Electronic Supplementary Information (ESI)

Mixed-valence dimolybdenum complexes containing hard oxo and soft carbonyl ligands: Synthesis, structure and electrochemistry $Mo_2(O)(CO)_2\{\mu\text{-}\kappa^2\text{-}S(CH)_nS\}_2(\kappa^2\text{-diphosphine})$

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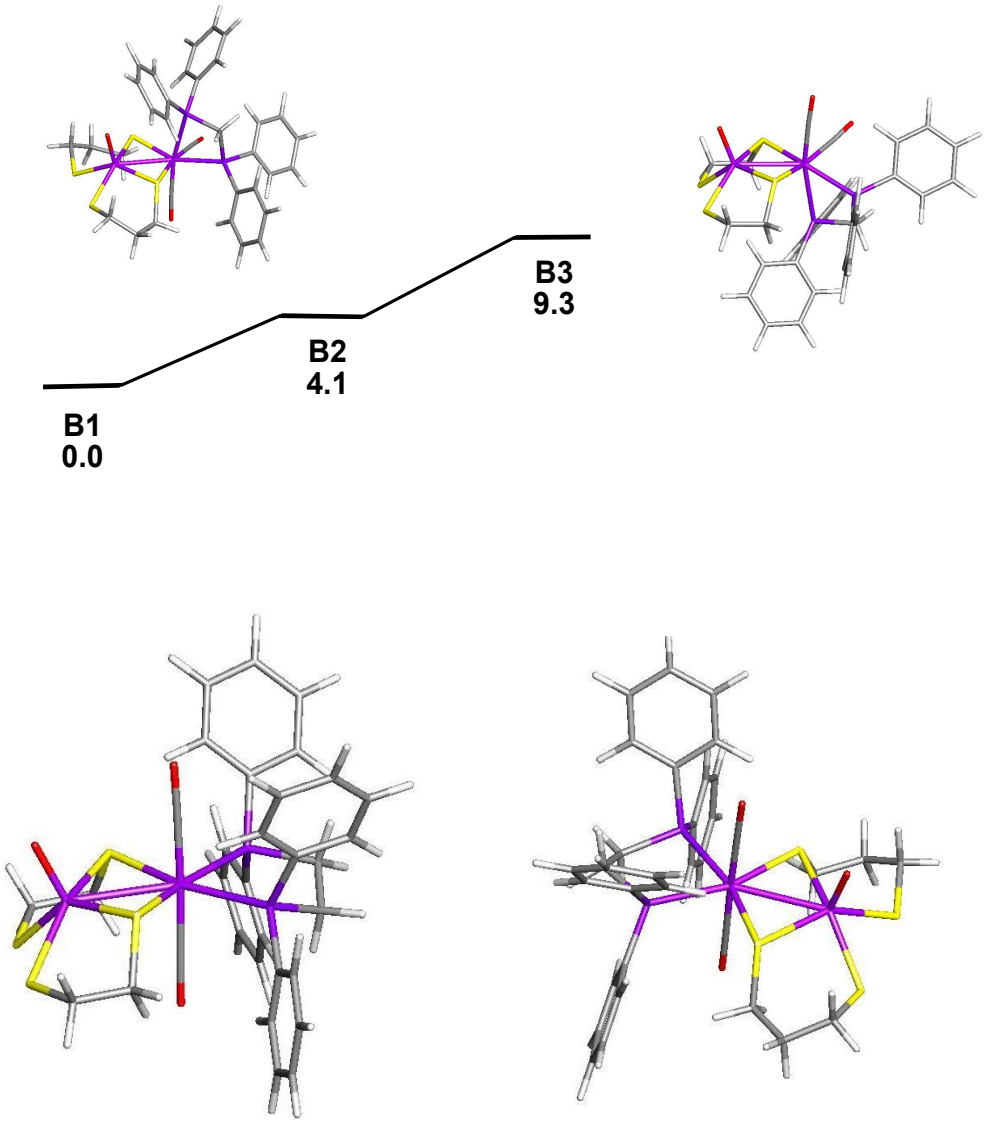


Figure S1. Top portion: B3LYP-optimized structures and ground-state energy ordering for the different diastereomers of $Mo_2(O)(CO)_2(\mu\text{-}\kappa^2\text{-}pdt)_2(\kappa^2\text{-}dppm)$ (**2**). The free energy (ΔG) values are in kcal/mol relative to *trans*-$Mo_2(O)(CO)_2(\mu\text{-}\kappa^2\text{-}pdt)_2(\kappa^2\text{-}dppm)$ (**B1**). Bottom portion: DFT-optimized structures of $Mo_2(O)(CO)_2\{\mu\text{-}\kappa^2\text{-}S(CH_2)_2S\}_2(\kappa^2\text{-}dppe)$ (**D**-left) and $[Mo_2(O)(CO)_2\{\mu\text{-}\kappa^2\text{-}S(CH_2)_3S\}_2(\kappa^2\text{-}dppe)$ (**E**-right)].

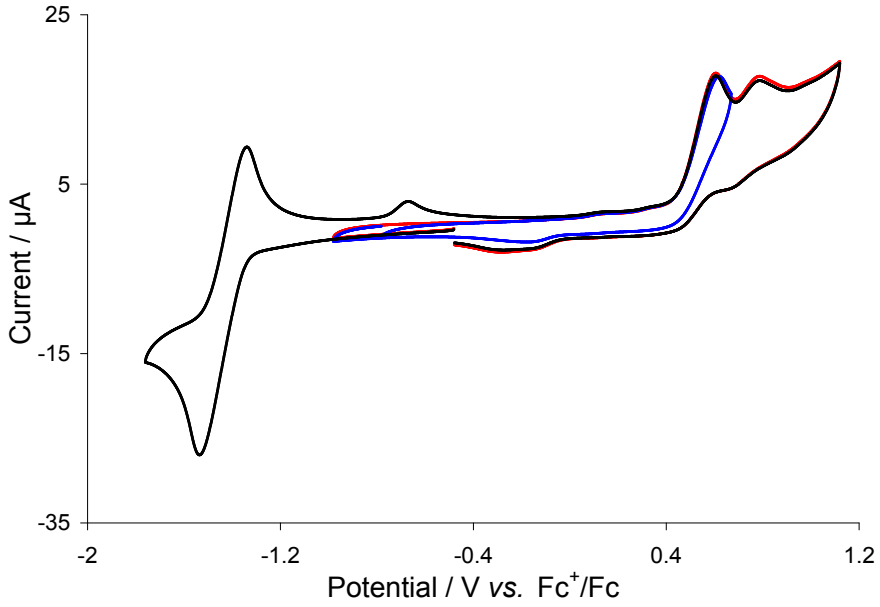


Fig. S2. CVs of $Mo_2(O)(CO)_2(\kappa^2\text{-dppm})(\mu\text{-}\kappa^2\text{-edt})_2$ (**1**) in MeCN (0.5 mM solution, supporting electrolyte $[NBu_4][PF_6]$, scan rate 0.1 Vs^{-1}, glassy carbon electrode, potential vs Fc^+/Fc).

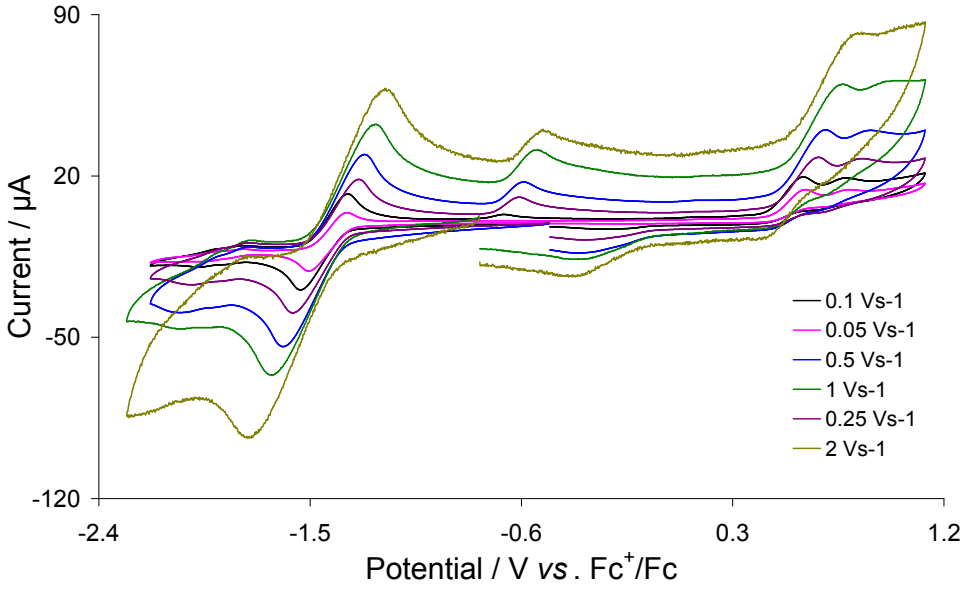
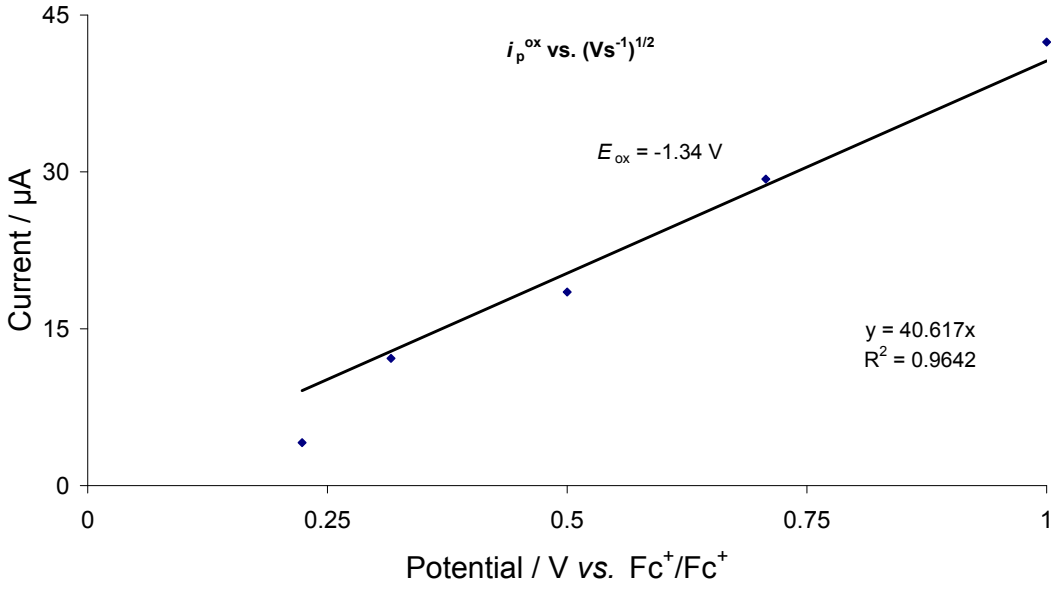


Fig. S3. CVs of $Mo_2(O)(CO)_2(\kappa^2\text{-dppm})(\mu\text{-}\kappa^2\text{-edt})_2$ (**1**) at various scan rates as shown in the legend (0.5 mM solution in MeCN, supporting electrolyte $[NBu_4][PF_6]$, scan rate 0.1 Vs^{-1}, glassy carbon electrode, potential vs Fc^+/Fc).

(a)



(b)

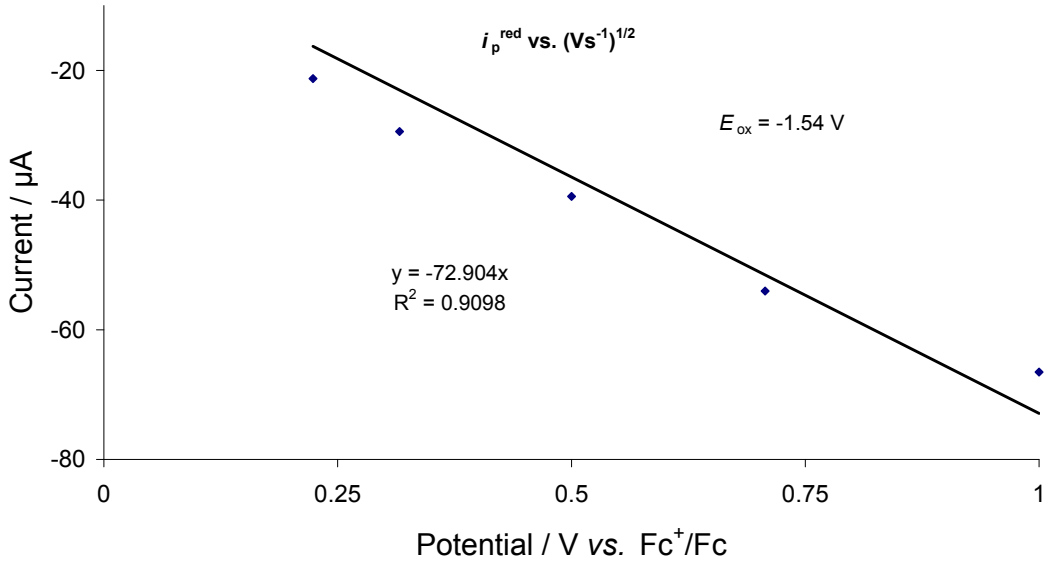


Fig. S4. Plots of peak current, i_p, *vs.* square root scan rate of the quasi-reversible reduction (at $E_{1/2}$ = –1.44 V) of $Mo_2(O)(CO)_2(\kappa^2\text{-dppm})(\mu\text{-}\kappa^2\text{-edt})_2$ (**1**). Line shows best linear fit of data through the origin – (a) for anodic wave; (b) for cathodic wave.

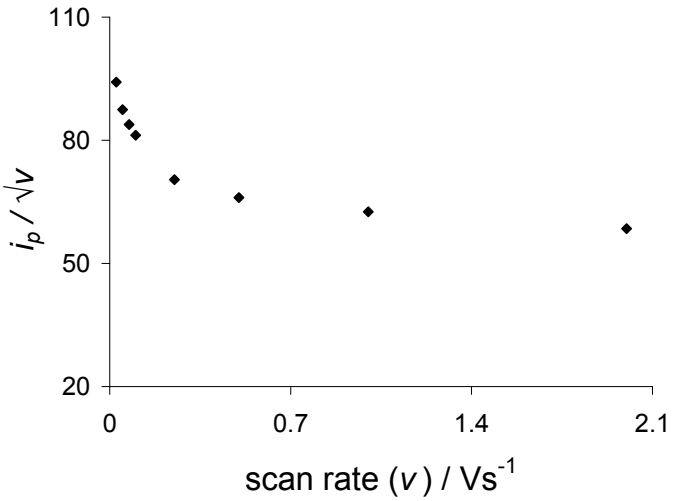


Fig. S5. Scan rate (ν) dependence of the current function ($i_p/\sqrt{\nu}$) for the reduction of $Mo_2(O)(CO)_2(\kappa^2\text{-dppm})(\mu\text{-}\kappa^2\text{-edt})_2$ (**1**) (0.5 mM solution in MeCN, supporting electrolyte $[NBu_4][PF_6]$, glassy carbon electrode).

Table S1. Crystallographic Data and Structure Refinement for*cis*-**1**, *trans*-**2** and **5**

Compound	*Cis*-**1**	*Trans*-**2**	**5**
CCDC registry	1400764	1400766	1400765
Empirical formula	$C_{31}H_{30}Mo_2O_3P_2S_4$	$C_{33}H_{34}Mo_2O_3P_2S_4$	$C_{31}H_{32}MoOP_2S_3$
Formula weight	832.61	860.66	674.63
Temp (K)	296(2)	293(2)	293(2)
Wavelength (Å)	0.71075	0.71075	0.71075
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_l/c$	$P2_1$/n	$P2_1$/c
a/ Å	16.1232(15)	12.152(3)	11.568(17)
b/ Å	11.4670(11)	15.879(3)	15.89(2)
c/ Å	19.7039(19)	18.565(4)	17.05(2)
α/ °	90	90	90
β/ °	108.445(8)	90.143(6)	103.363(15)
γ / °	90	90	90
V / Å^3	3455.8(6)	3582.2(13)	3049(7)
Z	4	4	4
D_{calc} (Mg m^{-3})	1.600	1.596	1.470
μ (Mo Kα) (mm^{-1})	1.090	1.055	0.764
F(000)	1672	1736	1384
Crystal size (mm^3)	0.20 × 0.18 × 0.08	0.22 × 0.14 × 0.05	0.20× 0.18 × 0.08
θ range (°)	3.10 to 27.00	3.04 to 27.00	2.22 to 27.00
Index ranges	$-20 \le h \le 20$	$-15 \le h \le 15$	$-14 \le h \le 14$
	$-14 \le k \le 14$,	$-20 \le k \le 20$	$-20 \le k \le 20$
	$-25 \le l \le 25$	$-23 \le l \le 23$	$-21 \le l \le 21$
Reflections collected	30335	26643	26844
Independent reflections	6321 (R_{int} = 0.1195)	7292 (R_{int} = 0.1148)	6627 (R_{int} = 0.0501)
(R_{int})	6321 / 0 / 379	7292 / 0 / 397	6627 / 0 / 343
Data/restraints/parameters	1.019	1.030	1.036
Goodness-of-fit on F^2	R_1 = 0.0546,	R_1 = 0.0567,	R_1 = 0.0416,
Final *R* indices [$I > 2\sigma(I)$]	wR_2 = 0.1105	wR_2 = 0.0900	wR_2 = 0.1034
	R_1 = 0.1021,	R_1 = 0.1132,	R_1 = 0.0524,
R indices (all data)	wR_2 = 0.1288	wR_2 = 0.1002	wR_2 = 0.1096
Largest difference in peak	1.274 and –0.531	0.482 and –0.504	0.385 and –0.661
and hole (e Å^{-3})			

Computational Details

B3LYP geometries and energies for all optimized structures

Species A1

HF energy= -3837.18727537
No Imaginary frequency
Zero-point correction = 0.537885 (Hartree/Particle)
Thermal correction to Energy = 0.581770
Thermal correction to Enthalpy = 0.582714
Thermal correction to Gibbs Free Energy = 0.456991
Sum of electronic and zero-point Energies = -3836.649390
Sum of electronic and thermal Energies = -3836.605506
Sum of electronic and thermal Enthalpies = -3836.604561
Sum of electronic and thermal Free Energies = -3836.730284

Coordinates: **A1**

Mo	2.31380000	0.79710000	5.29000000
Mo	1.37760000	1.40630000	7.94530000
S	3.50530000	2.16920000	6.95320000
S	2.76180000	1.23470000	9.94740000
S	0.03730000	0.38610000	6.11170000
S	0.38390000	-0.41850000	9.20700000
P	1.69530000	-0.35300000	3.10550000
P	4.21780000	0.93370000	3.58120000
O	0.51140000	2.86090000	8.02170000
O	3.37990000	-1.94590000	6.51270000
O	1.20850000	3.58670000	4.17710000
C	2.99140000	-0.94610000	6.07690000
C	5.76440000	-0.07040000	3.71110000
C	1.62550000	-2.19240000	2.99410000
C	1.60510000	2.57720000	4.57010000
C	0.32290000	0.19720000	2.00900000
C	4.80740000	2.54650000	2.90610000
C	3.25430000	0.13780000	2.18380000
C	5.16660000	2.70410000	1.55640000
C	6.24930000	-0.41880000	4.98020000
C	6.48540000	-0.47720000	2.57420000
C	5.73390000	5.02310000	1.95620000
C	0.33970000	-0.12250000	0.63830000
C	0.40640000	-2.85510000	2.77830000
C	2.72750000	-4.35000000	3.20300000
C	2.78480000	-2.95550000	3.21580000
C	-0.74110000	0.95260000	2.52280000
C	7.65950000	-1.21900000	2.70730000
C	0.35160000	-4.25140000	2.77440000
C	4.91450000	3.64590000	3.77250000
C	1.51070000	-5.00170000	2.98350000
C	-0.68320000	0.31730000	-0.20150000
C	4.79000000	1.43930000	8.06850000
C	-0.40940000	-1.30320000	6.71050000

C	5.37940000	4.87560000	3.29860000
C	-0.92780000	-1.14840000	8.13270000
C	7.42890000	-1.15730000	5.11320000
C	4.43440000	1.86770000	9.48360000
C	-1.73880000	1.07490000	0.31840000
C	5.62480000	3.93520000	1.08490000
C	-1.76820000	1.38720000	1.67810000
C	8.13400000	-1.56020000	3.97810000
H	1.14900000	-0.72330000	0.22670000
H	-0.65840000	0.06790000	-1.26030000
H	-2.53580000	1.41860000	-0.33790000
H	-2.58660000	1.97470000	2.08850000
H	-0.77050000	1.19870000	3.58040000
H	5.76010000	1.84250000	7.74630000
H	4.46420000	2.96080000	9.57310000
H	5.14890000	1.44550000	10.20230000
H	4.79590000	0.34820000	7.97890000
H	-1.82980000	-0.52470000	8.15140000
H	-1.18010000	-2.12780000	8.56040000
H	0.46350000	-1.96100000	6.66850000
H	-1.18340000	-1.68400000	6.03050000
H	2.99880000	0.88130000	1.42120000
H	3.76690000	-0.70270000	1.70410000
H	-0.50100000	-2.28290000	2.60190000
H	-0.59990000	-4.75070000	2.60290000
H	1.46680000	-6.08870000	2.97830000
H	3.63470000	-4.92610000	3.37230000
H	3.73870000	-2.46880000	3.40890000
H	6.13850000	-0.21160000	1.57770000
H	8.20540000	-1.52930000	1.81860000
H	9.04940000	-2.13920000	4.08040000
H	7.78940000	-1.42140000	6.10510000
H	5.69860000	-0.11820000	5.86600000
H	5.08900000	1.86950000	0.86240000
H	5.89460000	4.04480000	0.03640000
H	6.08800000	5.98320000	1.58690000
H	5.45180000	5.72000000	3.98050000
H	4.62000000	3.54670000	4.81450000

Species A2
HF energy= -3837.18106983
No imaginary frequency
Zero-point correction = 0.537856 (Hartree/Particle)
Thermal correction to Energy = 0.581726
Thermal correction to Enthalpy = 0.582670
Thermal correction to Gibbs Free Energy = 0.457022
Sum of electronic and zero-point Energies = -3836.643214
Sum of electronic and thermal Energies = -3836.599344

Sum of electronic and thermal Enthalpies = -3836.598400
Sum of electronic and thermal Free Energies = -3836.724048

Coordinates: **A2**

Mo	2.16110000	0.67790000	5.34940000
Mo	1.36520000	1.71640000	7.89990000
S	3.48200000	2.26590000	6.74940000
S	2.82780000	1.50940000	9.82670000
S	-0.12970000	0.70980000	6.21850000
S	0.16400000	0.22080000	9.38840000
P	1.74280000	2.63810000	3.59790000
P	4.06520000	0.92650000	3.66000000
O	0.67210000	3.27060000	7.85560000
O	3.31090000	-1.79150000	6.89040000
O	0.78970000	-1.50650000	3.47490000
C	2.85310000	-0.85960000	6.35930000
C	4.20720000	-0.18010000	2.19190000
C	0.71900000	2.16990000	2.13890000
C	1.29180000	-0.68210000	4.10660000
C	1.38900000	4.43990000	3.78300000
C	5.82690000	1.09380000	4.17470000
C	3.53390000	2.60250000	3.03550000
C	6.65540000	2.12650000	3.71040000
C	3.99270000	-1.55690000	2.36230000
C	4.60930000	0.29420000	0.93250000
C	8.52210000	1.21220000	4.95360000
C	1.36790000	5.29560000	2.66670000
C	-0.62350000	1.83430000	2.39400000
C	0.32280000	1.79690000	-0.23180000
C	1.18200000	2.14630000	0.81490000
C	1.15570000	4.96960000	5.06130000
C	4.77260000	-0.58710000	-0.13730000
C	-1.48140000	1.49580000	1.34720000
C	6.36190000	0.12040000	5.03460000
C	-1.00960000	1.47450000	0.03110000
C	1.13320000	6.66040000	2.83060000
C	4.79450000	1.59970000	7.87140000
C	-0.74720000	-0.84920000	6.99910000
C	7.70390000	0.17740000	5.41620000
C	-1.22530000	-0.48720000	8.39730000
C	4.16330000	-2.43900000	1.29250000
C	4.48540000	2.10850000	9.27030000
C	0.90910000	7.18470000	4.10890000
C	7.99530000	2.18680000	4.10270000
C	0.91730000	6.33950000	5.21890000
C	4.54770000	-1.95540000	0.04030000
H	1.51890000	4.89470000	1.66630000
H	1.11790000	7.31430000	1.96080000
H	0.72130000	8.24930000	4.23420000
H	0.73280000	6.73570000	6.21510000

H	1.14560000	4.32650000	5.93600000
H	5.75280000	1.97800000	7.49430000
H	4.52080000	3.20430000	9.30210000
H	5.22010000	1.72060000	9.98820000
H	4.79450000	0.50700000	7.83660000
H	-2.05870000	0.22430000	8.35140000
H	-1.57010000	-1.38420000	8.92820000
H	0.06130000	-1.58530000	7.02820000
H	-1.56380000	-1.22210000	6.36670000
H	4.03700000	3.34500000	3.66760000
H	3.74310000	2.85050000	1.98910000
H	-0.99490000	1.83130000	3.41740000
H	-2.51700000	1.24010000	1.56130000
H	-1.67660000	1.20260000	-0.78420000
H	0.69910000	1.77750000	-1.25270000
H	2.21530000	2.39130000	0.58470000
H	4.81000000	1.35240000	0.78040000
H	5.08000000	-0.20520000	-1.10870000
H	4.67470000	-2.64130000	-0.79460000
H	3.98880000	-3.50250000	1.43980000
H	3.69270000	-1.94350000	3.33340000
H	6.26430000	2.89030000	3.04170000
H	8.62620000	2.99620000	3.74100000
H	9.56550000	1.26040000	5.25790000
H	8.10620000	-0.58210000	6.08330000
H	5.72730000	-0.67720000	5.41590000

Species A3
HF energy= -3837.17464679
No Imaginary frequency
Zero-point correction = 0.538089 (Hartree/Particle)
Thermal correction to Energy = 0.581854
Thermal correction to Enthalpy = 0.582798
Thermal correction to Gibbs Free Energy = 0.457908
Sum of electronic and zero-point Energies = -3836.636558
Sum of electronic and thermal Energies = -3836.592793
Sum of electronic and thermal Enthalpies = -3836.591848
Sum of electronic and thermal Free Energies = -3836.716738

Coordinates: **A3**

Mo	2.13420000	0.84020000	5.26840000
Mo	1.43440000	1.38760000	8.07300000
S	3.30650000	2.36310000	6.84600000
S	3.08970000	1.39420000	9.88290000
S	0.08220000	0.13870000	6.44670000
S	0.82260000	-0.48920000	9.50270000
P	3.46490000	-1.48060000	5.44630000
P	4.16690000	0.75430000	3.75340000

O	0.42240000	2.72700000	8.28630000
O	0.84870000	3.53610000	4.30430000
O	0.49120000	-0.10570000	2.73210000
C	1.32430000	2.55450000	4.69910000
C	5.75060000	1.53060000	4.28710000
C	4.75510000	-1.96390000	6.67180000
C	1.11340000	0.17540000	3.66780000
C	2.64690000	-3.10820000	5.08880000
C	4.12280000	1.14370000	1.95410000
C	4.40660000	-1.09450000	3.86080000
C	5.07780000	0.60450000	1.07380000
C	5.89650000	2.91610000	4.09200000
C	6.78570000	0.81930000	4.91050000
C	4.04690000	1.77060000	-0.77990000
C	2.75080000	-4.19340000	5.97490000
C	4.53880000	-1.66170000	8.02540000
C	6.83080000	-3.07860000	7.28070000
C	5.90530000	-2.69020000	6.31090000
C	1.83620000	-3.24530000	3.94770000
C	7.94930000	1.47870000	5.32090000
C	5.46290000	-2.06150000	8.99710000
C	3.13600000	2.00470000	1.45130000
C	6.61130000	-2.76280000	8.62640000
C	2.06890000	-5.38670000	5.71920000
C	4.83800000	1.99440000	7.81470000
C	-0.08580000	-1.57060000	7.13140000
C	3.10200000	2.31850000	0.08870000
C	-0.48260000	-1.42360000	8.59200000
C	7.05780000	3.57010000	4.50240000
C	4.53090000	2.36520000	9.25810000
C	1.27760000	-5.51630000	4.57660000
C	5.03580000	0.91240000	-0.28580000
C	1.16440000	-4.44140000	3.69040000
C	8.08940000	2.85210000	5.11750000
H	3.36420000	-4.11300000	6.86790000
H	2.16220000	-6.21600000	6.41750000
H	0.74940000	-6.44660000	4.37840000
H	0.54680000	-4.52800000	2.79880000
H	1.71100000	-2.41740000	3.25530000
H	5.63430000	2.61610000	7.38640000
H	4.32560000	3.43900000	9.34550000
H	5.38530000	2.12680000	9.90570000
H	5.11020000	0.94080000	7.71820000
H	-1.44930000	-0.91450000	8.68470000
H	-0.56610000	-2.40780000	9.07160000
H	0.85280000	-2.11990000	7.02420000
H	-0.86420000	-2.06720000	6.53750000
H	3.85590000	-1.53610000	3.02240000
H	5.43870000	-1.45810000	3.80930000
H	3.65100000	-1.11640000	8.33770000

H	5.27570000	-1.81280000	10.03920000
H	7.33270000	-3.06910000	9.38130000
H	7.71810000	-3.63630000	6.98740000
H	6.07520000	-2.97340000	5.27390000
H	6.69550000	-0.24620000	5.09990000
H	8.74370000	0.91220000	5.80260000
H	8.99510000	3.36300000	5.43720000
H	7.15640000	4.64160000	4.34230000
H	5.10080000	3.48660000	3.61710000
H	5.86120000	-0.05100000	1.45030000
H	5.77610000	0.48630000	-0.95990000
H	4.01630000	2.01080000	-1.84070000
H	2.33140000	2.98680000	-0.28920000
H	2.39340000	2.43020000	2.12110000

Species B1
HF energy= -3915.80070076
No imaginary frequency
Zero-point correction = 0.596349 (Hartree/Particle)
Thermal correction to Energy = 0.642520
Thermal correction to Enthalpy = 0.643465
Thermal correction to Gibbs Free Energy = 0.513049
Sum of electronic and zero-point Energies = -3915.204351
Sum of electronic and thermal Energies = -3915.158180
Sum of electronic and thermal Enthalpies = -3915.157236
Sum of electronic and thermal Free Energies = -3915.287652

Coordinates: **B1**

Mo	-0.21760000	-0.06040000	-0.09350000
Mo	-3.00180000	-0.50600000	-0.76720000
S	-1.83020000	1.70430000	-0.59560000
S	-1.24110000	-2.25890000	-0.40230000
S	-4.51010000	-2.16510000	0.21360000
S	-4.94000000	0.73870000	0.06170000
P	2.07360000	-1.13370000	0.32170000
P	1.59210000	1.68830000	0.30460000
O	-3.12270000	-0.60620000	-2.45170000
O	-1.00340000	0.00120000	2.98580000
O	0.33710000	-0.10740000	-3.24980000
C	2.47930000	-2.35800000	1.65040000
C	-0.71160000	-0.02750000	1.85990000
C	1.80310000	-2.27180000	2.88090000
C	2.09680000	-3.16090000	3.91660000
C	3.05720000	-4.15970000	3.73360000
C	3.72340000	-4.26210000	2.51080000
C	3.43920000	-3.36790000	1.47500000
C	3.02860000	-1.74740000	-1.12700000
C	2.36160000	-2.57040000	-2.05090000

C	3.03990000	-3.08970000	-3.15520000
C	4.38920000	-2.78770000	-3.35590000
C	5.06250000	-1.97340000	-2.44150000
C	2.89400000	0.46330000	0.86680000
C	2.34930000	2.62230000	-1.08950000
C	1.55010000	2.98790000	-2.18400000
C	2.09440000	3.72250000	-3.24180000
C	3.44010000	4.09310000	-3.21890000
C	3.69890000	3.01610000	-1.06670000
C	1.49070000	2.95680000	1.64570000
C	1.37380000	2.55360000	2.98750000
C	1.23450000	3.49900000	4.00440000
C	1.19260000	4.86190000	3.69620000
C	1.29340000	5.27220000	2.36560000
C	1.44360000	4.32810000	1.34580000
C	-3.81740000	-3.85860000	-0.04040000
C	-2.68400000	-4.25240000	0.92070000
C	-1.66460000	-3.13630000	1.17270000
C	0.15370000	-0.09150000	-2.11190000
C	-2.50610000	2.57850000	0.89080000
C	-3.80120000	3.32160000	0.54470000
C	-4.75480000	2.52740000	-0.36260000
C	4.38860000	-1.46090000	-1.33020000
C	4.24200000	3.74080000	-2.12820000
H	-0.72830000	-3.53530000	1.57860000
H	-2.06280000	-2.39940000	1.87400000
H	-3.10260000	-4.54120000	1.89520000
H	-2.17550000	-5.13870000	0.51310000
H	-3.48840000	-3.94410000	-1.08070000
H	-4.66610000	-4.54090000	0.08850000
H	-5.76580000	2.94670000	-0.29400000
H	-4.44320000	2.60270000	-1.40890000
H	-3.56470000	4.27460000	0.04820000
H	-4.30240000	3.56740000	1.49150000
H	-1.72820000	3.26870000	1.23620000
H	-2.68190000	1.83570000	1.67180000
H	1.53060000	4.66440000	0.31610000
H	1.26020000	6.33060000	2.11520000
H	1.07870000	5.59790000	4.48920000
H	1.15050000	3.16790000	5.03730000
H	1.37700000	1.49840000	3.24910000
H	0.50160000	2.70240000	-2.20810000
H	1.46420000	3.99590000	-4.08520000
H	3.86500000	4.65710000	-4.04660000
H	5.28960000	4.03390000	-2.10250000
H	4.32910000	2.76940000	-0.21430000
H	3.90060000	0.64490000	0.47710000
H	2.94610000	0.46600000	1.96100000
H	4.93660000	-0.84590000	-0.62020000
H	6.11400000	-1.73660000	-2.59040000

H	4.91450000	-3.18360000	-4.22250000
H	2.50790000	-3.72050000	-3.86400000
H	1.30720000	-2.79800000	-1.90910000
H	3.96680000	-3.46060000	0.53040000
H	4.46820000	-5.04040000	2.35740000
H	3.27950000	-4.85810000	4.53770000
H	1.56390000	-3.07870000	4.86170000
H	1.03580000	-1.51820000	3.03240000

Species B2
HF energy= -3915.79365691
No Imaginary frequency
Zero-point correction = 0.596052 (Hartree/Particle)
Thermal correction to Energy = 0.642356
Thermal correction to Enthalpy = 0.643300
Thermal correction to Gibbs Free Energy = 0.512564
Sum of electronic and zero-point Energies -3915.197605
Sum of electronic and thermal Energies = -3915.151301
Sum of electronic and thermal Enthalpies = -3915.150357
Sum of electronic and thermal Free Energies = -3915.281093

Coordinates: **B2**

Mo	-0.42410000	0.18370000	0.03250000
Mo	-3.26980000	-0.08020000	-0.63260000
S	-2.02240000	2.05320000	-0.33440000
S	-1.57970000	-1.88790000	-0.51970000
S	-4.78230000	-1.76000000	0.30870000
S	-5.17070000	1.14720000	0.29690000
P	0.39280000	0.61390000	-2.44320000
P	1.47250000	1.87810000	-0.07730000
O	-3.44370000	-0.06290000	-2.31650000
O	-0.99400000	0.26780000	3.11190000
O	1.81830000	-1.89590000	0.91280000
C	1.58610000	-0.53930000	-3.24970000
C	-0.81500000	0.22070000	1.95950000
C	1.56510000	-1.90010000	-2.90860000
C	2.45620000	-2.79480000	-3.51050000
C	3.37880000	-2.33720000	-4.45290000
C	3.40260000	-0.98300000	-4.80560000
C	2.50760000	-0.09100000	-4.21380000
C	-0.60600000	1.21630000	-3.87600000
C	-0.84090000	0.37330000	-4.97530000
C	-1.65650000	0.79100000	-6.02880000
C	-2.25220000	2.05360000	-6.00000000
C	-2.03560000	2.89400000	-4.90540000
C	1.44530000	2.09350000	-1.93660000
C	1.37300000	3.56800000	0.64470000
C	0.80710000	3.72870000	1.92030000

C	0.76110000	4.99130000	2.51920000
C	1.26580000	6.10560000	1.84450000
C	1.88900000	4.69200000	-0.02080000
C	3.19920000	1.36940000	0.33920000
C	3.95040000	0.56370000	-0.53230000
C	5.22910000	0.13190000	-0.17190000
C	5.77170000	0.48900000	1.06420000
C	5.02840000	1.28360000	1.94030000
C	3.75220000	1.72200000	1.58200000
C	-4.17540000	-3.44820000	-0.13430000
C	-2.99840000	-3.96430000	0.70960000
C	-1.91480000	-2.91560000	0.98440000
C	1.03810000	-1.13120000	0.53760000
C	-2.66490000	2.84160000	1.21420000
C	-3.93730000	3.64730000	0.93030000
C	-4.92960000	2.95080000	-0.01360000
C	-1.22540000	2.47760000	-3.84730000
C	1.82820000	5.95420000	0.57360000
H	-0.96520000	-3.38570000	1.26440000
H	-2.21350000	-2.23330000	1.78330000
H	-3.36420000	-4.31860000	1.68330000
H	-2.55830000	-4.83170000	0.19590000
H	-3.92080000	-3.45480000	-1.19890000
H	-5.04080000	-4.10890000	-0.00470000
H	-5.92360000	3.40060000	0.09690000
H	-4.62780000	3.08310000	-1.05730000
H	-3.67170000	4.62290000	0.49660000
H	-4.41890000	3.84520000	1.89830000
H	-1.86670000	3.48650000	1.59400000
H	-2.85410000	2.05050000	1.94270000
H	3.19330000	2.34960000	2.27150000
H	5.44150000	1.56840000	2.90580000
H	6.76660000	0.14930000	1.34390000
H	5.79760000	-0.48870000	-0.86140000
H	3.54560000	0.25810000	-1.49340000
H	0.40110000	2.86630000	2.44480000
H	0.32320000	5.10200000	3.50900000
H	1.22170000	7.08930000	2.30700000
H	2.22540000	6.81870000	0.04570000
H	2.34720000	4.58660000	-1.00210000
H	0.88160000	3.00710000	-2.15560000
H	2.42460000	2.16620000	-2.42350000
H	-1.10180000	3.13660000	-2.99220000
H	-2.50290000	3.87590000	-4.86820000
H	-2.88630000	2.37880000	-6.82200000
H	-1.82440000	0.12550000	-6.87300000
H	-0.38370000	-0.61180000	-5.01550000
H	2.52000000	0.95580000	-4.51190000
H	4.11460000	-0.62350000	-5.54590000
H	4.07620000	-3.03200000	-4.91650000

H	2.42830000	-3.84740000	-3.23740000
H	0.84830000	-2.25860000	-2.17440000

Species B3
HF energy= -3915.78547613
No imaginary frequency
Zero-point correction = 0.595811 (Hartree/Particle)
Thermal correction to Energy = 0.642199
Thermal correction to Enthalpy = 0.643143
Thermal correction to Gibbs Free Energy = 0.512615
Sum of electronic and zero-point Energies = -3915.189665
Sum of electronic and thermal Energies = -3915.143277
Sum of electronic and thermal Enthalpies = -3915.142333
Sum of electronic and thermal Free Energies = -3915.272861

Coordinates: **B3**

Mo	-0.09270000	-0.22170000	-0.39840000
Mo	-3.00570000	-0.76010000	-0.49140000
S	-1.90790000	1.45460000	-0.57130000
S	-1.17090000	-2.42310000	-0.41640000
S	-4.20170000	-2.37730000	0.91510000
S	-4.84450000	0.46630000	0.58000000
P	0.29070000	0.08970000	2.25800000
P	1.55680000	1.62780000	0.14410000
O	-3.48500000	-0.96200000	-2.09860000
O	2.45400000	-1.96900000	-1.12030000
O	-0.07050000	0.01900000	-3.52110000
C	-0.93740000	0.55000000	3.56430000
C	1.54410000	-1.33730000	-0.78860000
C	-0.70980000	1.59150000	4.48320000
C	-1.65770000	1.89780000	5.46210000
C	-2.84910000	1.17040000	5.53740000
C	-3.09090000	0.14170000	4.62500000
C	-2.14410000	-0.16460000	3.64370000
C	1.48370000	-0.98230000	3.19880000
C	2.07010000	-2.08790000	2.56280000
C	2.99410000	-2.89430000	3.23500000
C	3.34150000	-2.60900000	4.55610000
C	2.75780000	-1.51570000	5.20400000
C	1.24610000	1.69270000	1.98690000
C	3.36790000	1.34170000	-0.05610000
C	3.98800000	1.73650000	-1.25440000
C	5.34100000	1.47320000	-1.47120000
C	6.09360000	0.81110000	-0.49700000
C	4.12850000	0.67020000	0.91350000
C	1.36340000	3.36090000	-0.44660000
C	1.89600000	4.43420000	0.28970000
C	1.76170000	5.74310000	-0.17400000

C	1.10530000	5.99400000	-1.38390000
C	0.58320000	4.93310000	-2.12600000
C	0.70630000	3.62030000	-1.65910000
C	-3.58250000	-4.07270000	0.52000000
C	-2.24790000	-4.45020000	1.18200000
C	-1.21520000	-3.31700000	1.20360000
C	-0.10550000	-0.07860000	-2.36430000
C	-2.42230000	2.46190000	0.89450000
C	-3.78210000	3.12750000	0.65070000
C	-4.81760000	2.21210000	-0.02140000
C	1.83500000	-0.71150000	4.53380000
C	5.48420000	0.41080000	0.69350000
H	-0.20680000	-3.70930000	1.37270000
H	-1.43940000	-2.59730000	1.99330000
H	-2.41930000	-4.75670000	2.22360000
H	-1.83190000	-5.32090000	0.65480000
H	-3.51630000	-4.16540000	-0.56810000
H	-4.37120000	-4.75630000	0.85560000
H	-5.82740000	2.59810000	0.16250000
H	-4.67020000	2.19530000	-1.10550000
H	-3.65240000	4.02330000	0.02600000
H	-4.15790000	3.46570000	1.62670000
H	-1.64240000	3.21720000	1.04900000
H	-2.46290000	1.80710000	1.76520000
H	0.28330000	2.80110000	-2.23350000
H	0.07180000	5.12150000	-3.06750000
H	1.00300000	7.01510000	-1.74540000
H	2.17330000	6.56680000	0.40590000
H	2.42450000	4.24950000	1.22330000
H	3.41630000	2.25880000	-2.01840000
H	5.80650000	1.78730000	-2.40300000
H	7.14850000	0.60660000	-0.66700000
H	6.06050000	-0.10840000	1.45640000
H	3.67330000	0.33300000	1.84100000
H	2.12920000	1.83600000	2.62080000
H	0.55530000	2.52600000	2.15820000
H	1.37510000	0.11900000	5.06280000
H	3.01560000	-1.29150000	6.23730000
H	4.05800000	-3.23680000	5.08190000
H	3.43730000	-3.74480000	2.72130000
H	1.81090000	-2.31840000	1.53480000
H	-2.37930000	-0.94390000	2.92280000
H	-4.02370000	-0.41620000	4.65520000
H	-3.58950000	1.41340000	6.29660000
H	-1.46500000	2.70730000	6.16350000
H	0.20790000	2.17470000	4.44020000

Species C

HF energy= -3221.38195134
No Imaginary frequency
Zero-point correction = 0.552756 (Hartree/Particle)
Thermal correction to Energy = 0.590774
Thermal correction to Enthalpy = 0.591719
Thermal correction to Gibbs Free Energy = 0.478362
Sum of electronic and zero-point Energies = -3220.829196
Sum of electronic and thermal Energies = -3220.791177
Sum of electronic and thermal Enthalpies = -3220.790233
Sum of electronic and thermal Free Energies = -3220.903590

Coordinates: **C**

Mo	-0.02240000	-0.26720000	-1.19310000
P	-1.62400000	0.50610000	0.69930000
S	-1.97250000	-0.79330000	-2.45020000
P	1.62200000	0.50660000	0.64770000
S	1.90700000	-0.91770000	-2.42190000
S	-0.11160000	-2.74440000	-0.49830000
C	-2.95550000	2.46630000	-0.80640000
O	0.02510000	2.54830000	-2.51670000
C	0.01420000	1.50600000	-1.98420000
C	-2.42010000	2.15980000	0.45790000
C	4.20520000	-2.84730000	2.63590000
C	2.64590000	-0.79290000	1.49110000
C	-3.04010000	-0.55890000	1.25100000
C	2.92520000	1.77310000	0.29270000
C	0.69440000	1.32730000	2.05580000
C	-0.66910000	0.66910000	2.29580000
C	3.14620000	2.24460000	-1.00830000
C	-4.37780000	-0.15900000	1.10830000
C	1.50100000	-3.41790000	-1.10050000
C	-2.48000000	-2.50540000	-1.94210000
C	-2.77300000	-1.82680000	1.80050000
C	3.83310000	-1.22670000	0.87170000
C	4.60470000	-2.24210000	1.44010000
C	-5.14290000	-2.24900000	2.07000000
C	4.12380000	3.21500000	-1.25240000
C	2.25710000	-1.40780000	2.69220000
C	-2.51340000	3.12270000	1.47690000
C	-3.81460000	-2.66000000	2.21370000
C	-3.11540000	4.36090000	1.23700000
C	-3.64750000	4.65130000	-0.02070000
C	1.99630000	-2.77630000	-2.38810000
C	3.71150000	2.28220000	1.34330000
C	-5.41960000	-0.99950000	1.51230000
C	-1.29360000	-3.44280000	-1.75090000
C	4.68180000	3.25370000	1.09870000
C	-3.57110000	3.69770000	-1.03890000
C	3.03020000	-2.42560000	3.26030000
C	4.88890000	3.72370000	-0.20250000

H	4.15530000	-0.76260000	-0.05730000
H	5.52330000	-2.55720000	0.94860000
H	4.80790000	-3.63760000	3.07880000
H	2.71240000	-2.88330000	4.19530000
H	1.35170000	-1.09490000	3.20540000
H	0.56030000	2.37260000	1.74980000
H	3.57750000	1.91010000	2.35710000
H	5.27950000	3.63980000	1.92230000
H	5.64740000	4.48020000	-0.39450000
H	4.28170000	3.56980000	-2.26870000
H	2.56130000	1.85230000	-1.83200000
H	1.42630000	-3.14040000	-3.25240000
H	3.04390000	-3.06160000	-2.54700000
H	2.19330000	-3.22190000	-0.27570000
H	1.38990000	-4.50500000	-1.20400000
H	-0.75030000	-3.56410000	-2.69400000
H	-1.61590000	-4.42780000	-1.39040000
H	-3.12340000	-2.89990000	-2.73880000
H	-3.08180000	-2.44780000	-1.02760000
H	-1.74850000	-2.17980000	1.89430000
H	-3.58590000	-3.63440000	2.64140000
H	-5.95500000	-2.90010000	2.38720000
H	-6.44990000	-0.67040000	1.39220000
H	-4.61130000	0.81220000	0.68180000
H	-0.54790000	-0.35650000	2.66170000
H	-1.24530000	1.20210000	3.06140000
H	1.29880000	1.33120000	2.97170000
H	-2.88940000	1.73660000	-1.60890000
H	-3.97840000	3.91380000	-2.02430000
H	-4.11570000	5.61580000	-0.20710000
H	-3.16900000	5.09610000	2.03770000
H	-2.12150000	2.92290000	2.47040000

Species D
HF energy= -3876.50852020
No Imaginary frequency
Zero-point correction= 0.567776 (Hartree/Particle)
Thermal correction to Energy= .612433
Thermal correction to Enthalpy= 0.613377
Thermal correction to Gibbs Free Energy= 0.487118
Sum of electronic and zero-point Energies= -3875.940744
Sum of electronic and thermal Energies= -3875.896087
Sum of electronic and thermal Enthalpies= -3875.895143
Sum of electronic and thermal Free Energies= -3876.021403

Coordinates: **D**

Mo	2.44830000	1.21430000	4.71480000
Mo	1.31250000	3.41940000	6.19210000

S	3.70490000	3.08490000	5.71330000
S	2.19600000	4.15300000	8.34370000
S	0.04810000	1.78970000	4.81360000
S	-0.46720000	2.93110000	7.77630000
P	1.71870000	-0.83720000	3.36090000
P	4.72040000	0.15280000	4.23090000
O	1.00230000	4.77890000	5.22780000
O	2.25720000	-0.42090000	7.43440000
O	2.55990000	2.97470000	2.04100000
C	2.33000000	0.18700000	6.44750000
C	6.01230000	0.07000000	5.55430000
C	0.61150000	-2.06290000	4.19780000
C	2.52330000	2.32450000	2.99280000
C	0.90670000	-0.64500000	1.71000000
C	5.65860000	0.74750000	2.75470000
C	3.24430000	-1.85020000	2.91280000
C	6.25940000	-0.11860000	1.82570000
C	5.70530000	-0.55650000	6.77620000
C	7.28860000	0.62950000	5.38570000
C	7.08150000	1.76920000	0.55010000
C	0.96150000	-1.68470000	0.76240000
C	-0.73410000	-2.20520000	3.82160000
C	0.26150000	-3.73180000	5.93680000
C	1.09600000	-2.83420000	5.26840000
C	0.20190000	0.52470000	1.38750000
C	8.23450000	0.56280000	6.41340000
C	-1.57060000	-3.09760000	4.49800000
C	5.78680000	2.13510000	2.56350000
C	-1.07620000	-3.86420000	5.55510000
C	0.34420000	-1.54710000	-0.48130000
C	4.48930000	2.92400000	7.38040000
C	-1.04840000	0.89350000	5.99970000
C	6.49930000	2.64060000	1.47430000
C	-1.73100000	1.94960000	6.85570000
C	6.65530000	-0.63020000	7.79600000
C	4.03720000	4.12870000	8.19060000
C	-0.34720000	-0.37290000	-0.79510000
C	6.95860000	0.38950000	0.72760000
C	-0.42130000	0.65800000	0.14250000
C	7.92280000	-0.06800000	7.61890000
H	1.47870000	-2.61310000	0.99330000
H	0.40070000	-2.35880000	-1.20380000
H	-0.82770000	-0.26550000	-1.76540000
H	-0.95990000	1.57410000	-0.08970000
H	0.12740000	1.33090000	2.11000000
H	5.57560000	2.91310000	7.22200000
H	4.38930000	5.05900000	7.72750000
H	4.44300000	4.07900000	9.20960000
H	4.18310000	1.98500000	7.84950000
H	-2.35280000	2.60860000	6.23750000

H	-2.37620000	1.47700000	7.60810000
H	-0.45940000	0.20080000	6.60710000
H	-1.76660000	0.32290000	5.39700000
H	3.54930000	-1.50960000	1.91590000
H	2.97690000	-2.91090000	2.83360000
H	-1.13210000	-1.62440000	2.99400000
H	-2.61030000	-3.19420000	4.19180000
H	-1.72830000	-4.55900000	6.08000000
H	0.65720000	-4.32130000	6.76120000
H	2.12720000	-2.73440000	5.59730000
H	7.55160000	1.11820000	4.45220000
H	9.21800000	1.00410000	6.26480000
H	8.66040000	-0.11980000	8.41700000
H	6.39860000	-1.11980000	8.73310000
H	4.71900000	-0.97770000	6.94910000
H	6.19340000	-1.19650000	1.94710000
H	7.40970000	-0.29660000	0.01360000
H	7.62650000	2.16330000	-0.30500000
H	6.58780000	3.71700000	1.34480000
H	5.32950000	2.82360000	3.27030000
C	4.39830000	-1.65670000	3.90290000
H	4.15630000	-2.09430000	4.87850000
H	5.30670000	-2.16440000	3.55600000

Species E

HF energy= -3955.12089479

No Imaginary frequency

Zero-point correction= 0.625712 (Hartree/Particle)

Thermal correction to Energy= 0.672898

Thermal correction to Enthalpy= 0.673842

Thermal correction to Gibbs Free Energy= 0.542276

Sum of electronic and zero-point Energies= -3954.495183

Sum of electronic and thermal Energies= -3954.447997

Sum of electronic and thermal Enthalpies= -3954.447053

Sum of electronic and thermal Free Energies= -3954.578619

Coordinates: **E**

Mo	-0.16260000	0.05780000	-0.01880000
Mo	-2.95280000	-0.44230000	-0.78180000
S	-1.88800000	1.76360000	-0.37870000
S	-1.15530000	-2.14720000	-0.45900000
S	-4.41520000	-2.17330000	0.14520000
S	-5.01000000	0.68440000	-0.07480000
P	2.05680000	-1.20210000	0.27230000
P	1.42040000	2.00210000	0.48150000
O	-3.00660000	-0.48600000	-2.47260000
O	-0.83320000	-0.18590000	3.08190000
O	0.42620000	0.28540000	-3.15760000

C	2.18010000	-2.43980000	1.64600000
C	-0.59720000	-0.09740000	1.94690000
C	2.14940000	-2.01240000	2.98480000
C	2.20140000	-2.93530000	4.03060000
C	2.26910000	-4.30420000	3.75680000
C	2.28920000	-4.74160000	2.43110000
C	2.24800000	-3.81780000	1.38240000
C	2.81120000	-2.12310000	-1.14420000
C	2.01230000	-2.61460000	-2.18780000
C	2.58630000	-3.32090000	-3.24970000
C	3.96340000	-3.54320000	-3.28410000
C	4.76870000	-3.06570000	-2.24550000
C	3.42000000	0.03300000	0.68000000
C	2.14450000	2.91820000	-0.95150000
C	1.28490000	3.31310000	-1.99270000
C	1.77520000	4.02330000	-3.09040000
C	3.13420000	4.33660000	-3.17480000
C	3.50670000	3.25060000	-1.04200000
C	0.91840000	3.36250000	1.63520000
C	0.56750000	3.04490000	2.96030000
C	0.18050000	4.04500000	3.85370000
C	0.12290000	5.37780000	3.43540000
C	0.45900000	5.70220000	2.12010000
C	0.85770000	4.70380000	1.22580000
C	-3.68960000	-3.83560000	-0.20730000
C	-2.54620000	-4.25230000	0.73270000
C	-1.56540000	-3.12190000	1.06080000
C	0.22110000	0.20210000	-2.02510000
C	-2.67810000	2.44040000	1.15620000
C	-3.96770000	3.19490000	0.81370000
C	-4.83130000	2.51190000	-0.25870000
C	4.19740000	-2.36630000	-1.18190000
C	3.99820000	3.94730000	-2.14910000
H	-0.62160000	-3.51280000	1.45500000
H	-1.99500000	-2.43740000	1.79530000
H	-2.95840000	-4.61370000	1.68550000
H	-2.00790000	-5.09520000	0.27430000
H	-3.36120000	-3.85710000	-1.25100000
H	-4.52300000	-4.54230000	-0.11540000
H	-5.85280000	2.90880000	-0.21820000
H	-4.44060000	2.72340000	-1.25920000
H	-3.72210000	4.20960000	0.46670000
H	-4.54230000	3.30270000	1.74430000
H	-1.94540000	3.10030000	1.63040000
H	-2.87800000	1.60160000	1.82740000
H	1.12300000	4.97600000	0.20860000
H	0.41570000	6.73600000	1.78330000
H	-0.18540000	6.15610000	4.13020000
H	-0.08610000	3.77870000	4.87440000
H	0.57540000	2.01320000	3.30080000

H	0.22690000	3.06650000	-1.94530000
H	1.09320000	4.32000000	-3.88430000
H	3.51810000	4.87940000	-4.03600000
H	5.05800000	4.18780000	-2.20540000
H	4.20050000	2.97420000	-0.25260000
H	3.87300000	0.31130000	-0.27930000
H	4.19460000	-0.45170000	1.28630000
H	4.83990000	-2.01890000	-0.37620000
H	5.84270000	-3.24010000	-2.26080000
H	4.40940000	-4.08790000	-4.11390000
H	1.95010000	-3.69040000	-4.05100000
H	0.93890000	-2.45680000	-2.16990000
H	2.27400000	-4.17420000	0.35630000
H	2.34100000	-5.80500000	2.20650000
H	2.30300000	-5.02380000	4.57200000
H	2.18060000	-2.58300000	5.05990000
H	2.07340000	-0.95470000	3.22300000
C	2.88740000	1.28410000	1.38500000
H	3.67760000	2.03310000	1.51780000
H	2.52270000	1.04040000	2.38930000