08090000
C	5.96360000	-0.76060000	-2.39020000
H	5.72150000	-1.75180000	-1.98860000
H	6.37970000	-0.88850000	-3.39710000
H	6.73420000	-0.31230000	-1.75290000

Species R

HF energy= -2359.72363500

No imaginary frequency

Zero-point correction= 0.284742 (Hartree/Particle)

Thermal correction to Energy= 0.325085

Thermal correction to Enthalpy= 0.326029

Thermal correction to Gibbs Free Energy= 0.208573

Sum of electronic and zero-point Energies= -2359.438893

Sum of electronic and thermal Energies= -2359.398550

Sum of electronic and thermal Enthalpies= -2359.397606

Sum of electronic and thermal Free Energies= -2359.515062

Coordinates: **R**

Os	-1.60220000	0.96160000	1.12370000
Os	1.19110000	-0.46650000	1.61540000
Os	0.82810000	2.39290000	0.56600000
O	-3.92900000	2.75600000	0.28220000
O	-2.63870000	0.75600000	4.02370000
O	-3.02980000	-1.59170000	0.04250000
O	-1.08170000	-2.22610000	2.77030000
O	1.62790000	0.95040000	4.29460000
O	3.01980000	-2.86560000	2.27520000
O	3.01960000	3.73340000	2.19480000
O	0.62340000	4.91160000	-1.13680000
O	-0.96650000	3.69170000	2.56860000
N	0.80960000	-0.97530000	-0.49860000
C	-0.43800000	0.26610000	-3.71090000
C	-1.08910000	1.43080000	-3.32200000
C	-1.16900000	1.80240000	-1.96550000
C	-0.59700000	1.05210000	-0.91550000
C	0.16340000	-0.49570000	-2.69920000
C	0.10970000	-0.10730000	-1.34910000
C	-3.05620000	2.07800000	0.60520000
C	-2.26360000	0.82840000	2.94080000
C	-2.41870000	-0.70770000	0.45340000
C	-0.34770000	-1.48260000	2.28130000
C	1.45230000	0.42010000	3.29020000
C	2.34880000	-1.97830000	1.98620000
C	2.20330000	3.21580000	1.56070000
C	0.72200000	3.96080000	-0.48800000
C	-0.62980000	2.86200000	1.78720000
H	4.26530000	0.24290000	2.75120000
S	1.07280000	-1.98790000	-2.86160000
C	1.33830000	-1.97950000	-1.15270000
H	1.92540000	-2.75390000	-0.67290000
H	-1.71890000	2.70860000	-1.72330000
H	-1.55730000	2.06040000	-4.07550000
H	-0.38800000	-0.03610000	-4.75340000
C	4.26920000	0.45810000	1.68350000
H	5.22150000	0.79450000	1.27330000
C	3.16040000	0.36060000	0.92320000
C	3.31090000	0.77460000	-0.49230000
O	2.48640000	1.47700000	-1.08040000
O	4.41780000	0.33720000	-1.10300000
C	4.65060000	0.80070000	-2.45960000
H	4.63730000	1.89640000	-2.46070000
H	3.82440000	0.45440000	-3.09170000

C	5.98870000	0.24090000	-2.90610000
H	5.98280000	-0.85510000	-2.89030000
H	6.20300000	0.57050000	-3.93000000
H	6.79700000	0.59200000	-2.25470000

Species TSRS

HF energy= -2359.71885780

Imaginary frequency= 30i

Zero-point correction= 0.284670 (Hartree/Particle)

Thermal correction to Energy= 0.324292

Thermal correction to Enthalpy= 0.325236

Thermal correction to Gibbs Free Energy= 0.209420

Sum of electronic and zero-point Energies= -2359.434188

Sum of electronic and thermal Energies= -2359.394566

Sum of electronic and thermal Enthalpies= -2359.393622

Sum of electronic and thermal Free Energies= -2359.509438

Coordinates: TSRS

Os	-1.38210000	0.95690000	1.21840000
Os	1.17640000	-0.61790000	1.43190000
Os	0.89400000	2.61960000	0.39510000
O	-3.75470000	2.87280000	0.77890000
O	-2.11490000	0.41170000	4.16710000
O	-2.95010000	-1.46730000	0.06790000
O	-0.85730000	-2.81470000	2.19690000
O	1.41400000	0.33430000	4.33240000
O	3.49450000	-2.64700000	1.69920000
O	3.11070000	4.46120000	1.35700000
O	-0.23550000	5.05920000	-0.97820000
O	-0.47160000	3.46270000	2.89920000
N	0.83590000	-0.88400000	-0.72180000
C	-0.61920000	0.52770000	-3.76920000
C	-1.30450000	1.62640000	-3.26240000
C	-1.31470000	1.90560000	-1.88380000
C	-0.63090000	1.13320000	-0.91660000
C	0.06940000	-0.26700000	-2.84680000
C	0.08030000	0.02970000	-1.46940000
C	-2.86340000	2.16180000	0.93450000
C	-1.84080000	0.61580000	3.06980000
C	-2.31830000	-0.61180000	0.50730000
C	-0.15180000	-1.95780000	1.89290000
C	1.30850000	-0.02940000	3.24670000
C	2.65810000	-1.87310000	1.54110000
C	2.28620000	3.74530000	0.97630000
C	0.20330000	4.12290000	-0.45860000

C	-0.31490000	2.75960000	1.95570000
H	3.56610000	1.35820000	2.81920000
S	1.00880000	-1.71540000	-3.16100000
C	1.35600000	-1.82340000	-1.47120000
H	1.97400000	-2.62030000	-1.07410000
H	-1.90280000	2.75800000	-1.55440000
H	-1.85490000	2.27530000	-3.94020000
H	-0.61820000	0.29690000	-4.83090000
C	3.76270000	1.28480000	1.75130000
H	4.73410000	1.66100000	1.42640000
C	2.84930000	0.80120000	0.87520000
C	3.24920000	0.87670000	-0.55850000
O	2.61290000	1.52120000	-1.38680000
O	4.35470000	0.18880000	-0.87110000
C	4.82320000	0.28210000	-2.24360000
H	4.97390000	1.33960000	-2.48750000
H	4.04060000	-0.10700000	-2.90580000
C	6.10810000	-0.51970000	-2.33960000
H	5.93710000	-1.57190000	-2.08330000
H	6.49720000	-0.47290000	-3.36400000
H	6.87090000	-0.11960000	-1.66220000

Species S

HF energy= -2359.76465596

No imaginary frequency

Zero-point correction= 0.286328 (Hartree/Particle)

Thermal correction to Energy= 0.325699

Thermal correction to Enthalpy= 0.326643

Thermal correction to Gibbs Free Energy= 0.211955

Sum of electronic and zero-point Energies= -2359.478328

Sum of electronic and thermal Energies= -2359.438957

Sum of electronic and thermal Enthalpies= -2359.438013

Sum of electronic and thermal Free Energies= -2359.552701

Coordinates: S

Os	2.95830000	1.24770000	1.11170000
Os	3.35570000	2.39000000	3.90100000
Os	5.45220000	4.37530000	3.59730000
S	2.41190000	7.98730000	3.91220000
N	3.74030000	5.77370000	3.78180000
C	3.15860000	0.74770000	-0.73260000
C	1.01010000	0.91680000	1.30160000
C	3.45740000	-0.48280000	1.68880000
C	1.89980000	1.17820000	4.22420000
C	4.69410000	0.96650000	4.11160000

C	3.57930000	2.96340000	5.73470000
C	6.88770000	3.12140000	3.53670000
C	5.99390000	4.98230000	5.40190000
C	6.39880000	5.58180000	2.44220000
O	3.29010000	0.45410000	-1.83750000
O	-0.12490000	0.75440000	1.34980000
O	3.77300000	-1.53720000	2.03040000
O	1.04570000	0.45210000	4.50380000
O	5.46170000	0.13360000	4.31130000
O	3.63680000	3.24270000	6.85200000
O	7.77370000	2.38670000	3.51230000
O	6.31960000	5.36540000	6.43610000
O	6.96550000	6.28780000	1.72720000
C	3.06260000	7.35760000	-0.23030000
H	2.41120000	7.83500000	-0.97230000
H	4.09690000	7.42380000	-0.58660000
H	2.97810000	7.91480000	0.70930000
C	2.64110000	5.91230000	-0.04980000
H	1.61980000	5.81730000	0.33410000
H	2.71590000	5.33810000	-0.97860000
C	3.43530000	4.01790000	1.14600000
C	4.39100000	3.32130000	2.05710000
C	4.93030000	2.19950000	1.18280000
H	5.72730000	1.62450000	1.65790000
H	5.26460000	2.52080000	0.18700000
C	1.94130000	4.04340000	3.71330000
C	0.54230000	3.91520000	3.65460000
H	0.09960000	2.92360000	3.60440000
C	-0.34340000	5.00890000	3.66650000
H	-1.41500000	4.82400000	3.62090000
C	0.11970000	6.31890000	3.75200000
H	-0.56030000	7.16570000	3.78300000
C	1.50450000	6.48700000	3.79800000
C	2.39020000	5.38380000	3.76220000
C	3.88000000	7.06920000	3.86600000
H	4.84660000	7.55850000	3.89360000
O	2.59580000	3.34340000	0.50330000
O	3.54300000	5.31120000	0.93040000
