Supplementary Information

Mechanism Study on Hydrogen Evolution Reaction Catalyzed by Molybdenum Disulfide Complexes

Ti-Long Yang,[b] Shao-Fei Ni,[b] Peng Qin[a] and Li Dang*[ab]

[a]Department of Chemistry and Key Laboratory for Preparation and Application of Ordered Structural Materials of Guangdong Province, Shantou University, Guangdong 515063, P. R. China

[b]Department of Chemistry, Southern University of Science and Technology, Shenzhen, 518055, P. R. China.

*Email: ldang@stu.edu.cn

Contents :

Text S1.
Computational details

Density functional theory (DFT) calculation using Gaussian 09 package[1] were performed to illuminate the mechanism of the molecular MoS_2 catalyzed hydrogen evolution reaction. To produce a good description of the structural, thermodynamic, and kinetic properties of the systems, a series of density functionals such as B3P86,[2] M06-L,[3] B3LYP,[4] BP86,[2b, 2c, 5] BP86G and PBE1PBE[6] were selected to optimize the structure of catalyst molecular $[MoS_2]^{2+}$. The effective core potentials (ECPs) of Hay and Wadt with a double-ζ valence basis set (LanL2DZ) were used for Mo,[7] setting the polarization functions with f = 1.043.[8] The all-electron 6-31G** basis set was used in describing all other atoms.[9] Geometric structures of all species in this work were optimized in gas phase at T = 298.15 K and 1 atm pressure. The harmonic vibrational frequencies and the number of imaginary frequencies determine the nature of all intermediates (no imaginary frequency) and transition state structures (only one imaginary frequency). The latter were also confirmed to connect appropriate intermediates, reactants, or products by intrinsic reaction coordinate (IRC) calculations.[10] The gas-phase Gibbs free energies, *G*, were calculated within the harmonic potential approximation at optimized structures. Solvent effects were computed by using C-PCM (conductor-like polarizable continuum) model[11] with Bondi atomic radii[12] and water as solvent. The newly developed M11-L functional[13] with a 6-311++G** basis set[14] (Lanl2dz basis set for Mo)[7a-c] was used to the solvent corrections to give more accurate energy information. The 3D molecular structures displayed in the supplementary material were generated by using CYL-view.[15]

Text S2.

Redox potential calculation

The stand redox potential E^0 is determined using the equation

$$E^0 = -\frac{\Delta G_{\text{solv}}^{\text{o,red}}}{nF} \qquad (1)$$

where,

$\Delta G_{\text{solv}}^{\text{o,red}}$ is the calculated free energy of reduction;

F is the Faraday constant;

n is the number of electrons being transferred.[16]

The $\Delta G_{\text{solv}}^{\text{o,red}}$ is defined as the free energy change associated with the following reduction process

$$\text{Ox}_{\text{solv}} + e^- \rightarrow \text{Red}_{\text{solv}} \qquad (2)$$

where Ox_{solv} and Red_{solv} are the oxidized and reduced species in solution.

The effect of the electron on the free energy is −0.868 kcal/mol at 298.15 K.[17] The Standard Hydrogen Electrode (SHE) potential in water was experimentally estimated to be 4.44 V.[18]

The E^0 versus SHE can be obtained via

$$E^0\text{vs SHE} = -\frac{\Delta G_{\text{solv}}^{\text{o,red}}}{nF} - 4.44\text{V} \qquad (3)$$

Text S3.

pK_a calculations

The pK_a is determined from the free energy of deprotonation, $\Delta G_{\text{solv}}^{\text{o,p}Ka}$, using the equation

$$\text{p}K_a = \frac{\Delta G_{\text{solv}}^{\text{o,p}Ka}}{\ln(10)\,\text{RT}} \qquad (4)$$

where,

R is the gas constant;

T is the temperature.

For a molecule HA, $\Delta G_{\text{solv}}^{\text{o,p}Ka}$ is defined to be the free energy change associated with the reaction

$$\text{AH}_{\text{solv}} \rightarrow \text{A}_{\text{solv}}^- + \text{H}_{\text{solv}}^+ \qquad (5)$$

the free energy of H^+ in water was determined to be −262.4kcal/mol.[19]

Scheme S1. Determination of the thermodynamic hydricity of $^{3}[MoS\text{-}SH]^{+}$, $^{2}[MoSH\text{-}SH]^{+}$, and $^{2}[Mo(SH)_2]^{+}$.

a: $^{3}[MoS\text{-}SH]^{+} \rightleftharpoons {}^{3}[MoS]^{2+} + H^{-}$

$^{4}[MoS\text{-}SH]^{2+} \rightleftharpoons {}^{4}[MoS\text{-}S]^{+} + H^{+}$ $\quad \Delta G = \ln(10)RTpK_a$ (6)

$^{4}[MoS\text{-}S]^{+} \rightleftharpoons {}^{3}[MoS_2]^{2+} + e^{-}$ $\quad \Delta G = FE^{0}$ (7)

$^{3}[MoS\text{-}SH]^{+} \rightleftharpoons {}^{4}[MoS\text{-}SH]^{2+} + e^{-}$ $\quad \Delta G = FE^{0}$ (8)

$H^{+} + 2e^{-} \rightleftharpoons H^{-}$ $\quad \Delta G$ (9)[20]

$^{3}[MoS\text{-}SH]^{+} \rightleftharpoons {}^{3}[MoS]^{2+} + H^{-}$ $\quad \Delta G_{H-}$ (10)

b: $^{2}[Mo(SH)_2]^{+} \rightleftharpoons {}^{4}[MoS\text{-}SH]^{2+} + H^{-}$

$^{3}[Mo(SH)_2]^{2+} \rightleftharpoons {}^{3}[MoS\text{-}SH]^{+} + H^{+}$ $\quad \Delta G = \ln(10)RTpK_a$ (11)

$^{2}[Mo(SH)_2]^{+} \rightleftharpoons {}^{3}[Mo(SH)_2]^{2+} + e^{-}$ $\quad \Delta G = FE^{0}$ (12)

$^{3}[MoS\text{-}SH]^{+} \rightleftharpoons {}^{4}[MoS\text{-}SH]^{2+} + e^{-}$ $\quad \Delta G = FE^{0}$ (13)

$H^{+} + 2e^{-} \rightleftharpoons H^{-}$ $\quad \Delta G$ (9)

$^{2}[Mo(SH)_2]^{+} \rightleftharpoons {}^{4}[MoS\text{-}SH]^{2+} + H^{-}$ $\quad \Delta G_{H-}$ (14)

c: $^{2}[MoSH\text{-}SH]^{+} \rightleftharpoons {}^{4}[MoS\text{-}SH]^{2+} + H^{-}$

$^{3}[MoSH\text{-}SH]^{2+} \rightleftharpoons {}^{3}[MoS\text{-}SH]^{+} + H^{+}$ $\quad \Delta G = \ln(10)RTpK_a$ (15)

$^{2}[MoSH\text{-}SH]^{+} \rightleftharpoons {}^{3}[MoSH\text{-}SH]^{2+} + e^{-}$ $\quad \Delta G = FE^{0}$ (16)

$^{3}[MoS\text{-}SH]^{+} \rightleftharpoons {}^{4}[MoS\text{-}SH]^{2+} + e^{-}$ $\quad \Delta G = FE^{0}$ (17)

$H^{+} + 2e^{-} \rightleftharpoons H^{-}$ $\quad \Delta G$ (9)

$^{2}[MoSH\text{-}SH]^{+} \rightleftharpoons {}^{4}[MoS\text{-}SH]^{2+} + H^{-}$ $\quad \Delta G_{H-}$ (18)

d: $^{2}[MoSH\text{-}SH]^{+} \rightleftharpoons {}^{4}[MoSH\text{-}S]^{2+} + H^{-}$

$^{3}[MoSH\text{-}SH]^{2+} \rightleftharpoons {}^{3}[MoSH\text{-}S]^{+} + H^{+}$ $\quad \Delta G = \ln(10)RTpK_a$ (19)

$^{2}[MoSH\text{-}SH]^{+} \rightleftharpoons {}^{3}[MoSH\text{-}SH]^{2+} + e^{-}$ $\quad \Delta G = FE^{0}$ (20)

$^{3}[MoSH\text{-}S]^{+} \rightleftharpoons {}^{4}[MoSH\text{-}S]^{2+} + e^{-}$ $\quad \Delta G = FE^{0}$ (21)

$H^{+} + 2e^{-} \rightleftharpoons H^{-}$ $\quad \Delta G$ (9)

$^{2}[MoSH\text{-}SH]^{+} \rightleftharpoons {}^{4}[MoSH\text{-}S]^{2+} + H^{-}$ $\quad \Delta G_{H-}$ (22)

Table S1. Crystal[21] and calculated gas phase structural parameters for the catalyst molecular $[MoS_2]^{2+}$. B3P86 functional reproduced the geometry of $[MoS_2]^{2+}$ best.

	Crystal	**B3P86**	BP86	BP86G	PBE1PBE	M06L	B3LYP
Mo-S	2.402 (2)	2.419	2.442	2.442	2.418	2.420	2.444
S-S	2.019 (1)	2.032	2.054	2.054	2.030	2.028	2.047
Mo-N	2.19 (2)	2.189	2.199	2.199	2.188	2.217	2.215
S-Mo-S	49.68 (3)	49.675	49.728	49.731	49.641	49.536	49.518

Table S2. The gas phase relative electronic energies (ΔE_{gas}), gas phase relative free energies (ΔG_{gas}), solvation corrected relative electronic energies (ΔE_{sol}), and solvation corrected relative free energies (ΔG_{sol}) for every intermediate in their high spin states, low spin states, side-on configuration and end-on configuration. The most thermodynamically stable species are set as the reference point at the given reduction and protonation state. The pre-superscript indicates a particular spin state of the complex, and the overall charge is shown in the superscript on the complex.

$[MoS_2]^{2+}$

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
$^3[MoS_2]^{2+}$	0.0	0.0	0.0	0.0
$^1[MoS_2]^{2+}$	15.8	16.5	16.4	17.1
$^3[MoS\text{-}S]^{2+}$	16.4	13.0	7.8	4.4
$^1[MoS\text{-}S]^{2+}$	29.2	27.6	32.1	30.4

After a reduction process [E].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
$^4[MoS\text{-}S]^{+}$	0.0	0.0	0.0	0.0
$^2[MoS\text{-}S]^{+}$	−2.8	−2.6	6.6	6.8
$^4[MoS_2]^{+}$	−1.7	−0.3	12.2	13.6
$^2[MoS_2]^{+}$	−17.0	−13.8	−0.6	2.6

After a reduction-protonation process [EC].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
$^4[MoS\text{-}SH]^{2+}$	0.0	0.0	0.0	0.0
$^2[MoS\text{-}SH]^{2+}$	6.9	7.5	9.6	10.2
$^4[MoSH\text{-}S]^{2+}$	25.7	26.2	12.6	13.2
$^2[MoSH\text{-}S]^{2+}$	31.1	31.4	26.4	26.8
$^4[MoS_2H]^{2+}$	----	----	----	----
$^2[MoS_2H]^{2+}$	12.0	15.4	14.2	17.6
$^4[MoHS\text{-}S]^{2+}$	----	----	----	----
$^2[MoHS\text{-}S]^{2+}$	37.5	38.4	33.7	34.7
$^4[MoHS_2]^{2+}$	----	----	----	----
$^2[MoHS_2]^{2+}$	----	----	----	----

---- structure could not be obtained.

After a reduction-protonation-reduction process [ECE].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
^{3}[MoS-SH]$^{+}$	0.0	0.0	0.0	0.0
^{1}[MoS-SH]$^{+}$	3.2	4.6	3.7	5.1
^{3}[MoSH-S]$^{+}$	18.4	20.1	10.2	11.9
^{1}[MoSH-S]$^{+}$	28.5	31.0	23.6	26.2
^{3}[MoS$_2$H]$^{+}$	----	----	----	----
^{1}[MoS$_2$H]$^{+}$	10.6	15.2	12.0	16.6
^{3}[MoHS-S]$^{+}$	32.4	33.5	21.1	22.3
^{1}[MoHS-S]$^{+}$	31.9	34.9	24.7	27.7
^{3}[MoHS$_2$]$^{+}$	----	----	----	----
^{1}[MoHS$_2$]$^{+}$	----	----	----	----

---- structure could not be obtained.

After a reduction-protonation-reduction-protonation process [ECEC].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
^{3}[MoSH-SH]$^{2+}$	0.0	0.0	0.0	0.0
^{1}[MoSH-SH]$^{2+}$	20.8	20.2	21.8	21.2
^{3}[MoHS-SH]$^{2+}$	10.3	9.4	8.9	8.0
^{1}[MoHS-SH]$^{2+}$	18.5	19.0	18.0	18.6
^{3}[Mo(SH)$_2$]$^{2+}$	0.1	1.9	−6.5	−4.6
^{1}[Mo(SH)$_2$]$^{2+}$	13.6	16.3	8.7	11.4
^{3}[MoHSH-S]$^{2+}$	33.7	34.3	18.1	18.7
^{1}[MoHSH-S]$^{2+}$	40.9	42.8	33.3	35.2
^{3}[MoHS$_2$H]$^{2+}$	----	----	----	----
^{1}[MoHS$_2$H]$^{2+}$	33.2	36.2	34.3	37.3

---- structure could not be obtained.

After a reduction-protonation-reduction-protonation-reduction process [ECECE].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
^{4}[MoSH-SH]$^{+}$	0.0	0.0	0.0	0.0
^{2}[MoSH-SH]$^{+}$	−3.5	−2.6	12.5	13.4
^{4}[MoHS-SH]$^{+}$	24.4	23.6	46.7	45.9
^{2}[MoHS-SH]$^{+}$	2.9	4.3	25.1	26.6
^{4}[Mo(SH)$_2$]$^{+}$	−16.9	−18.1	−6.0	−7.2
^{2}[Mo(SH)$_2$]$^{+}$	−9.1	−5.7	3.5	6.9
^{4}[MoHSH-S]$^{+}$	----	----	----	----
^{2}[MoHSH-S]$^{+}$	21.6	24.7	31.8	34.9
^{4}[MoHS$_2$H]$^{+}$	----	----	----	----
^{2}[MoHS$_2$H]$^{+}$	----	----	----	----

---- structure could not be obtained.

Table S3. The ΔE_{gas}, ΔG_{gas}, ΔE_{sol}, and ΔG_{sol} of the relative stable intermediates involved in the proposed mechanism. The most thermodynamically stable species are set as the reference point at the given reduction and protonation state. The pre-superscript indicates a particular spin state of the complex, and the overall charge is shown in the superscript on the complex. The dispersion corrected functional B3LYP-D3[22] with the 6-311++G** basis set[14] (Lanl2dz basis set for Mo)[7a-c] is applied in the solvent effect calculations by using PCM[23] solvent model.

$[MoS_2]^{2+}$

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
$^{3}[MoS_2]^{2+}$	0.0	0.0	0.0	0.0
$^{3}[MoS\text{-}S]^{2+}$	16.4	13.0		

After a reduction process [E].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
$^{4}[MoS\text{-}S]^{+}$	0.0	0.0	0.0	0.0
$^{2}[MoS\text{-}S]^{+}$	−2.8	−2.6	2.5	2.8
$^{4}[MoS_2]^{+}$	−1.7	−0.3	7.7	9.1
$^{2}[MoS_2]^{+}$	−17.0	−13.8	−8.2	−5.0

After a reduction-protonation process [EC].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
$^{4}[MoS\text{-}SH]^{2+}$	0.0	0.0	0.0	0.0
$^{2}[MoS\text{-}SH]^{2+}$	6.9	7.5	8.2	8.8

After a reduction-protonation-reduction process [ECE].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
$^{3}[MoS\text{-}SH]^{+}$	0.0	0.0	0.0	0.0
$^{1}[MoS\text{-}SH]^{+}$	3.2	4.6	3.4	4.8

After a reduction-protonation-reduction-protonation process [ECEC].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
$^{3}[MoSH\text{-}SH]^{2+}$	0.0	0.0	0.0	0.0
$^{3}[Mo(SH)_2]^{2+}$	0.1	1.9	−10.1	−8.2

After a reduction-protonation-reduction-protonation-reduction process [ECECE].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
$^{4}[MoSH\text{-}SH]^{+}$	0.0	0.0	0.0	0.0
$^{4}[Mo(SH)_2]^{+}$	−16.9	−18.1	−10.7	−11.9

Table S4. The ΔE_{gas}, ΔG_{gas}, ΔE_{sol}, and ΔG_{sol} of the relative stable intermediates involved in the proposed mechanism. The most thermodynamically stable species are set as the reference point at the given reduction and protonation state. The pre-superscript indicates a particular spin state of the complex, and the overall charge is shown in the superscript on the complex. The dispersion corrected functional ωB97X-D[24] with the 6-311++G** basis set[14] (Lanl2dz basis set for Mo)[7a-c] is applied in the solvent effect calculations by using PCM[23] solvent model.

$[MoS_2]^{2+}$

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
$^3[MoS_2]^{2+}$	0.0	0.0	0.0	0.0
^{3}[MoS-S]$^{2+}$	16.4	13.0		

After a reduction process [E].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
^{4}[MoS-S]$^+$	0.0	0.0	0.0	0.0
^{2}[MoS-S]$^+$	−2.8	−2.6	7.1	7.3
^{4}[MoS_2]$^+$	−1.7	−0.3	12.8	14.2
$^2[MoS_2]^+$	−17.0	−13.8	−5.7	−2.5

After a reduction-protonation process [EC].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
^{4}[MoS-SH]$^{2+}$	0.0	0.0	0.0	0.0
^{2}[MoS-SH]$^{2+}$	6.9	7.5	12.6	13.2

After a reduction-protonation-reduction process [ECE].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
^{3}[MoS-SH]$^+$	0.0	0.0	0.0	0.0
^{1}[MoS-SH]$^+$	3.2	4.6	7.7	9.0

After a reduction-protonation-reduction-protonation process [ECEC].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
^{3}[MoSH-SH]$^{2+}$	0.0	0.0	0.0	0.0
$^3[Mo(SH)_2]^{2+}$	0.1	1.9	−9.6	−7.7

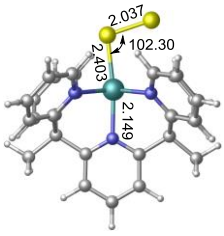
After a reduction-protonation-reduction-protonation-reduction process [ECECE].

	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
^{4}[MoSH-SH]$^+$	0.0	0.0	0.0	0.0
$^4[Mo(SH)_2]^+$	−16.9	−18.1	−13.8	−15.0

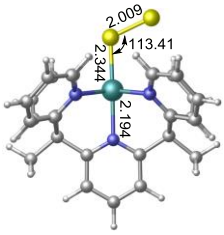
Optimized geometries

1. Calculated structure of the molecular $[MoS_2]^{2+}$ please see scheme 2 in the text.

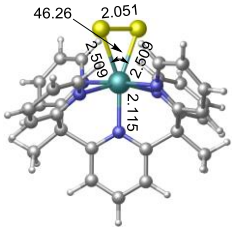
2. After a reduction process [E].



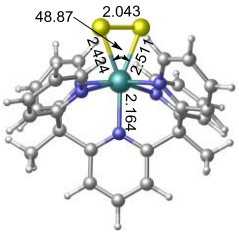
^{4}[MoS-S]$^+$ (*G* = 0.0)



^{2}[MoS-S]$^+$ (*G* = 6.8)

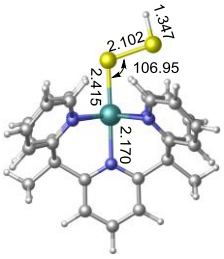


^{4}[MoS$_2$]$^+$ (*G* = 13.6)

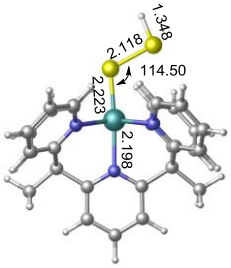


^{2}[MoS$_2$]$^+$ (*G* = 2.6)

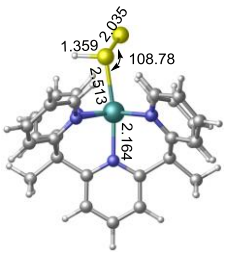
3. After a reduction-protonation process [EC].



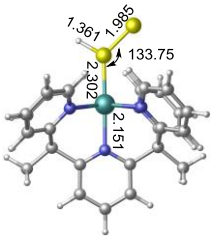
^{4}[MoS-SH]$^{2+}$ (*G* = 0.0)



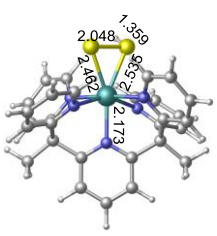
^{2}[MoS-SH]$^{2+}$ (*G* = 10.2)



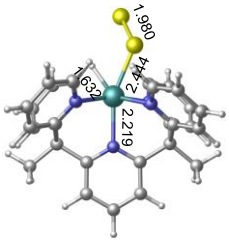
^{4}[MoSH-S]$^{2+}$ (*G* = 13.2)



^{2}[MoSH-S]$^{2+}$ (*G* = 26.8)

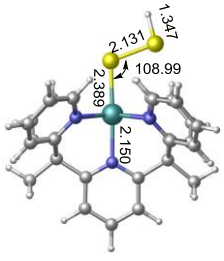


^{2}[MoS$_2$H]$^{2+}$ (*G* = 17.6)

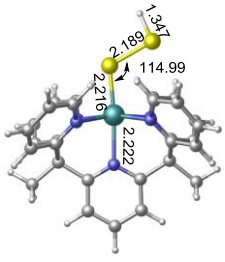


^{2}[MoHS-S]$^{2+}$ (*G* = 34.7)

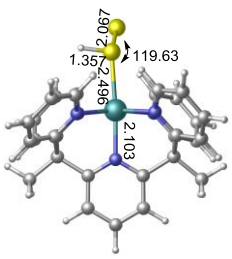
4. After a reduction-protonation-reduction process [ECE].



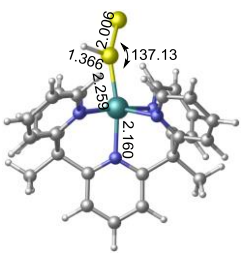
^{3}[MoS-SH]$^+$ (*G* = 0.0)



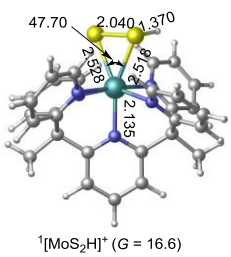
^{1}[MoS-SH]$^+$ (*G* = 5.1)



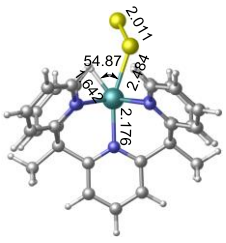
^{3}[MoSH-S]$^+$ (*G* = 11.9)



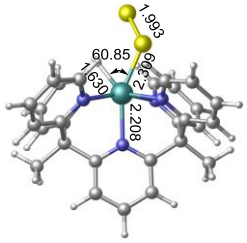
^{1}[MoSH-S]$^+$ (*G* = 26.2)



^{1}[MoS$_2$H]$^+$ (*G* = 16.6)

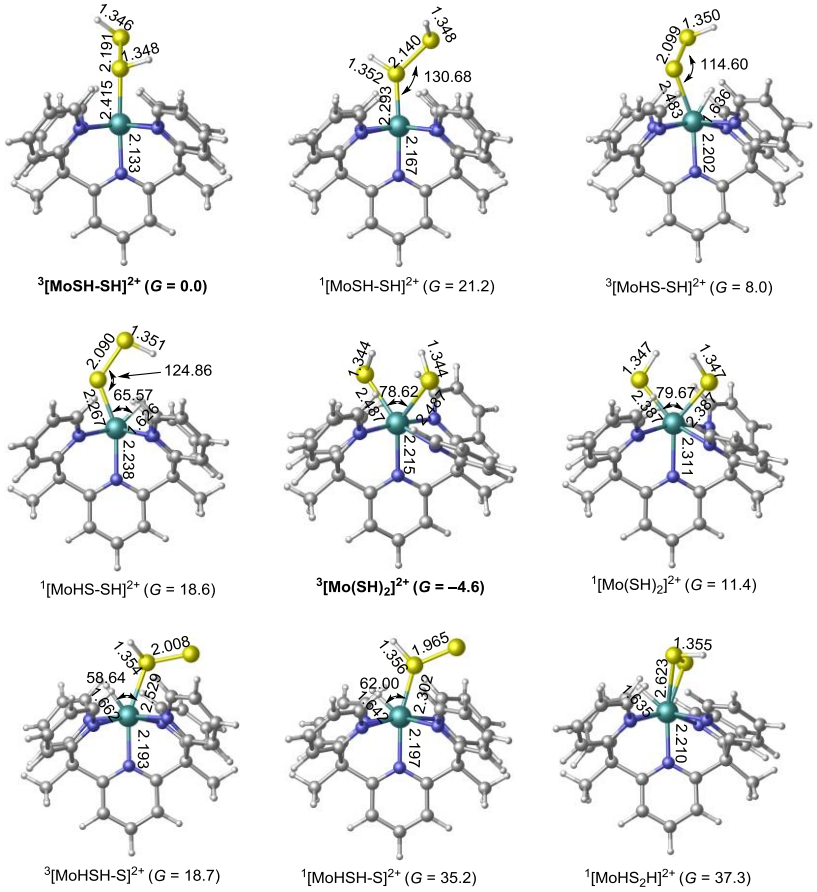


^{3}[MoHS-S]$^+$ (*G* = 22.3)

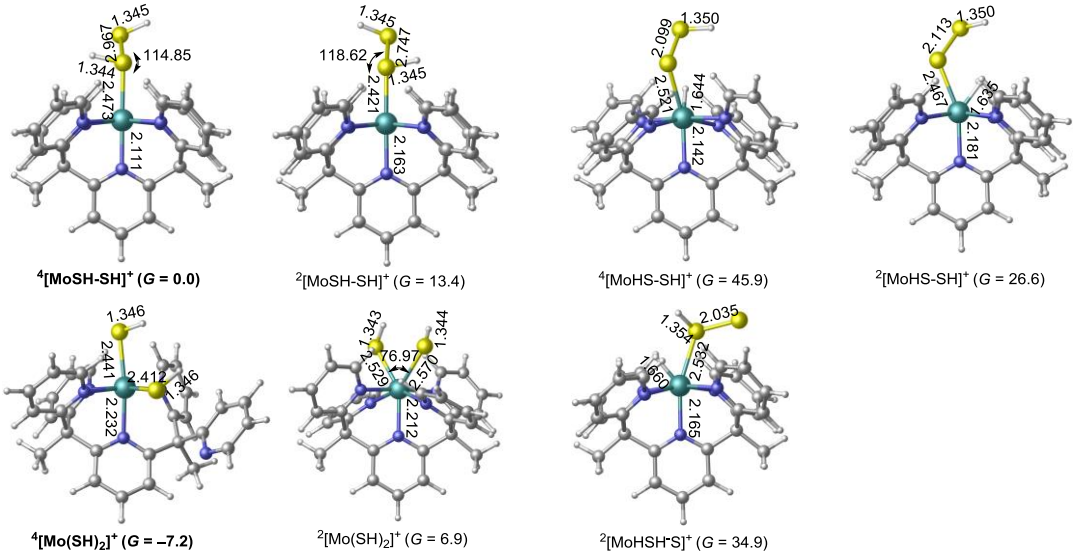


^{1}[MoHS-S]$^+$ (*G* = 27.7)

5. After a reduction-protonation-reduction-protonation process [ECEC].



6. After a reduction-protonation-reduction-protonation-reduction process [ECECE].



Scheme S2. Optimized geometries with selected structural parameters (distances in Å and angles in °) involved in Table S2. The relative Gibbs free energies are provided in kcal/mol.

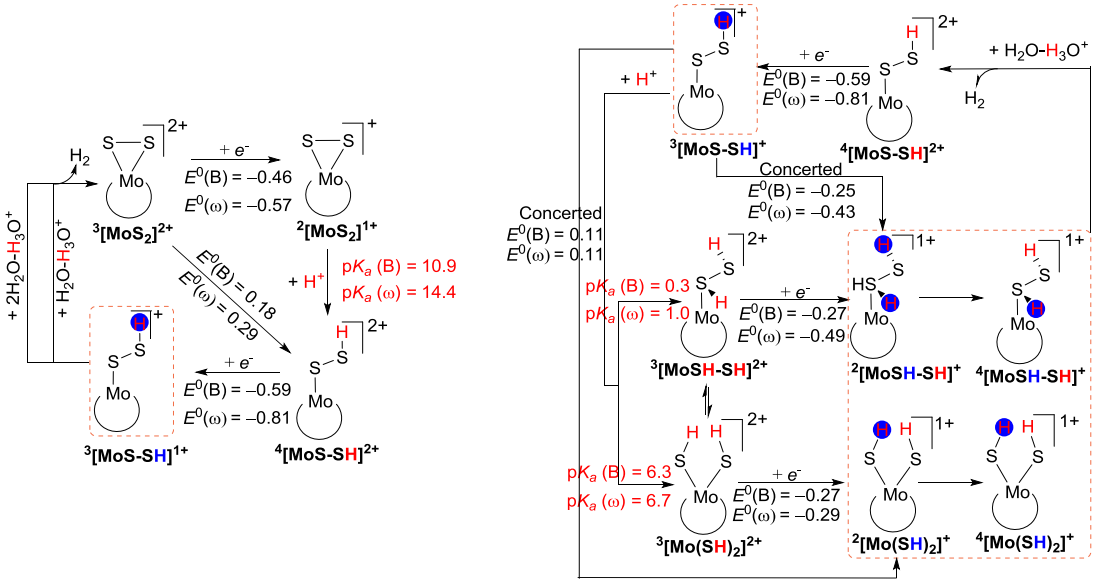


Figure S1. The reduction mechanism for $^{3}[MoS_2]^{2+}$ catalyzed hydrogen evolution reaction. The redox potentials (E^0) are reported in V with reference to the standard hydrogen electrode. The E^0 (B) and pK_a (B) refers to the data calculated using the B3LYP-D3 functional and E^0 (ω) and pK_a (ω) refers to the values calculated using the ωB97X-D functional. The pre-superscript indicates a particular spin state of the complex, and the overall charge is shown in the superscript on the complex.

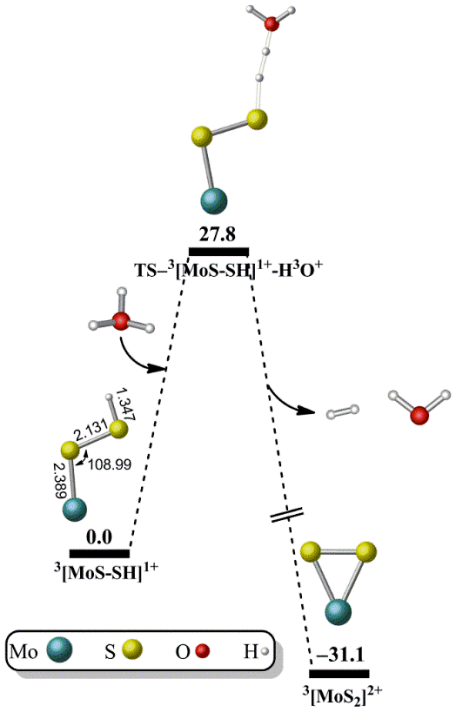


Figure S2. Energy profile for the hydrogen evolution reaction via direct H^+/H^- coupling between a proton hydrate and sulfur hydride of $^{3}[MoS\text{-}SH]^{+}$. Relative free energies in solvent are shown in kcal/mol. The distances are shown in Å and angles are shown in °. Ligand $PY5Me_2$ is eliminated for clear presentation.

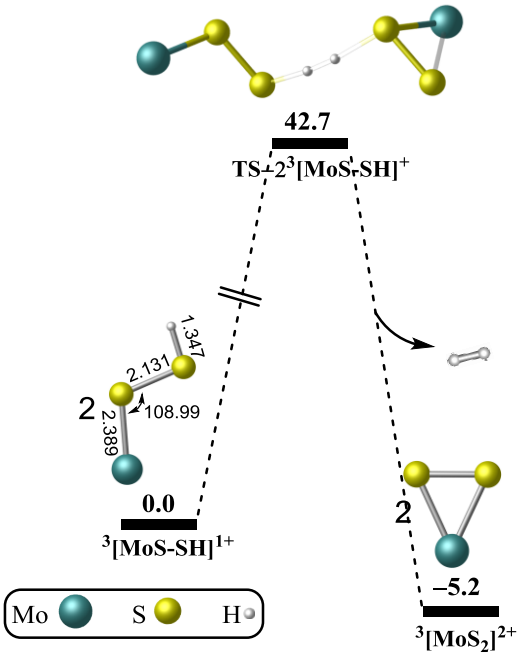


Figure S3. Energy profile of a bimolecular pathway where two ^{3}[MoS-SH]$^+$ come together to evolve hydrogen. Relative free energies in solvent are shown in kcal/mol. The distances are shown in Å. Ligand PY5Me$_2$ is eliminated for clear presentation.

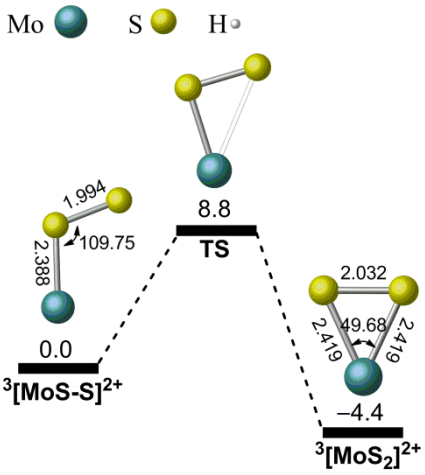


Figure S4. Transformation of the end-on ^{3}[MoS-S]$^{2+}$ to the side-on ^{3}[MoS$_2$]$^{2+}$. Relative free energies in solvent are shown in kcal/mol. The distances are shown in Å and angles are shown in °. Ligand PY5Me$_2$ is eliminated for clear presentation.

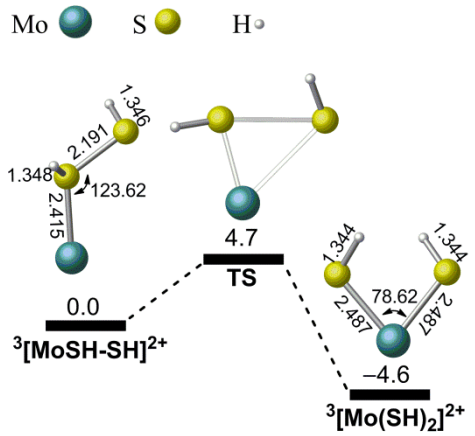


Figure S5. Isomerization between the end-on $^{3}[MoSH\text{-}SH]^{2+}$ and side-on $^{3}[Mo(SH)_2]^{2+}$. Relative free energies in solvent are shown in kcal/mol. The distances are shown in Å and angles are shown in °. Ligand $PY5Me_2$ is eliminated for clear presentation.

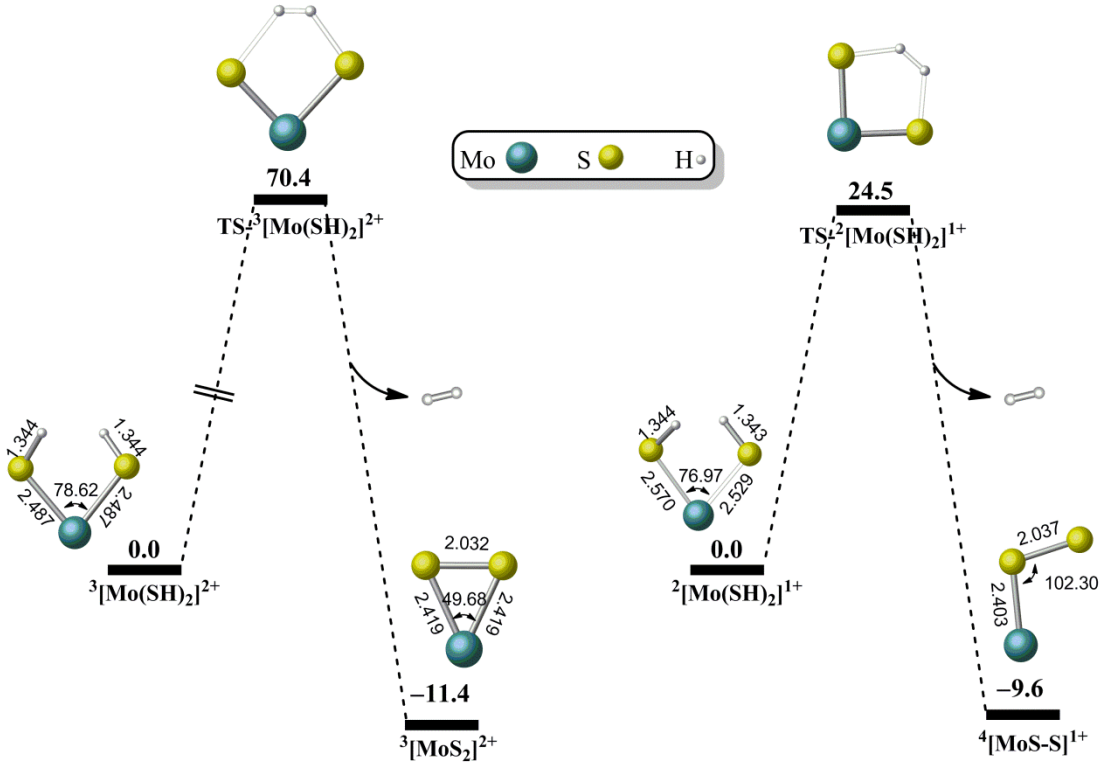


Figure S6. Energy profiles for the hydrogen evolution from the intramolecular coupling of the two sulfur bonded H of $^{3}[Mo(SH)_2]^{2+}$ (left) and $^{2}[Mo(SH)_2]^{+}$ (right). Ligand $PY5Me_2$ is eliminated for clear presentation.

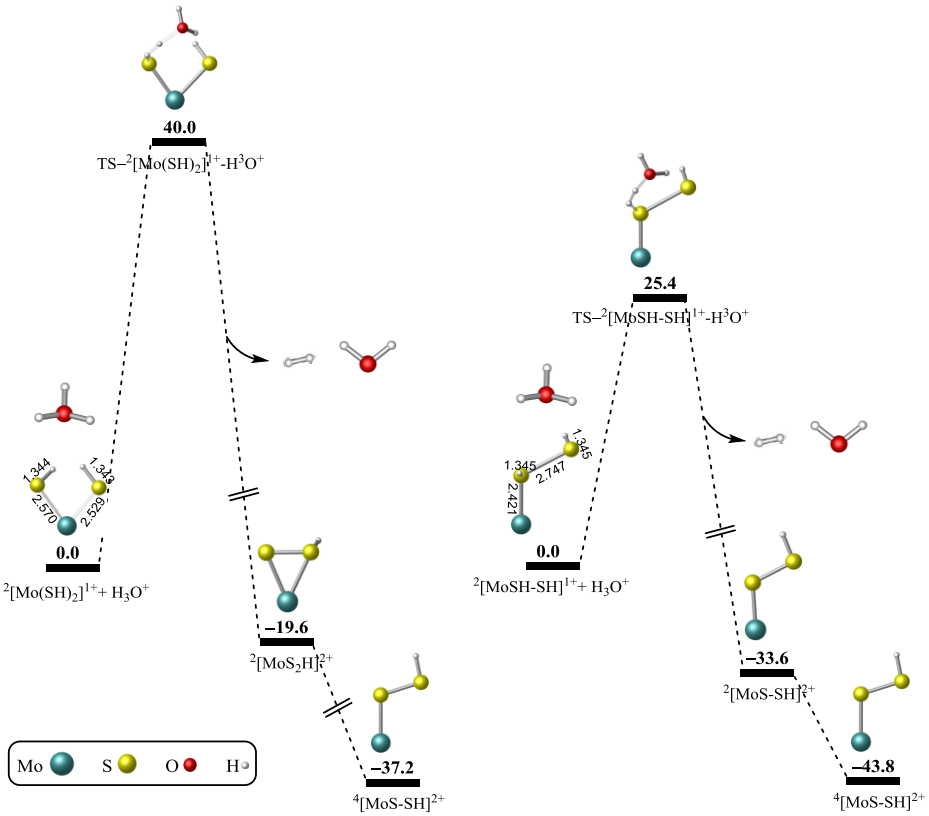


Figure S7. Energy profiles for the hydrogen evolution reaction via intermolecular H^+/H^- coupling between proton hydrate and the sulfur hydride of $^2[Mo(SH)_2]^+$ (left) or the intermolecular H^+/H^- coupling between proton hydrate and middle-sulfur bonded hydride of $^2[MoS\mathbf{H}\text{-}SH]^+$ (right). Ligand $PY5Me_2$ is eliminated for clear presentation.

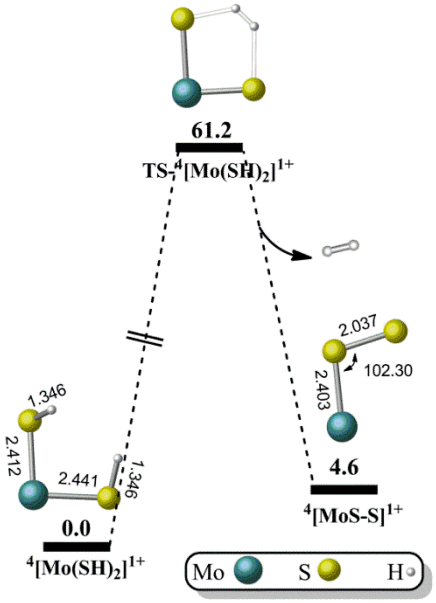


Figure S8. Energy profile for the hydrogen evolution from the coupling of the two sulfur-bonded H of $^4[Mo(SH)_2]^+$. Relative free energies in solvent are shown in kcal/mol. The distances are shown in Å and angles are shown in °. Ligand $PY5Me_2$ is eliminated for clear presentation.

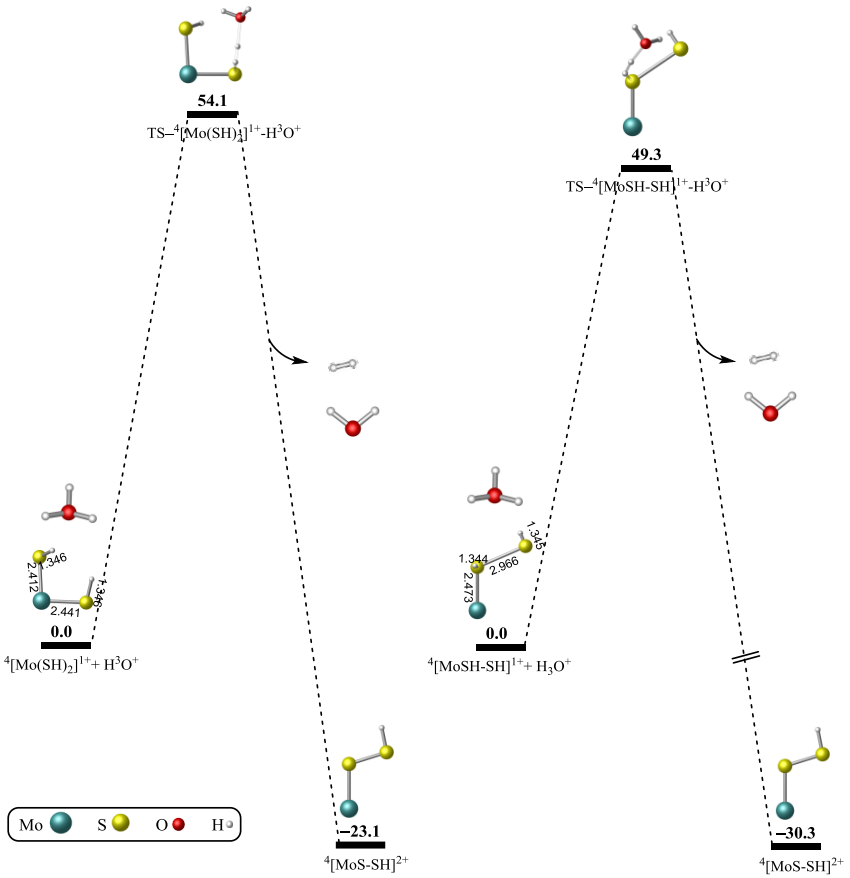


Figure S9. Energy profiles for the hydrogen evolution reaction via direct H^+/H^- coupling between a proton and sulfur hydride of $^4[Mo(SH)_2]^+$ (left) or the H^+/H^- coupling between a proton and the middle-sulfur hydride of $^4[MoS\mathbf{H}\text{-}SH]^+$ (right). Ligand $PY5Me_2$ is eliminated for clear presentation.

References

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. E. Hada, M.; , K. F. Toyota, R.; , J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. Montgomery, J. A.;, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09*, Gaussian, Inc., Wallingford CT, 2009.

2. (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652; (b) J. P. Perdew, *Phys. Rev. B*, 1986, **33**, 8822-8824; (c) J. P. Perdew, *Phys. Rev. B*, 1986, **34**, 7406.
3. Y. Zhao and D. G. Truhlar, *J. Chem. Phys.*, 2006, **125**, 194101.
4. P. Stephens, F. Devlin, C. Chabalowski and M. J. Frisch, *Chem. Phys.*, 1994, **98**, 11623-11627.
5. A. D. Becke, *Phys. Rev. A,*, 1988, **38**, 3098-3100.
6. M. Ernzerhof and J. P. Perdew, *J. Chem. Phys.*, 1998, **109**, 3313-3320.
7. (a) P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 270-283; (b) P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299-310; (c) W. R. Wadt and P. J. Hay, *J. Chem. Phys.*, 1985, **82**, 284-298; (d) C. E. Check, T. O. Faust, J. M. Bailey, B. J. Wright, T. M. Gilbert and L. S. Sunderlin, *J. Phys. Chem. A*, 2001, **105**, 8111-8116.
8. (a) A. Höllwarth, M. Böhme, S. Dapprich, A. Ehlers, A. Gobbi, V. Jonas, K. Köhler, R. Stegmann, A. Veldkamp and G. Frenking, *Chem. Phys. Lett.*, 1993, **208**, 237-240; (b) A. Ehlers, M. Böhme, S. Dapprich, A. Gobbi, A. Höllwarth, V. Jonas, K. Köhler, R. Stegmann, A. Veldkamp and G. Frenking, *Chem. Phys. Lett.*, 1993, **208**, 111-114.
9. (a) G. A. Petersson, A. Bennett, T. G. Tensfeldt, M. A. Allaham, W. A. Shirley and J. Mantzaris, *J. Chem. Phys.*, 1988, **89**, 2193-2218; (b) G. A. Petersson and M. A. Allaham, *J. Chem. Phys.*, 1991, **94**, 6081-6090.
10. (a) K. Fukui, *J. Phys. Chem.*, 1970, **74**, 4161-4163; (b) K. Fukui, *Acc. Chem. Res.*, 1981, **14**, 363-368.
11. (a) V. Barone and M. Cossi, *J. Phys. Chem. A*, 1998, **102**, 1995-2001; (b) M. Cossi, N. Rega, G. Scalmani and V. Barone, *J. Comput. Chem.*, 2003, **24**, 669-681.
12. A. Bondi, *Chem. Phys.*, 1964, **68**, 441-451.
13. R. Peverati and D. G. Truhlar, *J. Phys. Chem. Lett.*, 2012, **3**, 117-124.
14. (a) T. Clark, J. Chandrasekhar, G. W. Spitznagel and P. V. R. Schleyer, *J. Comput. Chem.*, 1983, **4**, 294-301; (b) R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Chem. Phys.*, 1980, **72**, 650-654; (c) A. McLean and G. Chandler, *J. Chem. Phys.*, 1980, **72**, 5639-5648.
15. C. Y. Legault, CYLVIEW, 1.0b, Université de Sherbrooke, 2009; http://www.cylview.org.
16. L. E. Roy, E. Jakubikova, M. G. Guthrie and E. R. Batista, *J. Phys. Chem. A*, 2009, **113**, 6745-6750.
17. B. H. Solis and S. Hammes-Schiffer, *Inorg. Chem.*, 2014, **53**, 6427-6443.
18. (a) S. Trasatti and S. Trasatti, *Pure Appl. Chem.*, 2009, **58**, 955-966; (b) S. Trasatti, *Electrochim. Acta*, 1987, **32**, 843-850.
19. C. G. Z. And and D. A. Dixon, *J. Phys. Chem. A*, 2001, **105**, 11534-11540.
20. E. S. Wiedner, M. B. Chambers, C. L. Pitman, R. M. Bullock, A. J. Miller and A. M. Appel, *Chem. Rev.*, 2016, **116**, 8655-8692.
21. H. I. Karunadasa, E. Montalvo, Y. Sun, M. Majda, J. R. Long and C. J. Chang, *Science*, 2012, **335**, 698-702.
22. (a) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465; (b) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
23. G. Scalmani and M. J. Frisch, *J. Chem. Phys.*, 2010, **132**, 114110.
24. J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615-6620.

Cartesian coordinates for the complexes calculated in this study:

$^3[MoS_2]^{2+}$
E= -2262.611297 a.u.
G= -2262.175766 a.u.

2 3

Mo	-0.00000400	0.00008900	-0.71714600
N	-1.73305700	-1.32187800	-0.62106200
N	1.46815500	-1.59651200	-0.22790800
N	1.73304400	1.32203100	-0.62074900
N	-1.46816000	1.59656800	-0.22748900
C	-2.63688100	-1.20529100	0.37523200
N	0.00001000	-0.00018200	1.47200400
C	-2.50030000	-0.01862000	1.35169500
C	-2.51274900	1.32011500	0.58209500
C	2.51274900	-1.32026600	0.58174300
C	-2.96061400	-3.17223100	-1.54321500
H	-3.05919000	-3.90438500	-2.33630700
C	-3.69590600	-2.10953600	0.46831200
H	-4.41235800	-2.04461100	1.27362900
C	2.63689400	1.20519000	0.37549200
C	3.68199400	0.04302100	2.33210700
H	3.65069200	-0.81004500	3.01069100
H	3.67761400	0.95462600	2.93155200
H	4.63018200	0.00542000	1.79493300
C	-3.53117400	2.25607500	0.75860000
H	-4.38599700	2.03102400	1.37935300
C	-3.68197000	-0.04360000	2.33213400
H	-3.65072100	0.80935800	3.01085500
H	-3.67752700	-0.95530300	2.93142900
H	-4.63016300	-0.00597200	1.79496900
C	3.69593100	2.10940100	0.46876600
H	4.41240100	2.04426900	1.27405000
C	1.19045200	0.07999000	3.53541600
H	2.11920300	0.14876100	4.08066400
C	-1.19040200	-0.08082800	3.53541500
H	-2.11914400	-0.14972700	4.08066100
C	1.17534200	0.05525300	2.14366400
C	1.38362600	-2.81705000	-0.79482600
H	0.51567300	-2.99869400	-1.41230700
C	2.50031900	0.01828100	1.35166800
C	-1.17531200	-0.05577100	2.14366800
C	-3.45939100	3.49921800	0.14091000
H	-4.25680400	4.22232400	0.27702800
C	3.53116600	-2.25627800	0.75801700
H	4.38599300	-2.03138700	1.37882300
C	1.91772200	2.26592600	-1.56957100
H	1.19782300	2.26003900	-2.38133900
C	0.00003000	-0.00049900	4.23733700
H	0.00003800	-0.00062300	5.32242500
C	3.85673500	3.10751000	-0.48467900
H	4.68183000	3.80768600	-0.40553500
C	2.96059900	3.17259900	-1.54247900
H	3.05916100	3.90494800	-2.33539300
C	2.34637600	-3.79701100	-0.63223600
H	2.22345600	-4.75850000	-1.11690600
C	-1.38364000	2.81724400	-0.79411000
H	-0.51568900	2.99903900	-1.41154700
C	-2.34639800	3.79715700	-0.63128000
H	-2.22348600	4.75876600	-1.11571400
C	3.45937300	-3.49926900	0.14002400
H	4.25678000	-4.22241600	0.27596500
C	-3.85672000	-3.10741500	-0.48537300
H	-4.68180300	-3.80762200	-0.40637800
C	-1.91775000	-2.26553800	-1.57011400
H	-1.19787200	-2.25942900	-2.38189800
S	-0.75555900	0.67994500	-2.91252700
S	0.75553000	-0.67920400	-2.91270000

$^1[MoS_2]^{2+}$
E= -2262.586091 a.u.
G= -2262.149515 a.u.

2 1

Mo	0.00017400	0.00851100	-0.71749000
N	1.68033200	1.39124600	-0.55529900
N	-1.44773800	1.60184900	-0.14037700
N	-1.76422700	-1.26058100	-0.68007700
N	1.46798200	-1.59535800	-0.31993600
C	2.61322200	1.20726800	0.40643500
N	0.03332300	-0.09936100	1.45358000
C	2.52527000	-0.04874600	1.29995600
C	2.54005000	-1.34362500	0.46230300
C	-2.47417700	1.30271900	0.68642200
C	2.85999900	3.33191000	-1.35455500
H	2.92751600	4.12842600	-2.08659800
C	3.66242100	2.11818200	0.54357600
H	4.40148300	2.00137400	1.32185500
C	-2.64427000	-1.19639000	0.34584300
C	-3.63146500	-0.12642000	2.38617100
H	-3.56653600	0.68558500	3.11142300
H	-3.63497300	-1.06994700	2.93342100
H	-4.58940200	-0.04075600	1.87235000
C	3.56824200	-2.27971300	0.56577100
H	4.44451400	-2.07065400	1.16228000
C	3.72700900	-0.06412600	2.25643600
H	3.72620900	-0.96124200	2.87617400
H	3.71591400	0.80345400	2.91794900
H	4.66532400	-0.04749900	1.70076200
C	-3.70967000	-2.09440200	0.42278600
H	-4.40367200	-2.05821700	1.24930200
C	-1.12328000	-0.31385500	3.53141400
H	-2.04473200	-0.40513500	4.08552600
C	1.25653000	-0.18843300	3.50325900
H	2.19530900	-0.16941000	4.03540600
C	-1.13005100	-0.18578900	2.14522200
C	-1.38083500	2.83771700	-0.67617800
H	-0.53032000	3.03842400	-1.30936000
C	-2.46856000	-0.07075400	1.38517600
C	1.21606200	-0.09261100	2.11540600
C	3.48070200	-3.49956100	-0.09516800
H	4.28795300	-4.22052200	-0.01933000
C	-3.48149500	2.23830600	0.92051500
H	-4.31897600	1.99662800	1.55793100
C	-1.99019400	-2.16549200	-1.66214400
H	-1.30080100	-2.14070200	-2.49629200
C	0.07816800	-0.31142300	4.21871800
H	0.09524600	-0.39621400	5.30016000
C	-3.90515400	-3.05021600	-0.56562700
H	-4.73256900	-3.74822200	-0.49616800
C	-3.03322700	-3.07179600	-1.64439200
H	-3.15087300	-3.77006600	-2.46512200
C	-2.33460000	3.81473600	-0.45910000
H	-2.22300900	4.78816800	-0.92213900
C	1.36388300	-2.80109900	-0.91998500
H	0.46275100	-2.97668100	-1.49175500
C	2.33700900	-3.77969800	-0.82888300
H	2.19682700	-4.72751400	-1.33541600
C	-3.42254700	3.50005400	0.34149000
H	-4.21046200	4.22273100	0.52663500
C	3.78433700	3.19368600	-0.32829300
H	4.60060100	3.89894700	-0.21064300
C	1.82901100	2.41453500	-1.42377000
H	1.09541400	2.46015900	-2.22308200
S	0.69452500	-0.55006700	-2.84654400
S	-0.73065400	0.83176000	-2.98087700

$^3[MoS\text{-}S]^{2+}$
E= -2262.585229 a.u.
G= -2262.155072 a.u.

2 3

Mo	0.00837600	-0.00207500	0.59289800
N	1.61118500	-1.41003500	0.17591500
N	-1.66662900	-1.41373700	0.67841800
N	-1.66638600	1.40933900	0.68697100
N	1.61069300	1.40895900	0.18438400
C	2.38133400	-1.25606100	-0.92496400
N	-0.31836800	0.00434700	-1.57865600
C	2.16925400	0.00543700	-1.79643500
C	2.38019100	1.26223600	-0.91793900
C	-2.71289100	-1.26037400	-0.16529700
C	2.79831200	-3.41287800	0.76312600
H	2.93836900	-4.22624900	1.46538100
C	3.36067700	-2.20050500	-1.22474000
H	3.97944600	-2.09732200	-2.10395500
C	-2.71174700	1.26206500	-0.15894300
C	-4.08077700	0.00582100	-1.84275000
H	-4.16093800	-0.87329300	-2.48316000
H	-4.15942200	0.88762900	-2.47963900
H	-4.93429500	0.00521400	-1.16347900
C	3.35815600	2.20961300	-1.21296600
H	3.97629900	2.11244000	-2.09329900
C	3.20634600	0.00908900	-2.92825600
H	3.09797800	0.89188300	-3.55970300
H	3.09950300	-0.87078900	-3.56400600
H	4.21936800	0.00889600	-2.52382400
C	-3.73093100	2.21321500	-0.17536300
H	-4.56915500	2.11627600	-0.84963100
C	-1.80577100	0.00735100	-3.43481700
H	-2.80624100	0.00782500	-3.84030400
C	0.56183900	0.00875500	-3.78835100
H	1.40011300	0.01040700	-4.46859900
C	-1.58059800	0.00499400	-2.06083900
C	-1.65136500	-2.45658100	1.53304100
H	-0.82459900	-2.48510900	2.23113100
C	-2.76030700	0.00313400	-1.05951300
C	0.74897900	0.00622700	-2.40889100
C	3.56407900	3.29552100	-0.36661400
H	4.32837200	4.02897500	-0.60183600
C	-3.73370800	-2.20971400	-0.18525600
H	-4.57277800	-2.10775400	-0.85771500
C	-1.65085500	2.44727600	1.54750500
H	-0.82509200	2.47050600	2.24701300
C	-0.72516800	0.00920500	-4.30272200
H	-0.88542900	0.01107600	-5.37593800
C	-3.69300400	3.30251800	0.68940300
H	-4.49109800	4.03750800	0.67198900
C	-2.63686100	3.41667300	1.58203600

H	-2.57450300	4.22741100	2.29852000
C	-2.63879400	-3.42463400	1.56368600
H	-2.57651900	-4.23951400	2.27546200
C	1.83763100	2.44057300	1.02064000
H	1.23538800	2.46697900	1.91902500
C	2.79616700	3.40949300	0.78258900
H	2.93595900	4.21882000	1.48955500
C	-3.69626800	-3.30374300	0.67352300
H	-4.49568000	-4.03723100	0.65345200
C	3.56712700	-3.29119500	-0.38470000
H	4.33245700	-4.02236300	-0.62362600
C	1.83862000	-2.44636700	1.00620800
H	1.23586300	-2.47865500	1.90404500
S	2.19312000	-0.01041700	3.44290000
S	0.25646700	-0.00904600	2.96758800

^{1}[MoS-S]$^{2+}$

E= -2262.564690 a.u.

G= -2262.131837 a.u.

2 1

Mo	0.00020100	0.59300100	0.00162400
N	1.62777300	0.33501900	1.43672500
N	-1.63142300	0.33863800	1.43384700
N	-1.62993600	0.35143400	-1.43448300
N	1.63380900	0.35354100	-1.43040700
C	2.58176900	-0.60531400	1.25571300
N	-0.00086900	-1.59765000	-0.01067300
C	2.49974500	-1.48704700	-0.00708900
C	2.58827800	-0.58772100	-1.25694100
C	-2.58436700	-0.60269300	1.25352800
C	2.74321000	1.07197000	3.44306600
H	2.76676700	1.76883700	4.27285300
C	3.61814500	-0.75276100	2.17942800
H	4.37255300	-1.51373000	2.04648400
C	-2.58801200	-0.58561100	-1.25922800
C	-3.68146800	-2.46754800	-0.01409000
H	-3.66061100	-3.11547900	0.86316100
H	-3.66602900	-3.09969000	-0.90289900
H	-4.62995700	-1.92980400	-0.00634700
C	3.63063000	-0.72037700	-2.17615300
H	4.38574300	-1.48171800	-2.04924300
C	3.67835300	-2.47142400	-0.01093400
H	3.66211400	-3.10467300	-0.89893700
H	3.65656100	-3.11838800	0.86702000
H	4.62750100	-1.93484800	-0.00393300
C	-3.63110500	-0.71512800	-2.17800200
H	-4.39026800	-1.47221700	-2.04959400
C	-1.19394000	-3.66271600	-0.03113500
H	-2.12520000	-4.20745400	-0.03678600
C	1.18985700	-3.66419100	-0.02989900
H	2.12060500	-4.20982500	-0.03449200
C	-1.17851500	-2.27108500	-0.01718600
C	-1.73506000	1.15844400	2.50339000
H	-0.97691700	1.92293600	2.59459200
C	-2.50187000	-1.48450200	-0.00904400
C	1.17587100	-2.27255700	-0.01612700
C	3.72320700	0.13244800	-3.26757200
H	4.53756700	0.02751900	-3.97652600
C	-3.62054400	-0.75059700	2.17744900
H	-4.37427500	-1.51243500	2.04541100
C	-1.73174000	1.18159000	-2.49607700
H	-0.96678000	1.93950800	-2.58486000
C	-0.00247600	-4.36611200	-0.03785400
H	-0.00319600	-5.45119700	-0.04893100
C	-3.71913200	0.13565400	-3.27145600
H	-4.53413700	0.03329300	-3.98006900
C	-2.75067500	1.11761600	-3.42661400
H	-2.77382100	1.82319600	-4.24900400
C	-2.74806600	1.07695600	3.43891600
H	-2.77285200	1.77490700	4.26775000
C	1.74117300	1.18663400	-2.48943400
H	0.98083500	1.94953500	-2.57609500
C	2.76014900	1.12029800	-3.41954800
H	2.78752300	1.82885100	-4.23926200
C	-3.70851600	0.08760400	3.28051600
H	-4.51782000	-0.02932500	3.99339400
C	3.70533700	0.08447500	3.28329800
H	4.51498500	-0.03203900	3.99583800
C	1.73002800	1.15311800	2.50776800
H	0.97021600	1.91570900	2.60078500
S	0.00275500	4.62934400	0.02421300
S	0.00120500	2.72184900	0.01355600

^{4}[MoS-S]$^{+}$

E= -2262.879419 a.u.

G= -2262.450748 a.u.

1 4

Mo	0.01869600	-0.00042000	0.58631200
N	1.62582500	-1.39542100	0.20925200
N	-1.64933300	-1.41632100	0.67261700
N	-1.64927900	1.41563000	0.67401100
N	1.62578600	1.39524100	0.21072600
C	2.38516200	-1.26112000	-0.89952700
N	-0.30759400	0.00059400	-1.53809500
C	2.17696200	0.00088100	-1.77032100
C	2.38494400	1.26208800	-0.89829400
C	-2.69903200	-1.26707100	-0.16635400
C	2.80018100	-3.39740900	0.80974400
H	2.94843300	-4.19703300	1.52587400
C	3.34712700	-2.22286000	-1.20494600
H	3.95663900	-2.13550100	-2.09253700
C	-2.69865900	1.26751600	-0.16552200
C	-4.07151100	0.00100500	-1.83271800
H	-4.14883700	-0.87899300	-2.47225900
H	-4.14844800	0.88127600	-2.47192100
H	-4.92462200	0.00107900	-1.15215600
C	3.34669600	2.22428000	-1.20295900
H	3.95604500	2.13789400	-2.09075100
C	3.21929800	0.00161200	-2.89566900
H	3.11335700	0.88304200	-3.52958300
H	3.11373300	-0.87930200	-3.53034900
H	4.22927700	0.00160400	-2.48270800
C	-3.70215200	2.23609100	-0.20693800
H	-4.54570200	2.13113400	-0.87356500
C	-1.78731600	0.00093100	-3.41630300
H	-2.78900600	0.00097500	-3.81964200
C	0.57411000	0.00123900	-3.76011500
H	1.41852200	0.00160600	-4.43321500
C	-1.56878800	0.00069400	-2.04284600
C	-1.61282600	-2.47851400	1.50153900
H	-0.79233800	-2.48506100	2.20799100
C	-2.75266500	0.00052700	-1.04915100
C	0.75929700	0.00087000	-2.38242200
C	3.54621400	3.30781600	-0.35249400
H	4.29573000	4.05459700	-0.59325000
C	-3.70307300	-2.23507400	-0.20803500
H	-4.54686900	-2.12914200	-0.87419900
C	-1.61259200	2.47709000	1.50383700
H	-0.79232600	2.48260700	2.21058300
C	-0.70874100	0.00124200	-4.28715100
H	-0.86498500	0.00154500	-5.36025400
C	-3.63883500	3.35144200	0.62098600
H	-4.42330500	4.10018700	0.58531400
C	-2.57439200	3.47166400	1.50299000
H	-2.49122200	4.30346800	2.19275800
C	-2.57511100	-3.47260900	1.50029200
H	-2.49200200	-4.30503500	2.18931600
C	1.86241800	2.40932800	1.06439300
H	1.29529300	2.39003500	1.98616300
C	2.79995100	3.39680000	0.81296600
H	2.94820200	4.19577100	1.52982500
C	-3.63996500	-3.35111300	0.61894500
H	-4.42487300	-4.09938500	0.58305800
C	3.54664700	-3.30720200	-0.35551000
H	4.29632400	-4.05362800	-0.59686700
C	1.86250500	-2.41029300	1.06200600
H	1.29531100	-2.39200300	1.98373800
S	2.08231800	-0.00207700	3.37068200
S	0.08139800	-0.00112600	2.98878000

^{2}[MoS-S]$^{+}$

E= -2262.883937 a.u.

G= -2262.454865 a.u.

1 2

Mo	-0.00601800	-0.58136300	-0.00492800
N	1.59452300	-0.16086900	-1.40896400
N	-1.64077400	-0.65630100	-1.40891800
N	-1.64126600	-0.68041100	1.39689700
N	1.59321300	-0.18253700	1.40653300
C	2.36508400	0.93962800	-1.24925400
N	-0.32362900	1.58895400	0.01283600
C	2.14967400	1.80745500	0.01445900
C	2.36453600	0.91982300	1.26437000
C	-2.71034000	0.16394800	-1.25120500
C	2.84528600	-0.76361000	-3.37300400
H	3.01107500	-1.47876200	-4.17011100
C	3.35411300	1.24691000	-2.18396000
H	3.95794000	2.13641400	-2.07965100
C	-2.71104900	0.14200600	1.25267700
C	-4.07995600	1.83896500	0.01516100
H	-4.16006400	2.48313200	-0.86172500
H	-4.16041800	2.46746900	0.90331300
H	-4.93081200	1.15707300	0.00897900
C	3.35331300	1.21203000	2.20416000
H	3.95763000	2.10271100	2.11383200
C	3.18649600	2.93953000	0.02357900
H	3.07796000	3.56489900	0.91099500
H	3.07667800	3.58035600	-0.85259700
H	4.19928900	2.53495800	0.01935800
C	-3.75116100	0.12122600	2.18545200
H	-4.59507900	0.78775800	2.08202700
C	-1.81822600	3.43953200	0.03001200
H	-2.82123100	3.83860900	0.03415300
C	0.54563100	3.80417000	0.03194700
H	1.38291000	4.48570700	0.03748700
C	-1.58743000	2.06523100	0.01750700
C	-1.64019300	-1.51481500	-2.45655200
H	-0.79601700	-2.18998500	-2.50260000
C	-2.75915900	1.05802300	0.00860600
C	0.73652200	2.42468400	0.01977600
C	3.59110400	0.34760800	3.26708500
H	4.36289600	0.57844000	3.99382500

C	-3.74948800	0.16018200	-2.18525100
H	-4.59313600	0.82533400	-2.07107900
C	-1.64122400	-1.55709800	2.42939400
H	-0.79689300	-2.23273300	2.46426500
C	-0.74309700	4.31308100	0.03721800
H	-0.90863000	5.38551000	0.04686400
C	-3.72424900	-0.75746000	3.25866800
H	-4.53228300	-0.76484100	3.98204600
C	-2.64717800	-1.63069900	3.37003200
H	-2.58096100	-2.36053500	4.16867700
C	-2.64532300	-1.57138500	-3.39927200
H	-2.57873900	-2.28712100	-4.21054500
C	1.86138900	-1.03895100	2.41238500
H	1.26211600	-1.93910800	2.43240900
C	2.84268800	-0.81624300	3.36171000
H	3.00762500	-1.54375100	4.14773800
C	-3.72196800	-0.69955400	-3.27367900
H	-4.52925600	-0.69375500	-3.99790800
C	3.59289100	0.39914400	-3.26001400
H	4.36485900	0.64166800	-3.98275100
C	1.86364200	-1.00152300	-2.42770500
H	1.26471500	-1.90151100	-2.46152600
S	2.21104800	-3.47224400	-0.02665700
S	0.28283600	-2.90735400	-0.02352900

$^{4}[MoS_2]^{+}$
E= -2262.882168 a.u.
G= -2262.451256 a.u.

1 4

Mo	0.00011900	-0.00022800	-0.68976100
N	1.75831900	1.29274100	-0.63672100
N	-1.47504400	1.58515200	-0.25026000
N	-1.75839400	-1.29287700	-0.63643700
N	1.47495600	-1.58514900	-0.25007600
C	2.67555200	1.16295200	0.34435800
N	0.00004200	0.00014600	1.42482500
C	2.50683200	0.00868500	1.34918500
C	2.48198400	-1.35046700	0.62392500
C	-2.48172600	1.35079800	0.62416500
C	3.02039700	3.09165600	-1.60917800
H	3.12188700	3.80980100	-2.41445500
C	3.76469500	2.03654700	0.40028100
H	4.49272300	1.95989900	1.19392700
C	-2.67581400	-1.16256200	0.34440500
C	-3.68879800	-0.03810400	2.32734400
H	-3.62584900	0.78086000	3.04328000
H	-3.70604600	-0.97365100	2.88875100
H	-4.63568900	0.05530700	1.79315600
C	3.41750800	-2.34704100	0.90383200
H	4.23817600	-2.15361100	1.57897400
C	3.68896000	0.03855800	2.32709100
H	3.62650800	-0.78072400	3.04270100
H	3.70580400	0.97388800	2.88887500
H	4.63583200	-0.05418400	1.79275200
C	-3.76542300	-2.03559100	0.40009300
H	-4.49364900	-1.95848300	1.19351100
C	-1.18683300	-0.11058500	3.51383300
H	-2.11670600	-0.19865300	4.05551700
C	1.18705400	0.10935800	3.51384000
H	2.11696100	0.19709200	4.05552300
C	-1.18168800	-0.07931900	2.13057300
C	-1.36256400	2.81651900	-0.79521700
H	-0.53674900	2.95744700	-1.47802100
C	-2.50676100	-0.00840100	1.34931900
C	1.18182000	0.07911800	2.13055100
C	3.31406300	-3.60126800	0.31581100
H	4.04984100	-4.36858100	0.53152100
C	-3.41681000	2.34767100	0.90452200
H	-4.23722300	2.15452900	1.58005500
C	-1.95075700	-2.21698800	-1.60168800
H	-1.20835900	-2.21399400	-2.39491500
C	0.00013900	-0.00087900	4.23161100
H	0.00017100	-0.00125700	5.31501000
C	-3.93766900	-3.01329700	-0.57012300
H	-4.78524500	-3.68886000	-0.51778400
C	-3.02105200	-3.09135600	-1.60898500
H	-3.12263700	-3.80957800	-2.41418100
C	-2.24760500	3.84635200	-0.53960700
H	-2.10512200	4.80801700	-1.01874800
C	1.36254900	-2.81663900	-0.79485800
H	0.53638900	-2.95790400	-1.47716700
C	2.24803800	-3.84616000	-0.53962600
H	2.10558600	-4.80790500	-1.01861400
C	-3.31323400	3.60184600	0.31641400
H	-4.04864800	4.36941000	0.53248200
C	3.93672900	3.01421500	-0.57001200
H	4.78394200	3.69022000	-0.51750900
C	1.95050700	2.21679100	-1.60206400
H	1.20828200	2.21335700	-2.39545300
S	0.69901400	-0.75067100	-2.97955900
S	-0.69931900	0.75020800	-2.97965000

$^{2}[MoS_2]^{+}$
E= -2262.906524 a.u.
G= -2262.472770 a.u.

1 2

Mo	-0.00725000	0.01056300	-0.69557000
N	-1.69973800	-1.27836900	-0.67012600
N	1.51570200	-1.53580800	-0.32481100
N	1.68614000	1.37086000	-0.55901500
N	-1.48637500	1.58158500	-0.13572400
C	-2.61599000	-1.23694800	0.32679300
N	0.01290300	-0.09903600	1.46505400
C	-2.48577900	-0.11047800	1.37049800
C	-2.51105300	1.26904200	0.68231000
C	2.55218900	-1.29727600	0.50792600
C	-2.90993600	-3.09307200	-1.69309100
H	-2.99806200	-3.77782800	-2.52895600
C	-3.66044800	-2.16077500	0.37036500
H	-4.37783900	-2.14521900	1.17818600
C	2.58708700	1.23982500	0.43504800
C	3.69310900	0.01230800	2.31485900
H	3.70898000	-0.88161100	2.93891500
H	3.65181300	0.88278200	2.97203200
H	4.63476900	0.04919800	1.76543900
C	-3.52999300	2.19373600	0.92073200
H	-4.36878900	1.93963100	1.55189600
C	-3.66241100	-0.19765600	2.35057700
H	-3.62433400	0.60810200	3.08505500
H	-3.65710500	-1.14781100	2.88648000
H	-4.61136500	-0.12420800	1.81802400
C	3.60990000	2.18163600	0.57932600
H	4.32152900	2.11293600	1.38889000
C	1.21243000	-0.20948500	3.53276000
H	2.14642400	-0.18701400	4.07347200
C	-1.16430000	-0.35435700	3.53138300
H	-2.09311600	-0.46134900	4.07057600
C	1.18839400	-0.08598700	2.14681400
C	1.47102400	-2.71826700	-0.97626000
H	0.61565700	-2.87022000	-1.61967500
C	2.50225900	-0.00547300	1.34677200
C	-1.15797500	-0.20609600	2.14859800
C	-3.47713700	3.45772300	0.34840800
H	-4.27118900	4.17362600	0.53385700
C	3.58474600	-2.22711400	0.64496900
H	4.42685900	-2.02170500	1.29000700
C	1.84412800	2.34963400	-1.47262100
H	1.12314300	2.33754200	-2.28732100
C	0.02864800	-0.35242900	4.23543200
H	0.03387200	-0.44855500	5.31579500
C	3.73667800	3.22359900	-0.33101300
H	4.53060500	3.95385100	-0.21290400
C	2.85098300	3.29513500	-1.39782200
H	2.93054000	4.06237000	-2.15939600
C	2.45245200	-3.68517400	-0.86648100
H	2.35544000	-4.61191300	-1.41992100
C	-1.42766500	2.81519800	-0.67043200
H	-0.58586000	3.00565100	-1.32046300
C	-2.39026400	3.78403300	-0.44983900
H	-2.28815700	4.75940300	-0.91092200
C	3.54814100	-3.42558500	-0.05370100
H	4.35743800	-4.14135300	0.04423500
C	-3.80696000	-3.11099800	-0.63284900
H	-4.61921200	-3.82857700	-0.59325300
C	-1.88723700	-2.16423200	-1.68029500
H	-1.17609900	-2.08838000	-2.49655000
S	-0.84981800	0.77351200	-2.93468600
S	0.78031700	-0.45791300	-2.93982600

$^{4}[MoS\text{-}SH]^{2+}$
E= -2263.224955 a.u.
G= -2262.786240 a.u.

2 4

Mo	0.00057200	0.00048200	-0.56819900
N	-1.60066500	-1.40934100	-0.14267600
N	1.67179300	-1.40396700	-0.71268200
N	1.67177900	1.40497200	-0.71013200
N	-1.59977600	1.40982700	-0.13899000
C	-2.34791200	-1.26263300	0.97511300
N	0.36302900	-0.00188000	1.57131600
C	-2.12163000	-0.00202500	1.84352700
C	-2.34702400	1.26103100	0.97849500
C	2.73338600	-1.26052300	0.11295200
C	-2.76796000	-3.43171900	-0.69621300
H	-2.91131900	-4.25028200	-1.39166700
C	-3.30845100	-2.21863300	1.29827900
H	-3.91078500	-2.12067400	2.18954000
C	2.73335300	1.26000100	0.11526000
C	4.13308200	-0.00172100	1.76928800
H	4.22567600	-0.88290300	2.40525800
H	4.22566800	0.87855100	2.40652200
H	4.97238400	-0.00120500	1.07248700
C	-3.30666300	2.21707900	1.30417600
H	-3.90884700	2.11744100	2.19533500
C	-3.13582700	-0.00320700	2.99562600
H	-3.01539200	0.87699200	3.62835700
H	-3.01601400	-0.88512300	3.62608100
H	-4.15646600	-0.00234100	2.61034200
C	3.75120200	2.21211500	0.11111200
H	4.60178300	2.11791400	0.77017100
C	1.88551400	-0.00378900	3.40125900
H	2.89405400	-0.00398100	3.78633100

C	-0.47307900	-0.00477700	3.80024900
H	-1.29876900	-0.00583700	4.49558200
C	1.63589600	-0.00226000	2.03197900
C	1.63841400	-2.43394600	-1.58158000
H	0.80187200	-2.43931300	-2.26944100
C	2.79819800	-0.00110500	1.01154700
C	-0.68791600	-0.00303200	2.42533800
C	-3.51288800	3.31622600	0.47510300
H	-4.26226500	4.05707700	0.73401400
C	3.75111500	-2.21273000	0.10719600
H	4.60169100	-2.11979600	0.76646700
C	1.63853200	2.43649800	-1.57723900
H	0.80204800	2.44327000	-2.26516100
C	0.82298700	-0.00511500	4.29094400
H	1.00394000	-0.00639500	5.36075100
C	3.69496800	3.29837300	-0.75717200
H	4.49154200	4.03521400	-0.75622800
C	2.62399300	3.40626800	-1.63263900
H	2.54952300	4.21355400	-2.35186800
C	2.62380000	-3.40371500	-1.63867200
H	2.54925200	-4.20975000	-2.35929200
C	-1.82618300	2.45547500	-0.95857000
H	-1.24255100	2.47424500	-1.87019300
C	-2.76560900	3.43444400	-0.68750800
H	-2.90848500	4.25475400	-1.38100300
C	3.69476300	-3.29746200	-0.76298500
H	4.49125500	-4.03439200	-0.76332500
C	-3.51543700	-3.31560100	0.46650400
H	-4.26551300	-4.05642400	0.72346600
C	-1.82769400	-2.45284600	-0.96475900
H	-1.24378600	-2.46968700	-1.87625800
S	-2.43197700	0.00435900	-3.26899300
S	-0.35293000	0.00266000	-2.95693900
H	-2.36871600	0.00522400	-4.61454600

^{2}[MoS-SH]$^{2+}$

E= -2263.214022 a.u.

G= -2262.774346 a.u.

2 2

Mo	0.02582200	0.00042700	-0.60200000
N	-1.64789600	-1.42706200	-0.68064200
N	1.62193000	-1.40908000	-0.14649400
N	1.62316200	1.40850900	-0.14624300
N	-1.64770500	1.42800400	-0.67975400
C	-2.73279300	-1.25976900	0.10744800
N	-0.36967200	-0.00001700	1.56052700
C	-2.80252100	-0.00007600	0.99967700
C	-2.73299500	1.25986700	0.10761000
C	2.35513900	-1.25908100	0.98015300
C	-2.58793900	-3.46162400	-1.56023700
H	-2.48795300	-4.29733100	-2.24302200
C	-3.76896000	-2.19495000	0.08569100
H	-4.64040700	-2.06875300	0.71083100
C	2.35701400	1.25714200	0.97979500
C	3.11770300	-0.00111800	3.00949900
H	2.99024100	-0.88169100	3.64026500
H	2.99234300	0.88038800	3.63938300
H	4.14257800	-0.00235800	2.63605600
C	-3.76960400	2.19457000	0.08553500
H	-4.64154200	2.06759900	0.70981400
C	-4.13703300	-0.00032500	1.75932900
H	-4.22950500	0.88135500	2.39474800
H	-4.22914700	-0.88201400	2.39479700
H	-4.97820100	-0.00060400	1.06517300
C	3.32778900	2.20065700	1.31354600
H	3.91718100	2.09490400	2.21233800
C	0.46081100	0.00212800	3.79219000
H	1.28230900	0.00329100	4.49203700
C	-1.89771900	0.00084700	3.38729100
H	-2.90634000	0.00046800	3.77160800
C	0.67738100	0.00060200	2.41688000
C	1.87551800	-2.45514300	-0.96022000
H	1.30456500	-2.48859800	-1.87850700
C	2.11441500	-0.00059700	1.84617200
C	-1.64149900	0.00017100	2.01838100
C	-3.69929100	3.30847300	-0.74153700
H	-4.50651500	4.03332200	-0.75022400
C	3.32375900	-2.20454100	1.31464200
H	3.91246400	-2.10025100	2.21404300
C	1.87773800	2.45449200	-0.95977300
H	1.30601400	2.48936600	-1.87752900
C	-0.83692400	0.00211100	4.27821600
H	-1.02033500	0.00304300	5.34783700
C	3.55978000	3.29631600	0.48828000
H	4.31471000	4.02818300	0.75622100
C	2.82642600	3.42173400	-0.68258000
H	2.98584500	4.23894400	-1.37624200
C	2.82230800	-3.42409000	-0.68246900
H	2.98112600	-4.24131300	-1.37624400
C	-1.59776900	2.50086000	-1.49754200
H	-0.73336400	2.56241500	-2.14440900
C	-2.58769000	3.46299200	-1.55840400
H	-2.48734600	4.29938800	-2.24029700
C	3.55451900	-3.30039600	0.48927900
H	4.30777100	-4.03377000	0.75783000
C	-3.69883500	-3.30826700	-0.74217700
H	-4.50568900	-4.03353200	-0.75060800
C	-1.59828700	-2.49921800	-1.49937900
H	-0.73432900	-2.55998800	-2.14692400
S	2.27267000	0.00049800	-3.48022400
S	0.26253800	0.00097600	-2.81222200
H	1.99431100	0.00092400	-4.79938900

^{4}[MoSH-S]$^{2+}$

E= -2263.184050 a.u.

G= -2262.744485 a.u.

2 4

Mo	0.00687600	0.35539900	0.42158900
N	-1.64018300	1.25004700	-0.67122100
N	1.65221800	1.19681100	-0.75333600
N	1.69559300	-0.66919300	1.35013200
N	-1.61904500	-0.80793900	1.31762700
C	-2.57331500	0.46857300	-1.26069700
N	-0.01925600	-1.20701300	-1.07514000
C	-2.51705400	-1.05192600	-0.99310900
C	-2.59601100	-1.31340800	0.52915000
C	2.55787400	0.35785100	-1.31205700
C	-2.68939500	3.21935700	-1.54956300
H	-2.70877400	4.30139700	-1.60972700
C	-3.56857100	1.04636500	-2.04520700
H	-4.31507300	0.43717000	-2.53398600
C	2.58989100	-1.31568500	0.56794400
C	3.65392800	-1.88010800	-1.62819900
H	3.62440900	-1.77554400	-2.71319600
H	3.63694100	-2.94570000	-1.39511600
H	4.60422600	-1.47461600	-1.27888000
C	-3.63483700	-2.05247600	1.09430800
H	-4.42692600	-2.45280300	0.47847000
C	-3.71499700	-1.72145100	-1.67960100
H	-3.72948200	-2.79586700	-1.49282000
H	-3.68470100	-1.56835100	-2.75913300
H	-4.65289200	-1.30490700	-1.31012000
C	3.61674800	-2.05378000	1.15473400
H	4.33124800	-2.59005900	0.54753000
C	1.15230200	-2.76424600	-2.44061200
H	2.07521900	-3.20158100	-2.79022700
C	-1.23820000	-2.68237400	-2.48982300
H	-2.17353800	-3.05257300	-2.88151300
C	1.15180800	-1.73162700	-1.50693900
C	1.74716300	2.52139900	-0.98848800
H	1.05794400	3.15109300	-0.43221400
C	2.47741300	-1.14893500	-0.96667600
C	-1.20553300	-1.66371000	-1.54230300
C	-3.67145400	-2.28634300	2.46468800
H	-4.48419000	-2.86073700	2.89695300
C	3.54676400	0.85788500	-2.15455700
H	4.27473500	0.20108300	-2.60746700
C	1.85218100	-0.68112900	2.68980200
H	1.15434800	-0.07511900	3.25638300
C	-0.05066800	-3.23861400	-2.93799600
H	-0.06289800	-4.03832600	-3.67133900
C	3.75104600	-2.09812000	2.53902300
H	4.55529300	-2.67194500	2.98780100
C	2.86277300	-1.37890400	3.32599200
H	2.94694500	-1.34687500	4.40601300
C	2.71128000	3.07365400	-1.81536900
H	2.74286700	4.14731400	-1.95962800
C	-1.65672500	-1.04285600	2.64584800
H	-0.85468300	-0.61192000	3.23284100
C	-2.65624400	-1.77420700	3.26074800
H	-2.63513300	-1.92539500	4.33375100
C	3.62213700	2.22278200	-2.41994600
H	4.39622200	2.60557400	-3.07711000
C	-3.62266500	2.42866200	-2.20396100
H	-4.39797500	2.87324800	-2.81949900
C	-1.71171400	2.59216200	-0.79610900
H	-0.98489400	3.17322800	-0.22574300
S	0.30597900	3.77522300	1.82313800
S	-0.33624500	1.91983400	2.35801400
H	-1.69465700	1.96279000	2.39023400

^{2}[MoSH-S]$^{2+}$

E= -2263.175445 a.u.

G= -2262.736139 a.u.

2 2

Mo	0.01821200	0.54650500	0.00031700
N	-1.64048700	0.64045100	-1.43222400
N	1.64247100	0.13197400	-1.40287000
N	1.64264400	0.13050900	1.40293200
N	-1.64035700	0.63870000	1.43310900
C	-2.72830100	-0.14254900	-1.26069600
N	-0.34157100	-1.57386600	-0.00092000
C	-2.78855600	-1.03339600	-0.00055800
C	-2.72808100	-0.14428900	1.26079200
C	2.38796300	-0.98570700	-1.25488500
C	-2.57177400	1.50492200	-3.47781700
H	-2.46455500	2.17368900	-4.32396000
C	-3.76559700	-0.12095500	-2.19454300
H	-4.64033200	-0.74092300	-2.06416200
C	2.38803000	-0.98707900	1.25371800
C	3.15121000	-3.01829300	-0.00171000
H	3.02752700	-3.64762600	-0.88399800

H	3.02748400	-3.64865200	0.87984000
H	4.17485500	-2.64193100	-0.00148100
C	-3.76507800	-0.12425000	2.19499300
H	-4.63972100	-0.74422300	2.06400900
C	-4.11541600	-1.80624200	-0.00100300
H	-4.20243700	-2.44267000	0.88051600
H	-4.20262400	-2.44124300	-0.88353500
H	-4.96277600	-1.11951200	-0.00035400
C	3.37561700	-1.30214000	2.18695600
H	3.97173500	-2.19666000	2.08163000
C	0.49711500	-3.80408200	-0.00238300
H	1.32242200	-4.49933000	-0.00275200
C	-1.86098900	-3.40967600	-0.00236300
H	-2.86784400	-3.79824700	-0.00277700
C	0.71008700	-2.42822300	-0.00143800
C	1.90596000	0.96003800	-2.43385300
H	1.32613800	1.87327000	-2.47126400
C	2.14583100	-1.85724400	-0.00105000
C	-1.61395600	-2.03976800	-0.00131100
C	-3.68972100	0.69396800	3.31552700
H	-4.49679800	0.70153600	4.04058200
C	3.37550700	-1.29972300	-2.18851100
H	3.97172400	-2.19427900	-2.08409800
C	1.90635500	0.95756500	2.43464900
H	1.32665600	1.87083900	2.47291500
C	-0.79723600	-4.29705200	-0.00288500
H	-0.97614100	-5.36733100	-0.00367600
C	3.61499400	-0.46323800	3.26985500
H	4.38244000	-0.71505100	3.99428300
C	2.87222800	0.70266900	3.39071000
H	3.03762900	1.40860100	4.19618500
C	2.87175800	0.70618100	-3.39025900
H	3.03695300	1.41290300	-4.19508500
C	-1.58283900	1.44208600	2.51585700
H	-0.70555900	2.07122800	2.59366400
C	-2.57120900	1.50005000	3.48021500
H	-2.46387000	2.16762500	4.32728300
C	3.61470200	-0.45973100	-3.27060400
H	4.38211600	-0.71073500	-3.99534400
C	-3.69041400	0.69884500	-3.31393100
H	-4.49771400	0.70762800	-4.03872500
C	-1.58314100	1.44538000	-2.51383200
H	-0.70577200	2.07448000	-2.59093100
S	0.35674500	2.82340700	0.00150400
S	1.97671300	3.97021800	0.00212200
H	-0.69097200	3.69264000	0.00186800

^{2}[MoS$_2$H]$^{2+}$

E= -2263.205772 a.u.

G= -2262.761661 a.u.

2 2

Mo	-0.00638600	0.00604000	-0.69713800
N	-1.75951400	-1.28094400	-0.59992600
N	1.45314800	-1.58813500	-0.23424700
N	1.76693400	1.29062400	-0.63546600
N	-1.39315000	1.63514500	-0.14496100
C	-2.66234500	-1.15017000	0.39927200
N	0.01862200	-0.02895300	1.47533500
C	-2.48809400	0.02549600	1.38105800
C	-2.46443500	1.37095900	0.63050100
C	2.51630800	-1.33638500	0.55820500
C	-3.00700500	-3.15752300	-1.46471500
H	-3.10497200	-3.91166500	-2.23725000
C	-3.73133700	-2.04043300	0.51297500
H	-4.44314000	-1.94802200	1.31985800
C	2.64314300	1.18480200	0.38713900
C	3.70256200	-0.00707200	2.32032100
H	3.68549900	-0.88096500	2.97227300
H	3.69401500	0.88367300	2.95044300
H	4.64660200	-0.01984200	1.77422300
C	-3.46791600	2.32766500	0.78746700
H	-4.34349500	2.11586700	1.38406600
C	-3.66169800	0.03359500	2.37117100
H	-3.59590200	0.88102200	3.05500800
H	-3.68471600	-0.88129100	2.96448000
H	-4.61242900	0.10321200	1.84142900
C	3.68626100	2.10537900	0.51787900
H	4.37083400	2.05413400	1.35144700
C	1.21681600	-0.04693400	3.54103900
H	2.14998400	-0.01565900	4.08233000
C	-1.16395400	-0.14911100	3.54634500
H	-2.09275600	-0.20753300	4.09268400
C	1.19438200	-0.00678000	2.14987000
C	1.35089900	-2.80125100	-0.81681400
H	0.46379100	-2.97492900	-1.40860900
C	2.51208900	-0.01478200	1.35012100
C	-1.15537800	-0.07544400	2.15655900
C	-3.34985600	3.57436200	0.18515000
H	-4.13300100	4.31534600	0.30775900
C	3.53036000	-2.28227000	0.70527600
H	4.39471100	-2.07252200	1.31869700
C	1.99170400	2.22448300	-1.58094100
H	1.31583300	2.21764600	-2.42751100
C	0.02961200	-0.13081800	4.24707800
H	0.03352500	-0.17238400	5.33119100
C	3.87386900	3.09984000	-0.43360800
H	4.68606400	3.81118500	-0.32614500
C	3.02322200	3.14317900	-1.53007200
H	3.14844600	3.86737500	-2.32672700
C	2.31308000	-3.78747700	-0.69327900
H	2.17406700	-4.73980800	-1.19160700
C	-1.25969100	2.85974500	-0.69000300
H	-0.35143300	3.03539400	-1.25141300
C	-2.20587000	3.85824600	-0.54949200
H	-2.04590400	4.82620300	-1.01016700
C	3.44247900	-3.51199400	0.06411100
H	4.23747300	-4.24240000	0.17155500
C	-3.90838800	-3.05905500	-0.41449300
H	-4.74186600	-3.74674200	-0.32044200
C	-1.95952400	-2.25713600	-1.51679100
H	-1.24278100	-2.29395700	-2.33041700
S	-0.93237700	0.55581300	-2.99235300
S	0.69370700	-0.68836600	-2.95285300
H	-0.37158300	1.71101100	-3.43717400

^{2}[MoHS-S]$^{2+}$

E= -2263.165218 a.u.

G= -2262.724973 a.u.

2 2

Mo	0.00026200	0.36193100	0.51790800
N	-1.62992200	1.39428300	-0.52772500
N	1.59191600	1.22060700	-0.71438000
N	1.56037300	-1.06495600	1.16711300
N	-1.70006400	-0.73214300	1.35456500
C	-2.61645400	0.69718500	-1.13032700
N	-0.17598400	-1.06868000	-1.16909600
C	-2.64514600	-0.83880000	-0.95087400
C	-2.69536700	-1.18008800	0.55787700
C	2.45991800	0.42498000	-1.37615100
C	-2.60658100	3.46241600	-1.25793100
H	-2.57935200	4.54581200	-1.24675800
C	-3.60171900	1.37013100	-1.85434600
H	-4.39254500	0.82630900	-2.34971200
C	2.47116100	-1.51606300	0.27397700
C	3.43418100	-1.78680800	-2.02562000
H	3.34937000	-1.54057700	-3.08473800
H	3.38712200	-2.87184500	-1.92755500
H	4.41915500	-1.46344500	-1.68681800
C	-3.75752600	-1.89610400	1.11177900
H	-4.55613900	-2.27176200	0.48940300
C	-3.90463000	-1.39590100	-1.62907700
H	-3.97045300	-2.47820600	-1.51118400
H	-3.90665500	-1.17659300	-2.69736100
H	-4.80447800	-0.95694400	-1.19607700
C	3.50061300	-2.35807200	0.69391300
H	4.24364800	-2.71233800	-0.00450500
C	0.86393300	-2.50191400	-2.76346600
H	1.75146000	-2.90846300	-3.22363700
C	-1.51762200	-2.39464500	-2.62675900
H	-2.48621200	-2.71826400	-2.97620600
C	0.94793000	-1.57137300	-1.73094300
C	1.71405100	2.55893500	-0.81230100
H	1.03995500	3.15144300	-0.20456000
C	2.32675700	-1.10411000	-1.20934800
C	-1.39432200	-1.45910900	-1.60293700
C	-3.81355500	-2.13068200	2.48077700
H	-4.64220300	-2.68986000	2.90271500
C	3.45077000	0.99158500	-2.17763700
H	4.15263400	0.37021300	-2.71377600
C	1.65302100	-1.46169900	2.45269900
H	0.91149100	-1.06474200	3.13204300
C	-0.37806300	-2.92017700	-3.21140100
H	-0.45653700	-3.64892400	-4.01151300
C	3.59227000	-2.75868800	2.02233600
H	4.39793400	-3.41288600	2.33898100
C	2.63935500	-2.30881600	2.92337000
H	2.65780000	-2.58934900	3.96993300
C	2.67551900	3.17706100	-1.59083000
H	2.72859200	4.25894100	-1.62534900
C	-1.78220600	-0.92032100	2.68789200
H	-1.00270800	-0.45833400	3.28180600
C	-2.81181900	-1.61639300	3.29268700
H	-2.82633700	-1.73602200	4.36974500
C	3.55913900	2.37286200	-2.29543100
H	4.33292800	2.80598300	-2.92068200
C	-3.58950900	2.75742100	-1.93901900
H	-4.35677800	3.27444900	-2.50584500
C	-1.65688400	2.74294800	-0.55668900
H	-0.91482300	3.24906000	0.05288900
S	1.09006000	1.56191400	2.34731600
S	0.64233400	3.48757300	2.45194700
H	-0.83371100	1.36508900	1.49776000

^{3}[MoS-SH]$^{+}$

E= -2263.516301 a.u.

G= -2263.080045 a.u.

1 3

Mo	0.01165500	0.55030500	0.00568900
N	-1.59593300	0.15950000	-1.40965700
N	1.64486300	0.69265800	-1.38972400
N	1.64424200	0.66215200	1.40511000
N	-1.59858200	0.13342100	1.41158300

C	-2.35171800	-0.95292700	-1.27167000
N	0.34392600	-1.57345300	-0.01564400
C	-2.13062200	-1.83266400	-0.01817500
C	-2.35329200	-0.97677900	1.25154100
C	2.72660400	-0.11458500	-1.25113700
C	-2.79719800	0.75117500	-3.40466400
H	-2.95126900	1.46396400	-4.20622600
C	-3.31843100	-1.26626400	-2.22799000
H	-3.91698900	-2.16112100	-2.13929200
C	2.72532100	-0.14310200	1.25045100
C	4.11012100	-1.80127800	-0.01892600
H	4.19700800	-2.42548100	-0.90955500
H	4.19606200	-2.44724400	0.85612200
H	4.95422500	-1.11085100	-0.01000000
C	-3.32110300	-1.30851500	2.20049700
H	-3.91911600	-2.20190700	2.09445800
C	-3.15453600	-2.97631500	-0.02937300
H	-3.03741700	-3.61759700	0.84532900
H	-3.03774100	-3.60005800	-0.91668300
H	-4.17216800	-2.58282400	-0.02539800
C	3.76106100	-0.12582400	2.18777900
H	4.61633100	-0.77595700	2.07227400
C	1.85717100	-3.41584100	-0.03771500
H	2.86470900	-3.80363900	-0.04315300
C	-0.50051500	-3.80485400	-0.03971000
H	-1.33145600	-4.49423000	-0.04663900
C	1.61564500	-2.04508100	-0.02182500
C	1.62462900	1.57054100	-2.42078400
H	0.77788700	2.24492100	-2.43309500
C	2.78300400	-1.03227600	-0.01048500
C	-0.70702000	-2.42931200	-0.02432700
C	-3.54315400	-0.48026700	3.29531500
H	-4.29857000	-0.74135500	4.02917800
C	3.76472300	-0.07409900	-2.18519200
H	4.62081700	-0.72519000	-2.08227900
C	1.62293600	1.51657500	2.45561700
H	0.77685900	2.19145300	2.48112900
C	0.79281700	-4.30379300	-0.04667900
H	0.96936700	-5.37410700	-0.05896300
C	3.71175400	0.72518900	3.28249700
H	4.51442300	0.72768400	4.01191200
C	2.61987300	1.57850100	3.40704300
H	2.53871000	2.28862800	4.22204600
C	2.62364700	1.65559600	-3.36819100
H	2.54321300	2.38388800	-4.16708100
C	-1.84704400	0.95362600	2.45117100
H	-1.25825100	1.86219400	2.47301700
C	-2.80297600	0.68723700	3.41531400
H	-2.95880600	1.38484200	4.22978200
C	3.71676500	0.80162600	-3.26030400
H	4.52130700	0.82208400	-3.98736700
C	-3.53843900	-0.41772200	-3.30754500
H	-4.29299500	-0.66459300	-4.04718300
C	-1.84253100	0.99893400	-2.43439200
H	-1.25350400	1.90753700	-2.43971400
S	-2.35676300	3.37041800	0.03162000
S	-0.27329800	2.92210900	0.03047700
H	-2.22571900	4.71073300	0.04435500

^{1}[MoS-SH]$^{+}$

E= -2263.511218 a.u.

G= -2263.072758 a.u.

1 1

Mo	0.03304200	-0.59629800	0.00112300
N	1.60073200	-0.11765500	-1.38427600
N	-1.62288200	-0.68594400	-1.42015000
N	-1.62338400	-0.68165000	1.42225400
N	1.60091800	-0.11338300	1.38484200
C	2.32024100	1.02425000	-1.24813800
N	-0.41569700	1.57946900	-0.00219000
C	2.05572000	1.89851700	-0.00283700
C	2.32073000	1.02785900	1.24489000
C	-2.73394800	0.06876200	-1.25595500
C	2.88969700	-0.68088100	-3.34357900
H	3.08974800	-1.39943500	-4.12994200
C	3.30318000	1.36113400	-2.18191300
H	3.86010600	2.28192800	-2.08630300
C	-2.73469100	0.07206700	1.25511400
C	-4.17487900	1.69423700	-0.00310400
H	-4.27980100	2.32582300	-0.88658100
H	-4.28080200	2.32758500	0.87898900
H	-4.99969700	0.98099000	-0.00285900
C	3.30435800	1.36719800	2.17703600
H	3.86165800	2.28743500	2.07821100
C	3.03732900	3.07916000	-0.00467100
H	2.89969100	3.70681000	0.87710400
H	2.89944600	3.70427900	-0.88821100
H	4.06754600	2.72205600	-0.00427000
C	-3.77945800	0.01861700	2.18304100
H	-4.66229300	0.62729800	2.05398900
C	-1.97655000	3.37559700	-0.00381000
H	-2.99293200	3.73933200	-0.00404100
C	0.37294800	3.82355200	-0.00455700
H	1.18318600	4.53639200	-0.00544300
C	-1.69281400	2.01101100	-0.00257100
C	-1.56761600	-1.51174100	-2.49050900
H	-0.67706100	-2.12130100	-2.55802700
C	-2.82455800	0.96408300	-0.00163300
C	0.61464900	2.45021600	-0.00321400
C	3.58935500	0.52659800	3.24376500
H	4.34915600	0.79871200	3.96837500
C	-3.77801200	0.01320500	-2.18455500
H	-4.66060100	0.62276500	-2.05796400
C	-1.56839100	-1.50409900	2.49522300
H	-0.67752500	-2.11290400	2.56535800
C	-0.93240600	4.28529000	-0.00479600
H	-1.13547600	5.35154800	-0.00579200
C	-3.70381800	-0.81787800	3.28648300
H	-4.51499000	-0.85153500	4.00583600
C	-2.57002900	-1.60806200	3.43846700
H	-2.45621200	-2.29486900	4.26928300
C	-2.56861900	-1.61797800	-3.43417700
H	-2.45463600	-2.30742600	-4.26278000
C	1.91672200	-0.94478800	2.40712700
H	1.36391800	-1.87406000	2.43487300
C	2.89057800	-0.67101200	3.34527500
H	3.09071500	-1.38718300	4.13378600
C	-3.70199900	-0.82658100	-3.28547300
H	-4.51262000	-0.86186900	-4.00537000
C	3.58796800	0.51735800	-3.24619200
H	4.34722600	0.78757400	-3.97208000
C	1.91639800	-0.95211200	-2.40412300
H	1.36390500	-1.88165500	-2.42879000
S	2.37760300	-3.47816800	0.00506200
S	0.29738700	-2.79664500	0.00440900
H	2.09041500	-4.79409600	0.00688500

^{3}[MoSH-S]$^{+}$

E= -2263.486926 a.u.

G= -2263.048026 a.u.

1 3

Mo	0.00040100	0.30073100	0.42642200
N	-1.64961900	1.22753900	-0.63212500
N	1.63468200	1.23959700	-0.65539600
N	1.69849800	-0.74049600	1.32200600
N	-1.60197700	-0.83974000	1.31970600
C	-2.58241000	0.44975400	-1.22613300
N	-0.00442400	-1.16443800	-1.08182700
C	-2.50014000	-1.07302500	-0.99167600
C	-2.55417800	-1.38437300	0.52093900
C	2.54115400	0.44911500	-1.27810500
C	-2.71207700	3.19975300	-1.48078900
H	-2.73604700	4.28252500	-1.52294500
C	-3.58643300	1.03221800	-1.99720200
H	-4.33381000	0.42405700	-2.48615600
C	2.60513800	-1.32958300	0.51024900
C	3.67763500	-1.74387300	-1.71006100
H	3.63584600	-1.58481900	-2.78796900
H	3.68273200	-2.82045100	-1.53404900
H	4.62077200	-1.33494200	-1.34396900
C	-3.53803700	-2.21047100	1.06659900
H	-4.30540300	-2.64000100	0.43884500
C	-3.69390500	-1.74187900	-1.68325800
H	-3.67985900	-2.82255400	-1.53787800
H	-3.67990000	-1.55001900	-2.75693400
H	-4.63418800	-1.35868200	-1.28342500
C	3.62894500	-2.10325600	1.05783000
H	4.35245500	-2.59211500	0.42164500
C	1.18176100	-2.65065500	-2.53604100
H	2.11337800	-3.04547200	-2.91362600
C	-1.20253800	-2.62401500	-2.55410100
H	-2.13737600	-2.99710300	-2.94561800
C	1.17191700	-1.65902300	-1.56332400
C	1.70502200	2.57769300	-0.80555600
H	1.03393700	3.16951800	-0.17837700
C	2.48935200	-1.07453200	-1.00868000
C	-1.18504600	-1.64192100	-1.57066400
C	-3.55387000	-2.49268700	2.42683300
H	-4.32456700	-3.13257600	2.84296700
C	3.49741000	1.01235200	-2.12084600
H	4.22424500	0.39419700	-2.62769900
C	1.84431300	-0.83626900	2.65763300
H	1.14692200	-0.25342600	3.24828100
C	-0.01281800	-3.13992800	-3.04424900
H	-0.01560400	-3.90735500	-3.81009100
C	3.74579900	-2.24272600	2.43630400
H	4.54702600	-2.84237400	2.85562200
C	2.84511300	-1.57946300	3.25777100
H	2.91608300	-1.61952100	4.33842800
C	2.63396600	3.18926000	-1.63214200
H	2.64800600	4.27025900	-1.71048800
C	-1.63915800	-1.10154500	2.64493100
H	-0.88556000	-0.60445300	3.24413300
C	-2.57694200	-1.92587900	3.23607500
H	-2.54862200	-2.09580600	4.30619600
C	3.53796600	2.39014600	-2.31456700
H	4.28471200	2.82347000	-2.97201500
C	-3.64708900	2.41552300	-2.13867100
H	-4.43008300	2.86477900	-2.74111200
C	-1.72872000	2.56941100	-0.73512700
H	-1.01787600	3.15353000	-0.14349100
S	-0.15433800	1.95868400	2.28607600
S	0.03330700	3.97548200	1.87535700
H	-1.45048700	1.80400700	2.65669100

^{1}[MoSH-S]$^+$

E= -2263.470941 a.u.

G= -2263.030624 a.u.

1 1

Mo	0.02311800	0.34783300	0.44836900
N	-1.46300000	1.10832000	-0.95587500
N	1.69208300	1.10092600	-0.70453700
N	1.61721800	-0.71293300	1.39323000
N	-1.68459000	-0.56819300	1.39222800
C	-2.46771300	0.32407100	-1.40375900
N	-0.05095600	-1.33538400	-0.90373900
C	-2.52587700	-1.12453500	-0.88715900
C	-2.67323100	-1.13309100	0.65084100
C	2.52125100	0.20879000	-1.30345600
C	-2.34337700	2.96548000	-2.20219200
H	-2.25769100	4.01263900	-2.46796300
C	-3.41682100	0.83241200	-2.29163800
H	-4.21340800	0.20683600	-2.66739300
C	2.59383000	-1.31096900	0.66653000
C	3.60478700	-2.04786900	-1.50030000
H	3.50686500	-2.08332400	-2.58646900
H	3.64394100	-3.07379800	-1.13102900
H	4.55704600	-1.57192300	-1.26438200
C	-3.78954400	-1.70572900	1.26477200
H	-4.57452500	-2.15098600	0.67073300
C	-3.73194300	-1.83144500	-1.51903800
H	-3.82199400	-2.85728000	-1.15998000
H	-3.64168400	-1.86045600	-2.60631100
H	-4.65813900	-1.31134700	-1.27133500
C	3.69691700	-1.88846900	1.29652600
H	4.46618600	-2.37482000	0.71365900
C	1.09733300	-3.12234200	-1.99024700
H	2.01784800	-3.60958400	-2.27394200
C	-1.28675800	-3.04993200	-2.01394500
H	-2.23074100	-3.47889800	-2.31476500
C	1.11093600	-1.92914000	-1.27186600
C	1.89880200	2.41678000	-0.93987500
H	1.30609900	3.10665800	-0.34315800
C	2.44319600	-1.27303600	-0.86343500
C	-1.23739800	-1.86709700	-1.28254600
C	-3.92089400	-1.71002400	2.64673300
H	-4.79212300	-2.15482200	3.11484700
C	3.46552600	0.63270100	-2.24146900
H	4.09741200	-0.08177600	-2.74929400
C	1.76314300	-0.65833100	2.74046400
H	0.97758200	-0.14475100	3.27793600
C	-0.10930300	-3.69055200	-2.36192400
H	-0.13163300	-4.61627200	-2.92734200
C	3.83220800	-1.83559900	2.67661400
H	4.69198700	-2.28386300	3.16225500
C	2.84373700	-1.18947600	3.41246900
H	2.89869600	-1.10099700	4.49132600
C	2.83305000	2.89550600	-1.83910600
H	2.93952900	3.96541100	-1.97790300
C	-1.83347100	-0.57503800	2.73972400
H	-1.03193700	-0.10864800	3.29979500
C	-2.91170400	-1.12663500	3.40264900
H	-2.95181300	-1.09219400	4.48548300
C	3.61329900	1.98140200	-2.53555700
H	4.34108500	2.30505100	-3.27197700
C	-3.35769700	2.15894400	-2.70032800
H	-4.09817800	2.55062300	-3.38985100
C	-1.41897400	2.40036100	-1.34352600
H	-0.62275600	3.00112200	-0.92179700
S	-0.30201500	2.16189500	1.75455200
S	0.14710000	4.11641100	1.69492700
H	-1.44511300	2.11354400	2.50081300

^{1}[MoS$_2$H]$^+$

E= -2263.499414 a.u.

G= -2263.055854 a.u.

1 1

Mo	0.01068500	-0.03779200	-0.66723800
N	1.46410700	1.55311000	-0.28680700
N	-1.67822600	1.27853600	-0.70773600
N	-1.47504300	-1.58402800	-0.11644600
N	1.67125200	-1.35099800	-0.50345000
C	2.50111500	1.34592500	0.55711500
N	-0.02683200	0.09210600	1.46368800
C	2.46844100	0.05755300	1.39401600
C	2.58935300	-1.18638100	0.48686400
C	-2.59934900	1.25551200	0.28975700
C	2.37444000	3.70673900	-0.86398400
H	2.26575400	4.62296500	-1.43290400
C	3.51346300	2.29787500	0.68867400
H	4.34988600	2.11944000	1.34934200
C	-2.54159200	-1.25557400	0.64225600
C	-3.71483300	0.21912700	2.28200200
H	-3.69532200	1.15479100	2.84263300
H	-3.71778700	-0.60472300	2.99692800
H	-4.65205500	0.18369400	1.72497200
C	3.62836600	-2.10259300	0.64912900
H	4.33833100	-1.99123400	1.45565200
C	3.64321800	0.07360400	2.38066900
H	3.61986000	-0.80022900	3.03372700
H	3.61882900	0.96578100	3.00754900
H	4.59433800	0.06757500	1.84642600
C	-3.58525400	-2.16348700	0.83151500
H	-4.45169500	-1.88986400	1.41604200
C	-1.23838000	0.26543300	3.52556700
H	-2.17866600	0.34102900	4.05047000
C	1.13690200	0.17132000	3.55914400
H	2.06434800	0.15816200	4.11147500
C	-1.20772300	0.17691200	2.13862800
C	-1.85809200	2.17907600	-1.70423200
H	-1.16578200	2.10044100	-2.53422200
C	-2.51572500	0.11929100	1.33062000
C	1.13917500	0.08893800	2.17091500
C	3.78451000	-3.17301700	-0.22584300
H	4.59543300	-3.87979500	-0.08872800
C	-3.61474300	2.21135400	0.34539800
H	-4.32630900	2.21263000	1.15844500
C	-1.40539800	-2.82877600	-0.62997100
H	-0.51784700	-3.05368300	-1.20298400
C	-0.05885900	0.25956700	4.25134600
H	-0.07164800	0.32064200	5.33400100
C	-3.52515300	-3.43054000	0.26713000
H	-4.34085900	-4.13181200	0.40817900
C	-2.39631800	-3.77841300	-0.46254400
H	-2.27960700	-4.76060800	-0.90570000
C	-2.85524300	3.13536200	-1.71555100
H	-2.92759800	3.82611900	-2.54811400
C	1.86077100	-2.37392800	-1.37774400
H	1.12333400	-2.44357900	-2.17528600
C	2.88856600	-3.29388600	-1.27879100
H	2.96991200	-4.08782100	-2.01310100
C	-3.74390300	3.17364100	-0.64909600
H	-4.53463500	3.91403200	-0.59811000
C	3.46584800	3.48284000	-0.03292900
H	4.25922900	4.21632500	0.06315600
C	1.40693400	2.72544200	-0.95752600
H	0.53945800	2.86826600	-1.58699400
S	-0.78573900	-0.82965600	-2.93236200
S	0.86418200	0.36875100	-3.00106600
H	1.88721100	-0.54139000	-3.05396200

^{3}[MoHS-S]$^+$

E= -2263.464742 a.u.

G= -2263.026619 a.u.

1 3

Mo	0.00378100	0.34000300	0.50066200
N	-1.61872800	1.38352300	-0.48433300
N	1.60778800	1.20244900	-0.65066200
N	1.58399200	-1.06074200	1.16594500
N	-1.67518600	-0.80048200	1.35349200
C	-2.62113200	0.71249100	-1.09228200
N	-0.18209900	-1.04179400	-1.16956600
C	-2.64862400	-0.82426300	-0.94377100
C	-2.68249800	-1.21306000	0.55419100
C	2.45968000	0.42230000	-1.35664400
C	-2.57532800	3.47165800	-1.18655000
H	-2.53219000	4.55433600	-1.16013500
C	-3.60159100	1.40539500	-1.80607000
H	-4.40139100	0.87489100	-2.30206900
C	2.46644100	-1.53783900	0.26027800
C	3.42042000	-1.78452300	-2.04128800
H	3.34148700	-1.51563900	-3.09504300
H	3.35984200	-2.87122800	-1.96637700
H	4.40636800	-1.47432700	-1.69228100
C	-3.74452400	-1.94463300	1.09319100
H	-4.55215800	-2.29203400	0.46609600
C	-3.91213000	-1.36667100	-1.62458700
H	-3.96958200	-2.45303600	-1.54095700
H	-3.92604600	-1.11214100	-2.68479900
H	-4.80848100	-0.94307000	-1.16903400
C	3.48611200	-2.40232400	0.66394200
H	4.20031900	-2.78508300	-0.04943000
C	0.84580200	-2.41632000	-2.83388100
H	1.73338500	-2.81234200	-3.30324600
C	-1.52954600	-2.28775600	-2.70403200
H	-2.50200700	-2.58368600	-3.06763600
C	0.93732700	-1.53967000	-1.75683200
C	1.75037100	2.54489100	-0.71516300
H	1.11569200	3.12668000	-0.05299200
C	2.31792800	-1.10711700	-1.21588500
C	-1.40263300	-1.41204500	-1.63025400
C	-3.78541000	-2.23246800	2.45125000
H	-4.61183400	-2.80361800	2.86136500
C	3.42775000	0.99847300	-2.17927100
H	4.10754800	0.38060400	-2.74748900
C	1.71490200	-1.42447700	2.45588200
H	1.00975800	-0.98063300	3.14546200
C	-0.39605000	-2.79951200	-3.31267100
H	-0.47859800	-3.49138200	-4.14390400
C	3.60491000	-2.78386200	1.99462600
H	4.39957900	-3.45699800	2.29916600
C	2.69755600	-2.28289100	2.91531700
H	2.74670200	-2.53393000	3.96835700
C	2.69308900	3.16848400	-1.51110800
H	2.75784900	4.25043900	-1.51123300
C	-1.74390400	-1.04180500	2.67641100
H	-0.95241700	-0.60000700	3.26969400

C	-2.76914700	-1.75627900	3.26819500
H	-2.76882700	-1.91843600	4.33975800
C	3.54522200	2.38003000	-2.27146700
H	4.30165500	2.82248500	-2.91076400
C	-3.57320400	2.79185100	-1.87430100
H	-4.33736600	3.32684000	-2.42811100
C	-1.63315000	2.73557800	-0.49410600
H	-0.88750100	3.22178700	0.13155700
S	1.00482000	1.57721500	2.40804800
S	0.58409300	3.54310600	2.37485600
H	-0.83537200	1.24178600	1.58691500

^{1}[MoHS-S]$^{+}$

E= -2263.465527 a.u.

G= -2263.024447 a.u.

1 1

Mo	-0.00364100	0.27281500	0.59466100
N	-1.62307500	1.40800500	-0.36983400
N	1.45718300	1.30992300	-0.67056700
N	1.62674900	-1.08095700	1.11247100
N	-1.65830500	-0.92596400	1.27415500
C	-2.56100600	0.75099800	-1.08711500
N	-0.13820500	-1.00520500	-1.20131600
C	-2.59994600	-0.79494600	-1.02356300
C	-2.68380500	-1.25144500	0.45061900
C	2.36161500	0.59919200	-1.38032800
C	-2.64721300	3.50948600	-0.92528800
H	-2.66522000	4.58465000	-0.78936700
C	-3.51685700	1.46941600	-1.81146600
H	-4.24994300	0.95829000	-2.41787700
C	2.55436500	-1.41967600	0.18246100
C	3.46853400	-1.50879500	-2.15116600
H	3.31950800	-1.23677400	-3.19724400
H	3.50736400	-2.59645800	-2.08797100
H	4.43914200	-1.12466200	-1.83491200
C	-3.78018200	-1.96827700	0.93626000
H	-4.59590200	-2.23219300	0.27904500
C	-3.84404400	-1.29082200	-1.77297000
H	-3.94259600	-2.37423000	-1.69774700
H	-3.79302800	-1.03314700	-2.83214000
H	-4.74924900	-0.84541800	-1.35792300
C	3.65090400	-2.20982400	0.53126000
H	4.39931100	-2.46559300	-0.20428600
C	0.93453700	-2.44300300	-2.77862900
H	1.83539000	-2.83303200	-3.22785700
C	-1.44524800	-2.37224700	-2.66040500
H	-2.40839500	-2.70606300	-3.01590700
C	0.99326500	-1.48408700	-1.77079500
C	1.49907000	2.65519000	-0.71560900
H	0.81481800	3.17517700	-0.05661400
C	2.34515800	-0.94170300	-1.27212000
C	-1.34465400	-1.41246900	-1.65726200
C	-3.85089500	-2.33914100	2.27132600
H	-4.70743100	-2.89115700	2.64258100
C	3.29078700	1.25921100	-2.18640200
H	4.01427700	0.70427300	-2.76460100
C	1.79258600	-1.54446800	2.37295200
H	1.04217600	-1.24044900	3.08918500
C	-0.29497400	-2.89979500	-3.22277300
H	-0.35588100	-3.64438600	-4.00934600
C	3.81301000	-2.67268500	1.83049000
H	4.67319500	-3.27876900	2.09327900
C	2.85178400	-2.33637200	2.77228900
H	2.91598800	-2.66519600	3.80303800
C	2.40098800	3.36264800	-1.49003200
H	2.38695400	4.44620200	-1.47467500
C	-1.74975800	-1.26660400	2.58146900
H	-0.94009600	-0.92204000	3.21178000
C	-2.81093300	-1.96797300	3.11603600
H	-2.81833500	-2.20520100	4.17360400
C	3.30927000	2.64713100	-2.25491000
H	4.03314900	3.15153800	-2.88634300
C	-3.54809700	2.85628100	-1.75538600
H	-4.28744600	3.40796700	-2.32668200
C	-1.71142300	2.74890500	-0.24862400
H	-1.02873500	3.20029900	0.46907300
S	1.05133400	1.42158400	2.29684400
S	0.52970600	3.30765400	2.67484500
H	-0.89420800	1.19498900	1.60083400

^{3}[MoSH-SH]$^{2+}$

E= -2263.818191 a.u.

G= -2263.370298 a.u.

2 3

Mo	-0.00564900	0.35289400	0.38603700
N	-1.66307500	1.16327900	-0.77324500
N	1.63715600	1.15398300	-0.79755400
N	1.62623600	-0.73037400	1.38499300
N	-1.68702200	-0.65889400	1.38115600
C	-2.56591400	0.31193300	-1.31430900
N	0.00919600	-1.28015600	-0.98627700
C	-2.48861700	-1.18260500	-0.91991400
C	-2.59505800	-1.31011800	0.61784700
C	2.59105500	0.32518200	-1.27872300
C	-2.72024900	3.01476300	-1.88612900
H	-2.75285400	4.08426600	-2.05870800
C	-3.54943400	0.79110000	-2.17908800
H	-4.27243700	0.12161700	-2.62148500
C	2.57313000	-1.33824900	0.63325900
C	3.69909800	-1.90479000	-1.53496800
H	3.69076600	-1.80556200	-2.62105800
H	3.67743200	-2.96874200	-1.29672900
H	4.64327500	-1.49877700	-1.16906000
C	-3.61712500	-2.04284300	1.22183100
H	-4.34259100	-2.57634800	0.62553400
C	-3.66961700	-1.92615400	-1.55941700
H	-3.65722800	-2.98485500	-1.29725800
H	-3.63959500	-1.85335800	-2.64694900
H	-4.61810800	-1.50600900	-1.22191500
C	3.57476100	-2.09684500	1.24149100
H	4.34035600	-2.57798500	0.65068900
C	1.21236000	-2.82303900	-2.35336600
H	2.14563200	-3.22386600	-2.71882400
C	-1.17420700	-2.84745500	-2.34202600
H	-2.10230200	-3.26946100	-2.69662600
C	1.18992900	-1.77956500	-1.43298700
C	1.70040100	2.46951900	-1.08447900
H	0.92689100	3.09167600	-0.65215900
C	2.50949800	-1.16972700	-0.90221900
C	-1.16491400	-1.79494500	-1.43180500
C	-3.72884000	-2.09091700	2.60694900
H	-4.52742400	-2.66206000	3.06893900
C	3.61277600	0.83054000	-2.08246900
H	4.38045200	0.18062500	-2.47588200
C	1.67653300	-0.87125400	2.72567000
H	0.91084300	-0.34886600	3.28537500
C	0.02240700	-3.36611400	-2.80877400
H	0.02745200	-4.18516300	-3.51995500
C	3.60854100	-2.24656200	2.62270400
H	4.39103600	-2.83636800	3.08850400
C	2.63260800	-1.62077800	3.38581700
H	2.61348400	-1.69433800	4.46702000
C	2.68868800	3.02847000	-1.87397200
H	2.68818300	4.09435800	-2.06971300
C	-1.82171400	-0.68201400	2.72198300
H	-1.10957100	-0.08848300	3.28055300
C	-2.81860200	-1.38173000	3.37732600
H	-2.87574000	-1.35949400	4.45938100
C	3.66524300	2.18627000	-2.38736200
H	4.46471900	2.57270900	-3.01091400
C	-3.62294100	2.14619900	-2.48263200
H	-4.38917400	2.51162200	-3.15828200
C	-1.76878900	2.48209300	-1.03439600
H	-1.08228400	3.13347500	-0.50485500
S	0.10051500	4.20246000	1.67455500
S	0.08128400	2.05307100	2.09876800
H	1.32113900	2.04707600	2.62848700
H	-0.88738400	4.49518000	2.54063500

^{1}[MoSH-SH]$^{2+}$

E= -2263.785084 a.u.

G= -2263.338136 a.u.

2 1

Mo	0.02903500	0.51862800	0.16451400
N	1.62946900	-0.27380300	1.39314300
N	-1.62879300	0.20712200	1.54748700
N	-1.62443700	0.98276500	-1.20334400
N	1.60010400	0.39042300	-1.33570200
C	2.37123000	-1.32406600	0.97707200
N	-0.37440200	-1.53858100	-0.38336100
C	2.11046300	-1.86557300	-0.44418300
C	2.36639200	-0.71779200	-1.44143100
C	-2.75416300	-0.43607600	1.16979100
C	2.90030500	-0.20090200	3.44212100
H	3.07876200	0.29045200	4.39159600
C	3.36552100	-1.86471000	1.79643500
H	3.94304000	-2.71791700	1.47256700
C	-2.72428500	0.19886700	-1.25342600
C	-4.15054500	-1.71164200	-0.47337300
H	-4.26384400	-2.53439500	0.23390900
H	-4.23058300	-2.11795500	-1.48257100
H	-4.98777100	-1.02937100	-0.32375100
C	3.37668600	-0.79457000	-2.40271200
H	3.97759300	-1.68660200	-2.50244100
C	3.09220300	-3.01023400	-0.73285200
H	2.95816300	-3.40130200	-1.74250600
H	2.95861000	-3.83317900	-0.02954900
H	4.12251000	-2.66494600	-0.64368900
C	-3.75471900	0.47061100	-2.15743200
H	-4.62700000	-0.16416400	-2.20820900
C	-1.91890400	-3.30126100	-0.81866400
H	-2.93139800	-3.66155700	-0.91466300
C	0.43143500	-3.72270600	-0.89508700
H	1.24751200	-4.41108100	-1.05154500
C	-1.65394300	-1.97262400	-0.50118100
C	-1.56246800	0.69918100	2.80458600
H	-0.64196200	1.20082400	3.07050300
C	-2.81406200	-0.98394200	-0.26904400
C	0.66565900	-2.38797900	-0.57660300
C	3.63068700	0.27828200	-3.24604600
H	4.41558400	0.21413000	-3.99208400
C	-3.82251600	-0.58391900	2.05753500

H	-4.72092000	-1.10388200	1.75866500
C	-1.56620100	2.04740200	-2.03421900
H	-0.67964100	2.66206200	-1.95484200
C	-0.86892500	-4.18204500	-1.01687500
H	-1.06314100	-5.22023700	-1.26645500
C	-3.67756100	1.56303700	-3.00925500
H	-4.47833400	1.76793400	-3.71175700
C	-2.55677500	2.38051900	-2.93674300
H	-2.44192600	3.25474600	-3.56716700
C	-2.58819100	0.59946200	3.72367800
H	-2.47047900	1.02539900	4.71336800
C	1.86051600	1.43036700	-2.15851100
H	1.23593700	2.30398700	-2.03055400
C	2.86170300	1.42711200	-3.10938500
H	3.02172400	2.30207200	-3.72863800
C	-3.74817900	-0.06328600	3.34196400
H	-4.57937000	-0.18039500	4.02907300
C	3.63262800	-1.31159100	3.04053600
H	4.40254600	-1.73642700	3.67550800
C	1.91678400	0.27192100	2.59710300
H	1.33298700	1.14021000	2.87603500
S	2.10445600	3.93134200	0.69265500
S	0.33823800	2.72387700	0.71217600
H	1.98571600	4.38221400	1.95791100
H	-0.60513800	3.68694900	0.61405100

^{3}[MoHS-SH]$^{2+}$

E= -2263.801701 a.u.

G= -2263.355330 a.u.

2 3

Mo	0.00178500	0.48971800	-0.31326600
N	1.65362000	0.95252300	1.02669800
N	-1.60894800	1.02684700	1.08946200
N	-1.69994400	-0.22903500	-1.47803100
N	1.57763400	-0.59198900	-1.42966700
C	2.50283100	-0.01272500	1.43480900
N	-0.13319800	-1.42590000	0.76504300
C	2.37186700	-1.41109900	0.79352300
C	2.50297600	-1.30456700	-0.74548300
C	-2.60737700	0.15973900	1.35915400
C	2.78187400	2.56815100	2.39704000
H	2.86884900	3.59827300	2.72219800
C	3.49417100	0.28208900	2.37114000
H	4.17655700	-0.48038100	2.71684500
C	-2.67166000	-0.96985900	-0.90241700
C	-3.85212400	-1.99684600	1.05544500
H	-3.85440200	-2.17357600	2.13160700
H	-3.89027300	-2.96657800	0.55751800
H	-4.76501700	-1.45563800	0.80308200
C	3.53603200	-1.94422900	-1.42894600
H	4.28999200	-2.50278500	-0.89472500
C	3.49957000	-2.30352500	1.33147600
H	3.47052800	-3.29609200	0.88101900
H	3.42255600	-2.42296300	2.41304800
H	4.47499600	-1.86716200	1.11333900
C	-3.71804500	-1.46645700	-1.68045000
H	-4.49755900	-2.07074500	-1.24035800
C	-1.43246100	-3.21626500	1.65243300
H	-2.39001900	-3.67321100	1.85085200
C	0.95164600	-3.28733600	1.78118800
H	1.85101000	-3.79924900	2.08757600
C	-1.33985200	-1.97876200	1.02133700
C	-1.61430400	2.24229900	1.67266000
H	-0.83663900	2.92686700	1.35792600
C	-2.61214900	-1.20090500	0.62595900
C	1.00716200	-2.05748400	1.13030800
C	3.61812500	-1.87411500	-2.81571600
H	4.42789800	-2.37238000	-3.33851200
C	-3.60801700	0.50685000	2.26846000
H	-4.41321500	-0.17773200	2.49157000
C	-1.78610200	0.08086000	-2.78802300
H	-1.01758100	0.74801600	-3.16337700
C	-0.27652100	-3.87399000	2.03766100
H	-0.33182800	-4.83667000	2.53522700
C	-3.78084400	-1.18299800	-3.04035900
H	-4.59609800	-1.57533000	-3.63940600
C	-2.80292600	-0.37613800	-3.60601000
H	-2.82427800	-0.09626400	-4.65287900
C	-2.57110900	2.63825400	2.58843700
H	-2.52253900	3.62827800	3.02664100
C	1.65845800	-0.53559100	-2.77434000
H	0.90346700	0.05457500	-3.27521600
C	2.65059300	-1.16239100	-3.50709900
H	2.66078400	-1.07584100	-4.58724800
C	-3.58797800	1.74531200	2.89818800
H	-4.36736700	2.00927700	3.60538700
C	3.62926700	1.57406800	2.86716600
H	4.40200100	1.79808200	3.59521300
C	1.81512300	2.21327200	1.47446300
H	1.15879800	2.96218500	1.04631700
S	0.24659200	4.19575200	-1.37011500
S	0.92173300	2.25484800	-1.79781500
H	-0.79904100	1.83779400	-0.78111700
H	-0.84324800	4.24070400	-2.16500800

^{1}[MoHS-SH]$^{2+}$

E= -2263.788663 a.u.

G= -2263.339947 a.u.

2 1

Mo	-0.03925100	-0.64414000	0.00085300
N	1.60579000	-0.36282700	-1.46484600
N	-1.60281000	-0.27625100	-1.48409600
N	-1.60241500	-0.27157000	1.48503100
N	1.60563200	-0.35840300	1.46581200
C	2.57395200	0.55848000	-1.26548400
N	0.01245900	1.59305200	-0.00259800
C	2.50545000	1.44230300	-0.00217500
C	2.57352500	0.56265800	1.26405300
C	-2.56601000	0.64709900	-1.27146900
C	2.70214700	-1.06568200	-3.49613400
H	2.70853000	-1.74224000	-4.34280700
C	3.61776900	0.69926100	-2.18348500
H	4.39160300	1.43582400	-2.02986700
C	-2.56552400	0.65127800	1.26982300
C	-3.64842300	2.51863600	-0.00368800
H	-3.62208800	3.15714300	-0.88762200
H	-3.62176200	3.16003400	0.87814400
H	-4.60426500	1.99379000	-0.00266800
C	3.61675200	0.70681500	2.18220600
H	4.39027300	1.44332700	2.02677000
C	3.69936600	2.40909800	-0.00354400
H	3.68821800	3.05133400	0.87781900
H	3.68873300	3.04820800	-0.88718000
H	4.64138300	1.86025500	-0.00230500
C	-3.61088300	0.79930200	2.18366700
H	-4.37907900	1.54197300	2.02849600
C	-1.14491900	3.68299200	-0.00649800
H	-2.06748900	4.24252000	-0.00750800
C	1.23703600	3.64278700	-0.00646100
H	2.17654800	4.17285900	-0.00744400
C	-1.14745900	2.29135800	-0.00384400
C	-1.69817600	-1.07810300	-2.56510600
H	-0.93464200	-1.83711700	-2.66180800
C	-2.47888000	1.52278100	-0.00227700
C	1.19658700	2.25040500	-0.00380800
C	3.68647000	-0.09676800	3.31119200
H	4.50016600	0.02206900	4.01870300
C	-3.61187600	0.79187700	-2.18525100
H	-4.38019600	1.53483700	-2.03209400
C	-1.69742200	-1.06986400	2.56869500
H	-0.93395200	-1.82867200	2.66753400
C	0.05833500	4.36636700	-0.00784900
H	0.07707400	5.45132200	-0.00992500
C	-3.68920500	-0.01167700	3.30867500
H	-4.50497200	0.11041500	4.01341500
C	-2.71417100	-0.98004200	3.50045600
H	-2.73244800	-1.65565800	4.34774000
C	-2.71539200	-0.99153800	-3.49666700
H	-2.73393300	-1.66992600	-4.34172700
C	1.69341600	-1.14655700	2.55978500
H	0.93651000	-1.90942100	2.66217600
C	2.70135400	-1.05462400	3.49971700
H	2.70767700	-1.72864400	4.34841200
C	-3.69057000	-0.02279500	-3.30756100
H	-4.50674100	0.09676700	-4.01226500
C	3.68769900	-0.10782300	-3.30996100
H	4.50188300	0.00837800	-4.01734800
C	1.69371400	-1.15429100	-2.55641000
H	0.93649800	-1.91709300	-2.65688500
S	-0.53669700	-4.47524400	0.00662900
S	0.69712100	-2.78836400	0.00380000
H	-1.22134300	-1.76116400	0.00282700
H	-1.73900100	-3.85991800	0.00599000

^{3}[Mo(SH)$_2$]$^{2+}$

E= -2263.818111 a.u.

G= -2263.367214 a.u.

2 3

Mo	-0.00003700	-0.00007000	-0.77645000
N	1.38242500	1.64077800	-0.10344300
N	-1.71137300	1.33788300	-0.66638900
N	-1.38246700	-1.64079700	-0.10305900
N	1.71130600	-1.33800600	-0.66633500
C	2.48097600	1.31222100	0.60970700
N	0.00007600	0.00009700	1.43842800
C	2.49544100	-0.06101700	1.31627900
C	2.63222600	-1.22320400	0.31145300
C	-2.63214700	1.22329300	0.31156400
C	2.18958500	3.88843200	-0.34411000
H	2.01352300	4.89224700	-0.71232400
C	3.50224500	2.24167600	0.78816900
H	4.40381300	1.97482700	1.32056600
C	-2.48095700	-1.31209400	0.61011800
C	-3.67941100	0.10712600	2.29289900
H	-3.68000600	1.03458800	2.86802600
H	-3.64662700	-0.72917800	2.99176600
H	-4.62646900	0.05169400	1.75541400
C	3.70551700	-2.11457500	0.36332100
H	4.44313700	-2.05153800	1.14955900
C	3.67965200	-0.10675300	2.29254200
H	3.68034600	-1.03415300	2.86776600
H	3.64690100	0.72962400	2.99132300

H	4.62665400	-0.05133800	1.75495600
C	-3.50226200	-2.24147500	0.78876100
H	-4.40378600	-1.97451000	1.32117300
C	-1.18410700	0.14611000	3.50004900
H	-2.10885700	0.26870600	4.04308900
C	1.18446600	-0.14576500	3.49994000
H	2.10927100	-0.26832000	4.04289700
C	-1.17103600	0.10430700	2.10848600
C	-1.87496500	2.26889000	-1.63148500
H	-1.12956100	2.25682400	-2.42125400
C	-2.49529900	0.06123200	1.31652500
C	1.17125700	-0.10405400	2.10837600
C	3.85113000	-3.09899100	-0.60662600
H	4.68837500	-3.78762800	-0.56003800
C	-3.70536300	2.11475200	0.36347100
H	-4.44285300	2.05189600	1.14984500
C	-1.23270700	-2.90714700	-0.53602300
H	-0.31962500	-3.13081400	-1.06915800
C	0.00021400	0.00019100	4.20216900
H	0.00026800	0.00022300	5.28724700
C	-3.36848900	-3.53526000	0.29491500
H	-4.16849100	-4.25544500	0.43129800
C	-2.18973800	-3.88844900	-0.34336100
H	-2.01374000	-4.89232400	-0.71144200
C	-2.92454800	3.16840500	-1.63848200
H	-3.00875200	3.89486900	-2.43849500
C	1.87479200	-2.26917100	-1.63129800
H	1.12925400	-2.25728900	-2.42094300
C	2.92443200	-3.16861900	-1.63832100
H	3.00854500	-3.89521600	-2.43822200
C	-3.85106800	3.09902200	-0.60661100
H	-4.68825200	3.78773100	-0.55999000
C	3.36838400	3.53538800	0.29415800
H	4.16835800	4.25563100	0.43040300
C	1.23258800	2.90706000	-0.53658100
H	0.31947000	3.13060900	-1.06970400
S	-1.24123300	-0.97051700	-2.70030300
S	1.24100400	0.97007700	-2.70055300
H	-1.01671900	-0.12109600	-3.71676500
H	1.01643800	0.12048400	-3.71686000

^{1}[Mo(SH)$_2$]$^{2+}$
E= -2263.796536 a.u.
G= -2263.344307 a.u.

2 1

Mo	0.00000600	0.00000400	-0.87976500
N	1.39762800	1.63482600	-0.16054900
N	-1.66863200	1.38031400	-0.55006900
N	-1.39766500	-1.63478700	-0.16061100
N	1.66863600	-1.38031100	-0.55007500
C	2.48606400	1.32587500	0.57108300
N	-0.00001700	-0.00006100	1.43100400
C	2.49198300	-0.01073200	1.34016700
C	2.60814300	-1.22086400	0.40136900
C	-2.60818300	1.22083200	0.40132400
C	2.26875800	3.84339600	-0.53572100
H	2.11962500	4.82399000	-0.97224900
C	3.53002400	2.24236100	0.70533300
H	4.42183700	1.98521500	1.25776700
C	-2.48607400	-1.32589200	0.57108300
C	-3.67576100	0.01991300	2.31843900
H	-3.67532000	0.92235400	2.93146800
H	-3.64577800	-0.84510600	2.98186100
H	-4.62275500	-0.00885300	1.77873700
C	3.66811200	-2.12567300	0.50398200
H	4.41466900	-2.01581800	1.27605400
C	3.67573000	-0.01992100	2.31845100
H	3.67537800	-0.92242800	2.93138100
H	3.64565900	0.84502300	2.98196600
H	4.62272100	0.00899400	1.77875300
C	-3.52996000	-2.24244700	0.70543700
H	-4.42173600	-1.98536100	1.25796000
C	-1.18565600	0.07748800	3.50767100
H	-2.11785100	0.14202200	4.04701700
C	1.18561500	-0.07724900	3.50768800
H	2.11781100	-0.14165900	4.04704700
C	-1.16760700	0.05031400	2.11559700
C	-1.81691200	2.38118200	-1.44865300
H	-1.08973200	2.40759200	-2.25042700
C	-2.49201600	0.01071700	1.34015100
C	1.16757200	-0.05030600	2.11561000
C	3.79224000	-3.17453000	-0.39603900
H	4.61977700	-3.87112100	-0.31258500
C	-3.66821200	2.12558200	0.50385600
H	-4.41481000	2.01568700	1.27588100
C	-1.29444200	-2.87209600	-0.67526100
H	-0.40123800	-3.08383300	-1.24112000
C	-0.00002200	0.00017400	4.21439800
H	-0.00002300	0.00027300	5.29941400
C	-3.43210000	-3.50748400	0.14045500
H	-4.24630900	-4.21697800	0.24458500
C	-2.26870200	-3.84340700	-0.53572100
H	-2.11954700	-4.82399100	-0.97226400
C	-2.85295800	3.29337500	-1.41136300
H	-2.91779900	4.06599900	-2.16863500
C	1.81692200	-2.38119400	-1.44864100
H	1.08979400	-2.40755400	-2.25046300
C	2.85292100	-3.29343900	-1.41127900
H	2.91777300	-4.06606700	-2.16854800
C	-3.79233900	3.17442200	-0.39618500
H	-4.61991900	3.87096700	-0.31279000
C	3.43219600	3.50740000	0.14034900
H	4.24646300	4.21683900	0.24439700
C	1.29443300	2.87214000	-0.67518700
H	0.40120300	3.08392100	-1.24098700
S	-1.45218400	-0.47967900	-2.71306200
S	1.45227500	0.47966900	-2.71300800
H	-0.73949400	-0.68297700	-3.83768700
H	0.73959900	0.68338800	-3.83756800

^{3}[MoHSH-S]$^{2+}$
E= -2263.764538 a.u.
G= -2263.315617 a.u.

2 3

Mo	0.02687400	0.06478000	-0.66312000
N	-1.55526900	-1.34467800	-0.32787000
N	1.63105400	-1.43236900	-0.85774200
N	1.72394700	1.45368100	-0.74359900
N	-1.40293400	1.49632800	0.22473100
C	-2.20608600	-1.39877300	0.85771600
N	0.55141900	-0.20344500	1.44875600
C	-1.91599600	-0.28832700	1.88609200
C	-2.18203600	1.09801900	1.25581400
C	2.79760000	-1.29041900	-0.19429200
C	-2.82854500	-3.22675800	-1.12555000
H	-3.06280700	-3.89373300	-1.94673900
C	-3.13754100	-2.40309400	1.09894100
H	-3.65006200	-2.46805300	2.04731500
C	2.83774800	1.23477100	-0.01366100
C	4.32726900	-0.16135300	1.44071700
H	4.45373600	-1.09764600	1.98557500
H	4.46414700	0.65856900	2.14693600
H	5.12334400	-0.09643700	0.69772900
C	-3.17227500	1.94531200	1.74882500
H	-3.81656000	1.63081400	2.55625800
C	-2.84637400	-0.47619400	3.09307400
H	-2.70899900	0.31764800	3.82823500
H	-2.66090900	-1.43051600	3.58789600
H	-3.89047500	-0.46304400	2.77846900
C	3.86988900	2.17410900	-0.01871800
H	4.76150200	2.02146700	0.57141700
C	2.17812100	-0.32329800	3.18767600
H	3.20746700	-0.31377500	3.51266200
C	-0.14613800	-0.47194200	3.71189900
H	-0.92934000	-0.58282000	4.44609500
C	1.84594900	-0.20076700	1.84194700
C	1.47011000	-2.47818200	-1.69228200
H	0.52792800	-2.52740600	-2.22086300
C	2.94900500	-0.09300900	0.76890500
C	-0.44483500	-0.33158800	2.35894000
C	-3.35213000	3.21300300	1.20694300
H	-4.13106900	3.86332200	1.59107800
C	3.82132800	-2.22212400	-0.37482700
H	4.76297300	-2.11458300	0.14316600
C	1.65522900	2.54360200	-1.53465500
H	0.77447400	2.61554200	-2.16341800
C	1.17360800	-0.46361100	4.13038600
H	1.41725400	-0.56486900	5.18285700
C	3.77197000	3.32310500	-0.79533600
H	4.57699700	4.05065700	-0.79316100
C	2.64658000	3.50567000	-1.58822400
H	2.53720700	4.36320600	-2.24194600
C	2.43929500	-3.44118600	-1.89887700
H	2.25036800	-4.26193800	-2.58092700
C	-1.56664300	2.73519700	-0.28065200
H	-0.91968800	3.00904200	-1.10213600
C	-2.51755000	3.62646300	0.17982200
H	-2.60459800	4.60668000	-0.27370700
C	3.64659400	-3.30526700	-1.22698300
H	4.44663400	-4.02526800	-1.36408700
C	-3.43517600	-3.34221800	0.11302300
H	-4.15567300	-4.12853900	0.31191600
C	-1.92081700	-2.19675400	-1.31028200
H	-1.44507900	-2.05362600	-2.27241600
S	-3.33224300	0.28454000	-2.58504500
S	-1.37933400	0.74884600	-2.65093500
H	-0.88379800	0.14563900	-3.75778900
H	0.62510200	-0.00819000	-2.21188600

^{1}[MoHSH-S]$^{2+}$
E= -2263.753058 a.u.
G= -2263.302042 a.u.

2 1

Mo	0.00875800	-0.03789600	-0.67406400
N	-1.51168700	-1.45063400	0.04177000
N	1.62841200	-1.53406400	-0.63567800
N	1.60124600	1.48124200	-0.76116700
N	-1.53310700	1.43375000	-0.15298800
C	-2.22522300	-1.17963300	1.15938700
N	0.53658300	0.08099700	1.45560900
C	-1.92094200	0.12427900	1.92760800
C	-2.20874000	1.33491100	1.01449900

C	2.80408000	-1.27013000	-0.02643500
C	-2.79254500	-3.47299000	-0.27179300
H	-2.98123600	-4.34711800	-0.88398400
C	-3.21831400	-2.05705700	1.59625900
H	-3.78412400	-1.84752100	2.49142100
C	2.78641800	1.27626200	-0.14683000
C	4.31327000	0.08642200	1.44431000
H	4.45353100	-0.76486400	2.11165300
H	4.43963100	1.00090600	2.02540800
H	5.10916600	0.05501600	0.69980300
C	-3.16335100	2.29116700	1.36397900
H	-3.69012400	2.22490100	2.30395100
C	-2.83451800	0.20198200	3.15955100
H	-2.64714400	1.11039200	3.73328800
H	-2.68023300	-0.65268900	3.81901500
H	-3.88319700	0.20751300	2.86161800
C	3.83804500	2.17609200	-0.32895100
H	4.78813200	2.02176700	0.16045300
C	2.17441100	0.14006600	3.19263500
H	3.20668100	0.14542500	3.50703900
C	-0.14363100	0.18192900	3.74152100
H	-0.92280900	0.21891500	4.48656900
C	1.83497100	0.08936900	1.84478400
C	1.51204000	-2.67257700	-1.34848100
H	0.56792900	-2.82095800	-1.85178700
C	2.93380200	0.04402300	0.77115900
C	-0.45141500	0.13040300	2.38401000
C	-3.46424000	3.34182900	0.50732000
H	-4.20687800	4.08125000	0.78732000
C	3.86288200	-2.17576200	-0.11440900
H	4.80353700	-1.97506600	0.37637400
C	1.46075600	2.56288900	-1.55300200
H	0.50229500	2.67583000	-2.03745800
C	1.17727400	0.18486400	4.15114600
H	1.42736500	0.22315000	5.20632800
C	3.68426600	3.28888900	-1.14628400
H	4.50694100	3.98255200	-1.28444500
C	2.46402500	3.48780100	-1.77532700
H	2.28413700	4.33469600	-2.42730700
C	2.52394400	-3.60499100	-1.47973600
H	2.36264000	-4.49829400	-2.07190500
C	-1.86352400	2.43783600	-0.99512100
H	-1.35760100	2.44402400	-1.95015000
C	-2.80918500	3.40469300	-0.71302700
H	-3.02132200	4.17778900	-1.44230500
C	3.72929600	-3.35227900	-0.84074200
H	4.55708100	-4.05041500	-0.90686000
C	-3.50729000	-3.21543300	0.88726500
H	-4.28143800	-3.89138200	1.23428300
C	-1.81812500	-2.56972800	-0.65082700
H	-1.26814300	-2.73413300	-1.56577100
S	-3.03694900	-0.24002100	-3.02083000
S	-1.10126500	-0.18227400	-2.68547300
H	-0.46850200	-0.24948100	-3.88305000
H	0.90651100	-0.09365400	-2.04758100

^{1}[MoHS$_2$H]$^{2+}$

E= -2263.765301 a.u.

G= -2263.312583 a.u.

2 1

Mo	0.03343000	-0.10288400	-0.75790700
N	-1.66119800	-1.49262300	-0.28871200
N	1.63169600	-1.57685900	-0.30063800
N	1.68414900	1.37205200	-0.60879700
N	-1.38424600	1.61308100	-0.27388500
C	-2.67349300	-1.12798900	0.52838100
N	0.02623100	0.03867800	1.44762600
C	-2.49554000	0.14791700	1.36301100
C	-2.45563800	1.42394200	0.51329500
C	2.63459800	-1.23563600	0.54265500
C	-2.78735800	-3.60148200	-0.67661700
H	-2.75162400	-4.58042800	-1.14077700
C	-3.80153900	-1.93780800	0.68451000
H	-4.62524500	-1.61569300	1.30355500
C	2.57046900	1.29323700	0.40596800
C	3.68565200	0.16327200	2.34047900
H	3.72368700	-0.71197000	2.98961200
H	3.60177100	1.04925100	2.97136400
H	4.63613000	0.22209000	1.80979900
C	-3.45261100	2.39841000	0.61125400
H	-4.32970600	2.23261000	1.21906400
C	-3.65352600	0.25741700	2.36721000
H	-3.54217300	1.13886000	3.00037000
H	-3.71247500	-0.62499800	3.00505800
H	-4.60772100	0.34360900	1.84737100
C	3.56392600	2.26746800	0.54569300
H	4.25154500	2.24111900	1.37760200
C	1.20814900	-0.01167200	3.52536400
H	2.13894700	-0.01829300	4.07042900
C	-1.16974000	-0.01012300	3.51626800
H	-2.10193800	-0.01702100	4.05865000
C	1.19211600	0.03760500	2.13338300
C	1.75299400	-2.73196300	-0.98790100
H	0.96050700	-2.96050600	-1.68385700
C	2.51129400	0.07474200	1.35233800
C	-1.15421000	0.04746600	2.12611100
C	-3.32373600	3.60534500	-0.06068200
H	-4.10064000	4.35911400	0.01175300
C	3.74918900	-2.06329500	0.69136900
H	4.55065300	-1.78869300	1.36012900
C	1.87328400	2.31304800	-1.56092300
H	1.22178700	2.23711900	-2.42531000
C	0.01754200	-0.04932300	4.22525200
H	0.01288200	-0.09409800	5.30933000
C	3.69948100	3.28212700	-0.39155200
H	4.47214600	4.03465700	-0.27405700
C	2.85611800	3.28178900	-1.49373900
H	2.95233000	4.00736200	-2.29334900
C	2.82794600	-3.59435100	-0.88259400
H	2.84910700	-4.50291500	-1.47313000
C	-1.24212900	2.80736500	-0.88149000
H	-0.34343900	2.94767100	-1.46301700
C	-2.17103600	3.82754200	-0.80049500
H	-1.99239900	4.76085500	-1.32163200
C	3.85715300	-3.25046400	-0.02025800
H	4.72944500	-3.88419900	0.09927100
C	-3.88230000	-3.17403800	0.06132200
H	-4.76349000	-3.79527400	0.17968300
C	-1.71951200	-2.73691600	-0.81748800
H	-0.85490400	-3.05981900	-1.37654800
S	-0.79596900	0.80666000	-2.99087900
S	-0.30743200	-1.16161100	-3.13360900
H	1.24190800	-0.12119300	-1.85867400
H	-1.54842300	-1.70099300	-3.06865900

^{4}[MoSH-SH]$^{+}$

E= -2264.102123 a.u.

G= -2263.659453 a.u.

1 4

Mo	0.00128900	0.25140000	0.44466200
N	-1.64952100	1.14334600	-0.61991300
N	1.62590400	1.19638500	-0.60786700
N	1.68348700	-0.82689800	1.33832800
N	-1.62254900	-0.89681000	1.34682900
C	-2.58345700	0.35597600	-1.20330900
N	0.00978400	-1.20897300	-1.07992000
C	-2.48443100	-1.16729700	-0.97337800
C	-2.53681400	-1.48164100	0.53944700
C	2.55713600	0.43003700	-1.22531900
C	-2.71364300	3.10254300	-1.50556000
H	-2.73072100	4.18417900	-1.57164500
C	-3.59345900	0.92717100	-1.97533800
H	-4.34416800	0.31053400	-2.44834900
C	2.59466200	-1.39744400	0.51847700
C	3.70116600	-1.74753600	-1.69859000
H	3.68094700	-1.54707400	-2.77017000
H	3.69719900	-2.83002000	-1.56363900
H	4.63914200	-1.35735600	-1.30014000
C	-3.50097000	-2.33258300	1.08100300
H	-4.23545200	-2.81009500	0.44879000
C	-3.67132500	-1.85038600	-1.66280000
H	-3.63138900	-2.93292800	-1.53521600
H	-3.67335900	-1.64235500	-2.73326300
H	-4.61519700	-1.49275800	-1.24786000
C	3.60011600	-2.20397900	1.05227800
H	4.32914200	-2.67712200	0.41063200
C	1.21479600	-2.60621500	-2.60620500
H	2.15152800	-2.96583900	-3.00572700
C	-1.16963100	-2.63212700	-2.60310100
H	-2.09996100	-3.01196000	-2.99903800
C	1.19291300	-1.66587200	-1.58424600
C	1.68942500	2.54101100	-0.71967300
H	0.98505100	3.12252600	-0.12420600
C	2.50322300	-1.09802900	-0.99554000
C	-1.16430400	-1.69477500	-1.57787200
C	-3.53921900	-2.57285700	2.45012400
H	-4.29327100	-3.23389100	2.86465700
C	3.53160700	1.02417700	-2.02503100
H	4.27694100	0.42419300	-2.52703700
C	1.79669200	-0.98424100	2.67079000
H	1.08858100	-0.41786500	3.26439700
C	0.02684600	-3.09810900	-3.12735600
H	0.03383800	-3.83446000	-3.92300100
C	3.68855900	-2.40101700	2.42610900
H	4.47452800	-3.02779700	2.83472200
C	2.77746500	-1.76541900	3.25713700
H	2.82400300	-1.85636600	4.33608200
C	2.63674600	3.18001000	-1.50113300
H	2.63800000	4.26281000	-1.55149200
C	-1.68463600	-1.10473100	2.67655600
H	-0.97082300	-0.54158700	3.26599100
C	-2.61610700	-1.93875300	3.26960200
H	-2.61910200	-2.06906000	4.34557300
C	3.56870800	2.40674500	-2.17808600
H	4.33138500	2.86390800	-2.79990800
C	-3.65988400	2.30771100	-2.13582600
H	-4.45304500	2.74726100	-2.73169400
C	-1.73038100	2.48375900	-0.75271300
H	-1.00084900	3.07284900	-0.20264400
S	-0.21185100	4.72649300	1.45266300
S	0.01578000	1.89065500	2.29598300
H	0.97451300	4.83075000	2.07721700
H	-1.29497900	2.05025400	2.54796700

^{2}[MoSH-SH]$^{+}$

E= -2264.107669 a.u.
G= -2263.663548 a.u.

1 2

Mo	-0.01061600	0.30146600	0.42025000
N	-1.62834300	1.10261700	-0.75756300
N	1.60375300	1.12068500	-0.76753300
N	1.62708500	-0.74152000	1.38541600
N	-1.64670500	-0.71868900	1.37658800
C	-2.54668500	0.25891400	-1.29022400
N	0.02225600	-1.35159300	-0.97498800
C	-2.46564200	-1.24002000	-0.91549400
C	-2.57320600	-1.36355400	0.62107200
C	2.55639500	0.30000600	-1.27108000
C	-2.76200500	2.97445300	-1.75115300
H	-2.81335300	4.04981000	-1.87729100
C	-3.56041500	0.75248300	-2.11296100
H	-4.28005700	0.08506200	-2.56430000
C	2.58897900	-1.33992700	0.64019900
C	3.70457500	-1.91392400	-1.53105700
H	3.67777600	-1.83403400	-2.61890700
H	3.71443700	-2.97333100	-1.27116500
H	4.64124900	-1.47612500	-1.18406100
C	-3.60694300	-2.08144100	1.22599100
H	-4.33213800	-2.61153400	0.62552300
C	-3.64573100	-1.97806700	-1.56088500
H	-3.63983500	-3.03640300	-1.29638600
H	-3.60919000	-1.90236400	-2.64878300
H	-4.59283900	-1.55465800	-1.22497800
C	3.62879000	-2.04154000	1.25397200
H	4.38973300	-2.52843000	0.66127800
C	1.23435700	-2.92905700	-2.28751100
H	2.17099200	-3.33771100	-2.63573700
C	-1.15431200	-2.94919800	-2.29423900
H	-2.08132100	-3.37509700	-2.64725800
C	1.20375300	-1.85172300	-1.40642400
C	1.68629000	2.44608300	-1.00837100
H	0.92779000	3.06693200	-0.54243000
C	2.50474300	-1.19966500	-0.89549000
C	-1.14904300	-1.87063100	-1.41354800
C	-3.73324400	-2.11603200	2.60777700
H	-4.53887500	-2.67490700	3.07127700
C	3.57080000	0.81526500	-2.07906800
H	4.32356700	0.16770900	-2.50445300
C	1.73133200	-0.80216000	2.73338500
H	0.96209700	-0.27483600	3.28242200
C	0.04583300	-3.48380300	-2.73325400
H	0.05480100	-4.32105600	-3.42332400
C	3.71478100	-2.11274700	2.63780400
H	4.52784700	-2.65443100	3.10895100
C	2.74599700	-1.46481500	3.39495600
H	2.76754000	-1.46881800	4.47868500
C	2.68357600	3.01485100	-1.78013400
H	2.69538000	4.08789800	-1.93205200
C	-1.80185700	-0.72834000	2.72276000
H	-1.08278600	-0.13806700	3.27584600
C	-2.81653300	-1.40189400	3.37137300
H	-2.87934600	-1.36196500	4.45281600
C	3.63708800	2.17832300	-2.34364000
H	4.42816700	2.57249700	-2.97293400
C	-3.66765300	2.11540800	-2.35991300
H	-4.45429800	2.49225600	-3.00507700
C	-1.76132500	2.43117900	-0.96705300
H	-1.05486900	3.08016700	-0.45343600
S	0.05087900	4.67424400	1.23149200
S	-0.01411500	2.06270400	2.08181200
H	1.29607700	2.26420200	2.30902500
H	-1.16338300	4.81340700	1.79320700

^{4}[MoHS-SH]$^{+}$
E= -2264.063257 a.u.
G= -2263.621818 a.u.

1 4

Mo	0.02325200	0.55132800	-0.21621600
N	1.78360100	0.91570500	1.02826900
N	-1.59524300	0.98260500	1.26029500
N	-1.74230500	0.02753600	-1.41111300
N	1.46260400	-0.54082500	-1.44798800
C	2.62123000	-0.09680300	1.33529100
N	-0.12691000	-1.38257900	0.69185600
C	2.38320600	-1.46733700	0.67251300
C	2.39544000	-1.33912900	-0.86163400
C	-2.60032300	0.09297200	1.44298300
C	3.09535700	2.43740000	2.34649000
H	3.25250600	3.45295800	2.69031800
C	3.69409700	0.12848200	2.20218800
H	4.36074800	-0.67659300	2.47270600
C	-2.66647800	-0.83271800	-0.91850900
C	-3.86281600	-2.00656100	0.92827200
H	-3.87852800	-2.26315300	1.98712400
H	-3.87914600	-2.94124300	0.36732700
H	-4.77321400	-1.45022000	0.69626100
C	3.28619200	-2.06733400	-1.65229700
H	4.04141100	-2.68681800	-1.19100800
C	3.50951400	-2.41461500	1.10690300
H	3.39442000	-3.39501400	0.64607000
H	3.50498300	-2.55400400	2.18881200
H	4.48369800	-2.01693600	0.81688600
C	-3.64993000	-1.35193500	-1.76178000
H	-4.37740700	-2.05660900	-1.38701400
C	-1.43854700	-3.22915500	1.50854800
H	-2.40123900	-3.68791300	1.67901700
C	0.94340300	-3.31512700	1.65134200
H	1.84270000	-3.83981000	1.93890900
C	-1.34799700	-1.98013000	0.92888800
C	-1.55033800	2.08279500	2.04472000
H	-0.74210900	2.77210700	1.83838700
C	-2.61653900	-1.18260800	0.58006600
C	1.01917000	-2.07338300	1.04586700
C	3.22854900	-2.00511000	-3.03716700
H	3.93556800	-2.56407200	-3.64042700
C	-3.56652000	0.32043100	2.42501600
H	-4.37718100	-0.37858000	2.56820600
C	-1.84991200	0.44441100	-2.69370200
H	-1.12565800	1.19646500	-2.99190400
C	-0.28710200	-3.91755400	1.89679500
H	-0.35006800	-4.88764000	2.37441500
C	-3.73017900	-0.95380700	-3.09092500
H	-4.50597500	-1.35605200	-3.73391600
C	-2.82173300	-0.01403100	-3.56146300
H	-2.85957000	0.36533200	-4.57607900
C	-2.47532700	2.35535500	3.03364300
H	-2.38470100	3.26225300	3.62015400
C	1.39961100	-0.50320100	-2.80025200
H	0.64243400	0.14265600	-3.22406800
C	2.24713400	-1.21081900	-3.62504600
H	2.14485800	-1.12430700	-4.70029500
C	-3.51263500	1.45265200	3.22700100
H	-4.27281600	1.62367300	3.98192700
C	3.92862100	1.39342700	2.72293900
H	4.76350200	1.55833200	3.39625600
C	2.04088600	2.15454200	1.49923700
H	1.37734700	2.93848000	1.15325000
S	0.27546800	4.28333200	-1.32793000
S	0.78319300	2.31496400	-1.85010200
H	-0.05781400	2.15134900	0.15203600
H	-1.04235000	4.26306700	-1.61854900

^{2}[MoHS-SH]$^{+}$
E= -2264.097568 a.u.
G= -2263.652607 a.u.

1 2

Mo	-0.00572900	0.41867100	-0.40871000
N	1.58064500	1.09755100	0.95132900
N	-1.61968900	1.14878900	0.89674400
N	-1.62942900	-0.56719700	-1.41900200
N	1.63094000	-0.64164900	-1.35291800
C	2.46786800	0.20774700	1.44353200
N	-0.09393400	-1.32289600	0.90145100
C	2.40093100	-1.25062300	0.93769900
C	2.55366200	-1.29245600	-0.59855000
C	-2.58230600	0.30119400	1.32015900
C	2.64413000	2.86471100	2.18630400
H	2.68303000	3.92104700	2.42546200
C	3.44350000	0.61972300	2.35554900
H	4.14980000	-0.08497600	2.76830300
C	-2.63084400	-1.17625000	-0.74114300
C	-3.78954000	-1.89514000	1.36121100
H	-3.76218300	-1.93041300	2.45153600
H	-3.83041800	-2.92115100	0.99411600
H	-4.71277400	-1.39805700	1.05990100
C	3.60029700	-1.99120800	-1.20313500
H	4.33642800	-2.50412000	-0.60167300
C	3.54967500	-2.04205700	1.57781700
H	3.56425500	-3.07350800	1.22531700
H	3.45443000	-2.05974800	2.66469000
H	4.51148300	-1.59249000	1.32782700
C	-3.67937600	-1.79156100	-1.43007800
H	-4.47577800	-2.28424600	-0.89122500
C	-1.34555100	-3.05574500	1.97679700
H	-2.29536700	-3.49412300	2.24369100
C	1.03453300	-3.09284300	2.04634100
H	1.95036000	-3.56313700	2.37020300
C	-1.28424600	-1.87242800	1.24741300
C	-1.69473700	2.44883800	1.24194500
H	-0.96076900	3.09829700	0.78016600
C	-2.56773300	-1.15595800	0.80053400
C	1.05952700	-1.90998700	1.31341100
C	3.72754200	-2.03127000	-2.58470300
H	4.54731200	-2.57184700	-3.04505300
C	-3.58679600	0.75611100	2.17959200
H	-4.35113200	0.08426800	2.54097600
C	-1.70284000	-0.51589400	-2.76987400
H	-0.92110200	0.05465100	-3.25642000
C	-0.17604100	-3.67677700	2.38039300
H	-0.20687600	-4.59400700	2.95859900
C	-3.72629800	-1.76782900	-2.81665000
H	-4.54424000	-2.24439500	-3.34587900
C	-2.71572300	-1.10065300	-3.50136900
H	-2.71164700	-1.02238000	-4.58253100
C	-2.66802200	2.95905800	2.08105100
H	-2.67174700	4.01539600	2.32347900
C	1.77583600	-0.67519700	-2.70000300
H	1.05777500	-0.09568000	-3.26369000
C	2.78888800	-1.35172800	-3.34943400

H	2.83808400	-1.32816200	-4.43196700
C	-3.62468800	2.08514600	2.57934700
H	-4.40371700	2.42989000	3.25138000
C	3.52838600	1.95077900	2.74222400
H	4.28495300	2.26391900	3.45417100
C	1.69697100	2.39411100	1.29584900
H	1.01049700	3.07167300	0.80663700
S	-0.07342700	4.03256400	-1.84514800
S	0.93209400	2.17459200	-1.86638000
H	-0.96641200	1.53070400	-1.12629400
H	-1.13406100	3.74085800	-2.62808400

^{4}[Mo(SH)$_2$]$^+$

E= -2264.129106 a.u.

G= -2263.688369 a.u.

1 4

Mo	0.34039700	0.10187200	-0.88674200
N	1.87943300	1.42998300	0.01530400
N	-1.25680400	1.57186300	-0.45159600
N	-3.57941600	-1.86671700	0.75455800
N	2.04467900	-1.26818900	-0.94814700
C	2.60133200	0.96858100	1.05738800
N	0.05364700	-0.43184900	1.26140200
C	2.55013400	-0.54602400	1.35758300
C	2.92010600	-1.31972200	0.07577500
C	-2.02836800	1.52591500	0.66738700
C	2.81386000	3.61909900	0.29236200
H	2.88818300	4.64013200	-0.06332900
C	3.40662200	1.84332400	1.78668500
H	3.96635100	1.49648600	2.64342800
C	-3.33909400	-0.61678200	0.36320800
C	-3.25764700	0.41715500	2.56974500
H	-2.70344600	0.93042200	3.36116200
H	-3.62258800	-0.53309300	2.95204300
H	-4.14859700	0.99279200	2.31304600
C	4.09554600	-2.05861800	-0.03850400
H	4.81092100	-2.09166300	0.77128700
C	3.56808800	-0.86944000	2.46157400
H	3.66846400	-1.94476900	2.60600300
H	3.26296800	-0.42958000	3.41312400
H	4.55662700	-0.48607000	2.20415500
C	-4.00677500	-0.02583000	-0.70961900
H	-3.82433700	1.00403200	-0.99281600
C	-1.36535300	-1.68187900	2.69744600
H	-2.36028900	-1.96006500	3.00606200
C	1.00779700	-1.95958100	2.81989200
H	1.86965000	-2.42744400	3.27297400
C	-1.18352200	-0.67704900	1.74374400
C	-1.20356700	2.71918500	-1.16270600
H	-0.62952300	2.65710800	-2.08383500
C	-2.39115300	0.17527900	1.30509700
C	1.14414900	-0.99142600	1.83270800
C	4.35640900	-2.76841400	-1.20641200
H	5.27146100	-3.34452800	-1.29824000
C	-2.60554100	2.70510100	1.14463600
H	-3.16934200	2.69870900	2.06511400
C	-4.44465100	-2.59937400	0.05469600
H	-4.59702100	-3.61947800	0.39943500
C	-0.26677700	-2.34631400	3.21030200
H	-0.39871600	-3.14125700	3.93701900
C	-4.92081400	-0.79379900	-1.42521400
H	-5.45405700	-0.36199400	-2.26661300
C	-5.13751700	-2.11405500	-1.05031300
H	-5.83367500	-2.74906800	-1.58679500
C	-1.82013200	3.89521200	-0.76890800
H	-1.74647900	4.77780800	-1.39399200
C	2.28881100	-1.96579900	-2.07383300
H	1.52934200	-1.88917500	-2.84104700
C	3.43033800	-2.73298100	-2.23852400
H	3.58172800	-3.27795500	-3.16275600
C	-2.49544200	3.89931200	0.44079300
H	-2.95769800	4.80260700	0.82571500
C	3.50664900	3.17915900	1.41131900
H	4.13544200	3.85658000	1.97982100
C	2.00832900	2.70983000	-0.37286900
H	1.45023200	2.99113200	-1.25893000
S	-1.02283600	-1.70143000	-1.72790400
S	0.93930000	0.96259600	-3.09063000
H	-1.88601200	-1.01467400	-2.49912600
H	-0.00137600	0.37970000	-3.85649500

^{2}[Mo(SH)$_2$]$^+$

E= -2264.116666 a.u.

G= -2263.668530 a.u.

1 2

Mo	-0.00684500	0.01157900	-0.76066300
N	1.44818900	1.58609200	-0.14601600
N	-1.70134000	1.30276100	-0.69008100
N	-1.37245700	-1.62523500	-0.03490700
N	1.68884600	-1.32642600	-0.66043400
C	2.51902400	1.27343600	0.61083400
N	-0.00469700	0.05391600	1.45138300
C	2.48348600	-0.08318000	1.34183100
C	2.59072500	-1.25312700	0.33924400
C	-2.63244200	1.23014400	0.28875700
C	2.30910300	3.80983900	-0.44196100
H	2.16339300	4.80059600	-0.85599700
C	3.54902800	2.19290500	0.80324800
H	4.42487500	1.92721700	1.37782400
C	-2.47144300	-1.29262000	0.66588500
C	-3.68194600	0.16571500	2.29895700
H	-3.69212700	1.10973000	2.84637800
H	-3.64339100	-0.65061700	3.02148200
H	-4.62541100	0.08925900	1.75752000
C	3.63958400	-2.17430400	0.40543300
H	4.34948400	-2.15339500	1.21935100
C	3.66407400	-0.15799700	2.31907400
H	3.62674000	-1.07393900	2.91194200
H	3.66544000	0.69200500	3.00191800
H	4.61102800	-0.14760800	1.77829600
C	-3.49387800	-2.22116900	0.85607700
H	-4.40074400	-1.94684400	1.37588900
C	-1.19168000	0.28950500	3.50814400
H	-2.11943400	0.43428000	4.04058000
C	1.17254100	-0.01277200	3.52578800
H	2.09556100	-0.12421300	4.07413100
C	-1.17585800	0.18265600	2.11978000
C	-1.87850000	2.21075000	-1.68155100
H	-1.12640600	2.18150600	-2.46545300
C	-2.49614600	0.10115400	1.32769000
C	1.16079000	-0.04594300	2.13347800
C	3.79812600	-3.13069100	-0.58978000
H	4.61448500	-3.84321500	-0.53385100
C	-3.69768400	2.13158600	0.32391900
H	-4.42846300	2.09209900	1.11869400
C	-1.21611200	-2.89305700	-0.45011700
H	-0.30013200	-3.11160300	-0.98282600
C	-0.00989600	0.17781300	4.21977000
H	-0.01166500	0.22754200	5.30357800
C	-3.35068000	-3.52080100	0.38450900
H	-4.14704900	-4.24333600	0.52956000
C	-2.16937700	-3.87635900	-0.24841900
H	-1.99047600	-4.88297200	-0.60737400
C	-2.92560400	3.11156300	-1.70839500
H	-3.00567500	3.81255600	-2.53156300
C	1.87313400	-2.22393200	-1.65258100
H	1.13795800	-2.17619600	-2.45286300
C	2.91119300	-3.13805800	-1.65823600
H	3.00950700	-3.83707500	-2.48089300
C	-3.84984200	3.08785600	-0.67168900
H	-4.68229400	3.78238100	-0.64172500
C	3.45696600	3.46748500	0.25720800
H	4.26186700	4.18115700	0.39803200
C	1.33840900	2.84054700	-0.62591700
H	0.44031100	3.05819900	-1.18713000
S	-1.25674200	-1.07994900	-2.72358700
S	1.18757300	0.94310600	-2.78588100
H	-1.37142300	-0.05688500	-3.58785400
H	0.77784900	0.13110000	-3.77378700

^{2}[MoHSH-S]$^+$

E= -2264.067640 a.u.

G= -2263.620094 a.u.

1 2

Mo	-0.01751700	0.07512500	-0.64009600
N	1.56166900	1.35944400	0.07939600
N	-1.57283600	1.64729700	-0.48531100
N	-1.69421400	-1.24044700	-1.01363700
N	1.42303200	-1.48543500	-0.21370500
C	2.21450400	1.05051700	1.22584000
N	-0.57942600	-0.17947400	1.43502100
C	1.87195500	-0.28532400	1.91926800
C	2.12309000	-1.45837400	0.94725800
C	-2.77236500	1.35070800	0.05843800
C	2.92872200	3.33206200	-0.15955100
H	3.19247800	4.19225600	-0.76321000
C	3.18950600	1.90337400	1.73460500
H	3.69698100	1.67675900	2.66018300
C	-2.83876900	-1.16729000	-0.29684300
C	-4.34969000	-0.08205900	1.37856300
H	-4.47837400	0.72102000	2.10609400
H	-4.50576400	-1.03135700	1.89209200
H	-5.13043600	0.01554600	0.62297300
C	3.03166600	-2.47293600	1.25086700
H	3.59064700	-2.44889500	2.17444300
C	2.77926200	-0.44997000	3.14622400
H	2.59119500	-1.39614700	3.65478100
H	2.61824800	0.35618100	3.86352300
H	3.82842200	-0.43310200	2.84917700
C	-3.86852200	-2.08754800	-0.50709100
H	-4.77577500	-2.04143500	0.07795800
C	-2.23680700	-0.41243800	3.14437800
H	-3.27376700	-0.43676200	3.44362000
C	0.07396900	-0.53023100	3.70681300
H	0.84756200	-0.64643800	4.45018800
C	-1.88139600	-0.21246500	1.81412700
C	-1.39295500	2.85509600	-1.04940000
H	-0.41455000	3.03082500	-1.47449300
C	-2.95930200	-0.02729800	0.73299200
C	0.39785200	-0.32791700	2.36836100
C	3.24862300	-3.52195400	0.36840900

H	3.96387300	-4.30115200	0.60806100
C	-3.81133600	2.28443400	0.01599200
H	-4.77858800	2.05390900	0.43747800
C	-1.61503600	-2.15992300	-2.00290700
H	-0.72386200	-2.11071700	-2.61727200
C	-1.25199900	-0.56984700	4.10383400
H	-1.51291200	-0.71291700	5.14691700
C	-3.75309800	-3.06589900	-1.48482500
H	-4.55634700	-3.77628900	-1.64720000
C	-2.60287400	-3.08720700	-2.26564800
H	-2.47054600	-3.79957900	-3.07186000
C	-2.37652300	3.82529500	-1.11249700
H	-2.16705000	4.77896100	-1.58287900
C	1.65073800	-2.50752800	-1.07016500
H	1.11117000	-2.47220700	-2.00590400
C	2.53920300	-3.53483300	-0.82393400
H	2.67353000	-4.31460200	-1.56443600
C	-3.61905800	3.52808700	-0.57102200
H	-4.43042800	4.24784500	-0.60137300
C	3.53204900	3.07136100	1.05540200
H	4.27911600	3.74130700	1.46775500
C	1.97931600	2.43336800	-0.62323600
H	1.49413000	2.59391400	-1.57595100
S	3.31161000	0.61484300	-2.63991800
S	1.35167500	0.08368100	-2.77040800
H	0.79883400	0.96585000	-3.63549300
H	-0.69656100	0.46635100	-2.10381300

Com-I
E= -2416.967691 a.u.
G= -2416.491013 a.u.

2 3

Mo	-0.09369700	-0.21823900	-0.15937200
N	0.30917000	1.51265300	-1.41136400
N	-1.42765100	-1.32239800	-1.49745000
N	-0.74893600	-1.82276600	1.17531900
N	0.98329700	1.00751600	1.27467700
C	0.02787800	2.75445200	-0.95559200
N	-1.86826200	0.85937400	0.49159000
C	-0.43659400	2.90514600	0.51253200
C	0.63581500	2.30256000	1.45118400
C	-2.67973800	-1.62635800	-1.08674600
C	0.98783000	2.41107300	-3.53028300
H	1.38942300	2.22934300	-4.52014400
C	0.18992600	3.85537100	-1.79390900
H	-0.03654800	4.85367000	-1.44923200
C	-2.07039600	-2.07148700	1.31853000
C	-4.47697300	-1.86429800	0.64571200
H	-5.20597800	-1.37792900	-0.00351400
H	-4.78164900	-1.68596800	1.67766000
H	-4.52656900	-2.93840500	0.46138000
C	1.26243000	3.06196400	2.43671500
H	0.99334000	4.09586800	2.59543800
C	-0.59641300	4.39731800	0.83233600
H	-0.91415000	4.54771400	1.86488800
H	-1.34024200	4.86228700	0.18417400
H	0.34818000	4.92485700	0.69214300
C	-2.50369700	-3.00499700	2.25876500
H	-3.55553000	-3.20992600	2.39395000
C	-4.17716200	0.86478600	1.07329900
H	-5.11392500	0.34646300	1.21187000
C	-2.91803600	2.89733000	1.13654700
H	-2.87438300	3.95962800	1.32439900
C	-3.03226400	0.18967500	0.65994000
C	-1.03478800	-1.65870900	-2.74194500
H	0.00509600	-1.46179000	-2.97346900
C	-3.06072300	-1.33241800	0.38538200
C	-1.79271400	2.19139800	0.72106600
C	2.25924700	2.49962300	3.22900200
H	2.74323200	3.09628600	3.99524300
C	-3.57422600	-2.22649700	-1.97154200
H	-4.58065100	-2.46939200	-1.66371000
C	0.14384700	-2.52846200	1.89766400
H	1.18551800	-2.33854800	1.66894400
C	-4.11870700	2.22852700	1.31346600
H	-5.00367100	2.76653500	1.63673400
C	-1.58178100	-3.70228700	3.03344300
H	-1.92560500	-4.42841100	3.76278700
C	-0.22758800	-3.47251000	2.83877200
H	0.53159800	-4.01414300	3.39080000
C	-1.87640100	-2.26160300	-3.66016600
H	-1.50836000	-2.51361200	-4.64784700
C	1.97808800	0.47828400	2.01322000
H	2.26004700	-0.53703300	1.76606200
C	2.63458600	1.18347800	3.00677400
H	3.42723500	0.70880900	3.57291800
C	-3.17874200	-2.53683100	-3.26913000
H	-3.87981800	-3.00490800	-3.95235000
C	0.66056800	3.68568900	-3.09274200
H	0.78469000	4.54702700	-3.74088500
C	0.80506900	1.35535000	-2.65450000
H	1.08457500	0.34490000	-2.92524000
S	3.43324800	-0.08138000	-1.00777900
S	1.84178200	-1.43758900	-0.87728500
O	9.06368500	-1.84286200	1.04753900
H	9.34798000	-2.74635000	1.23703300
H	9.75922000	-1.47629300	0.48641100
H	7.70933000	-2.10463700	-0.10006600
H	4.41750000	-1.05413700	-1.21509000
O	5.49376300	-2.31588000	-1.41605900
H	5.79485300	-2.43963700	-2.32369400
H	6.31708200	-2.23685400	-0.88093900

TS-I
E= -2416.952256 a.u.
G= -2416.477589 a.u.

2 3

Mo	0.01692300	-0.17910200	-0.05304600
N	-0.60432500	1.30887500	1.40369200
N	0.65663500	-1.76687900	1.31481100
N	0.92512600	-1.56190100	-1.48320700
N	-0.33293100	1.50365700	-1.37565500
C	-0.02889300	2.53249500	1.40145000
N	2.02677200	0.62416200	0.20194800
C	0.95248100	2.87603200	0.25499600
C	0.22298900	2.70467300	-1.09919500
C	1.92330800	-2.23582800	1.25282900
C	-1.91231700	1.89457100	3.32746900
H	-2.67398700	1.60872000	4.04310800
C	-0.35642300	3.45608300	2.39142900
H	0.09990600	4.43481300	2.41024500
C	2.16655900	-2.04614200	-1.25434000
C	4.17679600	-2.47859900	0.18051000
H	4.67770400	-2.29532600	1.13184600
H	4.84995500	-2.15687600	-0.61507600
H	4.02880400	-3.55493500	0.08073700
C	0.09198100	3.75547200	-2.00402800
H	0.53757600	4.71900100	-1.80444900
C	1.39217400	4.33916700	0.39944400
H	2.07914800	4.62478400	-0.39822200
H	1.89906000	4.50688300	1.35062200
H	0.53041000	5.00659700	0.35548500
C	2.79721200	-2.82815900	-2.22133900
H	3.79102600	-3.21802700	-2.05760500
C	4.37462000	0.28396700	0.41882500
H	5.23033400	-0.37289400	0.45862400
C	3.47096100	2.49649900	0.49026800
H	3.62266400	3.56128600	0.58454600
C	3.08709100	-0.21599200	0.24748600
C	-0.18382600	-2.24447700	2.25378300
H	-1.20327000	-1.88329000	2.19372500
C	2.83541300	-1.73599700	0.10670800
C	2.19715600	1.96215100	0.31843100
C	-0.63200000	3.58195700	-3.18051600
H	-0.72966500	4.40363100	-3.88240700
C	2.36682600	-3.16766000	2.19045500
H	3.37645600	-3.55015500	2.15821500
C	0.28536000	-1.88632600	-2.62404800
H	-0.73342400	-1.52822400	-2.70458600
C	4.56739900	1.65091800	0.54188300
H	5.56551200	2.05423200	0.67643800
C	2.14906600	-3.12975200	-3.41473200
H	2.64578600	-3.73874400	-4.16289300
C	0.85961000	-2.65953800	-3.61737100
H	0.30018500	-2.88979000	-4.51653900
C	0.19984400	-3.16935500	3.20883500
H	-0.51713500	-3.51974500	3.94206300
C	-1.07792800	1.35376800	-2.48718200
H	-1.57066400	0.39664000	-2.59846700
C	-1.24341400	2.36147700	-3.42196000
H	-1.85034800	2.18803300	-4.30262100
C	1.50777500	-3.63106400	3.18182500
H	1.85939200	-4.35577100	3.90886200
C	-1.29283700	3.13411300	3.36977400
H	-1.54325900	3.85760900	4.13866400
C	-1.54636600	1.01745800	2.32090500
H	-2.02919500	0.05499400	2.20975900
S	-3.54891900	0.39689300	-0.37995700
S	-2.16062300	-1.14483600	-0.30319800
O	-8.76568500	-2.38196100	0.88028300
H	-9.24236800	-1.59122700	1.17137700
H	-9.35388000	-2.82251000	0.24991700
H	-7.53182900	-1.79341400	-0.02750000
H	-5.01723700	-0.53914700	-0.83403200
O	-5.85535200	-1.04553100	-1.29961300
H	-5.50605900	-1.85239000	-1.71135100
H	-6.78405800	-1.43231600	-0.56210700

^{3}[MoS-S]$^{2+}$-2H$_2$O
E= -2415.825686 a.u.
G= -2415.352814 a.u.

2 3

Mo	-0.01307800	-0.05048400	0.44142200
N	-2.10774600	-0.18748400	1.02729100
N	0.48208900	1.84094100	1.44087700
N	1.97978900	0.28801000	-0.37971500
N	-0.60920200	-1.70916400	-0.81653800
C	-3.07393900	-0.25613400	0.08395000
N	-0.73556300	1.21002900	-1.20796600
C	-2.64273600	-0.39097400	-1.39511100
C	-1.74940800	-1.64551700	-1.54321300
C	0.94951000	2.87858100	0.70971700

C	-3.76566100	-0.17779400	2.76459900
H	-3.98495500	-0.17101300	3.82581200
C	-4.41543700	-0.24952400	0.46096300
H	-5.19984600	-0.29375100	-0.28033100
C	2.29394800	1.49144500	-0.91307000
C	1.88080100	3.92252100	-1.37142200
H	1.18987100	4.76320500	-1.29716200
H	2.13245600	3.79141700	-2.42439000
H	2.79469200	4.19025000	-0.83946700
C	-2.10641900	-2.70576400	-2.37097900
H	-3.01102500	-2.67007200	-2.95996500
C	-3.89526300	-0.56120200	-2.26574000
H	-3.63008500	-0.68179600	-3.31687000
H	-4.55363300	0.30475500	-2.18405500
H	-4.46158800	-1.44203000	-1.96070400
C	3.53154200	1.67851100	-1.52419600
H	3.79707200	2.63021800	-1.96036700
C	-0.46191800	3.10621500	-2.61745100
H	0.08894500	3.98367500	-2.92110200
C	-2.33964500	1.65088100	-2.90829200
H	-3.24682100	1.39680600	-3.43533500
C	-0.02724100	2.30423700	-1.56564700
C	0.28463600	1.99905400	2.76517400
H	-0.02424600	1.11482900	3.30805000
C	1.26618400	2.64282100	-0.78733500
C	-1.87483000	0.87135600	-1.85215900
C	-1.30317500	-3.84169300	-2.44448900
H	-1.58954100	-4.66563400	-3.09003100
C	1.16876500	4.11389600	1.31840800
H	1.53444600	4.95519600	0.74840200
C	2.88883200	-0.70954000	-0.39822800
H	2.62428500	-1.64437900	0.09169500
C	-1.62593200	2.77469300	-3.29245100
H	-1.97596700	3.39060900	-4.11439100
C	4.45623500	0.63857200	-1.57344600
H	5.41775700	0.79422000	-2.05210300
C	4.13540700	-0.57675500	-0.98880000
H	4.81867400	-1.42091700	-0.96723800
C	0.49205100	3.19741300	3.42392100
H	0.32030800	3.26529400	4.49179900
C	0.15641500	-2.81779200	-0.86863500
H	1.04638400	-2.85831100	-0.24810400
C	-0.15381800	-3.90148300	-1.67431300
H	0.50190800	-4.76391400	-1.67198200
C	0.93145200	4.28202400	2.67865700
H	1.10630900	5.24604500	3.14504800
C	-4.76785000	-0.19947300	1.80624400
H	-5.81428900	-0.19593100	2.09324000
C	-2.45225200	-0.17954400	2.32985700
H	-1.63437200	-0.19740000	3.03796400
S	-0.29561200	-2.93006100	2.58828800
S	0.84365100	-1.32852300	2.26081400
O	5.42432800	-3.65326300	-0.30667600
H	5.68746000	-4.28985300	-0.98169200
H	6.10664900	-3.71033600	0.37245100
H	2.68907200	-4.03379100	1.38985600
O	2.77394700	-3.70408300	0.48915700
H	3.71741600	-3.80147600	0.24903100

Com-II

E= -2493.585987 a.u.

G= -2493.089970 a.u.

2 3

Mo	0.37982200	-0.24458100	0.08538800
N	-0.29052100	1.27935300	1.48264300
N	1.68612800	-1.38996100	1.41207200
N	1.29452800	-1.60810400	-1.36165100
N	-0.68144900	1.06217800	-1.28783400
C	-0.08085200	2.58621500	1.20509100
N	2.10029900	1.04278500	-0.25969800
C	0.49843800	2.95477400	-0.18214700
C	-0.42870200	2.39057700	-1.28517700
C	2.99142400	-1.54372800	1.09352400
C	-1.23797800	1.85159000	3.61121800
H	-1.71121200	1.51734200	4.52685600
C	-0.41655500	3.55831400	2.14495900
H	-0.24986300	4.60644900	1.94386400
C	2.64026000	-1.73528800	-1.39815900
C	4.94841900	-1.42588400	-0.46925800
H	5.57053500	-0.96850600	0.30096100
H	5.32652500	-1.09816000	-1.43832700
H	5.07661200	-2.50745900	-0.40684400
C	-1.02603200	3.21321400	-2.23752300
H	-0.83010400	4.27532600	-2.25543200
C	0.54881700	4.48315900	-0.30933300
H	0.94503600	4.78526100	-1.27957000
H	1.18488000	4.92216900	0.46026000
H	-0.44925600	4.91092400	-0.20524900
C	3.23887900	-2.50474700	-2.39469800
H	4.31262400	-2.61099000	-2.44439000
C	4.44265500	1.30285500	-0.60404600
H	5.43092500	0.88118200	-0.70979500
C	3.01647800	3.22200000	-0.54997600
H	2.89419700	4.29283800	-0.61287100
C	3.33100900	0.49354600	-0.38853100
C	1.21792300	-1.90352400	2.56692400
H	0.14850300	-1.81880800	2.71686700
C	3.47272700	-1.04368500	-0.29070400
C	1.92654900	2.38292800	-0.33653900
C	-1.90006100	2.67666600	-3.17879000
H	-2.36165700	3.32217500	-3.91880600
C	3.85528400	-2.17411300	1.98792800
H	4.90214500	-2.29942600	1.75336200
C	0.53808100	-2.27881000	-2.25294900
H	-0.53270600	-2.19908600	-2.11058200
C	4.28347400	2.67727400	-0.68498100
H	5.14168600	3.31962900	-0.85205100
C	2.45746100	-3.16296600	-3.33926400
H	2.92964300	-3.76089200	-4.11188400
C	1.07625900	-3.06131600	-3.25943700
H	0.42169400	-3.58107100	-3.94926300
C	2.02684400	-2.54301200	3.48966200
H	1.59829800	-2.93904500	4.40288500
C	-1.56437900	0.55287900	-2.16839200
H	-1.78411100	-0.50113600	-2.05586700
C	-2.18717500	1.32087900	-3.13694300
H	-2.88792100	0.86080800	-3.82345200
C	3.37752700	-2.66690900	3.19822800
H	4.05522100	-3.15714800	3.88944900
C	-0.98680600	3.19206200	3.36074400
H	-1.24574900	3.95368600	4.08892100
C	-0.88309800	0.93047700	2.64110800
H	-1.09661700	-0.12391800	2.76149600
S	-3.20789900	-0.52581700	0.61729200
S	-1.48476700	-1.69984300	0.44554600
O	-10.04874300	0.69320100	-0.58485400
H	-10.69482700	0.39744200	-1.23907300
H	-10.54124900	0.74033400	0.24466700
H	-9.05951800	-0.79351800	-0.32137600
H	-4.11985200	-1.64697700	0.63735700
O	-4.95582700	-2.90840100	0.61781800
H	-4.96984800	-3.32206300	1.48805700
H	-8.06819600	-2.03073400	-0.02542800
O	-7.52765600	-2.83819200	0.11840500
H	-5.91464000	-2.80748700	0.36258200
H	-7.85739500	-3.48536400	-0.51391400

TS-II

E= -2493.570302 a.u.

G= -2493.074151 a.u.

2 3

Mo	-0.33191200	-0.23648900	-0.07006300
N	0.34257500	1.30604600	-1.43944500
N	-1.55234400	-1.42482300	-1.44504500
N	-1.26295100	-1.61385900	1.35471000
N	0.63011700	1.11832400	1.32476500
C	0.05624000	2.60317300	-1.18794700
N	-2.12036600	0.98985000	0.20111800
C	-0.59057400	2.95766700	0.17313600
C	0.31865300	2.43400500	1.31097700
C	-2.86197400	-1.62615600	-1.17559000
C	1.37133500	1.90512600	-3.52148200
H	1.91086200	1.58707700	-4.40568600
C	0.38363200	3.58117800	-2.12447200
H	0.15260700	4.62118700	-1.94594100
C	-2.60228300	-1.79679300	1.33367300
C	-4.88016300	-1.58219400	0.31003600
H	-5.48822100	-1.14772900	-0.48418700
H	-5.30708700	-1.26730800	1.26284100
H	-4.96593000	-2.66786800	0.24484700
C	0.84763400	3.28359600	2.28000600
H	0.60227700	4.33548300	2.29089000
C	-0.70104200	4.48344400	0.28766500
H	-1.14201000	4.77617500	1.24134400
H	-1.32634400	4.89386500	-0.50618200
H	0.28357600	4.94738200	0.21502200
C	-3.21304900	-2.57937200	2.31315400
H	-4.28228700	-2.73232000	2.31425600
C	-4.48302900	1.16422900	0.45642600
H	-5.45806300	0.70579600	0.52585200
C	-3.12826500	3.13443300	0.44992800
H	-3.04810400	4.20930700	0.51378100
C	-3.33435500	0.39711800	0.28559700
C	-1.02745200	-1.90776000	-2.58867600
H	0.04206300	-1.78015700	-2.70230700
C	-3.41410100	-1.14498100	0.18832200
C	-2.00098200	2.33569500	0.27945300
C	1.71707500	2.78783300	3.24755300
H	2.12312700	3.45323900	4.00236600
C	-3.67080700	-2.27963500	-2.10491700
H	-4.71996900	-2.44477500	-1.90845500
C	-0.52204600	-2.23563900	2.29304900
H	0.54933800	-2.10797200	2.20044000
C	-4.37873100	2.54384500	0.53935700
H	-5.26581000	3.15406600	0.67212900
C	-2.44973000	-3.18847600	3.30377400
H	-2.93127600	-3.79620300	4.06281000
C	-1.07223000	-3.02377400	3.28831600
H	-0.42938400	-3.50066500	4.01890900
C	-1.78033800	-2.56455900	-3.54581600
H	-1.30690600	-2.93247700	-4.44857300
C	1.51781100	0.65269800	2.22385500
H	1.79688700	-0.38738900	2.11513600
C	2.07315000	1.44886000	3.21125100
H	2.77639600	1.02287200	3.91691900
C	-3.13438700	-2.74271200	-3.30188800

H	-3.76935800	-3.25064600	-4.02033300
C	1.03059200	3.23146500	-3.30650600
H	1.28082800	3.99689700	-4.03374800
C	1.02003100	0.97711200	-2.55582500
H	1.30373500	-0.06362100	-2.64494200
S	3.27306800	-0.49106300	-0.46078800
S	1.56544200	-1.63855700	-0.35622400
O	9.11610000	0.80290500	0.34780800
H	9.89531900	0.62450700	0.89322200
H	9.46028200	0.96299700	-0.54226700
H	8.40288000	-0.74576900	0.16799500
H	4.58879400	-2.07933900	-0.28655700
O	5.14521600	-2.91757700	-0.23955300
H	4.85862100	-3.46110500	-0.98330500
H	8.02520000	-1.65907300	0.01284800
O	7.58219700	-2.79709800	-0.15027200
H	6.49942800	-2.79395900	-0.18675200
H	7.86169300	-3.29717100	0.63144400

^{3}[MoS-S]$^{2+}$-3H$_2$O
E= -2492.437168 a.u.
G= -2491.946937 a.u.

2 3

Mo	0.21128400	-0.16291400	0.37072200
N	-0.27558200	1.59348400	1.56585900
N	2.25758100	-0.47865400	1.11044000
N	0.87158900	-1.70749100	-1.02733300
N	-1.66385200	0.37176800	-0.56661500
C	-0.64152900	2.74377500	0.95700300
N	1.12326900	1.25993500	-1.03017500
C	-0.84397800	2.72720100	-0.57546600
C	-1.90058700	1.65448000	-0.93329700
C	3.29296600	-0.46005700	0.24092700
C	-0.40924900	2.65486800	3.71568200
H	-0.32854400	2.56352900	4.79244000
C	-0.86649900	3.89043100	1.71640800
H	-1.15033200	4.81962200	1.24448000
C	2.06730600	-1.58544300	-1.65132400
C	4.29585200	-0.50451600	-2.05583900
H	4.96882500	0.31957600	-1.81555700
H	4.11639600	-0.48531400	-3.13137600
H	4.80952600	-1.43722200	-1.81930100
C	-3.08274600	1.98699200	-1.58778200
H	-3.28182100	3.00468200	-1.89000500
C	-1.35416900	4.10358600	-1.02327100
H	-1.52742600	4.12745900	-2.09964200
H	-0.63544500	4.88818000	-0.78240700
H	-2.29547500	4.34543700	-0.52847400
C	2.46685300	-2.53936500	-2.58358400
H	3.41480700	-2.45416000	-3.09390100
C	2.87088300	1.82750400	-2.54034200
H	3.80463600	1.59652000	-3.03011500
C	1.03845700	3.32879600	-2.20067100
H	0.54830900	4.26391500	-2.42589900
C	2.29567900	0.94879600	-1.62645600
C	2.50193900	-0.63929700	2.42652100
H	1.63122600	-0.71924300	3.06435000
C	2.97972000	-0.39295900	-1.27312400
C	0.49050800	2.42528900	-1.29377000
C	-4.03719800	1.00861100	-1.85476200
H	-4.97005200	1.23727500	-2.36161000
C	4.60144200	-0.54343000	0.71589900
H	5.44003100	-0.52030900	0.03580300
C	0.09017200	-2.77812300	-1.28255400
H	-0.84388500	-2.88101700	-0.73395000
C	2.23468600	3.02427500	-2.82961200
H	2.67136900	3.71781300	-3.54079500
C	1.65119200	-3.63189800	-2.86600900
H	1.97098000	-4.37354400	-3.59082700
C	0.44573500	-3.75802500	-2.19538200
H	-0.21970100	-4.59851500	-2.35234800
C	3.77646900	-0.73694800	2.95451300
H	3.91217600	-0.86937100	4.02151900
C	-2.60170800	-0.57312800	-0.79874000
H	-2.41080200	-1.58680100	-0.45381400
C	-3.79416900	-0.29177400	-1.44433600
H	-4.52931400	-1.06824200	-1.61949900
C	4.85026900	-0.67189500	2.07829700
H	5.87115200	-0.73806000	2.44001600
C	-0.74122200	3.85328200	3.10169400
H	-0.91899400	4.74962500	3.68681300
C	-0.19190800	1.55156600	2.90976900
H	0.03654400	0.58700200	3.34306600
S	-2.40568400	-1.13710300	2.69880000
S	-0.68998100	-1.75376200	1.89101700
O	-6.63942600	-0.31843900	-2.78377900
H	-6.89650300	-0.54892300	-3.68275000
H	-7.47238900	-0.25719500	-2.30432600
H	-2.96173200	-3.59354600	2.87131200
O	-2.89288700	-4.39897700	2.33661200
H	-3.52141600	-5.02704900	2.70719200
O	-2.67004900	-3.63833300	-0.23292600
H	-2.78145600	-3.97565100	0.68821700
H	-3.27711300	-4.15311000	-0.77285200

Com-III

E= -2417.570020 a.u.
G= -2417.081581 a.u.

2 2

Mo	0.08605000	-0.18989100	0.30443200
N	1.06204500	-1.77090200	-0.82470200
N	-1.60924900	0.17679300	-1.00261800
N	-0.68611600	1.62351200	1.28186100
N	1.93348200	-0.39214900	1.48106200
C	2.34555500	-1.60785500	-1.22406600
N	1.16783700	1.17844200	-0.93479800
C	3.11782000	-0.36999800	-0.70947500
C	3.12240300	-0.37153300	0.83632600
C	-1.83636900	1.41805300	-1.48700800
C	0.93185300	-3.83774100	-2.04668000
H	0.34204800	-4.70402200	-2.32296200
C	2.94445300	-2.54822500	-2.06182800
H	3.96771900	-2.42891500	-2.38629600
C	-0.99499500	2.70081000	0.52388300
C	-1.38142500	3.87221600	-1.66150700
H	-1.34601000	3.80713600	-2.74976700
H	-0.75335500	4.71018700	-1.35761900
H	-2.40820700	4.10073500	-1.37222100
C	4.31214000	-0.38703000	1.56494500
H	5.26826900	-0.35849800	1.06363400
C	4.56807300	-0.44628000	-1.20699700
H	5.14790000	0.41160700	-0.86409400
H	4.61096800	-0.46070100	-2.29635600
H	5.05504500	-1.35136600	-0.84102200
C	-1.37797800	3.89987300	1.12659900
H	-1.63279900	4.76308000	0.52962800
C	1.22886400	3.15642900	-2.27054300
H	0.74331200	4.03353500	-2.67077900
C	3.16871300	1.77830800	-2.08965600
H	4.19867400	1.58270300	-2.34692400
C	0.55157500	2.28422800	-1.42365600
C	-2.44583700	-0.82601000	-1.33578500
H	-2.23885200	-1.78964500	-0.88673500
C	-0.91342100	2.56179000	-1.01407200
C	2.45892500	0.91557500	-1.26001900
C	4.28886700	-0.44991600	2.95360000
H	5.21834600	-0.46119900	3.51333600
C	-2.89735100	1.63829700	-2.36527400
H	-3.08502600	2.62140800	-2.77158100
C	-0.77924200	1.72831500	2.62249500
H	-0.56904400	0.82488900	3.18089400
C	2.54998500	2.90658100	-2.60291400
H	3.09199000	3.58376300	-3.25423500
C	-1.44138000	4.00562700	2.51069000
H	-1.73765600	4.94140800	2.97290100
C	-1.13527400	2.89168000	3.27953000
H	-1.18424700	2.91019400	4.36207300
C	-3.52694800	-0.66593100	-2.18365300
H	-4.18472800	-1.50565900	-2.37795100
C	1.91803500	-0.48913400	2.82510000
H	0.94074500	-0.57313400	3.28286500
C	3.06328500	-0.51807900	3.60026800
H	2.98644800	-0.59773000	4.67837300
C	-3.74550800	0.59514900	-2.72074300
H	-4.57380800	0.77779400	-3.39754100
C	2.23491900	-3.66467300	-2.49023300
H	2.70612700	-4.39137500	-3.14361500
C	0.39300000	-2.87630900	-1.21013100
H	-0.59751400	-3.00833500	-0.78998000
S	-2.14476600	-3.42997200	1.31078800
S	-1.15561100	-1.53980200	1.87381200
O	-5.80006800	-2.74583000	-1.00768800
H	-5.79458500	-3.65807100	-0.68960900
H	-6.73511100	-2.50903800	-1.06551600
H	-5.24618600	-1.80176600	0.48956600
H	-2.39627800	-0.92260800	2.10640300
O	-3.92918800	-0.36621600	2.25167700
H	-4.31040900	-0.56959800	3.11555700
H	-4.48319700	-0.86014400	1.60807300
H	-1.38700000	-4.20364200	2.10905800

TS-III
E= -2417.561924 a.u.
G= -2417.076587 a.u.

2 2

Mo	0.05124200	-0.27955200	0.09673800
N	1.38273400	-1.45604600	-1.15546800
N	-1.21993400	0.55433000	-1.45171100
N	-1.04301700	1.15633700	1.34654700
N	1.53746000	-0.89309900	1.60450600
C	2.71584000	-1.22495800	-1.12569700
N	1.36151000	1.36924000	-0.31427800
C	3.25963000	-0.23465400	-0.07097700
C	2.85091000	-0.70354700	1.34397300
C	-1.36875900	1.89409900	-1.56062100
C	1.68184400	-3.04691400	-2.93185000
H	1.23018300	-3.76741700	-3.60388100
C	3.56016100	-1.88274700	-2.02007600
H	4.62547700	-1.70500000	-2.00752600
C	-1.18789000	2.43089500	0.91715000
C	-1.03561700	4.25397000	-0.79494900
H	-0.70183000	4.54561400	-1.79117600

H	-0.55948100	4.92386200	-0.07829300
H	-2.11387800	4.41377000	-0.74204700
C	3.80419200	-0.96069700	2.33031900
H	4.85559000	-0.80572900	2.13823700
C	4.79162200	-0.20625700	-0.16063300
H	5.21607800	0.48914700	0.56450900
H	5.12209400	0.10744900	-1.15117700
H	5.20878900	-1.19553500	0.03413000
C	-1.76751800	3.38967200	1.74991300
H	-1.89102200	4.40971200	1.41736000
C	1.67561600	3.66848800	-0.88931400
H	1.26915000	4.64649100	-1.09866600
C	3.56363000	2.22970600	-0.66507600
H	4.63270800	2.08355400	-0.69728900
C	0.84450100	2.59935100	-0.57036600
C	-1.82438900	-0.25085900	-2.34873800
H	-1.71454400	-1.31634300	-2.18489300
C	-0.68913000	2.78796000	-0.50095200
C	2.70538800	1.17895400	-0.35671200
C	3.41750600	-1.43277700	3.57922800
H	4.16407400	-1.62955700	4.34162600
C	-2.11508600	2.43153300	-2.61006500
H	-2.24255400	3.49956600	-2.70834400
C	-1.49060600	0.82778800	2.57404300
H	-1.39366900	-0.21551300	2.84461200
C	3.04790700	3.48645300	-0.93629000
H	3.70674700	4.31335200	-1.17796100
C	-2.19759400	3.04890600	3.02682000
H	-2.64200100	3.80089300	3.67047900
C	-2.05871600	1.73461800	3.45016000
H	-2.39001800	1.40920900	4.42943900
C	-2.56787800	0.22493900	-3.41350600
H	-3.02440200	-0.47152200	-4.10716500
C	1.17426900	-1.39167800	2.80147500
H	0.11910500	-1.60253600	2.92003100
C	2.07124200	-1.66802100	3.81773300
H	1.71700900	-2.06657700	4.76125800
C	-2.71338800	1.59869300	-3.54847600
H	-3.29080100	2.02322800	-4.36306300
C	3.04541100	-2.78949600	-2.93976600
H	3.70788000	-3.29703500	-3.63300900
C	0.89410800	-2.36894400	-2.01865700
H	-0.16569600	-2.58427100	-1.93450700
S	-2.27623400	-3.41459100	-0.68070700
S	-1.39986200	-2.05753200	0.78175900
O	-7.23469700	-1.61878000	-0.06776100
H	-7.47508700	-2.52767100	-0.30420100
H	-7.93085300	-1.30337600	0.52867200
H	-5.94145500	-1.71616700	0.78813100
H	-3.13212700	-1.77853100	1.48595900
O	-4.04326900	-1.79775600	2.01142700
H	-4.07530300	-2.66365100	2.45280100
H	-5.06657000	-1.73912700	1.31982100
H	-1.58900600	-4.51504100	-0.31875200

^{2}[MoS-SH]$^{2+}$-2H$_2$O

E= -2416.438752 a.u.

G= -2415.960346 a.u.

2 2

Mo	0.07806600	-0.29985800	-0.36271600
N	1.79986800	0.40363100	-1.55926500
N	-1.38606300	1.14231400	-1.08517800
N	-1.50042600	-0.70711400	1.06422400
N	1.67660500	-1.43865400	0.60851800
C	2.93942500	0.79729400	-0.94787200
N	0.67761200	1.30724700	1.01865700
C	3.04351500	0.64014100	0.58632100
C	2.83876400	-0.84491800	0.95986200
C	-2.01154000	1.96744200	-0.21884000
C	2.73544700	0.99491400	-3.69852900
H	2.60833900	1.03580200	-4.77405600
C	4.00082600	1.30756000	-1.69746900
H	4.91532000	1.62217200	-1.21698700
C	-2.13410200	0.31235200	1.68519200
C	-2.65340000	2.73414100	2.07610500
H	-2.42115200	3.77054200	1.82819200
H	-2.51927600	2.61262000	3.15154600
H	-3.70507500	2.55982500	1.84568800
C	3.83165600	-1.57619500	1.61150100
H	4.76331300	-1.11172900	1.89865100
C	4.44325100	1.07890600	1.03967100
H	4.56167500	0.96434500	2.11782500
H	4.62854200	2.12469000	0.79163300
H	5.21331400	0.47827900	0.55419700
C	-3.10618300	0.04955900	2.64761600
H	-3.61491600	0.85490300	3.15572600
C	0.06292900	3.03958500	2.53356700
H	-0.69050500	3.63592500	3.02511900
C	2.36935600	2.50659200	2.19081800
H	3.40894400	2.68883500	2.41667400
C	-0.28238200	2.04284600	1.62466200
C	-1.65201800	1.25652100	-2.40408300
H	-1.17406800	0.52994000	-3.04730600
C	-1.76371900	1.76031400	1.29024900
C	1.98564300	1.51878600	1.28755600
C	3.63903300	-2.92197700	1.90047200
H	4.41297700	-3.48481800	2.41191100
C	-2.86578200	2.96299100	-0.69050000
H	-3.36412900	3.63370700	-0.00672500
C	-1.85213000	-1.97691400	1.35526000
H	-1.35710200	-2.77453800	0.81253100
C	1.39897700	3.27238100	2.81617800
H	1.68285300	4.04601800	3.52227700
C	-3.44595600	-1.25999900	2.96675800
H	-4.20095400	-1.45701500	3.72094200
C	-2.81259400	-2.29585500	2.29832900
H	-3.04727100	-3.33647600	2.48807800
C	-2.49250500	2.21809600	-2.93059200
H	-2.66242700	2.26167700	-4.00008000
C	1.50307000	-2.75449800	0.86298600
H	0.58704000	-3.21586200	0.50933500
C	2.45346100	-3.52530100	1.50828400
H	2.25946100	-4.57712700	1.68172100
C	-3.10191600	3.10220400	-2.05154700
H	-3.76509100	3.88151100	-2.41234100
C	3.90210600	1.41875700	-3.07869300
H	4.72981100	1.81959300	-3.65430200
C	1.72205200	0.49321500	-2.90362500
H	0.81166200	0.11735600	-3.35031300
S	-2.40329300	-2.41630800	-2.15662400
S	-0.34864700	-1.86856600	-1.89419800
O	-4.30965500	-0.07660900	-0.56761900
H	-4.12354800	-0.59625300	-1.35904200
H	-5.25474900	-0.19126700	-0.42261600
H	-1.49639500	-4.64814400	-0.73257900
O	-0.96950200	-4.71003600	0.07386400
H	-1.01050700	-5.63489900	0.33964300
H	-2.23545000	-3.03005900	-3.34457900

Com-IV

E= -2417.543403 a.u.

G= -2417.053769 a.u.

2 2

Mo	-0.21095400	-0.23954100	0.16167700
N	0.71423300	-1.27069400	-1.59538000
N	-1.34377100	1.13848400	-1.10427100
N	-0.13995100	1.45057800	1.60359200
N	1.03454500	-1.53999300	1.34997300
C	1.96342700	-1.76602100	-1.50124300
N	1.59754400	0.90890000	-0.34279200
C	2.83824500	-1.26383000	-0.33777500
C	2.32251700	-1.79094800	1.01590100
C	-0.94883200	2.42428200	-1.24075600
C	0.43293500	-2.34111100	-3.72535300
H	-0.19719400	-2.51327800	-4.58994800
C	2.45450800	-2.62863400	-2.48150000
H	3.44031800	-3.06184800	-2.39229200
C	-0.15294700	2.72389300	1.16496300
C	0.33740900	4.46520400	-0.56439100
H	0.65738900	4.67180100	-1.58690600
H	1.07670200	4.89347400	0.11299800
H	-0.60604100	4.98721300	-0.39897200
C	3.13960900	-2.54282600	1.86129500
H	4.17245200	-2.72874000	1.60612600
C	4.27733400	-1.75289500	-0.55207900
H	4.94702400	-1.36170900	0.21511700
H	4.65801800	-1.44248500	-1.52589800
H	4.32564300	-2.84150300	-0.50617400
C	-0.34217100	3.77815300	2.05923500
H	-0.39264600	4.79823900	1.70651200
C	2.66239700	2.98485900	-0.85143300
H	2.60186400	4.04572100	-1.04104300
C	3.96100100	0.99507700	-0.67205100
H	4.91968900	0.50058900	-0.70662900
C	1.52261100	2.24625600	-0.54454600
C	-2.41533300	0.70961300	-1.80138500
H	-2.74255300	-0.30251000	-1.59893800
C	0.17199200	2.95755800	-0.32383300
C	2.79414300	0.27719900	-0.42474800
C	2.64166900	-3.07573000	3.04409000
H	3.28432500	-3.65751400	3.69591200
C	-1.58350300	3.25825600	-2.16259600
H	-1.25833400	4.27797200	-2.30496900
C	-0.20846900	1.21586900	2.92820700
H	-0.15053700	0.18105400	3.23806800
C	3.89532500	2.35848100	-0.90140200
H	4.79408900	2.92500200	-1.12119400
C	-0.45701400	3.52753000	3.42127400
H	-0.60718400	4.34705900	4.11623800
C	-0.34982700	2.21855100	3.87009800
H	-0.39204000	1.96732700	4.92340300
C	-3.10575300	1.49664100	-2.70619500
H	-3.96566800	1.09140900	-3.22602100
C	0.54558000	-2.10264800	2.48133000
H	-0.50615300	-1.92812900	2.68601500
C	1.30551300	-2.86332300	3.35128400
H	0.84741400	-3.27840400	4.24182900
C	-2.65993300	2.79376600	-2.91066600
H	-3.14802500	3.44909800	-3.62470000
C	1.68365200	-2.92893700	-3.59811300
H	2.06737100	-3.59770600	-4.36157100
C	-0.01652000	-1.53629400	-2.69411000
H	-0.99934900	-1.08822200	-2.73606100
S	-2.28060900	-0.53125400	1.58772500
S	-1.67814300	-2.24463900	-0.24587400
H	-1.19375000	-3.11340900	0.66928100

O	-6.67435700	-3.97851600	0.58750600
H	-7.18166300	-4.22994500	-0.19558700
H	-7.33361000	-3.84438900	1.28124200
H	-6.10267800	-2.36554700	0.21602100
H	-5.43371600	0.47501500	0.19895500
O	-4.82492300	-0.18315600	-0.15892900
H	-5.30078200	-1.04594700	-0.05150800
H	-3.38162100	-0.28015100	0.77316200

TS-IV
E= -2417.498069 a.u.
G= -2417.011104 a.u.

2 2

Mo	-0.09452400	-0.34199200	0.23814300
N	1.00711000	-1.35372100	-1.43015400
N	-1.55147000	0.49953100	-1.10438100
N	-0.36272600	1.51927800	1.44438700
N	1.51282100	-1.09875300	1.48221200
C	2.34594100	-1.49194700	-1.37921600
N	1.34229100	1.14560200	-0.55056500
C	3.10691100	-0.61769000	-0.36688700
C	2.80592900	-1.05839500	1.07904100
C	-1.53732000	1.81740300	-1.42625300
C	0.92669100	-2.77611400	-3.36475900
H	0.32598800	-3.23397600	-4.14179800
C	3.00548300	-2.33678200	-2.27275200
H	4.07441600	-2.48067400	-2.20935400
C	-0.74123100	2.66502900	0.84737100
C	-0.80846400	4.19656900	-1.13021000
H	-0.60271000	4.32144800	-2.19441700
H	-0.17519300	4.89267200	-0.57958600
H	-1.84630600	4.48375800	-0.95570900
C	3.83420000	-1.44739400	1.93994500
H	4.86570500	-1.38927300	1.62579300
C	4.61315700	-0.74954600	-0.63184200
H	5.19017400	-0.09394500	0.02184800
H	4.85346200	-0.49688900	-1.66516100
H	4.94830600	-1.77156600	-0.45155300
C	-1.16476300	3.75557600	1.60781700
H	-1.50763100	4.66227400	1.12999000
C	1.80442800	3.32316400	-1.41974300
H	1.45938800	4.29375200	-1.74180600
C	3.58270500	1.77362700	-1.09033400
H	4.63443900	1.53682900	-1.13961700
C	0.91441900	2.37670700	-0.91946500
C	-2.50515500	-0.28344300	-1.66203400
H	-2.52845000	-1.31369700	-1.32707000
C	-0.56197300	2.74966200	-0.68050900
C	2.65677700	0.83019600	-0.65246000
C	3.55608200	-1.92681800	3.21317400
H	4.36134300	-2.22568800	3.87534500
C	-2.41410000	2.31829300	-2.38945600
H	-2.38334900	3.35897700	-2.67640900
C	-0.29187700	1.47788600	2.78859000
H	0.06584400	0.55275500	3.21978700
C	3.15406900	3.02692600	-1.49104300
H	3.86286500	3.76186200	-1.85781200
C	-1.13577000	3.69145200	2.99593400
H	-1.46439900	4.53890700	3.58843900
C	-0.65196600	2.53953800	3.60000500
H	-0.56568400	2.44932700	4.67651900
C	-3.41691100	0.16376700	-2.60180400
H	-4.14585800	-0.52473300	-3.01393500
C	1.25227500	-1.60757100	2.71256900
H	0.20351700	-1.66583700	2.98272900
C	2.22728700	-2.02777200	3.59831500
H	1.93746300	-2.42037900	4.56642000
C	-3.35245000	1.49156700	-2.99773400
H	-4.02351400	1.88904800	-3.75169500
C	2.29354000	-2.99529200	-3.26758700
H	2.80689600	-3.65089300	-3.96318800
C	0.32766000	-1.96335800	-2.41940200
H	-0.73842800	-1.78809200	-2.44508400
S	-1.85845900	-0.87041200	1.78629500
S	-0.98983500	-2.70974000	0.20962200
H	-0.24454000	-3.26922200	1.18817800
O	-7.52846500	-3.18549100	0.47457300
H	-7.93314200	-3.20719300	1.35837600
H	-7.36132100	-4.10774900	0.21655100
H	-6.31295800	-2.55089500	0.57769300
H	-4.83689200	-0.42308500	0.56120000
O	-4.40758300	-1.29433000	0.60112700
H	-5.25722900	-2.00558800	0.66123400
H	-3.22072200	-1.11257500	1.11568000

^{2}[Mo(SH)$_2$]$^{2+}$-2H$_2$O
E= -2416.394779 a.u.
G= -2415.915153 a.u.

2 2

Mo	-0.15416900	-0.05222500	-0.71672300
N	-0.58911000	-1.87866500	0.55380400
N	1.91467800	-0.08933900	-0.00902800
N	0.00579000	2.19747500	-0.76149900
N	-2.30009100	-0.04665500	-1.00670400
C	-1.76518600	-1.98906100	1.20625900
N	-0.57729700	0.71615600	1.35628400
C	-2.62807900	-0.72289500	1.35643100
C	-3.18186100	-0.28267600	-0.01008600
C	2.43376900	0.90526000	0.74446000
C	-0.06219300	-4.15386500	1.12236800
H	0.65864300	-4.95989600	1.05911300
C	-2.14753000	-3.20089600	1.78033900
H	-3.10289300	-3.30026600	2.27417600
C	0.92677200	2.83262200	-0.01468400
C	2.31918700	3.04019500	2.05277000
H	2.70136300	2.54974100	2.94941900
H	1.70662900	3.88903600	2.35852000
H	3.17380900	3.43390100	1.50234200
C	-4.55573400	-0.17165900	-0.23687400
H	-5.25853300	-0.33760600	0.56593300
C	-3.80368200	-1.02259800	2.29740900
H	-4.40708600	-0.13065600	2.47199700
H	-3.45312200	-1.39161100	3.26173300
H	-4.45662000	-1.78281000	1.86761700
C	1.23239500	4.17248400	-0.25768900
H	2.00355400	4.67456700	0.30864000
C	0.04834900	2.02389800	3.25434300
H	0.75845300	2.66423400	3.75456300
C	-2.02397200	0.85269600	3.25094100
H	-2.94580700	0.58671600	3.74409500
C	0.29239500	1.55562000	1.96608500
C	2.73997800	-1.05675700	-0.46779600
H	2.31267800	-1.81527900	-1.11161700
C	1.51636800	2.06191600	1.18313300
C	-1.71419800	0.34389900	1.99182300
C	-5.04732300	0.14004500	-1.49659400
H	-6.11582900	0.22224200	-1.66394900
C	3.78592700	0.89288700	1.09053800
H	4.20499400	1.67251000	1.70863300
C	-0.70027400	2.90174800	-1.66663400
H	-1.45873000	2.35725600	-2.21222700
C	-1.12862700	1.68572400	3.89722600
H	-1.34432900	2.06361800	4.89118500
C	0.53576600	4.88337300	-1.22728300
H	0.77622600	5.92375800	-1.41937400
C	-0.48425300	4.24447700	-1.91863900
H	-1.08900400	4.76000600	-2.65547800
C	4.08870600	-1.10865300	-0.17425700
H	4.71753100	-1.89877000	-0.56660100
C	-2.79059200	0.22643000	-2.24443300
H	-2.05138700	0.37285500	-3.02226000
C	-4.13879400	0.32403900	-2.52946300
H	-4.45549300	0.54283100	-3.54289800
C	4.62306800	-0.11908000	0.63685600
H	5.67959900	-0.15014500	0.88527000
C	-1.29613300	-4.29879500	1.73539400
H	-1.59646900	-5.24038100	2.18341300
C	0.24234000	-2.93735300	0.53684700
H	1.18217800	-2.83705400	0.01637700
S	0.58863400	0.41667900	-2.78189000
S	-0.04971600	-2.02725500	-2.32913300
H	-1.29707800	-1.94485500	-2.84066700
O	7.13037800	-1.79491500	0.04670400
H	7.78004100	-1.53701700	-0.61593900
H	7.62016800	-2.35792900	0.65549700
H	3.31279600	-4.65908800	-1.19083000
O	2.50927700	-4.13278500	-1.26317100
H	2.10157000	-4.41658300	-2.08894500

Com-V
E= -2417.569965 a.u.
G= -2417.082218 a.u.

2 4

Mo	0.08658300	-0.18965200	0.30443700
N	1.06068200	-1.77263300	-0.82374800
N	-1.60930800	0.17809100	-1.00213900
N	-0.68324400	1.62513600	1.28127100
N	1.93414300	-0.39286800	1.48036400
C	2.34424000	-1.61106400	-1.22361700
N	1.16883700	1.17661700	-0.93626500
C	3.11763500	-0.37326400	-0.71056500
C	3.12283700	-0.37331100	0.83521600
C	-1.83636200	1.41961000	-1.48569100
C	0.92847000	-3.84060300	-2.04363000
H	0.33786000	-4.70666100	-2.31888500
C	2.94216600	-2.55282000	-2.06050600
H	3.96546800	-2.43472300	-2.38530700
C	-0.99057500	2.70261600	0.52294800
C	-1.37790300	3.87292800	-1.66288100
H	-1.34453600	3.80673400	-2.75114700
H	-0.74789000	4.71012600	-1.36088900
H	-2.40376600	4.10350200	-1.37199700
C	4.31280100	-0.38878800	1.56346800
H	5.26877900	-0.36105400	1.06181900
C	4.56766600	-0.45106900	-1.20851100
H	5.14814600	0.40687100	-0.86684100
H	4.61021900	-0.46684800	-2.29786100
H	5.05419100	-1.35602900	-0.84161600
C	-1.37043100	3.90289700	1.12522900
H	-1.62383400	4.76629800	0.52792800
C	1.23041900	3.15256300	-2.27501600
H	0.74526900	4.02947600	-2.67614700

C	3.16922000	1.77302700	-2.09381300
H	4.19877700	1.57611500	-2.35170800
C	0.55317000	2.28237700	-1.42603500
C	-2.44726700	-0.82394600	-1.33389500
H	-2.23959700	-1.78800200	-0.88612200
C	-0.91098500	2.56232500	-1.01499200
C	2.45942500	0.91217100	-1.26224600
C	4.28992200	-0.45068600	2.95216800
H	5.21956100	-0.46196800	3.51163600
C	-2.89966600	1.64120700	-2.36087700
H	-3.08746200	2.62457900	-2.76648800
C	-0.77524800	1.73090600	2.62191200
H	-0.56668500	0.82734200	3.18071500
C	2.55096700	2.90097300	-2.60835300
H	3.09290600	3.57658600	-3.26135400
C	-1.43251200	4.00960900	2.50930100
H	-1.72636600	4.94630200	2.97120800
C	-1.12834100	2.89539500	3.27853700
H	-1.17659400	2.91459500	4.36110100
C	-3.53095900	-0.66259800	-2.17811100
H	-4.19035900	-1.50151600	-2.37058500
C	1.91903600	-0.48908100	2.82447600
H	0.94183300	-0.57245600	3.28253600
C	3.06451500	-0.51800700	3.59928300
H	2.98804500	-0.59698700	4.67746500
C	-3.75008200	0.59908100	-2.71378800
H	-4.58041400	0.78282200	-3.38780500
C	2.23158500	-3.66910000	-2.48762700
H	2.70203600	-4.39686300	-3.14037400
C	0.39065100	-2.87786600	-1.20791100
H	-0.59985300	-3.00863400	-0.78736300
S	-2.14792700	-3.42654800	1.31400600
S	-1.15681300	-1.53758300	1.87496100
O	-5.80684400	-2.74417300	-1.01289600
H	-5.80216100	-3.65814500	-0.69990700
H	-6.74174500	-2.50723000	-1.07182300
H	-5.25899600	-1.80543000	0.49505600
H	-2.39663700	-0.91964800	2.10688600
O	-3.93258800	-0.36397400	2.25246200
H	-4.31070500	-0.56594600	3.11799000
H	-4.48844400	-0.85963200	1.61216700
H	-1.39639700	-4.20023700	2.11814900

TS-V
E= -2417.563679 a.u.
G= -2417.079194 a.u.

2 4

Mo	0.03860000	-0.24638400	0.10136900
N	1.26606100	-1.47096600	-1.21211500
N	-1.22020000	0.69301000	-1.40051400
N	-0.94098300	1.23127800	1.39149600
N	1.49485600	-1.00704400	1.56376200
C	2.61284000	-1.33183800	-1.18889400
N	1.44083100	1.31867000	-0.29979500
C	3.23392400	-0.41188700	-0.11234200
C	2.81457500	-0.89655000	1.29316900
C	-1.26798500	2.03964400	-1.49988000
C	1.44428300	-3.00091100	-3.05881700
H	0.93885900	-3.65713500	-3.75789500
C	3.40432700	-2.01332400	-2.11354600
H	4.47950600	-1.91126300	-2.10241000
C	-1.01971300	2.51824400	0.98041200
C	-0.76962300	4.35889800	-0.70539500
H	-0.42132600	4.64488600	-1.69842500
H	-0.24938500	4.98557600	0.01964800
H	-1.83535400	4.58595900	-0.64492300
C	3.75792500	-1.24954900	2.25906100
H	4.81545600	-1.15620500	2.06072900
C	4.76348400	-0.48080200	-0.22141100
H	5.24117200	0.16094500	0.51992200
H	5.10343200	-0.15836000	-1.20587200
H	5.11598100	-1.50114000	-0.06242100
C	-1.53755300	3.49623500	1.83143900
H	-1.61084900	4.52524400	1.51172500
C	1.90049000	3.60645600	-0.81854000
H	1.55700400	4.61313000	-1.00299100
C	3.69305400	2.04410400	-0.63592500
H	4.75065200	1.83107400	-0.67531800
C	1.00308400	2.58528300	-0.52319200
C	-1.91619000	-0.06053600	-2.27444100
H	-1.89233600	-1.13039300	-2.10461600
C	-0.51461700	2.86908900	-0.43823800
C	2.77014700	1.04235800	-0.35340400
C	3.35153500	-1.73941100	3.49496400
H	4.09013600	-2.00975400	4.24246400
C	-1.99113700	2.63791700	-2.53240200
H	-2.03421600	3.71294700	-2.62809800
C	-1.38790400	0.91333400	2.62239600
H	-1.34308500	-0.13712500	2.88064000
C	3.25832200	3.33794100	-0.87376300
H	3.96848800	4.12665400	-1.09695500
C	-1.96931200	3.16373200	3.10971500
H	-2.36651800	3.93007800	3.76706500
C	-1.89303600	1.83895800	3.51700000
H	-2.22754300	1.52033600	4.49745000
C	-2.64723800	0.47541800	-3.31925300
H	-3.18144500	-0.17959600	-3.99759900
C	1.10815100	-1.52484700	2.74529700
H	0.04189600	-1.67047900	2.86499200
C	1.99490400	-1.89686100	3.73980000
H	1.62446800	-2.30556800	4.67271400
C	-2.67669200	1.85647700	-3.45562900
H	-3.23459600	2.32730200	-4.25835400
C	2.82301700	-2.84435100	-3.06430600
H	3.44477900	-3.37036800	-3.78104400
C	0.71143100	-2.30797900	-2.11184900
H	-0.36014700	-2.45119500	-2.03189100
S	-2.36775200	-3.36492000	-0.63426300
S	-1.59342600	-1.90499900	0.75701500
O	-7.24964500	-1.58859900	-0.26782100
H	-7.53168600	-2.48876200	-0.49027300
H	-7.95981800	-1.21404200	0.27509900
H	-6.01892000	-1.74643400	0.69412000
H	-3.27578900	-1.77766300	1.54363700
O	-4.20079500	-1.90205200	2.05223400
H	-4.20707400	-2.81261900	2.39264100
H	-5.11023700	-1.80750400	1.35084700
H	-1.56123400	-4.39258700	-0.30344300

^{4}[MoS-SH]$^{2+}$-2H_2O
E= -2416.459585 a.u.
G= -2415.978602 a.u.

2 4

Mo	-0.02138700	-0.16458400	-0.30451100
N	1.75423800	-0.34980000	-1.57911700
N	-0.84069500	1.64604500	-1.20934700
N	-1.60317600	0.22028000	1.13391700
N	1.02352400	-1.77103700	0.73016200
C	2.98113600	-0.30909100	-1.01130400
N	1.16649100	1.19817500	0.90762900
C	3.07633900	-0.36888200	0.53192900
C	2.33823000	-1.63637000	1.02724700
C	-1.07013900	2.73758700	-0.44664600
C	2.73901900	-0.41048000	-3.76820200
H	2.59470600	-0.48272800	-4.83987100
C	4.11846600	-0.26874100	-1.81645000
H	5.10529200	-0.22118700	-1.37979100
C	-1.80242100	1.47225300	1.60818200
C	-1.30500500	3.92796000	1.74655000
H	-0.67684400	4.75330800	1.40865500
H	-1.22189200	3.86585900	2.83227400
H	-2.33979300	4.17385900	1.50489800
C	2.99952200	-2.64023200	1.72884000
H	4.04636200	-2.54699000	1.97784300
C	4.55519300	-0.46284000	0.93271600
H	4.66574700	-0.54193200	2.01478400
H	5.10972800	0.41724900	0.60443300
H	5.02183400	-1.34074600	0.48400800
C	-2.81631100	1.71472000	2.53138400
H	-2.98860900	2.70814700	2.91888100
C	1.31535500	3.15415600	2.25498000
H	0.86901300	4.03991400	2.68094100
C	3.21766900	1.72735600	1.99143500
H	4.25028000	1.50385100	2.21320500
C	0.58648100	2.30570000	1.42668800
C	-1.06737500	1.70316000	-2.53581500
H	-0.92513400	0.77568000	-3.07576200
C	-0.89199900	2.60719300	1.08308100
C	2.46089700	0.90008900	1.16626400
C	2.31999000	-3.79400400	2.11321100
H	2.84271400	-4.57387300	2.65749200
C	-1.48656200	3.92763200	-1.04136500
H	-1.66787900	4.81102000	-0.44673300
C	-2.39786400	-0.78701600	1.55111600
H	-2.23057900	-1.78465600	1.15130300
C	2.63873000	2.85966200	2.54186200
H	3.21704500	3.51113200	3.18875100
C	-3.63412500	0.67521800	2.96656500
H	-4.42538800	0.87189900	3.68269800
C	-3.42101600	-0.59878900	2.46570900
H	-4.02803100	-1.44741900	2.75755500
C	-1.48234700	2.85386900	-3.18178800
H	-1.64731400	2.84597000	-4.25286000
C	0.36987400	-2.89716700	1.08225200
H	-0.67357000	-2.99939300	0.79908600
C	0.98330000	-3.92804200	1.77596600
H	0.40462200	-4.80873000	2.02752900
C	-1.68521800	3.99349800	-2.41664000
H	-2.00830200	4.92276600	-2.87436300
C	4.00142800	-0.30607000	-3.20228100
H	4.89097500	-0.27583400	-3.82298500
C	1.64590800	-0.43081100	-2.92022200
H	0.63932300	-0.55416700	-3.30041500
S	-3.24869800	-0.97756600	-1.86371100
S	-1.27293100	-1.69615600	-1.72400600
O	-4.22817200	-4.09141700	-0.88851200
H	-4.20168600	-3.24407700	-1.35768400
H	-4.14562400	-4.77437900	-1.56237200
H	-3.11511400	-4.02013200	0.38160600
O	-2.53173100	-3.83923900	1.15755100
H	-2.90746200	-4.35162700	1.87995200
H	-3.35647100	-1.03020200	-3.20673800

Com-VI

E= -2417.545339 a.u.
G= -2417.063820 a.u.

2 4

Mo	0.58470000	0.16822000	0.78679700
N	2.03974100	-1.57454700	0.66895200
N	-1.06454100	-1.03140000	1.62883800
N	-3.58179600	0.54742300	-0.66141000
N	2.25529300	1.23772900	-0.15551200
C	2.70961900	-1.79707700	-0.47949600
N	0.13041900	-0.75901500	-1.13006700
C	2.58391000	-0.74117100	-1.59589500
C	3.04341500	0.62844600	-1.06827400
C	-2.14258400	-1.44607400	0.92800600
C	2.88495200	-3.61880400	1.59216900
H	2.92971700	-4.29837100	2.43519400
C	3.48168500	-2.94762400	-0.62884700
H	4.01753300	-3.14190900	-1.54681300
C	-3.58062700	-0.75917600	-0.94547700
C	-2.23400800	-2.95881200	-1.01304100
H	-1.26795200	-3.40086000	-0.75648000
H	-2.38755100	-3.07551000	-2.08827400
H	-3.00732200	-3.52302500	-0.48897600
C	4.21828000	1.23347800	-1.50466900
H	4.85952200	0.74073800	-2.22174500
C	3.45258400	-1.15459200	-2.79292600
H	3.48445500	-0.37215900	-3.55090500
H	3.06765500	-2.06423700	-3.25773700
H	4.48134700	-1.33907200	-2.48109600
C	-4.68263000	-1.41518000	-1.48908000
H	-4.65704000	-2.47396400	-1.72178400
C	-1.51693800	-0.62609400	-2.83603300
H	-2.55963400	-0.66182200	-3.12547300
C	0.80054000	-0.44164000	-3.39569500
H	1.57580200	-0.33473900	-4.14060600
C	-1.16613100	-0.85522500	-1.50240500
C	-1.07018900	-1.20003700	2.97850600
H	-0.17904300	-0.86518600	3.49248900
C	-2.25157700	-1.45642500	-0.60386600
C	1.11450600	-0.63648800	-2.05931100
C	4.57891100	2.48612700	-1.01757200
H	5.49592800	2.95758800	-1.35567900
C	-3.24630600	-1.98686700	1.60006900
H	-4.11691600	-2.28049600	1.02642000
C	-4.69195500	1.24512600	-0.89820700
H	-4.65592500	2.30271200	-0.64885700
C	-0.53556100	-0.38426500	-3.77756000
H	-0.80119000	-0.19744800	-4.81309100
C	-5.84028700	-0.67430000	-1.73453500
H	-6.71694600	-1.15594700	-2.15579100
C	-5.85054700	0.68041900	-1.43176900
H	-6.73026900	1.29067800	-1.60343400
C	-2.12056000	-1.74730900	3.68295200
H	-2.05039700	-1.84792600	4.75975800
C	2.60663900	2.45217500	0.31270500
H	1.94845900	2.89113500	1.04827200
C	3.74882300	3.11459800	-0.10131500
H	3.97679800	4.09308500	0.30372100
C	-3.25152300	-2.13729200	2.97478000
H	-4.11713800	-2.55322600	3.47974700
C	3.57176500	-3.86664100	0.41242100
H	4.17657100	-4.76015700	0.29668200
C	2.13047000	-2.46034900	1.67598900
H	1.58959100	-2.20936200	2.58004500
S	-0.84895400	1.91791600	0.83321400
S	1.78165700	0.51254000	2.85075600
H	-0.23097100	3.01243800	0.18893800
H	0.84212100	1.20957900	3.51709600
O	-2.01489400	7.54810400	1.05220200
H	-0.80036300	6.40562500	0.60308900
H	-1.82048300	8.33418200	0.52414300
H	-1.79182900	7.79292600	1.96028000
O	0.38169100	4.41736600	-0.43492700
H	0.14229600	4.54104000	-1.36211900
H	-0.03369600	5.19248600	0.03039600

TS-VI
E= -2417.532834 a.u.
G= -2417.050876 a.u.

2 4

Mo	0.54860000	0.35119900	0.64213900
N	2.11031600	-1.28860100	0.99481800
N	-1.04941700	-0.71368100	1.71966300
N	-3.55611500	0.14685700	-0.89636700
N	2.19402600	1.24923300	-0.51614400
C	2.82366600	-1.74861200	-0.05191300
N	0.22095100	-1.04489400	-0.99693900
C	2.68345400	-1.00453800	-1.39652400
C	3.05509300	0.47620900	-1.20997800
C	-2.07452600	-1.35732100	1.12486400
C	3.02884300	-2.99536700	2.40503000
H	3.08253400	-3.44482700	3.38972500
C	3.65404800	-2.85834400	0.09680200
H	4.22394200	-3.24279200	-0.73694900
C	-3.48616100	-1.18764300	-0.87879800
C	-2.05210700	-3.28079600	-0.41627500
H	-1.07194100	-3.60568200	-0.05808500
H	-2.18030400	-3.64945500	-1.43654600
H	-2.80825900	-3.74560800	0.21870300
C	4.22689000	1.01567100	-1.73656800
H	4.92669800	0.39425600	-2.27737000
C	3.61405600	-1.64435800	-2.43811200
H	3.63643900	-1.06462500	-3.36101700
H	3.28923600	-2.65814600	-2.68002700
H	4.63869800	-1.69479300	-2.06788800
C	-4.54358300	-2.00185100	-1.28004900
H	-4.46395900	-3.08315000	-1.26691900
C	-1.37219300	-1.42666500	-2.71745900
H	-2.40156700	-1.59007300	-3.01096800
C	0.95158200	-1.25696200	-3.25536300
H	1.74498900	-1.29195600	-3.98774200
C	-1.05434100	-1.30358100	-1.36165700
C	-1.08600300	-0.54887200	3.06735700
H	-0.23661200	-0.02915600	3.49198200
C	-2.13955600	-1.72707200	-0.36454800
C	1.22842000	-1.10058400	-1.90560400
C	4.50686600	2.36707000	-1.56943300
H	5.42111900	2.78775400	-1.97518300
C	-3.16180500	-1.79895200	1.89023700
H	-3.99461500	-2.27998800	1.39179000
C	-4.68808800	0.71763600	-1.30380200
H	-4.70610000	1.80470100	-1.29795500
C	-0.37205900	-1.36709100	-3.66829100
H	-0.61059100	-1.45208500	-4.72356300
C	-5.72512100	-1.39409300	-1.70722200
H	-6.56704600	-2.00114700	-2.02450400
C	-5.80472000	-0.00823100	-1.71794400
H	-6.70529600	0.50358300	-2.03868200
C	-2.11816200	-0.98749000	3.86887700
H	-2.07546500	-0.82103700	4.93893800
C	2.46388000	2.56089700	-0.36405100
H	1.73904400	3.12933000	0.20161400
C	3.59869800	3.15977500	-0.88139800
H	3.76588100	4.21927100	-0.72751300
C	-3.19802700	-1.61746600	3.26068400
H	-4.04892800	-1.96173100	3.83922100
C	3.75838500	-3.48855300	1.33313100
H	4.40695100	-4.35071000	1.44974700
C	2.21647500	-1.89385900	2.18925800
H	1.63754800	-1.45876700	2.99513200
S	-0.91213400	1.99788300	0.30338300
S	1.68994000	1.25732000	2.58832800
H	-0.62383400	3.93042000	-0.24706800
H	0.73194700	2.08537900	3.04242400
O	-2.46461800	7.88014200	0.54752200
H	-1.53414700	6.66092700	0.13747200
H	-2.09387600	8.65741100	0.10148700
H	-2.30856100	8.01585900	1.49488200
O	-0.26147400	4.79524900	-0.61671500
H	-0.49368400	4.79124100	-1.56025800
H	-1.03933900	5.97271200	-0.10128400

$^4[Mo(SH)_2]^{2+}$-2H_2O
E= -2416.412644 a.u.
G= -2415.935280 a.u.

2 4

Mo	-0.78155500	-0.24267700	-0.73986400
N	-2.91571500	-0.50833400	-0.41658000
N	-0.15123500	-2.33079900	-0.50257200
N	2.79704400	-0.01107100	0.06149000
N	-1.36521100	1.84819000	-0.70792000
C	-3.49940700	0.12842600	0.62078500
N	-0.61955300	-0.09702700	1.40183100
C	-2.71079700	1.27042900	1.30129000
C	-2.24873500	2.27987400	0.22038800
C	1.02036100	-2.49210300	0.13992400
C	-4.92224600	-1.74672300	-0.83865200
H	-5.45346800	-2.45857700	-1.45962100
C	-4.79847200	-0.20850200	0.99729700
H	-5.27478100	0.26992500	1.84113800
C	2.74037700	-0.91787400	1.08542500
C	1.58155800	-2.73730100	2.48122300
H	0.61857000	-3.23765800	2.60656600
H	1.86582300	-2.33195500	3.45040100
H	2.31427900	-3.49507000	2.20653200
C	-2.70385100	3.59521300	0.19167400
H	-3.42058300	3.95140600	0.91764300
C	-3.63414200	1.98190300	2.30010400
H	-3.15569000	2.86443300	2.72478500
H	-3.90604900	1.31835200	3.12309900
H	-4.55175100	2.31122700	1.81083000
C	3.86892000	-1.09488400	1.87703400
H	3.83948900	-1.82358100	2.67699400
C	0.85027400	-0.09962200	3.26236300
H	1.78200000	-0.40324100	3.72012200
C	-1.16639000	1.18006600	3.33698900
H	-1.83134000	1.84117700	3.87252800
C	0.48490900	-0.58190200	2.00372500
C	-0.53432700	-3.24435100	-1.41693100
H	-1.49280500	-3.07127700	-1.88817300
C	1.42592700	-1.64969200	1.37365500
C	-1.46003500	0.74871900	2.04900300
C	-2.23956000	4.47273700	-0.78467800
H	-2.60000400	5.49596000	-0.80857200
C	1.89259600	-3.51268900	-0.24406400

H	2.87006500	-3.59438800	0.21655100
C	3.91335700	0.73251100	-0.14610700
H	3.89571500	1.45582400	-0.97010600
C	0.02243300	0.78257700	3.93225600
H	0.29423100	1.15211800	4.91542500
C	5.03000700	-0.35787600	1.66003700
H	5.90135500	-0.51890600	2.28607200
C	5.04090000	0.58364900	0.64057100
H	5.90210400	1.20961600	0.42063500
C	0.25159700	-4.32106400	-1.78670100
H	-0.10612700	-5.02743600	-2.52651000
C	-0.90551300	2.70043100	-1.64572000
H	-0.20405900	2.28492500	-2.35910500
C	-1.31610700	4.02092000	-1.71593600
H	-0.92155100	4.66643300	-2.49171900
C	1.51657900	-4.42578800	-1.22054500
H	2.19813000	-5.21487300	-1.52094400
C	-5.51020300	-1.16220100	0.27513700
H	-6.52170700	-1.42122100	0.57045800
C	-3.62131800	-1.39065500	-1.14875200
H	-3.11565500	-1.77793000	-2.02646100
S	1.58916300	0.19892900	-1.24871800
S	-0.92429700	-0.30229600	-3.16671800
H	4.63922800	2.95378600	-2.94111900
H	0.04266600	-1.18618900	-3.47628100
O	7.09037700	2.88890200	-0.72714500
H	7.87838500	2.65425100	-1.23081500
H	7.31938000	3.70616500	-0.26932900
O	4.58997300	2.95133400	-1.98051200
H	5.50934800	3.03903000	-1.66701300