

**Supplementary Information for
Eight-Electron Reduction of CO₂ to CH₄ by a Bioinspired Mo-Fe-S Cubane Catalyst**

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This file contains following materials:

Materials and Methods including supplementary notes,

Supplementary Figs. 1 to 26,

Supplementary Tables 1 to 6,

Additional References, and

Cartesian coordinates of the optimized structures.

Materials and Methods

General considerations. Unless otherwise noted, all reactions were performed under an inert nitrogen or argon atmosphere using Schlenk techniques and glove boxes. Hexane, toluene, and tetrahydrofuran (THF) were dried and deoxygenated by passing over columns of activated alumina and supported copper catalyst purchased from Hansen & Co., Ltd. ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were recorded on a Bruker Avance II 400M spectrometer. Detected ^1H NMR signals were referenced to the residual peaks of the deuterated solvents. Fourier transform-infrared (FT-IR) spectra were measured using Bruker ALPHA spectrometer equipped with a diamond ATR accessory. Elemental analysis was performed using a J-SCIENCE MICRO CORDER JM11 analyzer for C and H determinations and a Thermo Fisher Scientific DIONEX ICS-1600 ion chromatograph equipped with Mitsubishi Chemical Analytech AQF-2100 H furnace for S determination, where crystalline samples were sealed in tin capsules under an inert atmosphere. Synthetic procedures for $[\text{Cp}^{\text{R}}_3\text{Mo}_3\text{S}_4\text{FeCl}]$ ($\text{Cp}^{\text{R}} = \text{C}_5\text{Me}_5$ (Cp^* , **1**)¹⁶, $\text{C}_5\text{Me}_4\text{SiMe}_3$ (Cp^{L} , **2**), and $\text{C}_5\text{Me}_4\text{SiEt}_3$ (Cp^{XL} , **3**))¹⁷ and $\text{Cp}^*_3\text{Mo}_3\text{S}_4$ ¹⁶ were described elsewhere. Potassium graphite (KC_8) was prepared according to the literature procedure⁴². SmI_2 was used as a solid prepared by the literature procedure⁴³ or a solution in THF purchased from Tokyo Chemical Industry Co., Ltd. Deuterated solvents (C_6D_6 , and $\text{THF-}d_8$) were dried over sodium metal and distilled before use. $[\text{N}^i\text{Bu}_4][\text{PF}_6]$ was recrystallized from THF prior to use. All other chemicals were purchased from commercial sources and used without further purification.

Catalytic evaluations

General procedure for the catalytic reduction of CO₂ into CH₄. Catalytic CO₂ reduction reactions were carried out in THF under 1 atm of CO₂ in 13.6 mL crimp-sealed assay vials fitted with butyl rubber septa. Unless otherwise noted, the reaction mixture (1.0 mL) contained a precatalyst (10 nmol), SmI₂ (50 μmol, 5000 equiv.), and H₂O (1.5% v/v). Reactions were initiated by the addition of SmI₂ and stirred at room temperature. Reaction progress was monitored by the disappearance of the characteristic deep blue color of SmI₂. Control experiments were conducted under identical conditions using FeCl₂, Fe(TPP)Cl (5,10,15,20-tetraphenyl-21*H*,23*H*-porphine iron(III) chloride), Fe₂(CO)₉, FeCp₂ (Cp = C₅H₅), and [Cp*₃Mo₃S₄] as catalyst precursors. Reaction products were quantified by headspace gas analysis using gas chromatographs (GCs). Product amounts were determined from calibration curves prepared using authentic standards. CH₄ was analyzed using a Shimadzu GC-2030 equipped with a flame ionization detector (FID). Gas separation was achieved on an Agilent DB-1 capillary column (0.320 mm internal diameter (ID) with 50 m length), which was held at 35 °C for 6.5 min, heated to 280 °C at 30 °C/min, and held at 280 °C for another 5 min. H₂ and CO were analyzed by a Shimadzu GC-2014 equipped with a thermal conductivity detector (TCD). Gas separation was achieved on a molecular sieve 13X packed column (3.00 mm ID with 2.0 m length) held at 40 °C.

Time course analysis of the catalytic reduction of CO₂ to CH₄ and H⁺ to H₂. Time course analysis was conducted in the presence of a precatalyst (**1** or **3**) by terminating the catalytic reduction at target reaction times by the addition of acetone (50 μL) that quenches SmI₂. The reaction conditions and product quantification methods are similar to those described above as the general procedure.

¹³C-labeling experiment of CO₂-to-CH₄ conversion. ¹³C-labeling experiment was performed using ¹³CO₂ (1 atm) as a substrate. The reaction was conducted under the following conditions: solvent, THF; precatalyst, cluster **1** (10 nmol); reductant, SmI₂ (50 μmol); proton source, H₂O (1.5% v/v). Produced ¹³CH₄ was identified by a headspace gas analysis using a Shimadzu GCMS-QP2020 NX instrument with a mass spectrometry detector (GC-MS). Gas separation conditions were similar to those applied for GC-FID analysis. CH₄ produced by a reaction performed with unlabeled CO₂ was also analyzed as a control experiment.

Scale-up catalytic reduction of CO₂ into CH₄. Scale up reactions of catalytic CO₂ reduction to CH₄ were carried out in 13.6 mL crimp-sealed assay vials fitted with butyl rubber septa. Unless otherwise noted, the reaction mixture (320 μL) contained a precatalyst (0.040 nmol), SmI₂ (0.16 mmol), and H₂O (20 μL, 6.25% v/v). Reactions were conducted at room temperature or 0 °C in a BAS TB-1 isothermal chamber. As the reaction proceeded, white insoluble solids gradually formed. When the reaction mixture became highly heterogeneous, small portions of THF and H₂O were added as needed to maintain efficient stirring. Products were quantified by GC-FID and GC-TCD analyses as described above.

Supporting experiments for CO₂-to-CH₄ conversion mediated by the [Cp*₃Mo₃S₄Fe] cluster

Mass spectrometry analysis of the reaction mixture after catalytic CO₂ reduction. The solution phase obtained by filtration of the reaction mixture after catalytic CO₂ reduction through a syringe filter was analyzed by electrospray ionization quadrupole time-of-flight mass spectrometry (ESI-QTOF-MS). The spectra were recorded using a Bruker Compact QTOF spectrometer. Catalytic reactions were carried out as described in the general procedure using cluster **1** as the precatalyst. Samples for ESI-MS analysis were prepared by diluting the filtrate with anhydrous THF.

Formation of [Cp*₃Mo₃S₄Fe(CO)]⁻ (4**) by reduction of cluster **1** under a CO₂ atmosphere.** Cluster **1** (11 mg, 12 μmol) and KC₈ (10 eq., 16 mg, 0.12 mmol) were suspended in THF (5 mL) and stirred for 10 min. The color of the suspension turned from dark reddish brown to yellowish-brown. The suspension was subsequently exposed to CO₂ (1 atm) and stirred for an additional 10 min, resulting in the color change to dark brownish green. The resulting mixture was filtered, and the filtrate was evaporated to give a black residue. A small portion of this material was used for FT-IR analysis. The remaining material was dissolved in C₆D₆ containing cyclododecane as an internal standard (11.9 mM, 800 μL, 9.5 μmol). Cluster **4** was quantified by its characteristic signal observed at 2.11 ppm (*Me*, 45H) and was afforded with 33% NMR yield. The ¹H NMR spectrum of pure **4** was recorded using crystalline material prepared by the procedure described below.

Synthesis of ¹³C-labeled **4 from reduction of cluster **1** under ¹³CO₂.** Cluster **1** (10 mg, 11 μmol) and KC₈ (10 eq., 16 mg, 0.12 mmol) were suspended in THF (5 mL) and stirred for 10 min. The color of the suspension turned dark yellowish brown from dark red. Subsequently, the mixture was stirred under a ¹³CO₂ atmosphere for 10 min to give a dark green suspension. Insoluble materials were removed by filtration, and the filtrate was evaporated to dryness. A small portion of this material was used for FT-IR analysis. The remaining material was dissolved in C₆D₆ containing cyclododecane as an internal standard (11.9 mM, 800 μL, 9.5 μmol). ¹³C-labeled **4** was obtained with 39% NMR yield. ¹H NMR (C₆D₆, 400 MHz, ppm): δ 2.12 (br, 45H, *Me*). FT-IR (ATR, cm⁻¹): 1646 (¹³CO).

Independent Synthesis of [Cp*₃Mo₃S₄Fe(CO)] (5**) from cluster **1** and CO.** A reddish-brown solution of **1** (97.6 mg, 0.107 mmol) in THF (30 mL) was frozen with liquid nitrogen, followed by the addition of KC₈ (1.2 eq., 18.2 mg, 0.135 mmol). The reaction vessel was subsequently charged with CO (1 atm) while the reaction mixture remained frozen and then allowed to warm gradually to room temperature under stirring overnight. The resulting brown suspension was filtered to remove insoluble materials. The brown filtrate was evaporated in vacuo to give a black residue. The residue was extracted with a mixture of hexane (4 mL) and THF (8 mL). Crystallization of the extract at -30 °C over two days gave black needle crystals of [Cp*₃Mo₃S₄Fe(CO)] (**5**, 69 mg, 0.076 mmol) with 71% yield. Single crystals suitable for X-ray diffraction analysis were obtained by recrystallization from toluene. ¹H NMR (THF-*d*₈, 400 MHz, ppm): δ 7.85 (br, 45H, *Me*). ¹³C NMR (THF-*d*₈, 400 MHz, ppm): δ 113.4 (*CMe*), 40.1 (*CMe*). FT-IR (ATR, cm⁻¹): 1857 (CO). Anal. Calcd. for C₃₁FeH₄₅Mo₃OS₄: C, 41.11; H, 5.01; S, 14.16. Found: C, 40.73; H, 4.82; S, 13.73.

Synthesis of [K(THF)][Cp*₃Mo₃S₄Fe(CO)] ([K(THF)]4**) by reduction of cluster **5**.** A mixture of cluster **5** (60 mg, 66 μmol) and KC₈ (11 mg, 81 μmol) in THF (30 mL) was stirred,

leading to the formation of a greenish-brown suspension. Insoluble materials were removed by filtration, and the filtrate was evaporated to dryness in vacuo. The resultant black residue was washed with a mixture of THF (1 mL) and pentane (5 mL), followed by extraction with a mixture of THF (3 mL) and pentane (0.5 mL). The extract was stored at $-30\text{ }^{\circ}\text{C}$ for a week to give black crystals. The crystals were collected, washed with pentane (1 mL), and dried under vacuum to give $[\text{K}(\text{THF})][\text{Cp}^*\text{Mo}_3\text{S}_4\text{Fe}(\text{CO})]$ ($[\text{K}(\text{THF})]\mathbf{4}$, 27 mg, 26 μmol) with 40% yield. Single crystals suitable for X-ray diffraction analysis were grown by layering pentane onto a THF solution of $[\text{K}(\text{THF})]\mathbf{4}$. X-ray analysis revealed that these crystals crystallized as $[\text{K}(\text{THF})][\text{K}(\text{THF})_3]\mathbf{4}_2$ as described below. ^1H NMR (C_6D_6 , 400 MHz, ppm): δ 3.58 (m, 4H, $\text{CH}_2(2,5)$ of THF), 2.11 (br, 45H, *Me*), 1.42 (m, 4H, $\text{CH}_2(3,5)$ of THF). ^{13}C NMR (C_6D_6 , 400 MHz, ppm): δ 101.5 (*CMe*), 67.9 ($\text{CH}_2(2,5)$ of THF), 25.9 ($\text{CH}_2(3,5)$ of THF) 13.8 (*CMe*). FT-IR (ATR, cm^{-1}): 1692 (CO). Anal. Calcd. for $\text{C}_{35}\text{FeH}_{53}\text{KMo}_3\text{O}_2\text{S}_4$: C, 41.34; H, 5.01; S, 12.61. Found: C, 40.86; H, 4.82; S, 12.41.

Redox properties of cluster 5. A cyclic voltammogram of cluster **5** was recorded on a BAS ALS660A analyzer using the following conditions: Solvent, THF; sample concentration, 0.5 mM; working electrode, glassy carbon; counter electrode, Pt wire; reference electrode, Ag/AgCl; supporting electrolyte, $[\text{N}^n\text{Bu}_4][\text{PF}_6]$ (0.1 M); scan rate, 100 mV/s. Potentials were referred to the ferrocene/ferrocenium (Fc/Fc^+) redox couple measured as an internal standard.

Stability test of cluster 5 under a CO_2 atmosphere. Cluster **5** and cyclododecane (internal standard) were dissolved in THF- d_8 and transferred to an NMR tube with a J. Young valve. The internal atmosphere was then displaced by CO_2 (1 atm) from Ar. ^1H NMR analyses were performed both before the gas replacement and after standing at room temperature for one day following the replacement. Cluster **5** remained after the exposure to CO_2 was quantified by a comparison of peak areas of **5** (7.83 ppm, *CMe*) relative to the internal standard before and after the gas replacement.

CH_4 formation from cluster 5. Cluster **5** (4.5 mg, 5.0 μmol), solid SmI_2 (32 equiv., 0.16 mmol) and THF (0.30 mL) were placed in a crimp-sealed vial fitted with a butyl rubber septum under an argon atmosphere. After 3 minutes of stirring, H_2O (20 μL) was added to the mixture. The mixture changed from deep blue to red within approximately 20 seconds at room temperature, indicating rapid consumption of SmI_2 . Gas-phase products were then quantified by the GC-FID and GC-TCD analyses as described above.

X-ray crystallographic analysis

Single-crystal X-ray diffraction data of **4** and **5** were collected on a Rigaku RA-Micro 7HFMR diffractometer equipped with a HyPix-6000HE detector using graphite-monochromated MoK α radiation ($\lambda = 0.710690$ Å) at -150 °C under a cold N₂ stream. Crystals were coated with oil (Perfluoro(polyoxypropylene ethyl ether) 8,400, Wako pure chemical industries, Ltd) and placed on polyimide crystal mount tools. Preliminary cell parameters were obtained from thirty frames collected with 0.5° increments of ω . Full data sets were subsequently collected with 0.5° intervals of ω . Data reduction and integration were carried out with CrysAlisPro. Empirical absorption corrections were applied using SCALE3 ABSPACK scaling algorithm. All structures were solved by direct methods (SHELXT) and refined by full-matrix least squares (SHELXL). Cluster **4** crystallized as [K(THF)][K(THF)₃][**4**]₂, as described above. Methyl groups of a Cp* ligand and three of four THF molecules were disordered over two positions. Occupancies for the disordered moieties were refined as follows: 50:50 ((C58-C62):(C58A-C62A), Cp*), 55:45 ((C67-C70):(C67A-C70A), THF), 60:40 ((O5 and C71-C74):(O5A and C71A-C74A), THF), and 55:45 ((O6 and C76-C78):(O6A and C76A-C78A), THF). EADP constraints were applied to all disordered pairs. In addition, SIMU restraints were applied to the disordered methyl groups of the Cp* ligand (C58-62 and C58A-62A), and RIGU restraints were applied to O6, C75-C78, O6A, and C75A-C78A. The asymmetric unit of cluster **5** contains two crystallographically independent molecules. SIMU restraints were applied to one cyclopentadienyl ring (C2A-C6A). Hydrogen atoms were placed using a riding model. Crystallographic data have been deposited with Cambridge Crystallographic Data Centre. Deposition numbers CCDC 2586720 ([K(THF)][K(THF)₃][**4**]₂) and 2586721 (**5**) contain the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service.

Computational analysis

Computational methods. Geometry optimizations were performed using density functional theory (DFT), as implemented in the ORCA program (Version 6.1)⁴⁴. The TPSS density functional⁴⁵, including Grimme's dispersion and Becke-Johnson damping⁴⁶, def2-TZVP⁴⁷ basis sets and def2/J⁴⁸ auxiliary basis sets were employed for all atoms. A conductor-like continuum polarization model (C-PCM)^{49,50} was used as the implicit solvent model, with tetrahydrofuran as the solvent. Harmonic vibrational frequencies were computed to obtain zero-point energies and to confirm that the optimized structures are local minima (i.e., no imaginary frequency) or transition states (i.e., one imaginary frequency). The thermal corrections for the reported energies were evaluated at 298.15 K and 1 atm.

Geometry optimizations of cluster 4. Geometry optimizations of $[\text{Cp}^*_3\text{Mo}_3\text{S}_4\text{Fe}(\text{CO})]^-$ (**4**) identify the $S = 0$ (closed-shell) state as the ground state of the cluster, with the $S = 1$ and $S = 2$ states lying 18.8 and 18.6 kcal/mol higher in energy, respectively (relative energies computed as potential energies plus zero-point energy corrections). The optimized $S = 0$ structure closely reproduces the key structural parameters of the X-ray crystal structure, including the Fe1–C1, C1–O1, and Fe–S bond lengths (within 0.05 Å) as well as the Fe–Mo distances. In contrast, the higher-spin $S = 1$ and $S = 2$ states show more pronounced deviations from the crystallographic geometry, most notably in the Fe1–Mo3 distance, which elongates to 3.05 ($S = 1$) and 3.18 Å ($S = 2$), respectively, compared to 2.77 Å in the crystal structure and 2.74 Å in the $S = 0$ optimized geometry. These results support assignment of the $S = 0$ state as the electronic ground state of the cluster. This is consistent with the diamagnetic nature of **4** observed by ^1H NMR spectroscopy. The computed ground state showed a CO stretching frequency at 1745 cm^{-1} , comparable to the experimental value (1690–1692 cm^{-1} for **4**).

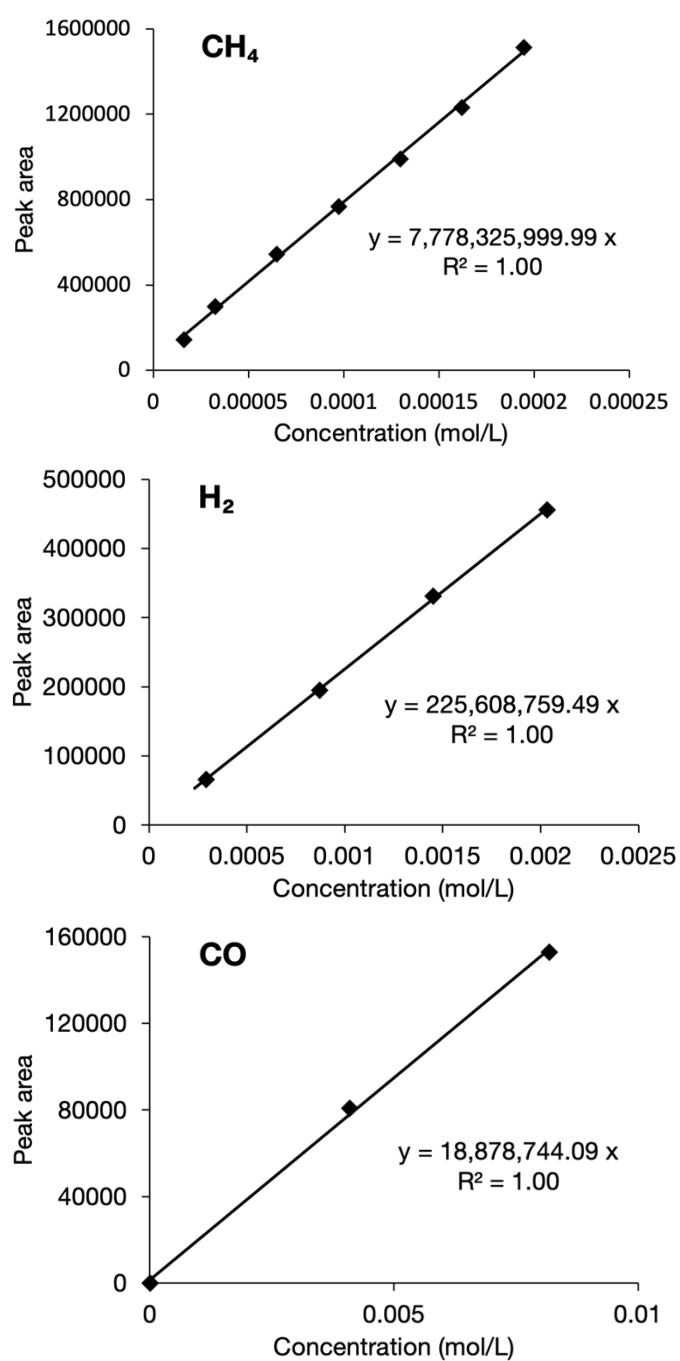
Geometry optimizations of cluster 5. Geometry optimizations of $[\text{Cp}^*_3\text{Mo}_3\text{S}_4\text{Fe}(\text{CO})]$ (**5**) identify the $S = 1/2$ state as the ground state, with the $S = 3/2$ and $S = 5/2$ states lying 17.6 and 42.1 kcal/mol higher in energy, respectively (relative energies computed as potential energies plus zero-point energy corrections). The optimized $S = 1/2$ structure agrees well with the X-ray crystal structure, reproducing the Fe1–C1, C1–O1, Fe–S, and Fe–Mo bond lengths within 0.05 Å. The higher-spin states show larger structural deviations: in the $S = 3/2$ state, the Fe1–Mo1 distance elongates to 3.15 Å (vs. 2.73 Å in the crystal structure and 2.68 Å for $S = 1/2$), while in the $S = 5/2$ state both the Fe1–Mo1 (3.15 Å) and Fe1–Mo1 (3.03 Å) distances are significantly elongated. These systematic distortions in the excited spin states further support assignment of $S = 1/2$ as the electronic ground state. Löwdin population analysis of the $S = 1/2$ ground state confirms that the unpaired electron is localized mainly on the Fe center, which carries a spin density of 0.79. In contrast, the three Mo centers carry only small spin densities (0.04–0.05), and the coordinating S and C/O atoms show negligible spin population (< 0.02), indicating minimal radical character on the ligand framework. The computed ground state showed a vibrational CO stretching frequency of 1820 cm^{-1} , which is in qualitative agreement with the observed value (1857 cm^{-1} for **5**).

Supplementary note on DFT-calculated Fe-CO binding energies. The CO binding energy calculated for the anionic cluster **4** (70.8 kcal/mol) is markedly larger than that for the neutral cluster **5** (53.5 kcal/mol). This charge-dependent difference reflects the added electron density in **4**, which strengthens $\text{Fe}(3d) \rightarrow \text{CO}(2\pi^*)$ backdonation and stabilizes the Fe-CO bond. Together with the preferential CO binding over CO_2 discussed in the main text, this charge-

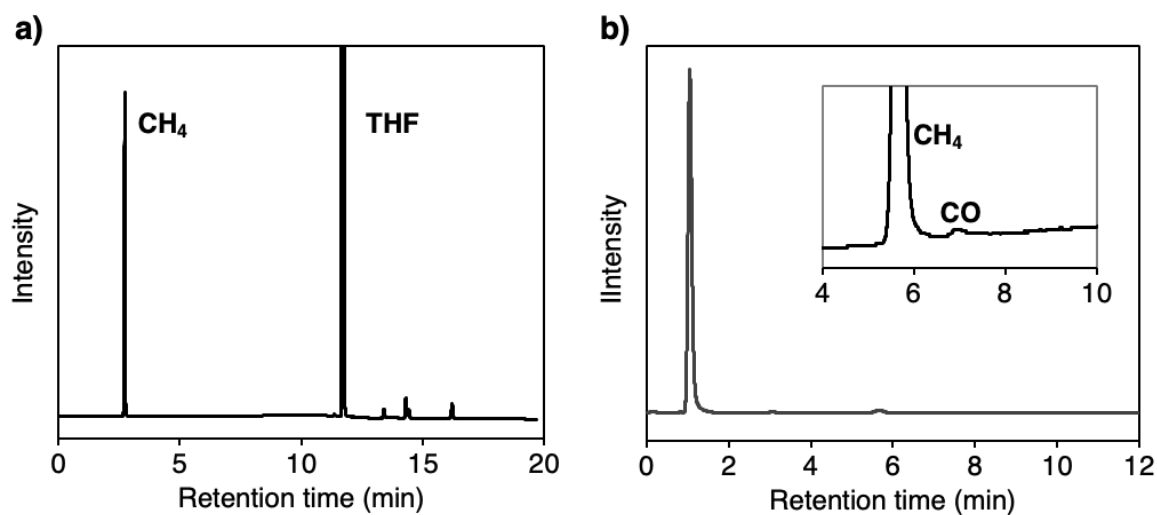
dependent modulation of Fe-CO affinity could contribute to the productive retention of the CO intermediate.

Computational analysis of CO₂ coordination to [Cp*₃Mo₃S₄Fe] cluster. The ground state of the precursor, [Cp*₃Mo₃S₄FeCl] (**R**, described as **1** in the main text), is triplet ($S = 1$, **R**³), which was set as the reference energy (0.0 kcal/mol). The quintet ($S = 2$, **R**⁵) and singlet ($S = 0$, **R**¹) states lie 15.3 and 24.5 kcal/mol higher in energy, respectively, indicating a well-isolated triplet ground state for **R**. Upon reduction and dissociation of Cl[−], the intermediate **I1** is formed, where the spin ordering changes: the quartet state ($S = 3/2$, **I1**⁴) becomes the ground state, and is 40.1 kcal/mol below the reference, while the doublet ($S = 1/2$, **I1**²) and sextet ($S = 5/2$, **I1**⁶) states are less stable, at −33.5 and −26.6 kcal/mol, respectively. The stabilization of the higher-spin quartet state reflects the reduced ligand field upon loss of Cl[−] ligand. Coordination of THF gives rise to **I2**, where the doublet state ($S = 1/2$, **I2**²) becomes the ground state at −42.5 kcal/mol, while the quartet ($S = 3/2$, **I2**⁴) and sextet ($S = 5/2$, **I2**⁶) states are higher in energy, at −37.8 and −22.6 kcal/mol. The spin-state crossing from quartet (**I1**) to doublet (**I2**) is observed upon THF binding. The CO₂ coordination can yield **I3**, which favors a doublet ground state ($S = 1/2$, **I3**²), and is substantially stabilized at −60.4 kcal/mol relative to **R**. The corresponding quartet (**I3**⁴, −43.5 kcal/mol) and sextet (**I3**⁶, −24.9 kcal/mol) states are relatively unstable. We note that the optimized ground-state structure of **I3**² shows CO₂ binding in a side-on (η^2) manner (Supplementary Fig. 26a), whereas end-on binding via an O atom (Supplementary Fig. 26b) is 30.6 kcal/mol higher in energy. Comparing the ground-state energies along the pathway (**R**³ → **I1**⁴ → **I2**² → **I3**²), CO₂ binding is thermodynamically favorable. The CO₂-bound complex **I3** (−60.4 kcal/mol) is more stable than the THF adduct **I2** (−43.0 kcal/mol) by 17.4 kcal/mol. This preference for CO₂ over THF coordination, despite THF being present in large excess as solvent, indicates that CO₂ binding to the Fe center is thermodynamically favorable, allowing an accessible and efficient entry point for the subsequent CO₂ reduction chemistry.

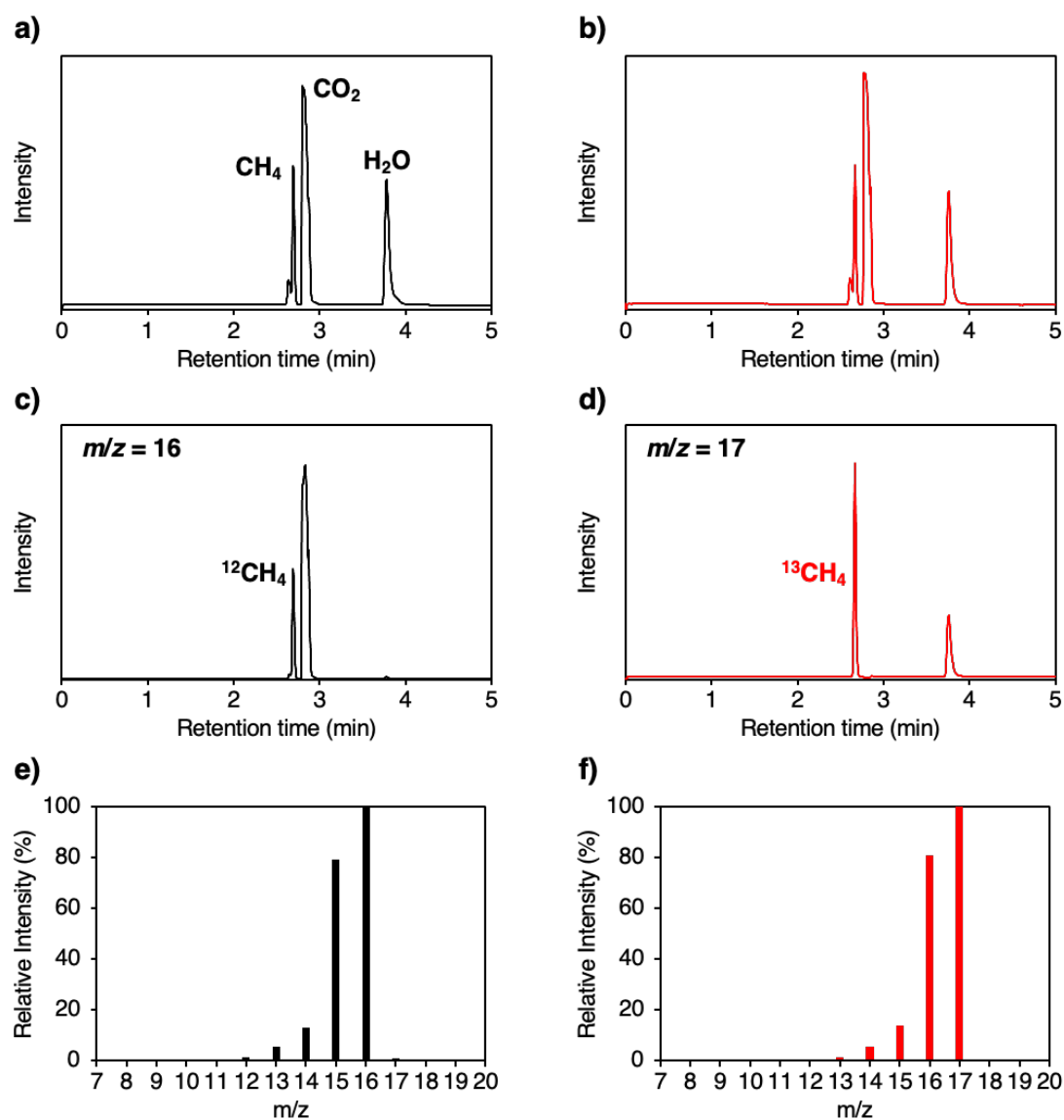
Supplementary Figures



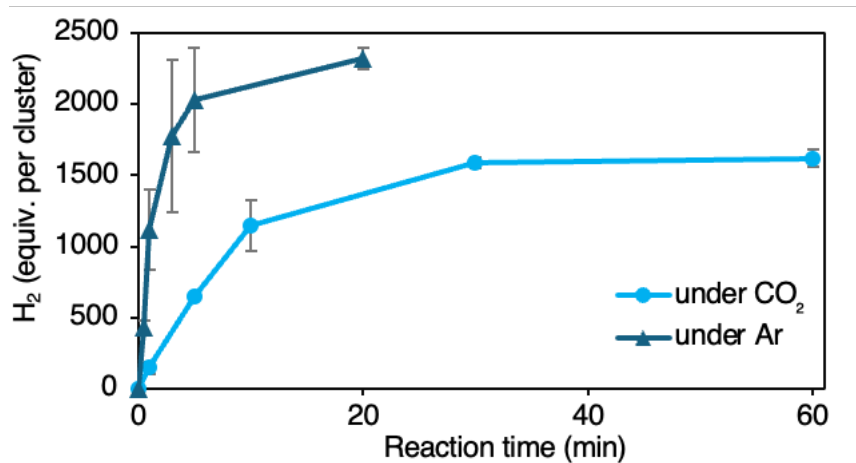
Supplementary Fig. 1. Calibration curves for quantification of CH₄, CO, and H₂.



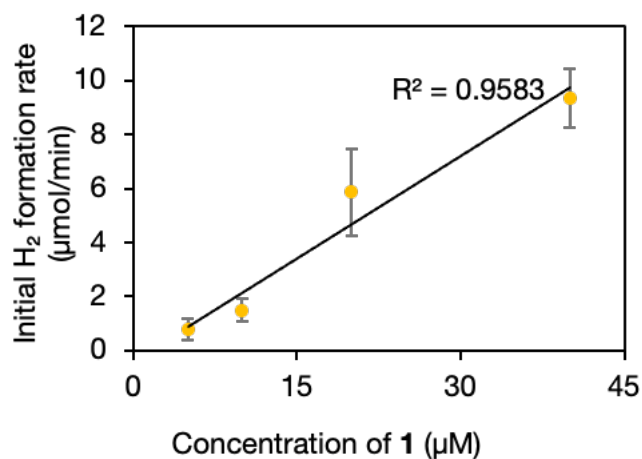
Supplementary Fig. 2. Representative GC-FID (a) and GC-TCD (b) charts of the headspace gas obtained from the experiment, Supplementary Table 1, entry 1, run 1. The inset of (b) displays an enlarged view of the retention time region where CH_4 and CO were detected.



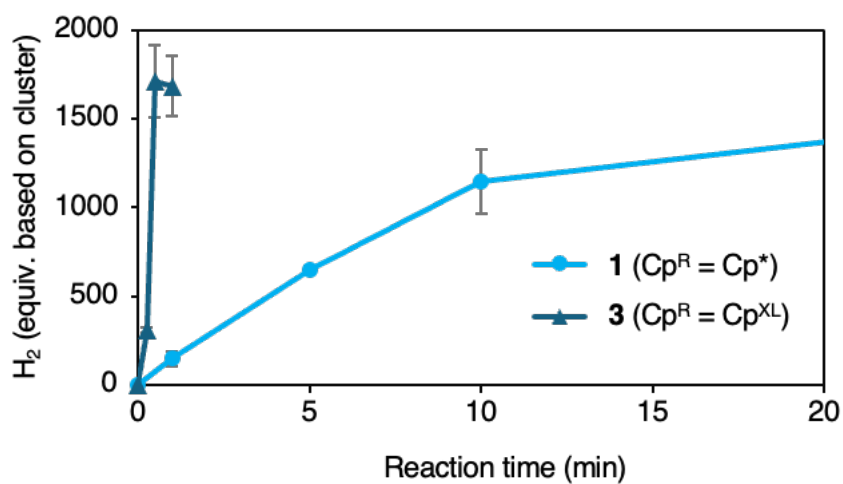
Supplementary Fig. 3. GC-MS analysis of the gas phase obtained from catalytic reduction of CO_2 to CH_4 under unlabeled CO_2 (a, c, e) and $^{13}\text{CO}_2$ (b, d, f) atmospheres in the presence of **1**. Shown are full GC-MS charts (a, b), extracted ion chromatograms at $m/z = 16$ (c) and 17 (d), and mass spectra of the generated CH_4 (e, f).



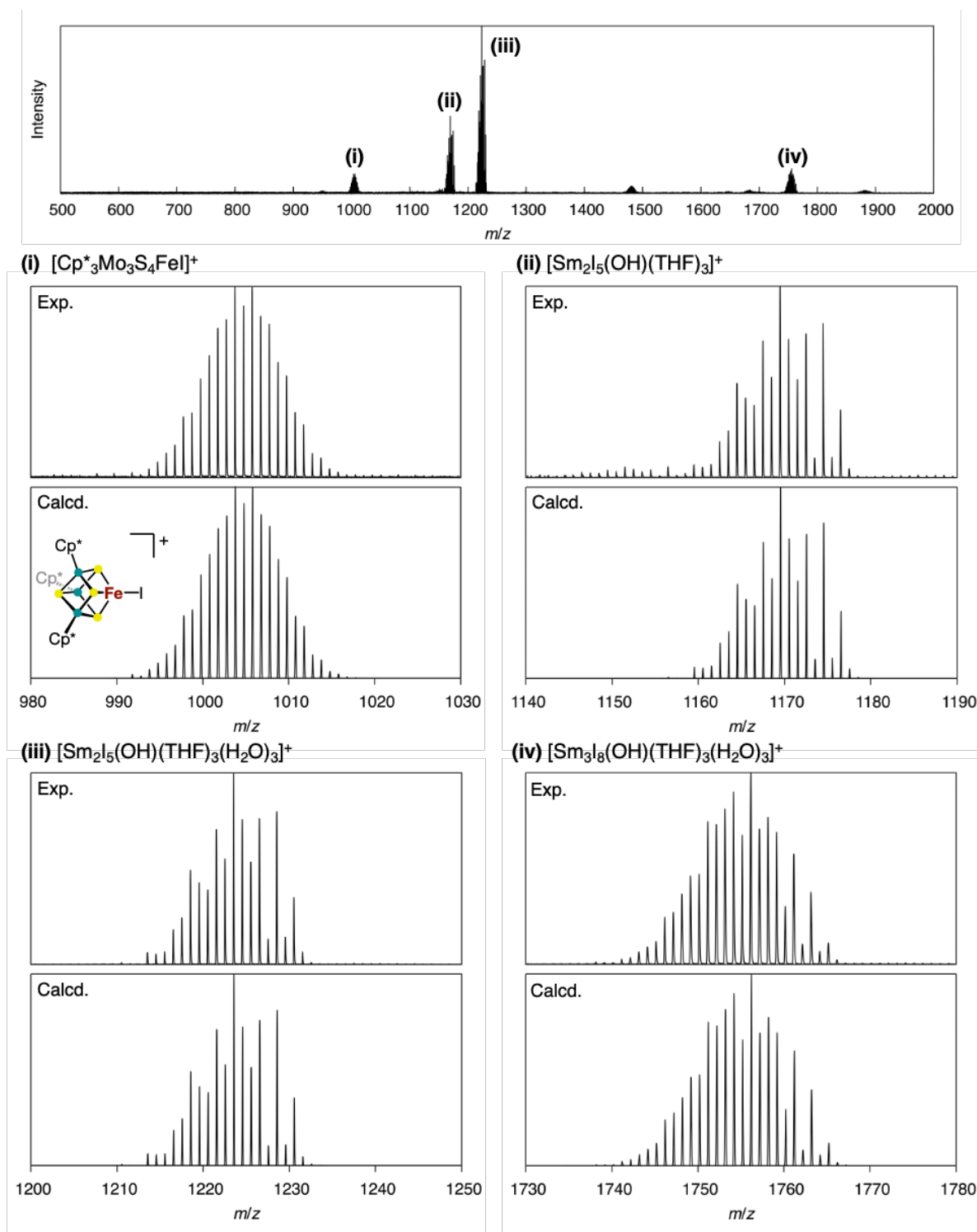
Supplementary Fig. 4. Time course analysis of the H₂ formation during the catalytic reactions under CO₂ (blue) and Ar (navy) by **1**. Data were obtained from three independent experiments and shown as average $\pm$ standard deviation.



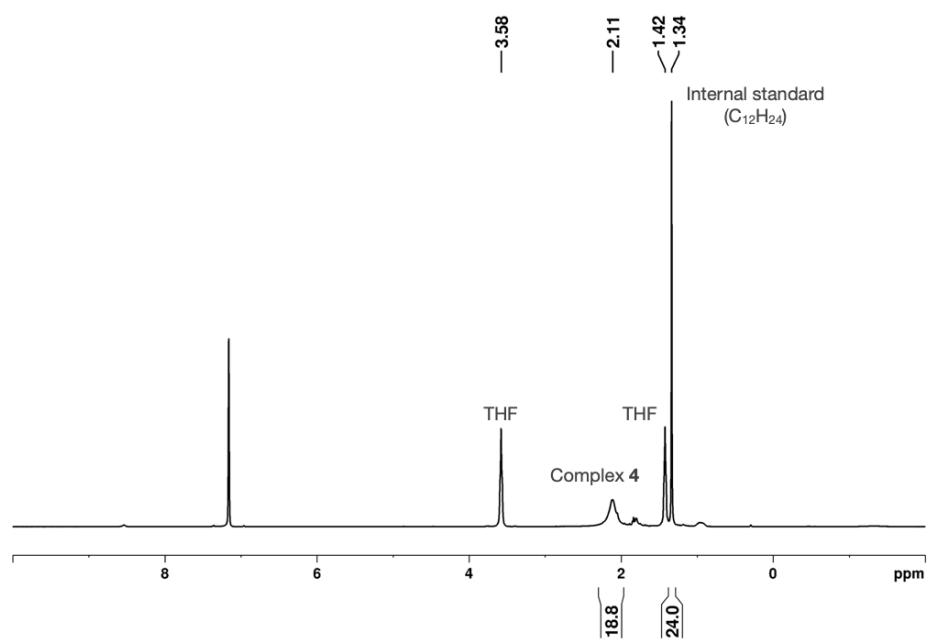
Supplementary Fig. 5. Plot of initial rates of H₂ production versus precatalyst concentrations in the CO₂ reduction reaction by **1**. Data were obtained from three independent experiments and shown as average $\pm$ standard deviation.



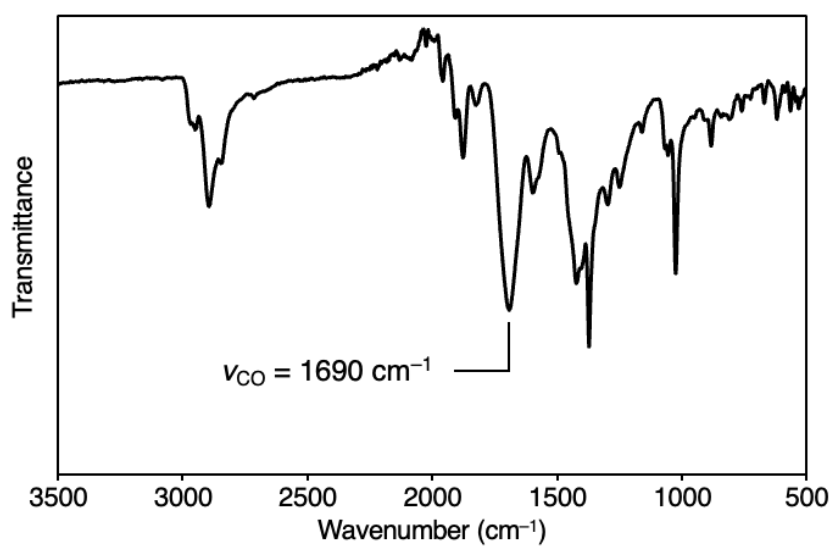
Supplementary Fig. 6. Time course analysis of the H₂ formation during the catalytic reactions under CO₂ using cluster **1** (blue) and **3** (navy) as precatalysts. The time points for **3** were taken at 0.25, 0.5, and 1 min. Data were obtained from three independent experiments and presented as average $\pm$ standard deviation.



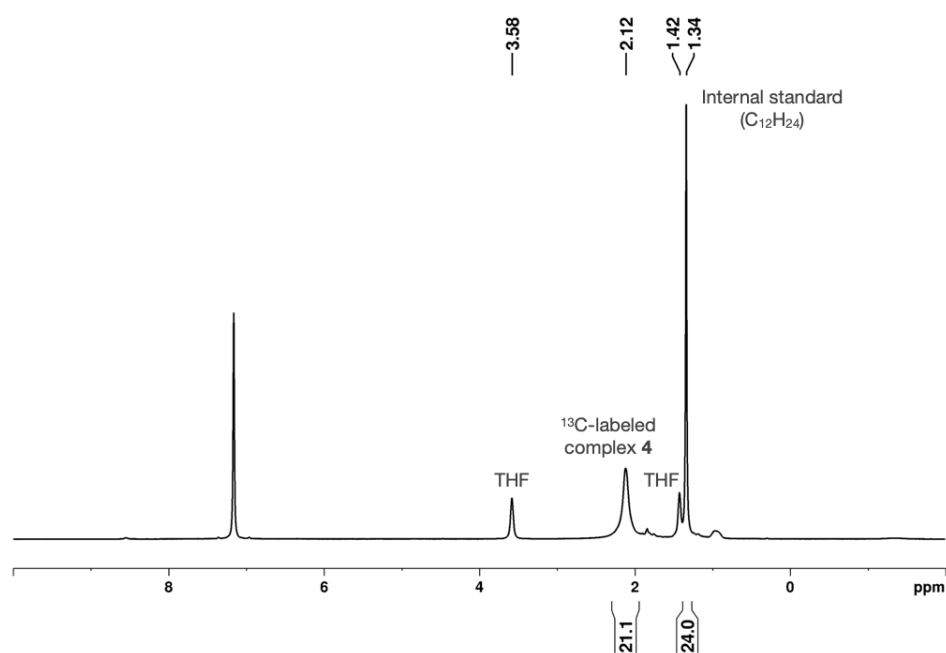
Supplementary Fig. 7. Post-catalytic mass spectrum of the reaction solution, showing an intact $[\text{Cp}^*_3\text{Mo}_3\text{S}_4\text{Fe}]$ cluster and SmI_2 -derived species. Major species (i-iv) were assigned to $[\text{Cp}^*_3\text{Mo}_3\text{S}_4\text{Fe}]^+$ (i), $[\text{Sm}_2\text{I}_5(\text{OH})(\text{THF})_3]^+$ (ii), $[\text{Sm}_2\text{I}_5(\text{OH})(\text{THF})_3(\text{H}_2\text{O})_3]^+$ (iii), and $[\text{Sm}_3\text{I}_8(\text{OH})(\text{THF})_3(\text{H}_2\text{O})_3]^+$ (iv), based on comparison of the experimental and calculated isotope patterns.



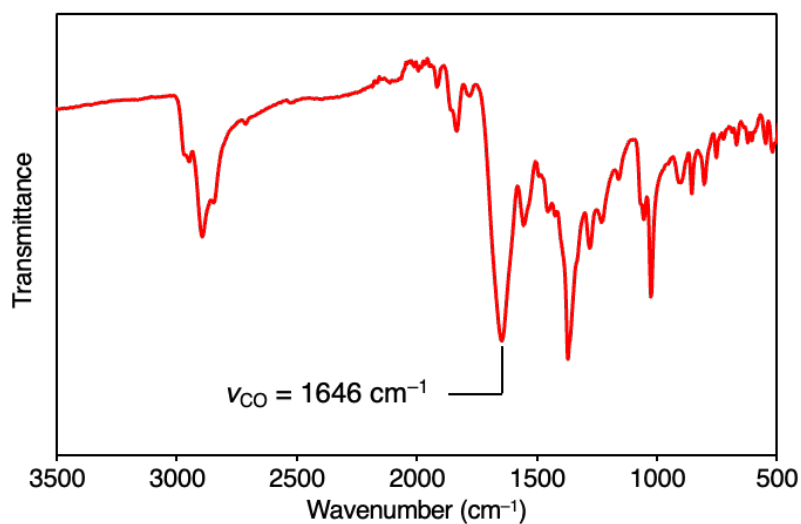
Supplementary Fig. 8. ^1H NMR spectrum of $[\text{Cp}^*_3\text{Mo}_3\text{S}_4\text{Fe}(\text{CO})]^-$ (**4**) formed by reduction of cluster **1** under a CO_2 atmosphere. The spectrum was measured in C_6D_6 containing cyclododecane ($\text{C}_{12}\text{H}_{24}$) as an internal standard.



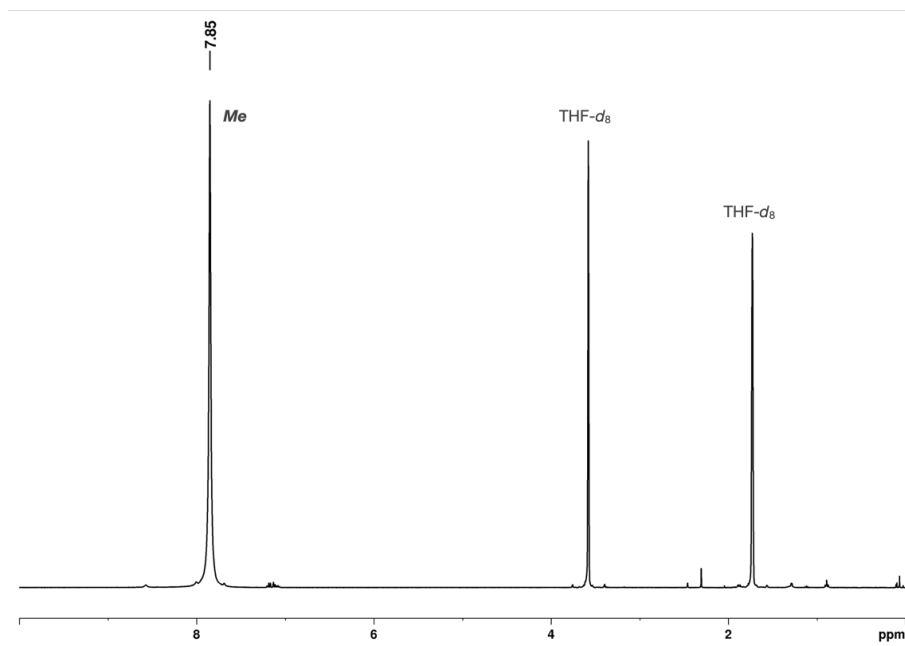
Supplementary Fig. 9. Solid-state FT-IR spectrum of **4** formed by reduction of cluster **1** under a CO_2 atmosphere.



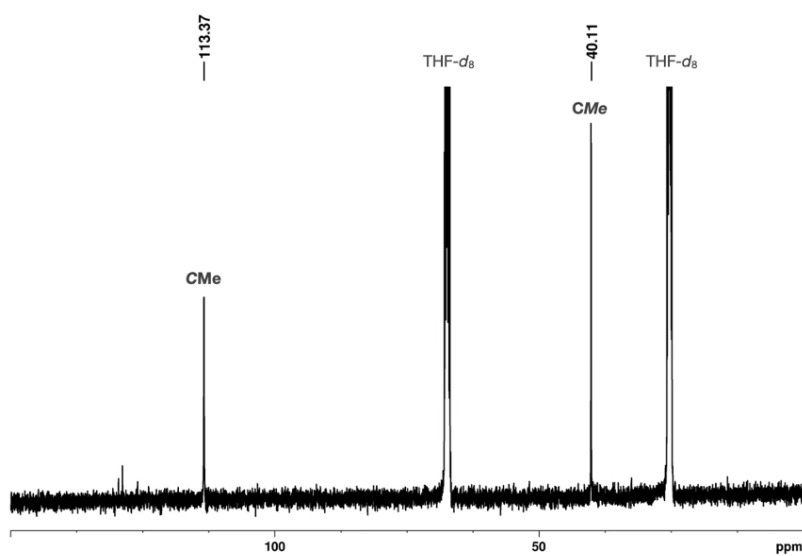
Supplementary Fig. 10. ^1H NMR spectrum of **4** formed by reduction of cluster **1** under a $^{13}\text{CO}_2$ atmosphere. The spectrum was measured in C_6D_6 containing cyclododecane ($\text{C}_{12}\text{H}_{24}$) as an internal standard.



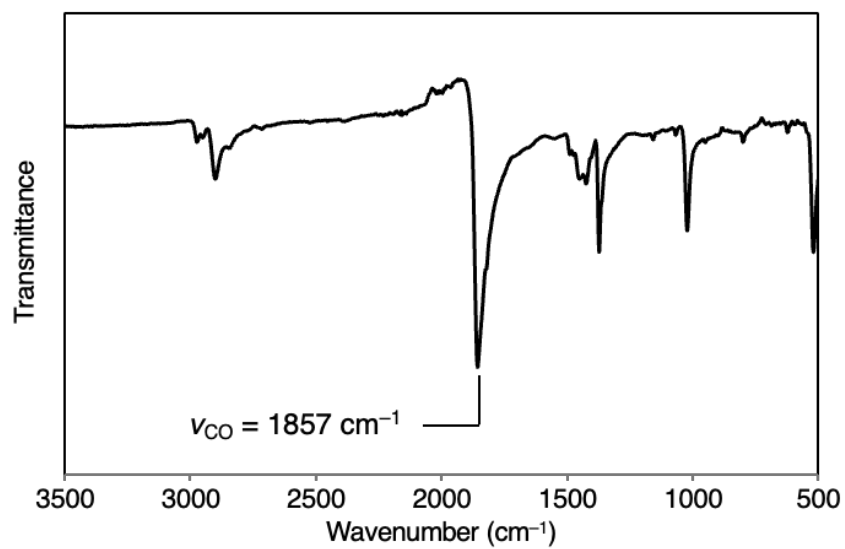
Supplementary Fig. 11. Solid-state FT-IR spectrum of **4** formed by reduction of cluster **1** under a $^{13}\text{CO}_2$ atmosphere.



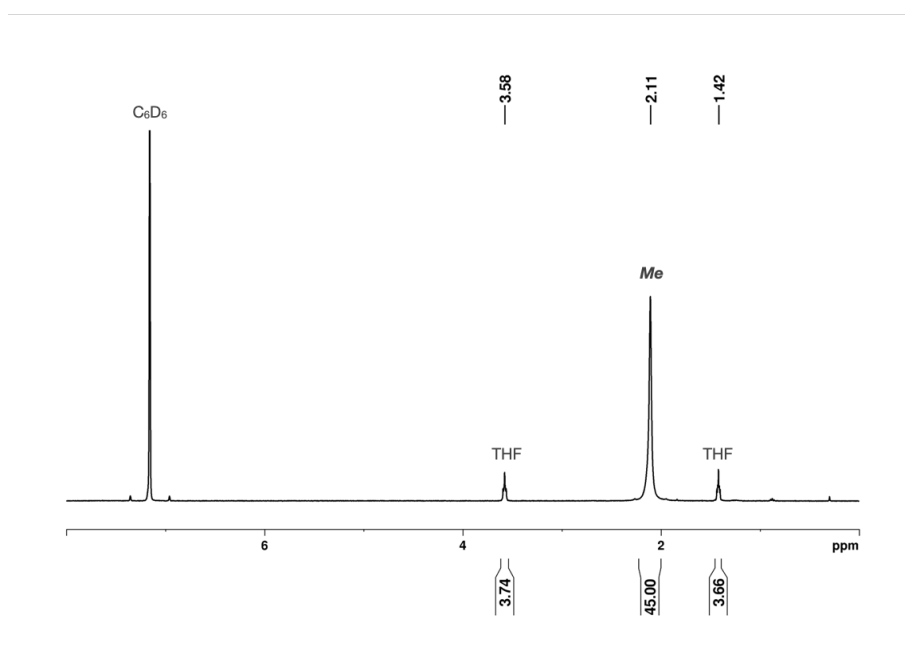
Supplementary Fig. 12. ^1H NMR spectrum of $[\text{Cp}^*_3\text{Mo}_3\text{S}_4\text{Fe}(\text{CO})]$ (**5**) in $\text{THF-}d_8$.



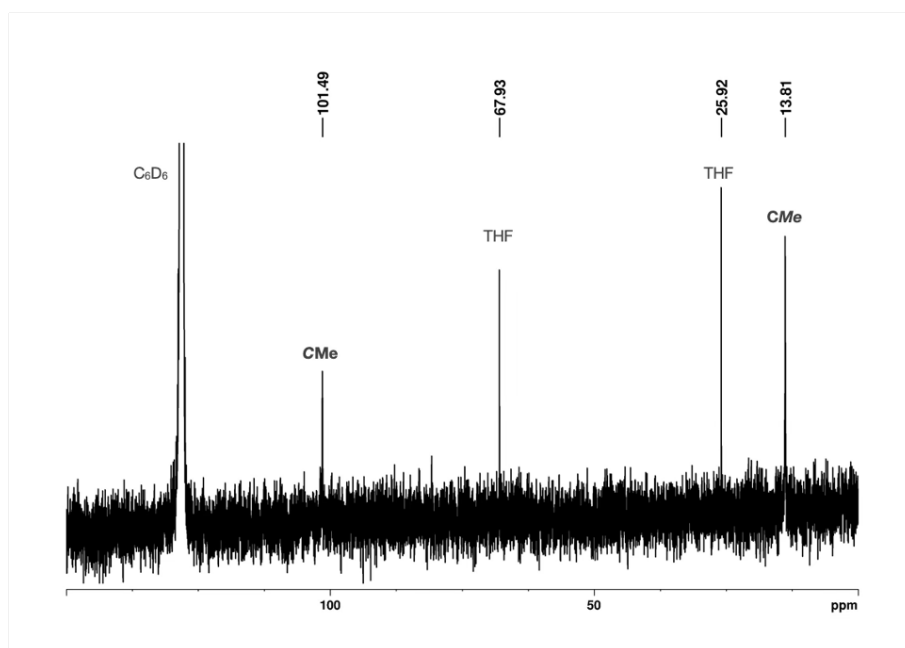
Supplementary Fig. 13. ^{13}C NMR spectrum of **5** in $\text{THF-}d_8$.



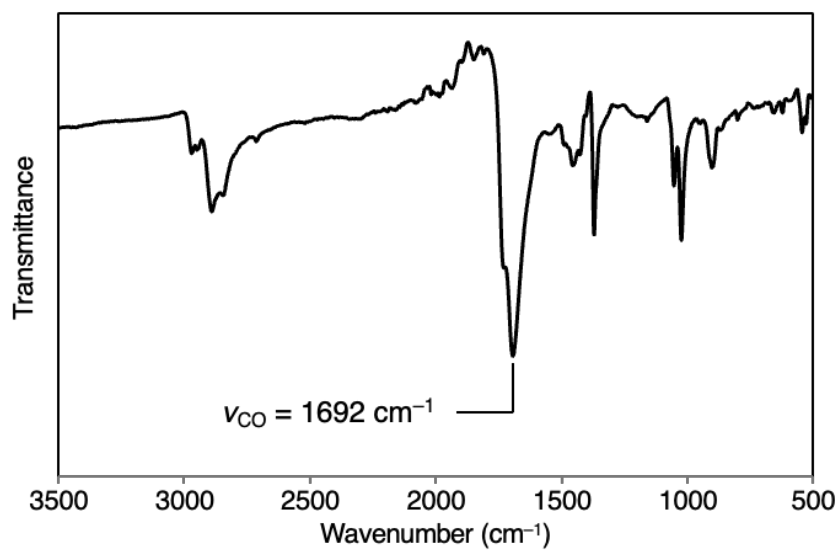
Supplementary Fig. 14. Solid-state FT-IR spectrum of **5**.



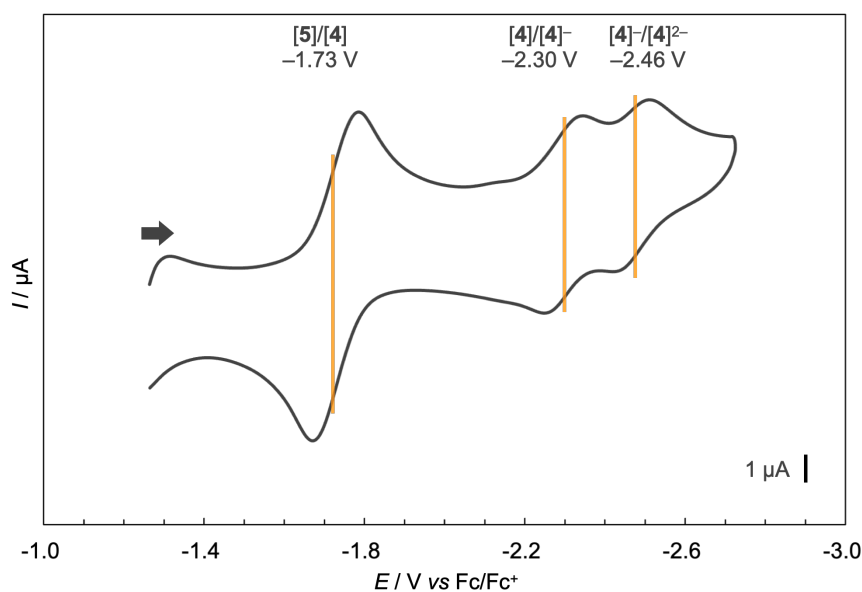
Supplementary Fig. 15. ^1H NMR spectrum of $[\text{K}(\text{THF})][\text{Cp}^*_3\text{Mo}_3\text{S}_4\text{Fe}(\text{CO})]$ ($[\text{K}(\text{THF})]\mathbf{4}$) in C_6D_6 .



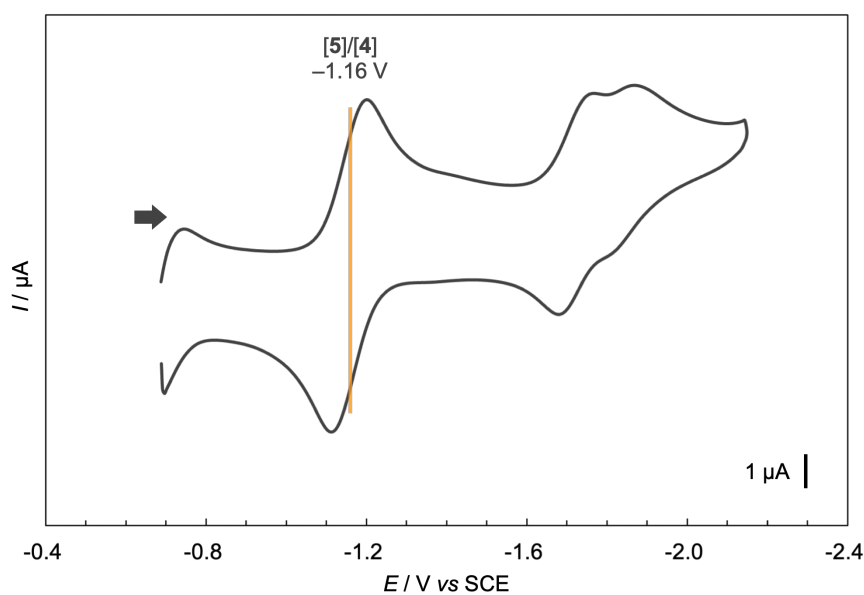
Supplementary Fig. 16. ^{13}C NMR spectrum of $[\text{K}(\text{THF})]\mathbf{4}$ in C_6D_6 .



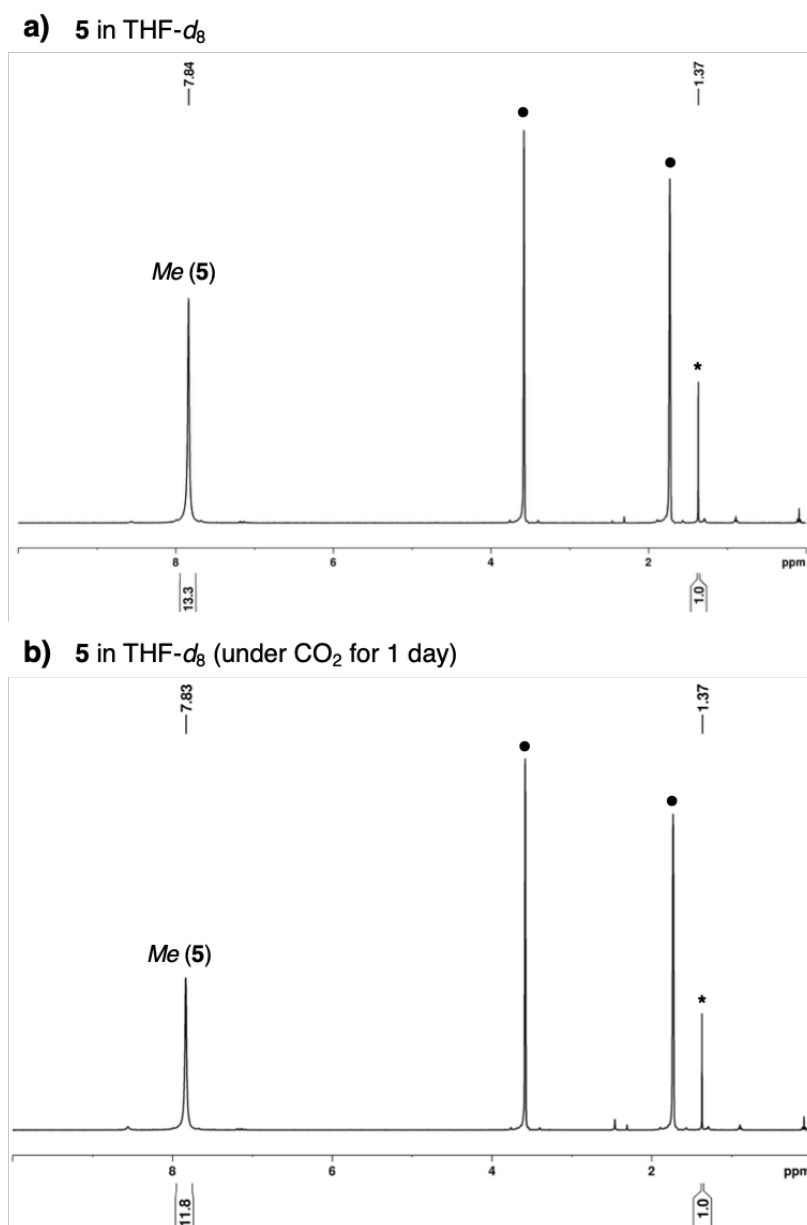
Supplementary Fig. 17. Solid-state FT-IR spectrum of [K(THF)]₄.



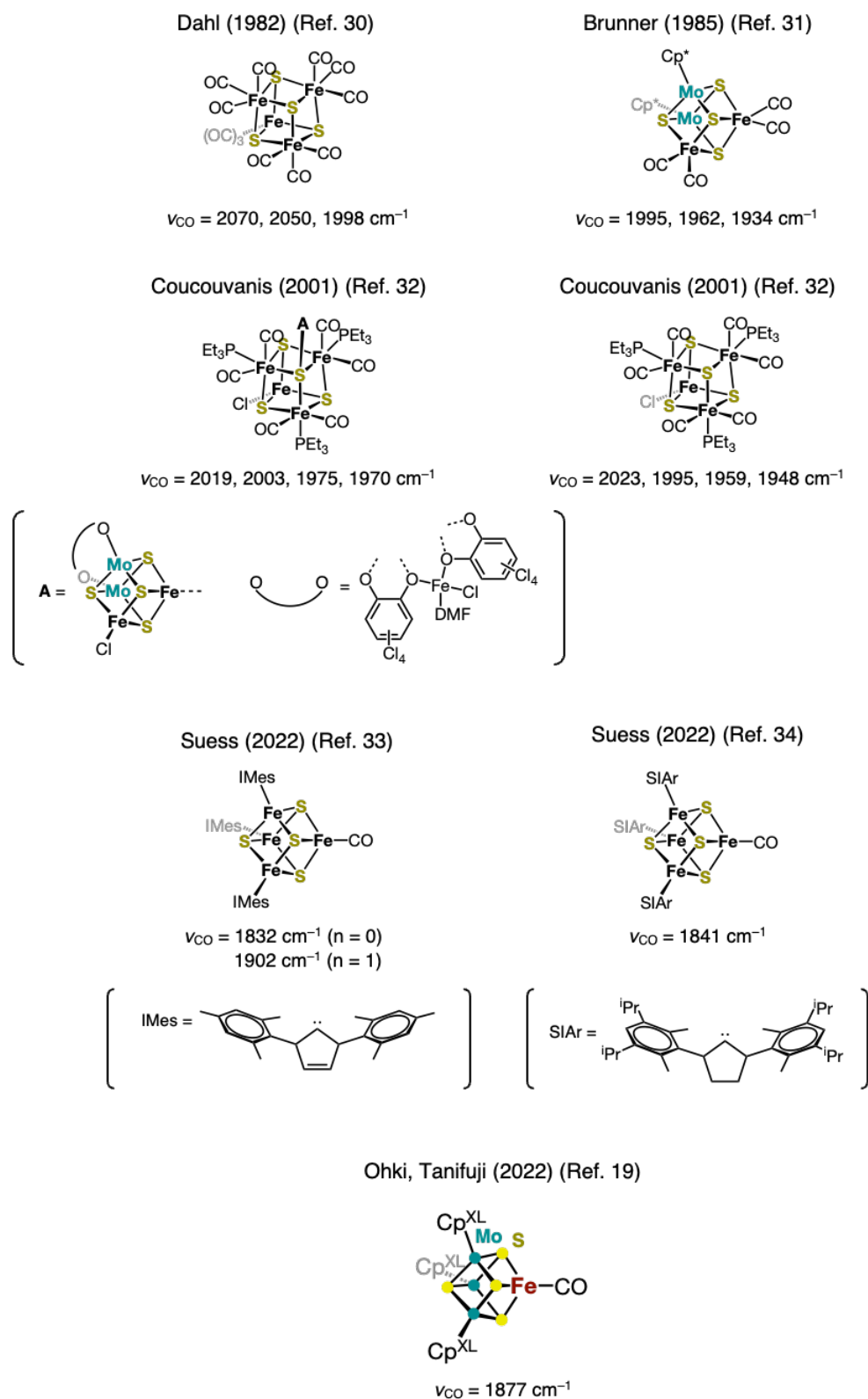
Supplementary Fig. 18. Cyclic voltammogram of **5** (0.5 mM) recorded in THF under a N_2 atmosphere. One electron reduced form of **5** is described as **4** ($[\text{Cp}^*_3\text{Mo}_3\text{S}_4\text{Fe}(\text{CO})]^-$) in the voltammogram.



Supplementary Fig. 19. Cyclic voltammogram of **5** shown with potentials versus standard calomel electrode (SCE). The original voltammogram is similar to the one shown in Supplementary Fig. 18, where the potentials were converted from Fc/Fc^+ ($\text{Fc} = \text{FeCp}_2$) to saturated calomel electrode (SCE) references based on the following equation: $E \text{ (V vs. SCE)} = E \text{ (V vs. Fc/Fc}^+) - 0.56 \text{ V}$ (ref. 28). One electron reduced form of **5** is described as **4** ($[\text{Cp}^*_3\text{Mo}_3\text{S}_4\text{Fe}(\text{CO})]^-$) in the voltammogram.

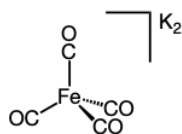


Supplementary Fig. 20. ^1H NMR spectra of **5** with cyclododecane ($\text{C}_{12}\text{H}_{24}$, internal standard) at room temperature under Ar (upper) and after a day-exposure of CO_2 (lower) in $\text{THF-}d_8$. Legend: * = Internal standard (cyclododecane, $\text{C}_{12}\text{H}_{24}$), ● = solvent ($\text{THF-}d_8$).



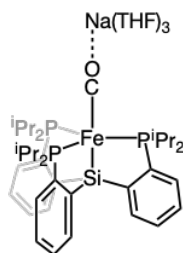
Supplementary Fig. 21. Structures and terminal Fe-CO stretching frequencies of structurally characterized cuboidal metal-sulfur clusters. References are indicated in the figure.

Edgell (1965) (Ref. 35)



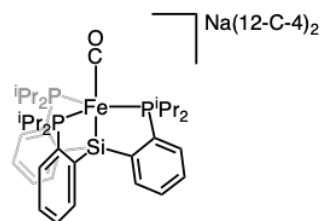
$\nu_{\text{CO}} = 1730 \text{ cm}^{-1}$

Peters (2011) (Ref. 36)



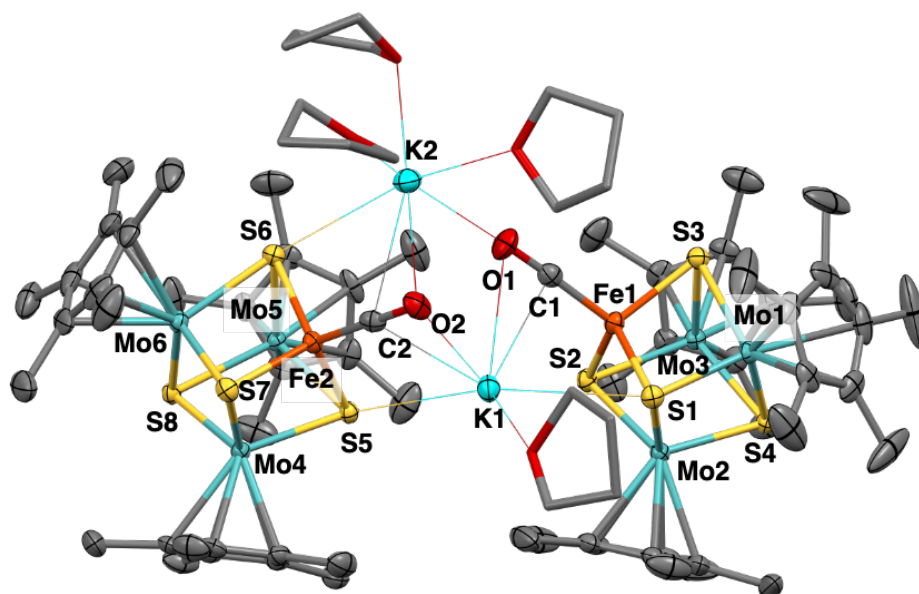
$\nu_{\text{CO}} = 1711 \text{ cm}^{-1}$
 $1676 \text{ cm}^{-1} (^{13}\text{CO})$

Peters (2011) (Ref. 36)

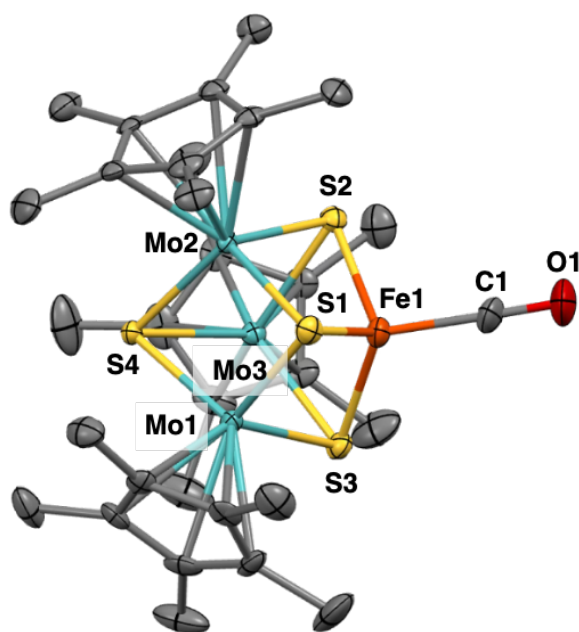


$\nu_{\text{CO}} = 1757 \text{ cm}^{-1}$
 $1711 \text{ cm}^{-1} (^{13}\text{CO})$

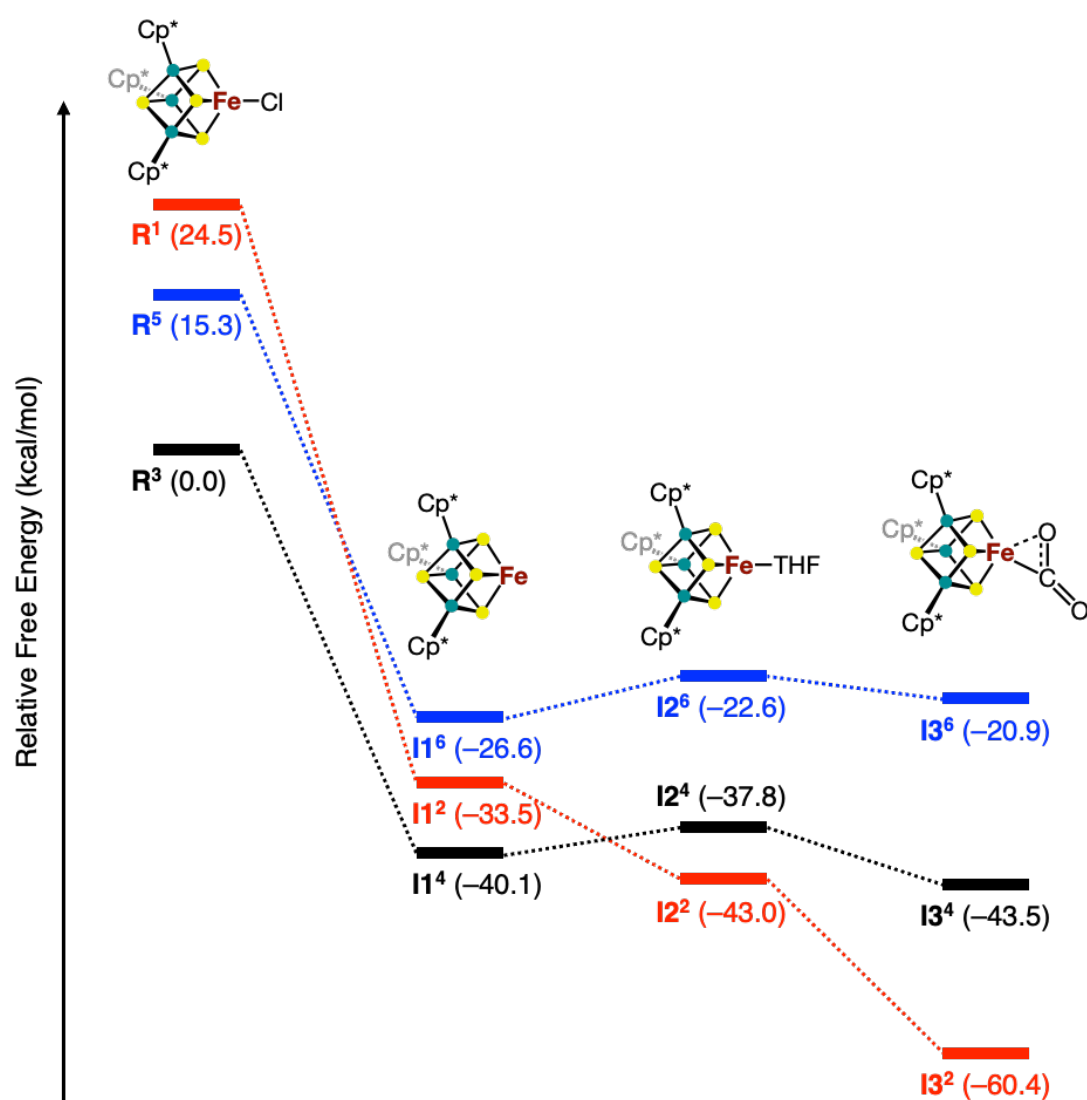
Supplementary Fig. 22. Representative examples of structurally characterized terminal Fe-CO complexes with notably low CO stretching frequencies. References for ν_{CO} values and crystal structures are indicated in the figure. For $\text{K}_2[\text{Fe}(\text{CO})_4]$, the ν_{CO} value and crystal structure (ref. 51) were reported separately.



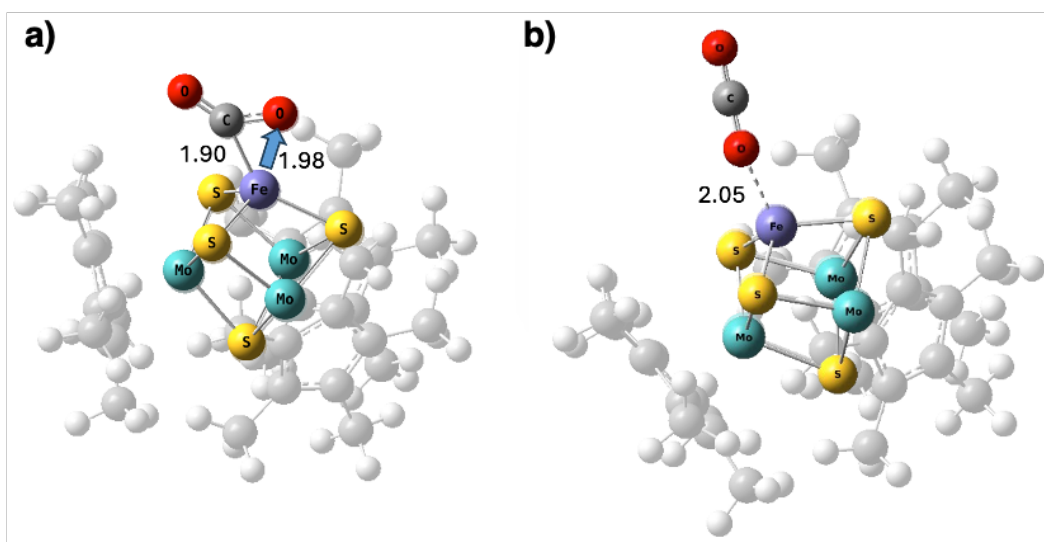
Supplementary Fig. 23. Crystal structure of $[K(THF)][K(THF)_3][4]_2$ with thermal ellipsoids set at the 50% probability level. For disordered Me groups of a Cp^* ligand and three THF molecules, each one of disordered pairs is shown. Hydrogen atoms are omitted for clarity. THF molecules are shown with capped stick description. Color legend: C, grey; O, red; K, turquoise; S, yellow; Mo, teal; and Fe, orange. Selected bond distances (Å) and angles (°): Fe1-C1 1.721(3), C1-O1 1.196(4), Fe1-S1 2.1912(8), Fe1-S2 2.1928(8), Fe1-S3 2.1801(9), Fe1-Mo1 2.7809(5), Fe1-Mo2 2.8149(5), Fe1-Mo3 2.7864(5), Mo1-S1 2.3506(8), Mo1-S3 2.3399(8), Mo1-S4 2.3410(8), Mo2-S1 2.3527(7), Mo2-S2 2.3538(7), Mo2-S4 2.3482(8), Mo3-S2 2.3547(8), Mo3-S3 2.3420(8), Mo3-S4 2.3353(7), Fe2-C2 1.713(3), C2-O2 1.205(3), Fe2-S5 2.1957(8), Fe2-S6 2.1932(8), Fe2-S7 2.1864(9), Fe2-Mo4 2.7866(5), Fe2-Mo5 2.8086(5), Fe2-Mo6 2.7884(5), Mo4-S5 2.3542(8), Mo4-S7 2.3423(8), Mo4-S8 2.3384(7), Mo5-S5 2.3500(7), Mo5-S6 2.3515(7), Mo5-S8 2.3458(8), Mo6-S6 2.3564(8), Mo6-S7 2.3407(8), Mo6-S8 2.3391(8), O1-C1-Fe1 176.9(3), C1-Fe1-S1 112.63(10), C1-Fe1-S2 114.26(10), C1-Fe1-S3 109.68(11), O2-C2-Fe2 176.6(3), C2-Fe2-S5 113.32(10), C2-Fe2-S6 113.01(10), C2-Fe2-S7 110.31(10).



Supplementary Fig. 24. Crystal structure of **5** with thermal ellipsoids set at the 50% probability level. Hydrogen atoms are omitted for clarity. Shown is one of two molecules of **5** in the asymmetric unit. Color legend: C, grey; O, red; S, yellow; Mo, teal; and Fe, orange. Selected Bond lengths (Å) and angles (°): Fe1-C1 1.768(8), C1-O1 1.157(8), Fe1-S1 2.187(2), Fe1-S2 2.197(2), Fe1-S3 2.195(1), Fe1-Mo1 2.725(1), Fe1-Mo2 2.801(1), Fe1-Mo3 2.768(1), Mo1-S1 2.354(1), Mo1-S3 2.360(2), Mo1-S4 2.343(1), Mo2-S1 2.343(1), Mo2-S2 2.341(2), Mo2-S4 2.331(1), Mo3-S2 2.347(2), Mo3-S3 2.351(1), Mo3-S4 2.337(2), O1-C1-Fe1 176.7(6), C1-Fe1-S1 119.0(2), C1-Fe1-S2 101.2(2), C1-Fe1-S3 113.6(2).



Supplementary Fig. 25. Computed free energy profile for CO₂ coordination to [Cp*₃Mo₃S₄Fe] cluster.



Supplementary Fig. 26. Optimized ground-state structure of CO₂-bound [Cp*₃Mo₃S₄Fe] clusters: (a) CO₂ binding in the side-on (η^2) fashion, and (b) CO₂ binding in the end-on fashion.

Supplementary Tables

Supplementary Table 1. GC analysis profiles of catalytic reduction of CO₂ to CH₄ using [Cp*₃Mo₃S₄Fe] clusters and relevant cluster and iron compounds. Reaction conditions: precatalyst (10 nmol), SmI₂ (50 μmol), H₂O (1.5% v/v).

Entry	Precatalyst	Run	Product (equiv. per precatalyst)		
			CH ₄	CO	H ₂
1	1	1	200	3.3	1742
		2	198	2.8	1758
		3	250	4.2	1649
		Ave. ^{a,b}	216 ± 29	3.4 ± 0.9	1720 ± 60
		[Sel.] ^c	[35]	[0.14]	[69]
2	2	1	10.0	n.d.	2204
		2	11.6	n.d.	2123
		3	9.3	n.d.	2195
		Ave. ^{a,b}	10 ± 1.1	n.d.	2170 ± 40
		[Sel.] ^c	[1.6]	[0]	[87]
3	3	1	0.6	n.d.	2145
		2	0.4	n.d.	2082
		3	0.2	n.d.	2356
		Ave. ^{a,b}	0.4 ± 0.2	n.d.	2190 ± 140
		[Sel.] ^c	[0.06]	[0]	[88]
4	[Cp* ₃ Mo ₃ S ₄] ^d	1	n.d.	n.d.	2189
		2	n.d.	n.d.	2151
		Ave. ^a	n.d.	n.d.	2170
		[Sel.] ^c	[0]	[0]	[87]
5	Fe(TPP)Cl ^e	1	n.d.	4.4	1657
		2	n.d.	5.6	1538
		Ave. ^a	n.d.	4.9	1600
		[Sel.] ^c	[0]	[0.2]	[64]
6	FeCp ₂ ^f	1	6.1	3.2	1182
		2	8.1	1.0	1570
		Ave. ^a	7.0	2.1	1380
		[Sel.] ^c	[1.1]	[0.08]	[55]
7	Fe ₂ (CO) ₉	1	5.5	0.2	1960
		2	6.4	7.7	1965
		Ave. ^a	5.9	6.3	1960
		[Sel.] ^c	[0.94]	[0.25]	[78]
8	FeCl ₂	1	2.6	n.d.	1710
		2	3.4	n.d.	2171
		Ave. ^a	3.0	n.d.	1940
		[Sel.] ^c	[0.48]	[0]	[78]
9	4	1	271	3.0	1273
		2	308	4.6	1130
		3	239	9.4	1340
		Ave. ^a	281 ± 41	3.7 ± 1.2	1170 ± 160
		[Sel.] ^c	[45]	[0.15]	[47]
10	5	1	283	3.3	1118
		2	240	2.8	1353
		3	323	5.1	1050
		Ave. ^{a,b}	272 ± 35	5.7 ± 3.4	1250 ± 110
		[Sel.] ^c	[44]	[0.23]	[50]

^a Ave.: Averaged value. ^b Data are shown as average ± standard deviation. ^c Sel.: SmI₂-based selectivity. Values are presented in brackets. Selectivity was calculated on an electron-balance basis, requiring 8, 2, and 2 electrons per molecule of CH₄, CO, and H₂, respectively. ^d Cp* = C₅Me₅. ^e Fe(TPP)Cl = 5,10,15,20-tetraphenyl-21*H*,23*H*-porphine iron(III) chloride. ^f Cp = C₅H₅.

Supplementary Table 2. GC analysis profiles of CH₄ formation from cluster **5**.

Reactant	Run	Product (equiv. per cluster)		
		CH ₄	CO	H ₂
5	1	1.03	0.022	13.5
	2	0.97	0.054	12.6
	3	0.88	0.064	13.2
	Ave. ^a	0.96 ± 0.08	0.047 ± 0.022	13.1 ± 0.4

^a Ave.: Averaged value. Data are presented as average ± standard deviation.

Supplementary Table 3. GC analysis profiles of catalytic reduction of CO₂ to CH₄ using [Cp*₃Mo₃S₄Fe] clusters. Reaction conditions: precatalyst (0.040 nmol), SmI₂ (0.16 mmol), H₂O (6.25% v/v), reaction temperature (0 °C or room temp.).

Entry	Precatalyst	Run	Product (equiv. per cluster)		
			CH ₄	CO	H ₂
1 ^a	1	1	20842	n.d.	1451720
		2	19349	n.d.	1369374
		3	16636	n.d.	1298570
		Ave. ^b [Sel.] ^c	1.9·10 ⁴ ± 2·10 ³ [3.8]	n.d.	1.4·10 ⁶ ± 8·10 ⁴ [69]
2	1	1	125566	1039	1343881
		2	123979	528	1108389
		3	132851	1215	1094444
		Ave. ^b [Sel.] ^c	1.27·10 ⁵ ± 5·10 ³ [25]	9.3·10 ² ± 3.6·10 ² [0.05]	1.18·10 ⁶ ± 1.4·10 ⁵ [59]
3	5	1	162360	1761	1020609
		2	155875	1973	1107058
		3	151742	1638	1135122
		Ave. ^b [Sel.] ^c	1.57·10 ⁵ ± 5·10 ³ [31]	1.8·10 ³ ± 2·10 ² [0.09]	1.1·10 ⁶ ± 6·10 ⁴ [55]

^a Reactions were performed at room temperature. ^b Ave.: Averaged value. Data are shown as average ± standard deviation. ^c Sel.: SmI₂-based selectivity. Values are presented in brackets. Selectivity was calculated on an electron-balance basis, requiring 8, 2, and 2 electrons per molecule of CH₄, CO, and H₂, respectively.

Supplementary Table 4. Crystal data and refinement summary for [K(THF)][K(THF)₃][4]₂ and 5.

	[K(THF)][K(THF) ₃][4] ₂	5
Formula	C ₇₈ H ₁₂₂ Fe ₂ K ₂ Mo ₆ O ₆ S ₈	C ₃₁ H ₄₅ FeMo ₃ OS ₄
Formula weight (g/mol)	2177.77	905.67
Crystal system	Triclinic	Monoclinic
Space group	<i>P</i> -1 (#2)	<i>P</i> 2 ₁ / <i>c</i> (#14)
<i>a</i> (Å)	15.1694(3)	20.9534(11)
<i>b</i> (Å)	17.2445(3)	17.3538(7)
<i>c</i> (Å)	17.9990(3)	20.5697(10)
<i>α</i> (°)	85.702(2)	90
<i>β</i> (°)	89.358(2)	114.468(6)
<i>γ</i> (°)	69.858(2)	90
<i>V</i> (Å ³)	4407.42(15)	6807.9(6)
<i>Z</i>	2	8
<i>D</i> _{calcd} (g/cm ³)	1.641	1.767
Max 2θ (°)	52.744	51.7400
No. of reflections (measured)	17944	13906
No. of data (used) (<i>I</i> > 2.00σ(<i>I</i>))	13722	8919
No. of parameters refined	1032	751
<i>R</i> ₁ ^a	0.0306	0.0550
<i>wR</i> ₂ ^b	0.0640	0.0863
GOF ^c	1.004	1.003
^a <i>I</i> > 2σ(<i>I</i>), <i>R</i> ₁ = Σ <i>F</i> _o - <i>F</i> _c /Σ <i>F</i> _o . ^b refined with all data, <i>wR</i> ₂ = [Σ <i>w</i> (<i>F</i> _o ² - <i>F</i> _c ²) ² /Σ <i>w</i> (<i>F</i> _o ²) ²] ^{1/2} . ^c GOF = [Σ <i>w</i> (<i>F</i> _o ² - <i>F</i> _c ²) ² /(<i>N</i> _o - <i>N</i> _p)] ^{1/2} , where <i>N</i> _o and <i>N</i> _p denote the numbers of reflection data and parameters.		

Supplementary Table 5. Selected bond distances (Å), angles (°), and relative energies of $[\text{Cp}^*_3\text{Mo}_3\text{S}_4\text{Fe}(\text{CO})]^-$ (**4**) optimized for $S = 0, 1$, and 2 states. Bond distances and angles are shown alongside the corresponding values from the crystal structure of $[\text{K}(\text{THF})][\text{K}(\text{THF})_3][\text{4}]_2$.

	Optimized structure			Crystal structure
Spin state	$S = 0$	$S = 1$	$S = 2$	-
Relative energy (kcal/mol)	0.0	+18.8	+18.6	-
Bond distance (Å)				
Fe1-C1	1.72	1.73	1.75	1.77
C1-O1	1.20	1.19	1.19	1.16
Fe1-S1	2.16	2.17	2.17	2.19
Fe1-S2	2.16	2.25	2.35	2.20
Fe1-S3	2.16	2.22	2.28	2.20
Fe1-Mo1	2.74	2.71	2.73	2.73
Fe1-Mo2	2.74	2.78	2.83	2.80
Fe1-Mo3	2.74	3.05	3.18	2.77
Mo1-S1	2.35	2.37	2.36	2.35
Mo1-S3	2.35	2.37	2.39	2.36
Mo1-S4	2.35	2.36	2.38	2.34
Mo2-S1	2.35	2.36	2.38	2.34
Mo2-S2	2.35	2.33	2.43	2.34
Mo2-S4	2.35	2.36	2.37	2.33
Mo3-S2	2.35	2.42	2.41	2.35
Mo3-S3	2.35	2.40	2.41	2.35
Mo3-S4	2.35	2.35	2.34	2.34
Bond angle (°)				
O1-C1-Fe1	179.8	178.5	178.0	176.7
C1-Fe1-S1	110.5	112.2	119.5	119.0
C1-Fe1-S2	111.1	106.5	111.6	101.2
C1-Fe1-S3	110.5	119.4	110.6	113.6

Supplementary Table 6. Selected bond distances (Å), angles (°), and relative energies of [Cp*₃Mo₃S₄Fe(CO)] (**5**) optimized for $S = 1/2$, $3/2$, and $5/2$ states. Bond distances and angles are shown alongside the corresponding values from the crystal structure of **5**.

	Optimized structure			Crystal structure
Spin state	$S = 1/2$	$S = 3/2$	$S = 5/2$	-
Relative energy (kcal/mol)	0.0	+17.6	+42.1	-
Bond distance (Å)				
Fe1-C1	1.77	1.74	1.76	1.80
C1-O1	1.16	1.18	1.18	1.17
Fe1-S1	2.19	2.17	2.27	2.34
Fe1-S2	2.20	2.19	2.16	2.27
Fe1-S3	2.20	2.17	2.27	2.26
Fe1-Mo1	2.73	2.68	3.15	3.03
Fe1-Mo2	2.80	2.76	2.71	3.10
Fe1-Mo3	2.77	2.77	2.70	2.72
Mo1-S1	2.35	2.37	2.41	2.43
Mo1-S3	2.36	2.37	2.40	2.38
Mo1-S4	2.34	2.35	2.33	2.36
Mo2-S1	2.34	2.35	2.36	2.42
Mo2-S2	2.34	2.35	2.37	2.39
Mo2-S4	2.33	2.34	2.36	2.35
Mo3-S2	2.35	2.35	2.37	2.36
Mo3-S3	2.35	2.34	2.35	2.35
Mo3-S4	2.34	2.34	2.36	2.38
Bond angle (°)				
O1-C1-Fe1	176.7	179.0	179.8	178.5
C1-Fe1-S1	119.0	114.3	109.9	131.0
C1-Fe1-S2	101.2	102.7	118.6	110.8
C1-Fe1-S3	113.6	113.9	109.9	105.9

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Cartesian Coordinates of the optimized structures and their electronic energies (E)

[Cp*₃Mo₃S₄Fe(CO)]⁻ (4)

S = 0

E = -4346.725450 AU

Mo	11.58096972493724	4.99283812738619	9.25697165252696
Mo	12.17160368317212	2.97955787136967	11.19308217099196
Mo	11.67463150477581	2.24882041151743	8.47565825065060
Fe	13.94650597359485	3.60445600198196	9.19643645792294
S	10.18106801826818	3.25513459084405	9.97859006117973
S	13.47895306126088	1.58984133242811	9.82292839849998
S	13.36927375090813	4.95653436097039	10.77991587055181
S	12.75817717427317	4.06524552167741	7.45174301815024
C	10.89512394855780	2.94123700664920	13.17992706518827
O	16.78713928714364	3.84687543301287	8.58902223980846
C	11.77247557665068	7.18558618255727	8.45141892532285
C	10.69784732989381	6.56318499799960	7.71846258651463
C	9.99554905138342	1.55384849905407	6.97591529743625
C	12.11209917500362	3.61732998612897	13.47438244717642
C	11.32719466708186	-0.04794798812072	7.99942518230647
C	12.08016119250586	0.54106021693860	6.91959017830446
C	11.36387889759218	7.28797963678312	9.82363880188267
C	11.21434769810925	1.57942379818082	12.81956024637314
C	10.05276877381826	0.58347707102903	8.04378938290166
C	9.66608440888384	6.23509035764846	8.64175143544411
C	15.62259993531289	3.74935260881400	8.83979041729742
C	11.77945793352491	-1.19752125252309	8.84812230681025
H	11.23050515063405	-1.23178943573959	9.79284938879046
H	11.61191555140717	-2.15018567246481	8.32655424848435
H	12.84555630953800	-1.12059845816491	9.07965040488226
C	13.44708560843560	0.11468124560558	6.47164116345810
H	14.04867362713630	-0.22182367627006	7.32122215474039
H	13.38826533087801	-0.71356192558042	5.75100104935219
H	13.97963254877290	0.93997249797034	5.99016304833709
C	10.64429679473267	6.38924240385888	6.23074792877142
H	10.01296295357291	5.54089431748008	5.95170452848564
H	10.23367645409594	7.28907766345710	5.75182337465884
H	11.64216640003665	6.21191838236532	5.82138919307235
C	13.19789049877458	2.68744669815159	13.28084391119403
C	8.30907707190879	5.69043966988352	8.31256822356161
H	7.98307750792281	4.95953427307311	9.05875843884196
H	7.56733411903515	6.50105865142205	8.28826496080146
H	8.30413853283636	5.20306566018039	7.33516970161507
C	11.23431412656018	1.49818051340443	6.26793663764312
C	8.90182133690843	0.20675746039284	8.92738737218558
H	8.32632062094964	1.08788674804301	9.22541612965306
H	8.22304040719389	-0.47992681961365	8.40254705039904
H	9.24826939942892	-0.29229716197049	9.83518054845277

C	13.02930389262290	7.74938461000064	7.85600532694684
H	13.34691562598937	7.16100525881683	6.99025925368105
H	12.88304425642756	8.78715042022887	7.52401041038217
H	13.84588362129156	7.74158380294280	8.58374452742966
C	12.63062122682154	1.42160642726981	12.91961807202603
C	10.08329896401926	6.67322911423347	9.95366402358565
C	9.50815076939882	3.47827191195502	13.36324811695214
H	8.83180747074454	3.09556923871987	12.59353168041945
H	9.10911222471355	3.18040619492450	14.34297876049706
H	9.49441233893030	4.56921621907790	13.31239518078669
C	10.21063844656653	0.49607784539986	12.55954619662736
H	10.63600844467940	-0.29637239052540	11.93751534685244
H	9.87139254685627	0.03766094973107	13.49978879399969
H	9.33096301909121	0.89326831046904	12.04562758648616
C	9.22810522882838	6.63265807884709	11.18452470058871
H	9.83645867868534	6.67989150867378	12.09177928305409
H	8.52982685470912	7.48178822007373	11.20539076434537
H	8.63689571747524	5.71320165789541	11.22031793747652
C	8.78066140444413	2.34313519241590	6.59091150587730
H	9.05443729170940	3.24601627708875	6.03827884533635
H	8.11173757228148	1.74932254683084	5.95121167246930
H	8.21401149822826	2.64715858609488	7.47528626331933
C	12.25341233181739	5.01358802436444	14.00025030003360
H	11.39012290971424	5.62959423636813	13.73452204014709
H	12.33592775310704	5.00503385056126	15.09607565752787
H	13.14817845136627	5.49595159903273	13.59679274011822
C	13.38063769463452	0.13193433236793	12.78249325272692
H	14.40060749117095	0.29967779653889	12.42729142831357
H	13.43894944676526	-0.37481442214551	13.75600922289871
H	12.88575353997466	-0.54300309406654	12.07935470847918
C	11.55114066709792	2.23209200530269	5.00064637082465
H	12.62447769077961	2.41474828736205	4.90515895536198
H	11.22720164451427	1.64192864780617	4.13194164564223
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C	12.10720118135195	8.00674419247311	10.90762419047614
H	13.18757361224281	7.95032491142678	10.75270925572277
H	11.81951991595636	9.06729309395868	10.92415539733024
H	11.88589687437613	7.58061807838996	11.88964688788103
C	14.64660575393577	2.96273306350875	13.55652682239371
H	14.89707071776800	4.00350587941926	13.33051957812945
H	14.89182145068804	2.77921157720356	14.61246630627327
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Mo	11.66100031470660	2.28327405415618	8.43953987631381
Fe	13.97450087038036	3.74640884602972	8.89865834789552
S	10.15002611576098	3.28103763507567	9.95171268945234
S	13.49504346516288	1.72637887665939	9.76892700879850
S	13.47262406037509	4.97355003895599	10.67925377269304
S	12.58874955554147	4.11673496073503	7.27622385885781
C	10.86354450159430	2.93654812745631	13.15868912766109
O	16.73592000989767	3.61962138070189	7.94729962304993
C	11.77526804647571	7.22964957911666	8.51808342318949
C	10.69755068909412	6.63851405563162	7.76523219936626
C	10.03032793602593	1.50585927721844	6.95602803349116
C	12.08048507408257	3.63041441148409	13.46053903746306
C	11.32794149422604	-0.04326981336071	8.09419056189669
C	12.11137635030968	0.48528352556050	7.00426688641635
C	11.36810281894584	7.27651198086269	9.89513279993665
C	11.19447753907570	1.57785309176850	12.79818224531160
C	10.05143184913296	0.58717288135846	8.06533194598866
C	9.67327532996067	6.26289223040169	8.67675286817367
C	15.61441871832016	3.67175915792161	8.35371889396582
C	11.76085316714459	-1.15372094669985	9.00120303987728
H	11.15825229187577	-1.18174929587994	9.91231719073038
H	11.65351564306941	-2.12430049725699	8.49714127841368
H	12.80918371148903	-1.03567469172337	9.29044126348755
C	13.48786787615682	0.02955540434764	6.62206310132032
H	14.07998492609040	-0.20127579969269	7.51242566060145
H	13.44442797115094	-0.87404500094215	5.99787995783129
H	14.01605830302231	0.80375149737355	6.05843497784750
C	10.62139243789663	6.53925623557160	6.27219018257959
H	10.03803261340074	5.66806996034710	5.96032441137582
H	10.13952711105842	7.43583430178169	5.85799963635475
H	11.61644929138485	6.45236140444982	5.82943520955941
C	13.17017038179454	2.70591343838315	13.25508712730714
C	8.32168314545378	5.71953839118022	8.32446338762445
H	7.98186549777293	4.99372538585017	9.06911599772480
H	7.58154245382205	6.53076704492642	8.27986513725895
H	8.33551509871347	5.22464699396311	7.35032160241003
C	11.29122278232307	1.41027033990755	6.28280186692833
C	8.87199760356479	0.25517565590911	8.92882435545148
H	8.28496643397427	1.14902750647668	9.15769708956851
H	8.21514650919907	-0.45906593547653	8.41341560630029
H	9.18362276539980	-0.19622921056108	9.87304284004481
C	13.02820229892381	7.82490285686920	7.94547628484024
H	13.33019547467158	7.29327794779689	7.03869454802804
H	12.88681684929417	8.88402783772336	7.68691812587393
H	13.85252396975833	7.75942557179068	8.66154138844145
C	12.60916086010346	1.43837012381766	12.87814682781915

C	10.09268986261939	6.65216592849167	10.00438616990613
C	9.46997293918752	3.45210887795397	13.35908594295331
H	8.79486090809105	3.07959166797677	12.58295220269333
H	9.07702511867129	3.12890970568423	14.33343094347462
H	9.44223726466777	4.54349564921661	13.33123809064177
C	10.20011542532250	0.48536316870461	12.54611591430520
H	10.62671697924288	-0.30242813280706	11.91957252155291
H	9.87695309768550	0.02270135048812	13.49012139894244
H	9.30954863789017	0.87391169709001	12.04491435189932
C	9.24222300218855	6.56219124493783	11.23467594276778
H	9.85555575290389	6.55243944397193	12.13947329586856
H	8.55849633098917	7.42043508375819	11.30049071921745
H	8.63753747541430	5.65107506781031	11.22517465938348
C	8.84679556051347	2.31196610388517	6.51119467874602
H	9.16385368044820	3.22743248864772	6.00342865522729
H	8.21680034496520	1.74125140585045	5.81382374019168
H	8.22802474713257	2.59795272884617	7.36600060106013
C	12.21744478658320	5.02059384116230	14.00401907117732
H	11.32178874885051	5.61499180004074	13.80404394741167
H	12.37202317645506	5.00190766400045	15.09234128910973
H	13.07128211009857	5.53426621253935	13.55073558558447
C	13.37569531696022	0.16504919582860	12.69337261075430
H	14.38835105940960	0.36055163082670	12.33154544317807
H	13.45306146357345	-0.37106475159218	13.64958689679788
H	12.88305502113170	-0.49475969507829	11.97456770969568
C	11.63686296218435	2.05977638218720	4.97862015062050
H	12.71087649544275	2.24730341122358	4.89957762909688
H	11.34249626829361	1.40561033480520	4.14610217096274
H	11.11829321899988	3.01488498771779	4.86072007934797
C	12.11349673805760	7.95415213727010	11.00277617288904
H	13.19317191765909	7.90393767633834	10.84192005019031
H	11.82398411400015	9.01292575198192	11.05696762276100
H	11.89541048361763	7.49260648266944	11.96915826773589
C	14.61847912528794	2.98224832269171	13.53206615488665
H	14.85716857100545	4.03366525837292	13.34853973934224
H	14.87173387970238	2.75545236252196	14.57803703024682
H	15.26581372591038	2.37491324635159	12.89253511489693

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E = -4346.664513 AU

Mo	11.57603464009041	5.01267370786397	9.21419825674234
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Mo	11.63730559416393	2.26879932018045	8.41031134952135
Fe	13.98626082309390	3.81597985758135	8.73548571346816
S	10.14524671029091	3.26459318284848	9.95776653387034
S	13.60163981165719	1.71582557145212	9.72622597352513
S	13.46259931285271	4.89862701932305	10.67687220705317
S	12.47754471414071	4.14793949935276	7.20731756803544
C	10.88252330895570	2.86248394252230	13.14978986357395
O	16.81823348353069	4.23497135155752	8.08898925132186
C	11.74943576189148	7.23378239063314	8.53326196721013
C	10.64581360884916	6.66805206323243	7.79949296107932
C	10.06137537064955	1.54440130908383	6.86391497710376
C	12.08011951985452	3.59375520203875	13.41932077934664
C	11.22000232795287	-0.01995406635935	8.14186830895365
C	12.07240467457479	0.40135737242286	7.05694447968465
C	11.38632943058716	7.24846771868492	9.92491765614839
C	11.24856715209519	1.51424732846377	12.79902379286706
C	9.98185997864806	0.68569407547800	8.02143528443433
C	9.64606595950689	6.27637263783765	8.73264994261173
C	15.67162294195757	4.04236934445669	8.34201392087972
C	11.55827529381263	-1.10276799154083	9.11827868377651
H	10.81799659792373	-1.15644535004215	9.92019019319087
H	11.58598272823320	-2.08176350498349	8.62046986069418
H	12.54039347255159	-0.92437898345360	9.57037137911596
C	13.42811003282265	-0.16110730530411	6.75175615092783
H	13.96685858329855	-0.39469730857751	7.67406779319432
H	13.34140795470342	-1.08468419981521	6.16170984758988
H	14.03087143860781	0.54887723541930	6.17812265915780
C	10.52984217152873	6.61065662902281	6.30760671875684
H	9.87917054538409	5.79154476541656	5.98960496179366
H	10.10429903565266	7.54950129282714	5.92689712152288
H	11.50710185658657	6.46606904201696	5.84019349856890
C	13.19627939859284	2.70069131027272	13.21913881922841
C	8.28745137812350	5.73490994115485	8.40506122520907
H	7.96252380338327	5.00738638295548	9.15445479792805
H	7.54674604991791	6.54629701466972	8.37710168446714
H	8.28224850744511	5.24236329932384	7.42963420859678
C	11.34549858128588	1.33530739822247	6.25963391625454
C	8.75228844602334	0.45721038064304	8.84737192994356
H	8.14660874117367	1.36466003295882	8.91382073765222
H	8.13391936650163	-0.33299996317734	8.39937971643098
H	9.00731625419925	0.15110865398204	9.86476402962673
C	12.98168139927116	7.84537583533693	7.93371094336029
H	13.25003376163510	7.34073092170244	7.00149530444775
H	12.82860920307987	8.91134670805407	7.71142156531521
H	13.83202803885799	7.76220966410169	8.61643251021404

C	12.67280590615927	1.41375778358320	12.86340641187487
C	10.10501208656683	6.63320367106670	10.05469385866168
C	9.47635835909106	3.34107847794656	13.34980253368313
H	8.80927103445484	2.93826392173174	12.58215105260116
H	9.09888229855193	3.01820892721725	14.33002703746990
H	9.41639070831399	4.43035766116819	13.30844397556315
C	10.28208574139651	0.38957666824505	12.58023743072809
H	10.72303277312659	-0.40149033589719	11.96934067946552
H	9.98242353321251	-0.05670644487920	13.53952263111148
H	9.37504333307160	0.74175615802493	12.08131729829391
C	9.28644370537246	6.52812167415494	11.30497366953474
H	9.92307688862318	6.47969945706317	12.19188837215380
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H	8.65916525929438	5.63277126259423	11.28707120946001
C	8.95031249099278	2.38714180424937	6.31187096977174
H	9.34387554163971	3.26548646922458	5.79153732720371
H	8.33602209415163	1.82133190501547	5.59595988182213
H	8.29316525834009	2.73618809364973	7.11282341480155
C	12.18788897798747	4.99593356964679	13.93626142384805
H	11.25946758091995	5.55094800437724	13.77921098074249
H	12.40035470747788	4.99467371439399	15.01436444146376
H	12.99553187971944	5.53679722020172	13.43269025033965
C	13.47548261454727	0.15976711879041	12.69926213156383
H	14.46601812758552	0.37624836670957	12.29120060030849
H	13.60605664497568	-0.33507573776406	13.67176745120042
H	12.98043694508520	-0.54310444066873	12.02468147520827
C	11.79818376047383	1.91308487943582	4.95429666549736
H	12.88528046095449	2.02532482902636	4.92310785486075
H	11.50026465751256	1.25096743174983	4.12954432306390
H	11.35167782300258	2.89523475175269	4.77991490300750
C	12.16354497768098	7.90747846493055	11.02113672271019
H	13.23854091576238	7.84685688302079	10.83372154140461
H	11.88674704832431	8.96852961372761	11.09406907269884
H	11.96497389141341	7.43634534357331	11.98682858520002
C	14.63642995992264	3.02731721476265	13.48080308918418
H	14.83858799838039	4.08202612120837	13.27531524902868
H	14.90141031719556	2.82724241688250	14.52899419027738
H	15.29682526577410	2.42799099470701	12.84739923914724

[Cp*₃Mo₃S₄Fe(CO)] (5)

S = 1/2

E = -4346.621719 AU

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Mo	11.63306073402302	2.32515497750310	8.44486968195211
Fe	13.92089884930670	3.69614191560069	9.16988699725497
S	10.14012694432354	3.26896132153815	9.98390892440511
S	13.42342859846583	1.66358556404939	9.81499566186830
S	13.37104790288188	5.02877354486481	10.78895812489352
S	12.74311041938871	4.10642681862376	7.39363330000465
C	10.92330027042286	2.97044992223383	13.18103838397526
O	16.79863565366225	3.51643599901692	8.70399076846478
C	11.73488615848706	7.19002140545227	8.46113705081472
C	10.66340971283465	6.56325966323009	7.72638545522501
C	10.01858388549835	1.54736279275568	6.96142040694572
C	12.16650306505855	3.61222261903184	13.46867744279414
C	11.33684996334583	-0.01123841978092	8.05704952723059
C	12.11290548777932	0.55331061549062	6.97912330085565
C	11.32370465020962	7.28199023882722	9.83258057853358
C	11.20665397431821	1.61343402357156	12.78259873326821
C	10.05339993217363	0.60326817844855	8.04919259495929
C	9.63944904981751	6.21064045730077	8.64773418945804
C	15.63628625496914	3.59925985146055	8.88590134947241
C	11.77706270031083	-1.13754467687683	8.93965195727081
H	11.19871279363859	-1.16714760700892	9.86572313579775
H	11.63379121911298	-2.09514436888892	8.42188645742462
H	12.83548982803868	-1.04994629638406	9.19895123005278
C	13.49665610590912	0.13203427508170	6.58569441294734
H	14.08228723491059	-0.15373579026242	7.46383437764458
H	13.46094230077149	-0.73031523430842	5.90668775122544
H	14.02442758647986	0.94190171891660	6.07512172379721
C	10.60816992534522	6.39970666275804	6.23867139704969
H	9.97433104843684	5.55612789993501	5.95387340790322
H	10.19436124146361	7.30593432127058	5.77716410139970
H	11.60412945100799	6.23193732203877	5.82154406599629
C	13.22501641671031	2.66575965155619	13.23011899101586
C	8.28870816939985	5.65359242072473	8.31726963188571
H	7.96251212781928	4.92844903772173	9.06836141488379
H	7.54737721306692	6.46308013048293	8.28652946407589
H	8.28915192156261	5.16099296774188	7.34300807528495
C	11.27897206927128	1.48300001184199	6.28062999116337
C	8.88203268484166	0.23875643388740	8.90880146838215
H	8.27667921039003	1.11720796130382	9.14778460102107
H	8.24124735105275	-0.48064678074937	8.38202237496912
H	9.20309656326317	-0.21965574779917	9.84594031768551
C	12.98044987019881	7.77834614162732	7.86681046740909
H	13.29655510048312	7.21150335093342	6.98686990662428
H	12.81409368025978	8.81898363180876	7.55752928342928

H	13.80215437027475	7.76776879387684	8.58810356709018
C	12.62033210100247	1.42274552577640	12.84939402690252
C	10.05644218083070	6.64131585295807	9.96343275299161
C	9.55385968672235	3.53128816433170	13.41275083742088
H	8.84796410707640	3.17939096266411	12.65542900026757
H	9.18066310609347	3.21505103716583	14.39596580887680
H	9.56227741624833	4.62255953417885	13.39107976010939
C	10.17619019175014	0.55838461482728	12.51855742646314
H	10.58281655365274	-0.24153393449927	11.89544924520260
H	9.83594859143048	0.10931495865377	13.46147141294624
H	9.30296871524392	0.97769593660680	12.01233314644270
C	9.20798703457607	6.57944148068163	11.19700581508648
H	9.82021673260901	6.63022429613381	12.10092916070083
H	8.50202571931914	7.42065328452338	11.22086064483752
H	8.62716938595751	5.65360080243671	11.22837721825289
C	8.81439064197255	2.32698449705248	6.52822537407064
H	9.10284957672191	3.23869396664436	5.99928083457128
H	8.19154343689674	1.72769037100704	5.85019075701601
H	8.20052971082422	2.60948910970225	7.38709580252557
C	12.34293469575914	4.99369340476945	14.02141050329977
H	11.51753226392807	5.64874459300209	13.73138382760673
H	12.37513710761184	4.95547929303789	15.11827840810359
H	13.27490647856000	5.44300111371929	13.66984300235704
C	13.33763829029741	0.12271190250359	12.66124025955211
H	14.36223515937049	0.27809322283269	12.31501608754294
H	13.38002983948308	-0.41450976890565	13.61805211476515
H	12.82572511639136	-0.51494661196465	11.93670441579372
C	11.61486075697155	2.17844891851852	4.99763340368981
H	12.68953484096536	2.35439944005200	4.90917823198798
H	11.29972698708495	1.55702375166689	4.14889067077541
H	11.10402014515676	3.14144114075974	4.92040561730453
C	12.05701226282932	7.99996124336955	10.92243585706852
H	13.13494142156314	8.00071873938345	10.74532949447925
H	11.71770311175099	9.04337668357127	10.96773959193368
H	11.87201345903804	7.54111287162483	11.89697360414135
C	14.68656563592655	2.90272734868477	13.46543379833218
H	14.94785478435826	3.94872253233090	13.28301257260660
H	14.95823104030111	2.66243848233523	14.50204829671372
H	15.29741781948709	2.28177015024829	12.80456536509527

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E = -4346,592799 AU

Mo	11.57247936377763	4.96749665879709	9.16189859644660
Mo	12.07351844978019	2.98007056260734	11.19031740019090
Mo	11.67951215021605	2.32248895313245	8.41246878756938
Fe	13.95331027574196	3.73786103743010	8.77634139732552
S	10.13264220143243	3.26109785952037	9.92835031274841
S	13.52843719566036	1.72812905009442	9.74315833663246
S	13.40560828238068	4.90578785715070	10.63981484019679
S	12.55828922852091	4.14263496501019	7.17223962605481
C	10.83967381238992	2.93527461962532	13.17463321420491
O	16.83135718682454	3.99582746193879	8.24271856071468
C	11.78228183000962	7.21519427466983	8.51707242164301
C	10.69391610097978	6.64725097133238	7.76552936629388
C	10.04565881753858	1.51027665234024	6.96406473357427
C	12.06721338364516	3.62212569883755	13.43287182554869
C	11.35266343302896	-0.02345250321065	8.10710091478174
C	12.12790123670000	0.49268734014088	7.00282264104509
C	11.38975311858697	7.23945103832811	9.89810967149110
C	11.15348626660742	1.57586900758357	12.82100571839928
C	10.07456966663600	0.59890187679603	8.07998129087599
C	9.67544856976624	6.25602625599912	8.68375036766950
C	15.67771776641806	3.89430095670737	8.45493747926383
C	11.79591764386061	-1.11726519052535	9.02691793187050
H	11.21272631683918	-1.12263913252665	9.95025056331398
H	11.66672122672473	-2.09244840542560	8.53918111793973
H	12.85182785230493	-1.00727377246067	9.28868420483113
C	13.50038690818051	0.03207352829616	6.61502324797080
H	14.10493393011771	-0.17729511803631	7.50200193978058
H	13.44459021130469	-0.88715073582824	6.01679503389492
H	14.01711799234626	0.79126900164978	6.02215261246550
C	10.59648583960105	6.57461622990043	6.27279888642087
H	10.03301107239507	5.69420847700860	5.95203305905251
H	10.07907928562012	7.46601050749206	5.89440765393135
H	11.58500196913002	6.53324950278765	5.81029288659478
C	13.14786360346711	2.68999522979098	13.22561876531956
C	8.31805838278202	5.72834776279481	8.33190426511804
H	7.96320024936614	5.01531865869933	9.08117582507689
H	7.59577428485478	6.55392043958104	8.28139834028833
H	8.32673807861125	5.22873137707707	7.36070504662646
C	11.29812764469157	1.40009362770480	6.27420461863055
C	8.90257555506876	0.26937081980939	8.95204132666762
H	8.29422004759157	1.15518731606696	9.15227988091047
H	8.26618876511991	-0.47103538264113	8.44971025698385
H	9.22032100197909	-0.15248840976924	9.90716648854905
C	13.03816581955264	7.80499667229576	7.94700278693152
H	13.31168537329996	7.30767669781206	7.01295689333776
H	12.90764809134691	8.87515094544241	7.73800077699137
H	13.87262691905450	7.69600091399114	8.64524783261635
C	12.57440456994315	1.42264987733031	12.87123378053968

C	10.11212257543171	6.61980868805508	10.01143438325481
C	9.45396144753154	3.46446918972808	13.38572764668898
H	8.76559862872019	3.09228348012825	12.62179383174643
H	9.07590707779475	3.14230459553521	14.36514431902132
H	9.43428182331455	4.55493894490906	13.36015903386719
C	10.14712888831390	0.48771984128716	12.60118602892650
H	10.55857871941484	-0.31572679456838	11.98583955757204
H	9.84420643757275	0.05021711256345	13.56244858428584
H	9.24872792102367	0.87320226750232	12.11280480897013
C	9.27650861882598	6.52011967427003	11.24964590349417
H	9.90088791453812	6.46961639362766	12.14429636011201
H	8.62610313196272	7.40018659095313	11.34210952214437
H	8.63923534377753	5.63260207812186	11.22390524200302
C	8.85881274183185	2.31216512912575	6.52096041730407
H	9.17073514497135	3.22074654148984	5.99882766189670
H	8.22878014979327	1.72817485932274	5.83653561505195
H	8.24561563150258	2.60543066457069	7.37685245330347
C	12.22432483174472	5.02374272288067	13.93672297137947
H	11.34137475631598	5.62903030848874	13.71759233811371
H	12.37005599410567	5.02165234655543	15.02503569070296
H	13.09224856572705	5.50967677962202	13.48146495456119
C	13.32427526104234	0.13859968221318	12.69196488345405
H	14.33901918274810	0.31835345099800	12.32907115435709
H	13.39421598083282	-0.38894464688032	13.65249521202117
H	12.82028831598751	-0.52008279938553	11.98062279859140
C	11.62555511251045	2.02950496790737	4.95642176106397
H	12.69969130823237	2.19957870567013	4.85002911650542
H	11.30353722100824	1.36300645674962	4.14529478133540
H	11.11342032201209	2.98699650569732	4.83273628534093
C	12.15338769748805	7.88998172010817	11.00737945343803
H	13.23015254490351	7.84191315003894	10.82930737096717
H	11.86600582721741	8.94749983843127	11.07813305625297
H	11.94390292958929	7.41548690074701	11.96850600947003
C	14.60255820256608	2.96278146029231	13.46589368918867
H	14.84312231624572	4.01173710666085	13.27367137858687
H	14.86994206515934	2.73952044407796	14.50775684190833
H	15.23079992644401	2.34598235935542	12.81758064779145

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E = -4346.552224 AU

Mo	11.64238016819877	4.96997939713106	9.23889221277774
Mo	12.14852944599988	2.98071818055815	11.23309733468203
Mo	11.62118317360761	2.22467594247906	8.44241373881177
Fe	14.10869076131704	3.86002571195051	9.00250438215752
S	10.17101902320580	3.25370550433885	9.99175447217295
S	13.59105867014215	1.70704238616277	9.76027189461927
S	13.38154576890133	4.98751741904739	10.83305340350726
S	12.62565717372417	4.06434687761516	7.30979544904868
C	10.87066454258569	2.88955290015237	13.19510504502656
O	16.64220498688676	5.03802191108364	7.99061377259984
C	11.82561863229585	7.18099863554231	8.48136354368622
C	10.75084684812678	6.57473820334788	7.73925998966631
C	9.98168744044606	1.52481393405371	6.93152823622439
C	12.08507324035378	3.57984554994867	13.48827798917225
C	11.24232126016352	-0.04782278320008	8.09468447761433
C	12.03585051914843	0.44824239309805	6.99787598023365
C	11.42315424534328	7.24691091759929	9.85707412901514
C	11.20069888218570	1.53983159210753	12.81885884554056
C	9.97876021890471	0.62487292876702	8.05720451720602
C	9.72890059817600	6.20460995653298	8.65954720407570
C	15.65405625980220	4.55861080486782	8.39245576357981
C	11.64726626933395	-1.15780541930458	9.01446963013808
H	11.01728342926504	-1.18421074199660	9.90618938826674
H	11.55159925448669	-2.12655136823791	8.50605338898921
H	12.68782841865815	-1.04483679655415	9.33292184737568
C	13.39934086269429	-0.04477939821254	6.61553811446267
H	13.97633071892003	-0.31994886937735	7.50237916467572
H	13.32025473074282	-0.93110009057025	5.97142640347746
H	13.95715992607554	0.72052661800122	6.06931134454111
C	10.67504343993422	6.45895124406764	6.24854318961576
H	10.07764073305808	5.59543580401831	5.94538176371167
H	10.20523540615765	7.36024994748074	5.83290520938141
H	11.66853320526910	6.35923220036589	5.80559507542443
C	13.17796414866704	2.65825506155623	13.28321846763305
C	8.37588296387504	5.66165059737149	8.31643562809626
H	8.03529085451784	4.94131392174958	9.06537182490197
H	7.64480296664104	6.48008981491912	8.27720394212396
H	8.38139383449240	5.16809306877306	7.34273711508628
C	11.24236744757074	1.39414224076583	6.27015343226518
C	8.78837660620814	0.32833908054136	8.91872728015480
H	8.19389233594556	1.22815782214517	9.09739491097938
H	8.14442311177504	-0.41020137290445	8.42299741569169
H	9.08632900608523	-0.08079332631460	9.88602980524743
C	13.08217368665055	7.75746919410690	7.89945937313798
H	13.38082429898726	7.21060702315608	7.00136034260535
H	12.93709566639187	8.81069303906214	7.62447847402387
H	13.90503595272646	7.70509498315606	8.61732216223093
C	12.62129160904205	1.39310173362794	12.89645598477540

C	10.15074926678347	6.61011745762525	9.98040384829394
C	9.47956178417023	3.41339744446393	13.38022250749176
H	8.80428197400350	3.02361991098018	12.61360629516044
H	9.09157026012489	3.10655489227376	14.36061344759686
H	9.45474042695210	4.50361649637724	13.33369461661487
C	10.20695651773838	0.45096565056478	12.55299193067538
H	10.63292550210069	-0.32830940822716	11.91707761998818
H	9.89500566378830	-0.01882931501372	13.49580877735260
H	9.31264896354885	0.84523315634706	12.06417088668458
C	9.30624930346136	6.53548175340873	11.21545876972411
H	9.92391433416469	6.52729592716688	12.11669365786976
H	8.63526669608689	7.40310146493307	11.27356193344130
H	8.69017646668682	5.63254888830483	11.21349616422234
C	8.82097724165577	2.35155506382529	6.46892197535601
H	9.16037660480987	3.25045588185697	5.94762880510284
H	8.18892906190500	1.77927344490179	5.77585134740873
H	8.19938840840494	2.65908476369147	7.31340399502583
C	12.21766600532118	4.96788928376088	14.03569561106476
H	11.33814607581742	5.57439287133017	13.80596188290525
H	12.32944594663438	4.93476917882318	15.12750855933295
H	13.09561896307432	5.47192630703078	13.62173222583108
C	13.38194971343802	0.11673428878640	12.70975164920381
H	14.40567113475292	0.30979231281603	12.38053455213050
H	13.42675236093462	-0.43224653387483	13.65985489124703
H	12.90247062354999	-0.52678026482873	11.96818492884942
C	11.62057735681875	2.04584476931793	4.97690723305433
H	12.70086380783062	2.19501817196658	4.90625439842127
H	11.30880492310637	1.40769157256002	4.13947045620768
H	11.13315411169660	3.01732964511689	4.86161197022954
C	12.15781555621702	7.95702783440022	10.95004255796346
H	13.23766058405625	7.93239870809274	10.78669539602656
H	11.83992080396184	9.00776682829475	10.97900264071782
H	11.94954422717616	7.51016585417229	11.92488868144346
C	14.62409565281965	2.93728100991716	13.56496189062421
H	14.86280669092958	3.98938437355489	13.38781240081683
H	14.86457036122844	2.70728955447551	14.61202507667442
H	15.27409141055850	2.32959513622894	12.92952864881114

R ([Cp*₃Mo₃S₄FeCl], **1**)

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E = -4693.463601 AU

Mo	0.00407669924051	0.73159101220255	-0.13767175206145
Mo	-0.03376931794820	-0.83340304386681	2.13996324510837
Mo	-1.14406971833378	-1.77651282471551	-0.39690696942668
Fe	-2.29856885311263	0.25384385474612	1.03978915236790
S	1.10377374964794	-1.33441001006513	0.14362699621873
S	-0.73326248728110	1.37631308603777	2.01992896422963
S	-2.08971054290187	0.22042474380021	-1.11396175914938
S	-2.16612979244281	-1.75053783155317	1.73015312538757
C	1.10995748025991	2.84952129944381	-0.14207653082841
C	1.67854813308827	1.26359428036216	-1.73824726350024
C	2.06318687994175	1.84217188553151	-0.46918933740197
C	0.09331239784185	2.85354508994129	-1.15396263174217
C	0.48098708833110	1.89910159142132	-2.16402581973344
C	-0.16902725647785	-0.89111487263407	4.47996600490109
C	1.08872941016175	-0.30230055417239	4.10799383283566
C	1.19476065269935	3.78803207755597	1.02111982717988
H	0.20720179216239	4.15572957328550	1.30967073266957
H	1.81457670840506	4.65345949719163	0.75187436518285
H	1.64752581701923	3.30668724010082	1.89244592676083
C	3.33134135528208	1.54401024941502	0.27189507641725
H	3.23333938452424	1.79028566523835	1.33227998580988
H	4.16492893226790	2.13238722014458	-0.13477300678885
H	3.59653423109113	0.48649418299806	0.19067146341261
C	-0.15125054901648	-2.26235715384844	4.05874849248051
C	1.85728553593593	-1.29405398109508	3.41732565584674
C	1.08324785673025	-2.50501446829351	3.37776288212342
C	-2.25536001784089	-2.76274960599381	-2.21052538300257
C	2.49774863445074	0.28303423008699	-2.52021628757914
H	2.97564926566517	-0.44795728066791	-1.86200522678954
H	3.28882597495270	0.80851695625059	-3.07143721765222
H	1.88623966909232	-0.25803113595618	-3.24549191607448
C	-0.85033205462106	-3.06144070991823	-2.29974668903139
C	-1.81417192458449	-5.00470782747599	0.77971387217008
H	-0.86538313323703	-5.11781774022777	1.30785345381637
H	-2.12839822831233	-5.99991167388647	0.43797152238990
H	-2.56309568645277	-4.64163409502451	1.48778859420687
C	-1.67781599920262	-4.08663226699750	-0.39472454187184
C	1.55816110182235	1.07118423681200	4.47964212681349
H	2.25300579513843	1.46974421985992	3.73614955176764
H	2.07762684894792	1.03635993552284	5.44636867703681
H	0.71833216205862	1.76376877167653	4.56850280110141
C	-0.50267553250690	-3.89822988546081	-1.18566279247816
C	-2.76144363081221	-3.37092139509357	-1.02375570973133
C	-0.22906132640857	1.67612362994552	-3.46343239911913
H	-0.05602276486967	0.66614146270636	-3.84301140965207
H	0.13072368472778	2.38866332216863	-4.21704845095070

H	-1.30724984323932	1.81827186396555	-3.35185167829333
C	-3.06447717342433	-2.04945442649172	-3.24855333399638
H	-3.93138262695591	-1.55314091152727	-2.80540166102836
H	-3.42814366148911	-2.77194323771431	-3.99110293774493
H	-2.46925113311829	-1.29615761092561	-3.77067745742881
C	-1.18644672090469	-3.28823147787073	4.39830553235256
H	-2.18334534686488	-2.84458222402023	4.45538181030259
H	-0.95556492702298	-3.72766284493745	5.37769640029159
H	-1.20963906407366	-4.09458080140717	3.66223858662375
C	0.82254794716036	-4.56491444849069	-0.97714265189578
H	1.64154942897746	-3.94054679443899	-1.34243998176657
H	0.85097356754384	-5.51641091176609	-1.52423120550909
H	0.99941499810897	-4.77758766580484	0.07901273961949
C	1.57886550072121	-3.82095506865711	2.86218052245258
H	0.75227441503284	-4.48907226867697	2.61205369830717
H	2.19287484449094	-4.31827532813773	3.62489115329820
H	2.19685502590360	-3.68561815353166	1.97107066147831
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H	3.43491315248430	-1.68205533474997	2.00417963609857
H	3.95669399069554	-1.58913097005486	3.69520476754742
H	3.54827485815404	-0.10989888103555	2.81192616782878
C	0.05683818274867	-2.68688394350429	-3.43309150838356
H	-0.23042905939030	-1.72646570277872	-3.86789248613036
H	0.00577531200990	-3.44456067154479	-4.22663128460875
H	1.09530031815855	-2.61801748888917	-3.10043707890446
C	-1.07310972633012	3.79349731479459	-1.23325068573654
H	-0.79492921091502	4.71900268154454	-1.75531250065927
H	-1.90668447576409	3.33920094625395	-1.77609517450060
H	-1.42779197044713	4.06339870344639	-0.23474963844556
C	-4.19059057720282	-3.37001404605674	-0.57302443094483
H	-4.73444248445278	-4.21002653766712	-1.02491613452127
H	-4.26100386520922	-3.46790472885535	0.51341565523437
H	-4.69413066736178	-2.44499570211526	-0.86575021538178
C	-1.25756521371720	-0.22860221223799	5.26996541029941
H	-2.23676161014407	-0.63710778771308	5.00556988861401
H	-1.10475798111438	-0.38298506602371	6.34630100628329
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Cl	-4.27632050147754	1.14162902464356	1.56115513546799

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Mo	-1.25340846049171	-1.80741190626604	-0.28511751273988
Fe	-2.38178149550640	0.25337894210298	1.09762320948021
S	0.99498341361572	-1.35089849103352	0.18409194893003
S	-0.68759683535433	1.37822696975754	2.01019178525951
S	-2.07345986393750	0.23083922082961	-1.11046147701453
S	-2.27077944422831	-1.85011961968045	1.82935247623999
C	1.10589429854786	2.83753450610609	-0.15716078271984
C	1.68162543051509	1.22293325857493	-1.72394269473020
C	2.05617282697031	1.81369574054084	-0.46155287027992
C	0.10877303581292	2.84437117030519	-1.18475657284939
C	0.49143006803393	1.86505698013417	-2.17047323108260
C	-0.13609070301433	-0.90392865626495	4.51986026238952
C	1.09143440772470	-0.28378242672078	4.09373839349502
C	1.20129698158021	3.80753359986898	0.97943291064111
H	0.21642491727329	4.17973888151685	1.27116986932997
H	1.81312503846105	4.66697760686636	0.67483332312407
H	1.66925219861082	3.35240664637985	1.85595561055690
C	3.32508632807214	1.52993967674047	0.28312556045373
H	3.22643388339598	1.78118945850938	1.34176030634949
H	4.15116196531446	2.12593666039008	-0.12811048838228
H	3.60152581658489	0.47565052208837	0.20565704080000
C	-0.09649452046306	-2.27563794878268	4.10241163576198
C	1.84918925698180	-1.24594603776599	3.36603531850700
C	1.10402109213411	-2.48217524607765	3.35638097700590
C	-2.25173199337814	-2.73831393995363	-2.21821404759091
C	2.51059901255119	0.23623716099821	-2.48660385293694
H	2.94755653317665	-0.51250178515874	-1.81999518841900
H	3.33304480894237	0.75461596241119	-2.99711092224453
H	1.91884427410405	-0.28153525327339	-3.24342023534603
C	-0.84348672438527	-3.00757536351724	-2.24814909928651
C	-1.91610327926012	-5.04835110625624	0.73558072191299
H	-0.98765476791167	-5.15865215811965	1.30049320986807
H	-2.21384361508371	-6.04261739784930	0.37728628267857
H	-2.69160304652438	-4.69035911828958	1.41773634665026
C	-1.74278080700756	-4.11931218404319	-0.42591550599497
C	1.53351506268435	1.10324136000423	4.44675381558458
H	2.19110543476541	1.52057758424081	3.68027036918445
H	2.08513983369228	1.08641160305706	5.39585696864077
H	0.67861662254814	1.77318994639546	4.56381949935012
C	-0.53831259509150	-3.88684633293231	-1.14812621826049
C	-2.80603311369561	-3.38748008462700	-1.07224692968163
C	-0.19529259086037	1.64815379857731	-3.48376386239129
H	-0.04360325761641	0.63110935641094	-3.85147074922347
H	0.20713138997842	2.34290505584037	-4.23252613472849
H	-1.27013400505500	1.82521319259058	-3.40011398500056
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H	-2.08296359739739	-2.91035048142640	4.63244765236893
H	-0.77188330295866	-3.81810544297737	5.40715701291708
H	-1.16183857598548	-4.10209067189673	3.70109063369416
C	0.78312723971982	-4.55297524317996	-0.91664861625610
H	1.61266701719886	-3.88040075869242	-1.14932171311366
H	0.87150268553455	-5.43686517919043	-1.56196836957639
H	0.88901875014602	-4.88033085721412	0.11926824810503
C	1.61117475884398	-3.78519213874438	2.81812202458947
H	0.78968938389525	-4.46881698675927	2.59110154894143
H	2.26218720619854	-4.27577963128944	3.55431116996018
H	2.19279232459080	-3.63063767308685	1.90571700330572
C	3.25128288378390	-1.08773326165250	2.86405835739729
H	3.38220524078858	-1.54960230836677	1.88123016650735
H	3.95106436271693	-1.57104616678170	3.55860563704909
H	3.52832704681973	-0.03503121374962	2.78780286620117
C	0.11076121625682	-2.61078676652630	-3.33354119043383
H	-0.15790413192470	-1.64227052607023	-3.76191523603767
H	0.10141503876626	-3.35130353424805	-4.14474374361387
H	1.13189455687255	-2.54520866368325	-2.95080443230605
C	-1.04822294655914	3.79271756901842	-1.28846816220819
H	-0.75434206525016	4.70736144487870	-1.82059991715519
H	-1.88027863821382	3.33915069013348	-1.83390820131474
H	-1.40883005855936	4.08043378636742	-0.29726871622396
C	-4.25374885867485	-3.42105915707925	-0.68364239091540
H	-4.76067209475629	-4.27346325542833	-1.15525609660253
H	-4.36480569024817	-3.51990542544550	0.39948278025006
H	-4.76640310151885	-2.50802218920744	-0.99742580964847
C	-1.19746512746069	-0.26694398318210	5.36712696697900
H	-2.17317452501796	-0.72459309367818	5.18335867140161
H	-0.96519956159352	-0.38178888457164	6.43427912459740
H	-1.27957364452511	0.80214777371277	5.15341880437302
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Mo	-0.05684519773402	0.76275433769460	-0.20133244307155
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Mo	-1.30295924754573	-1.77594806999457	-0.35113351018292
Fe	-2.54231276286545	0.34119327516350	0.69194217056711
S	0.97098643457088	-1.33760444681821	0.12059997508185
S	-0.86705856094295	1.32523915888003	1.93206477817730
S	-1.96408568342325	0.19548293569179	-1.44475877382321
S	-2.34357896094033	-1.69629338326932	1.75574561787208
C	1.09122406652443	2.84296495574616	-0.05838823108779
C	1.69833065933376	1.28752985701676	-1.67281493787263
C	2.03637275323029	1.82043845707960	-0.37344376467393
C	0.13459526118501	2.91301170994262	-1.12357098853862
C	0.54282236733108	1.97909067023554	-2.13939456665058
C	-0.09267540508492	-0.89779396328106	4.46586184047353
C	1.14576907504124	-0.30657170532945	4.02484999539144
C	1.14665696996129	3.75966820494894	1.12277864372793
H	0.14693400120591	4.07685422647037	1.42855144810406
H	1.72290158864921	4.65669225360651	0.85978415932408
H	1.63184867094311	3.28362818562894	1.97785895067110
C	3.28081647981533	1.49601562226179	0.39259501110744
H	3.15817708057969	1.71206770319454	1.45572171972199
H	4.11971556256682	2.10003038263416	0.02157190778492
H	3.55179951118647	0.44365802842403	0.28312533572724
C	-0.08666787197545	-2.27956693215808	4.07251863017873
C	1.89015645512970	-1.31086313828332	3.33478458273485
C	1.12395055061623	-2.53044615277732	3.35628319836683
C	-2.32409876448629	-2.83380495282895	-2.18566731520772
C	2.52985473345185	0.31568855720592	-2.45237787675073
H	2.96456911505656	-0.44482275844390	-1.79811126515096
H	3.35247517138304	0.84210498010101	-2.95432102933908
H	1.93734495353645	-0.18958727776016	-3.21824320244320
C	-0.90546741357752	-3.05792894086913	-2.25458290940073
C	-1.81370153401959	-5.00532027956485	0.84349521552667
H	-0.84796602740332	-5.12921278952566	1.33727100211691
H	-2.16821223879170	-5.99937091791297	0.54092608791992
H	-2.52235881799990	-4.60027396195481	1.57079934938664
C	-1.70288269365176	-4.11693406612055	-0.35547941159205
C	1.59905056687195	1.08503472343235	4.34382996087043
H	2.35210192617565	1.43373621016492	3.63316513293485
H	2.04099572892716	1.11732466465212	5.34839459665676
H	0.76093398785289	1.78680569973671	4.32138347858306
C	-0.53547629014910	-3.88351435540904	-1.13683471068340
C	-2.81249474573060	-3.45244830262977	-0.99479611261209
C	-0.07192179627764	1.84495054129360	-3.49806404666304
H	0.02033682643655	0.82600624206596	-3.88133819128043
H	0.43975680209914	2.51870111243237	-4.19779840730586
H	-1.13079639015072	2.11201563633132	-3.48367163816868
C	-3.16389062989036	-2.18732904775532	-3.24293979365221

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H	-1.15462488111441	-4.11320089027799	3.72090076075909
C	0.81192567982677	-4.49973787591081	-0.92316494881436
H	1.60988555575585	-3.84728940231818	-1.28542834124583
H	0.87223148784470	-5.44774288372730	-1.47360478881170
H	0.99334267570216	-4.71028271046600	0.13234697986100
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H	0.79107849313964	-4.53761963608324	2.64995660728548
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H	2.21583546182202	-3.74076052841679	1.95665868932798
C	3.29647900250079	-1.20233425868945	2.82875487510512
H	3.40564299571207	-1.65640448025904	1.83945487071243
H	3.97745142903660	-1.72427781963885	3.51396474185319
H	3.61815553258487	-0.16198511675919	2.76599501561542
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H	-0.32743648292325	-1.68365977494442	-3.80193377905634
H	0.00732833400080	-3.38364529270979	-4.17268344834679
H	1.02652359616695	-2.51076286780176	-3.01519824638543
C	-1.00491010068878	3.88313465643338	-1.22295328970003
H	-0.67854661223987	4.81466479561585	-1.70411574938860
H	-1.82511133364668	3.46739110070626	-1.81381190931198
H	-1.39288859080423	4.13315860425416	-0.23206907577552
C	-4.24231222127249	-3.53171281685027	-0.55412312903882
H	-4.71057172525645	-4.44630048575222	-0.94126881617833
H	-4.31350752549117	-3.55138900121351	0.53696924081427
H	-4.81592151931205	-2.67621707686129	-0.91920378263835
C	-1.14150693177723	-0.22321852142916	5.29950018254741
H	-2.13052975254854	-0.64827904119026	5.10818508276694
H	-0.92227733615557	-0.34595931563296	6.36889108069092
H	-1.18434744504431	0.84782040963369	5.08482757286800
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Fe	-2.35947587016035	0.21640656150245	1.06232981508627
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S	-0.75932920392453	1.41122082721842	2.02472810145588
S	-2.12156234953433	0.26102010319797	-1.11464536110307
S	-2.33441583796697	-1.82974799650758	1.84643399894707
C	1.12360202174724	2.84693143632622	-0.17067072416945
C	1.68412770881020	1.21891958609850	-1.72791758554741
C	2.06568714584467	1.81607643805496	-0.47054429412483
C	0.12839109882393	2.85838644473054	-1.20160417205302
C	0.49986643210369	1.86743231452459	-2.18064570227016
C	-0.13877555432386	-0.91423795252091	4.53830042699082
C	1.08798891953570	-0.29384044942906	4.10691933842709
C	1.22583918341842	3.81964471192434	0.96390549464125
H	0.24393076961564	4.20597001690189	1.24756439114091
H	1.85352012516328	4.67034638851331	0.66608662929793
H	1.67718453419756	3.35776363768995	1.84580992409564
C	3.33175590312788	1.52560239021521	0.27702390791463
H	3.23227712103592	1.77849568684324	1.33557506494306
H	4.16494359213077	2.11403102368633	-0.13169238141438
H	3.60022889595883	0.46881844543273	0.20320985829317
C	-0.10656977411472	-2.28469106248121	4.11164352804366
C	1.83975018508534	-1.25656116539595	3.37513673687946
C	1.09073013445281	-2.49019421792187	3.36291443705745
C	-2.26310692334560	-2.74105343976297	-2.21118932976517
C	2.50487256450361	0.21864631386133	-2.48204577299718
H	2.92031794059230	-0.53875567630957	-1.81101686351237
H	3.34312494390333	0.72062235834238	-2.98373654364585
H	1.91252076804221	-0.28838836436701	-3.24566985115401
C	-0.85045320960643	-2.98721373484576	-2.24476810521806
C	-1.88540499592577	-5.04771902878169	0.73941102422076
H	-0.94923619619380	-5.16372792726510	1.29024711843419
H	-2.19268298010525	-6.04024102548549	0.38368320548739
H	-2.64807774491200	-4.68754227221455	1.43499495253147
C	-1.72600065860439	-4.11345745574583	-0.42033105586566
C	1.53455426186590	1.09176574492979	4.46206370443753
H	2.19944993314503	1.50428585059864	3.69880087918704
H	2.07865425511668	1.07924700973229	5.41589726730176
H	0.68079569450947	1.76555243506568	4.56666100457095
C	-0.52871281338833	-3.86296351567667	-1.14714599342088
C	-2.80397646390411	-3.40200231965333	-1.06625460968868
C	-0.18855822719958	1.65184582264636	-3.49336914323457
H	-0.02771560900535	0.63814280624874	-3.86691476620019
H	0.19893989956718	2.35454249568328	-4.24299922747844

H	-1.26566619105168	1.81305293314784	-3.40203246974255
C	-3.04797406251679	-2.01889727996297	-3.26258314944607
H	-3.94564514670098	-1.55703873290011	-2.84395621556168
H	-3.36092025838826	-2.72809788566764	-4.04063163002033
H	-2.45110638314576	-1.23627953114070	-3.73718659250978
C	-1.09997833324848	-3.34255708421518	4.48035158989501
H	-2.09098653563850	-2.91569743677282	4.65142502889016
H	-0.78093427289980	-3.84426191833625	5.40377870811866
H	-1.18649559417308	-4.09903291211726	3.69642528375021
C	0.80300098215564	-4.51074404434848	-0.92315790658595
H	1.62202587404910	-3.82190492793372	-1.14591953947842
H	0.90697747186571	-5.38515279305126	-1.57930069762842
H	0.91356343918877	-4.84913808652454	0.10878442822777
C	1.59383403765145	-3.79108793056002	2.81596947595085
H	0.77058765017078	-4.47384321412366	2.59225757765340
H	2.25147418424816	-4.28671607420558	3.54334307224529
H	2.16796999307751	-3.63215604856071	1.89938587315219
C	3.23851911713832	-1.09889164706646	2.86314129351012
H	3.36138416869431	-1.56149933243045	1.87943772596056
H	3.94581667023448	-1.58045835039138	3.55173152954535
H	3.51459702166735	-0.04600574484079	2.78245050813422
C	0.09468909002387	-2.57821598076453	-3.33355963147702
H	-0.19318643342267	-1.61732922423694	-3.76683306009082
H	0.10160828916076	-3.32228449460762	-4.14194833125253
H	1.11421574217595	-2.48937364807138	-2.95106909862789
C	-1.01285029179476	3.82479554127325	-1.31918204858221
H	-0.70605570746672	4.72807585876344	-1.86423461724272
H	-1.85230511824347	3.37673108415234	-1.85827504427668
H	-1.36878053891278	4.13337767737383	-0.33226361596152
C	-4.24986904499638	-3.46967243740355	-0.67572539811237
H	-4.73664984377950	-4.34091718007556	-1.13472597142892
H	-4.35446006079358	-3.55695807405375	0.40925006573329
H	-4.78717254053835	-2.57396794850622	-0.99873729530029
C	-1.18705421303470	-0.27939825815032	5.40400402645203
H	-2.16580330779193	-0.73729195694701	5.23595799374997
H	-0.93969828529184	-0.39379471855410	6.46830125446955
H	-1.27280045932533	0.79013660242053	5.19231723357525

$S = 3/2$

E = -4233.157116 AU

Mo	-0.01305645205185	0.74398984712055	-0.13276331864171
Mo	-0.16858508099771	-0.89199097638198	2.17337167276583
Mo	-1.26323881825285	-1.79533201772606	-0.27575543055963
Fe	-2.35696148416081	0.24529541609373	1.09497944755813
S	0.98108207666173	-1.34338587440511	0.19046168464170
S	-0.76297145713036	1.41643679691515	2.03295474368155
S	-2.15084945454967	0.27192698318990	-1.08505358767997
S	-2.34910758612958	-1.80973721434324	1.85200693802829
C	1.10889477560783	2.83043477135673	-0.15213402083371
C	1.68075347792429	1.20864633671609	-1.71117439007828
C	2.05706125302044	1.80474091884502	-0.45218957734701
C	0.11128153714075	2.83677831615875	-1.17949658686138
C	0.49014815192698	1.84765857715572	-2.15989808186563
C	-0.13650571801184	-0.90552065851411	4.51252010962930
C	1.09052490696251	-0.28457138268411	4.07993022575683
C	1.20831831447082	3.80186891568895	0.98315243778697
H	0.22681174694997	4.19238410672910	1.26178515656671
H	1.84081043929366	4.64935592388439	0.68637390656448
H	1.65477623624020	3.33925185521223	1.86700037360446
C	3.32838411086209	1.52541498832826	0.28982179386572
H	3.23337623490046	1.78137097708956	1.34777942252093
H	4.15452088680115	2.11858315101153	-0.12608244166106
H	3.60407557393575	0.47042501879215	0.21753023141813
C	-0.09771562205620	-2.27713849131919	4.09219097788022
C	1.84650349183041	-1.24818217440929	3.35370784550018
C	1.10090250611898	-2.48379467094935	3.34554448155635
C	-2.25153997322043	-2.73389675704447	-2.21493423646920
C	2.50862359005602	0.21719424615103	-2.46873165615990
H	2.93645310695241	-0.53434581442934	-1.79901287854492
H	3.33789963903662	0.72891421133359	-2.97549913385865
H	1.91786928521634	-0.29767100222518	-3.22844773571251
C	-0.84232931701314	-2.99266187994726	-2.24637388622912
C	-1.89854608048132	-5.02744376625728	0.74955447790357
H	-0.96054839076643	-5.15870556507914	1.29381171768079
H	-2.22803646271436	-6.01526175194225	0.40075744041061
H	-2.64846152761905	-4.64940067876298	1.44991222886328
C	-1.72957840277596	-4.10009779290571	-0.41402425240797
C	1.53421942186821	1.10150859625459	4.43481422437518
H	2.20873438502877	1.51127109583854	3.67890056348601
H	2.06696767791609	1.08941290798239	5.39502337702253
H	0.68037513587771	1.77657726408968	4.52873797280669
C	-0.52906058028425	-3.86461258457783	-1.14265643975581
C	-2.80103526203014	-3.38158908195206	-1.06681030174473
C	-0.19706858299349	1.62871116929452	-3.47270796875813
H	-0.02376268998047	0.61892272595698	-3.85096941720634
H	0.18346564438041	2.33967010075981	-4.21815832537061
H	-1.27565573347659	1.77793177133823	-3.38040853438736
C	-3.02437304881412	-2.00308732327988	-3.26912048960621

H	-3.92776655838277	-1.54646610598470	-2.85758697010358
H	-3.32578544453680	-2.70584773208973	-4.05760428625427
H	-2.42240717346740	-1.21553580884838	-3.72895251671824
C	-1.08925876778062	-3.33618240889307	4.46177940593416
H	-2.08093831494779	-2.91105429708614	4.63198217555167
H	-0.76738474568420	-3.83390955150564	5.38641469823084
H	-1.17303961509663	-4.09492433057395	3.67998154954093
C	0.79599256899305	-4.52587961724529	-0.91718936606727
H	1.62226257390483	-3.84759142096621	-1.14575708525253
H	0.88903040804816	-5.40551161236804	-1.56799564080392
H	0.90507561451596	-4.85892089215085	0.11666437002173
C	1.60853147205356	-3.78599008561363	2.80624513082296
H	0.78741571313281	-4.47168427292295	2.58355966762483
H	2.26525828405548	-4.27585856402627	3.53828156017610
H	2.18466285503811	-3.63018565488747	1.89041522367631
C	3.24806203097826	-1.09319604892029	2.84938768254781
H	3.37341628530877	-1.54747144073075	1.86217223468773
H	3.94861447604697	-1.58557346628664	3.53711950693069
H	3.53029997688241	-0.04130703683766	2.78039569148588
C	0.10619678301745	-2.60245065053952	-3.33919705075498
H	-0.17322922321868	-1.64340945386932	-3.78205634629942
H	0.10542333478036	-3.35465839035200	-4.14018482150438
H	1.12707459043168	-2.51959868385562	-2.95885015119092
C	-1.03635916491833	3.79508883753622	-1.29483950305859
H	-0.73719040503321	4.70266012085163	-1.83685478047642
H	-1.87236242048457	3.34141141971150	-1.83473575605335
H	-1.39548343941283	4.09693650236168	-0.30688456885299
C	-4.24857403560430	-3.43100296255386	-0.67918844291544
H	-4.74777551508166	-4.29378853395247	-1.14086711587309
H	-4.35593808207803	-3.51887426085508	0.40547973792709
H	-4.77289691463962	-2.52692326478448	-1.00092193163342
C	-1.18860841487042	-0.27127963849844	5.37325417991791
H	-2.16681543311216	-0.72763151634376	5.19730781138652
H	-0.94879779933599	-0.38754062303721	6.43900670016991
H	-1.27252538097188	0.79854091596717	5.16202324704514

$S = 5/2$

E = -4233,134384 AU

Mo	-0.07751904188460	0.76224692395271	-0.21551561081117
Mo	-0.13625513933924	-0.93986846290080	2.14596746050723
Mo	-1.30421754183392	-1.77656858442286	-0.36865518989141
Fe	-2.51556691608940	0.27211339644242	0.74705157338025
S	0.95786713787374	-1.32458919883995	0.11805431965327
S	-0.92380108430748	1.33656935779295	1.94032233419775
S	-2.11322754850345	0.24912451632897	-1.41163859476993
S	-2.37830369397926	-1.74408458020198	1.75595115519132
C	1.08807236926919	2.83364146572869	-0.04724955484058
C	1.68314078095602	1.28976404276746	-1.67435606114067
C	2.03307610257724	1.82020902009192	-0.37768212491441
C	0.11891009206986	2.90695828522572	-1.10362437666958
C	0.51792673605555	1.97467842697217	-2.12825024054954
C	-0.09696426775370	-0.84503961112869	4.46204664537817
C	1.14947644514329	-0.29368120619627	3.98986431940550
C	1.14914238392047	3.74261147734014	1.13977677464434
H	0.14892297300872	4.03625317480820	1.46745658488772
H	1.70243665694671	4.65399937882400	0.87573096134966
H	1.65899282499846	3.26944600938762	1.98223590551576
C	3.28191185303770	1.48774240127735	0.37758171072041
H	3.16940310864588	1.70385950977144	1.44205065990245
H	4.12421845207670	2.08414697419170	0.00118068726182
H	3.54350657280452	0.43284070994666	0.26655290290779
C	-0.13110381270287	-2.23372161686779	4.09974053213622
C	1.85873928572630	-1.33197366073197	3.31293711592309
C	1.06320609395158	-2.53040454629589	3.37157818836925
C	-2.28201603648306	-2.84001802146886	-2.22603740132580
C	2.51191394934154	0.32183740883769	-2.46210101896282
H	2.94205147812457	-0.44707778022751	-1.81407914172123
H	3.33849705919183	0.84751328448178	-2.95893025549015
H	1.91785032609223	-0.17428871046061	-3.23277309639587
C	-0.86169335973315	-3.04616231494744	-2.27797698168771
C	-1.78709907516497	-5.01611073827374	0.80435944805083
H	-0.82403367699005	-5.14700677361668	1.30179537193814
H	-2.14446997328395	-6.00749806026154	0.49492624620391
H	-2.49633490993378	-4.61331035037335	1.53306390554430
C	-1.66751981023782	-4.11605927501549	-0.38535451155371
C	1.64196426770947	1.09094782411793	4.27875017545769
H	2.41071676867552	1.39848962556876	3.56611223556632
H	2.07716025397400	1.13702638902258	5.28603074373489
H	0.82515664283664	1.81649241252999	4.23026139076841
C	-0.49570444219080	-3.86802652990677	-1.15457872374974
C	-2.77843498305627	-3.46315308432963	-1.04149745165158
C	-0.10793940973527	1.84427822584325	-3.48271415008513
H	-0.01577228904978	0.82670072111726	-3.87023159353437
H	0.39101655801589	2.52267727951708	-4.18770106981274
H	-1.16885304238215	2.10243285792541	-3.45480915395775
C	-3.11347877863157	-2.20041704849236	-3.29464017320537

H	-4.00746008424611	-1.73048435274932	-2.87719004744653
H	-3.43445219007598	-2.96621520406092	-4.01363956515181
H	-2.55010463078113	-1.43889125851334	-3.83894796665104
C	-1.17891753158214	-3.22156366005329	4.51057853171659
H	-2.15633423919241	-2.74366352461621	4.61239022216652
H	-0.91385969889387	-3.66619576138543	5.47917902413315
H	-1.27150481097365	-4.02982374742960	3.78095851586761
C	0.85590236673376	-4.47178150006264	-0.92985149351574
H	1.65199799005442	-3.80095414253084	-1.26193997703914
H	0.94063925617594	-5.40733868100642	-1.49853753739549
H	1.02053665563318	-4.70221440115687	0.12443304458489
C	1.51879949822420	-3.88160963908664	2.91089321386094
H	0.67210858206177	-4.54776952971087	2.73222000436414
H	2.15594615298084	-4.34956178980411	3.67428612723487
H	2.10244728664355	-3.80835139115947	1.98975873422156
C	3.25919668248950	-1.27252807598285	2.78289930012878
H	3.33850327425413	-1.76229806786724	1.80797184091865
H	3.94024070975374	-1.78677241872732	3.47408252098095
H	3.60321864932529	-0.24271093896814	2.67802517358253
C	0.05249944868841	-2.62165965141079	-3.38843482407782
H	-0.27374654309821	-1.67484980792723	-3.82660346231000
H	0.07052441062886	-3.37431255643041	-4.18861670023124
H	1.07467598950082	-2.49447997275936	-3.02360457605612
C	-1.01975428694785	3.87922814185029	-1.19011487447676
H	-0.70257985566189	4.81367980844661	-1.67294648895798
H	-1.84644820703362	3.46287794814572	-1.77235283396718
H	-1.39821736934963	4.12661186745428	-0.19425112845056
C	-4.21350211460409	-3.56151873510912	-0.62059770323310
H	-4.67172827427209	-4.47698267848001	-1.01880389782001
H	-4.29630239014836	-3.58813498602214	0.46963621786300
H	-4.79102154713631	-2.70830921203657	-0.98622964299722
C	-1.11261862131951	-0.12438190201855	5.29811716220246
H	-2.11411071904615	-0.53525055596870	5.14328472096900
H	-0.87148739025058	-0.21653480419287	6.36614420323968
H	-1.14002878829189	0.93984323647889	5.04884628986713

I2 ([Cp*₃Mo₃S₄Fe(THF)])**S = 1/2**

E = -4465.776148 AU

Mo	0.03642402043585	0.86524641985713	-0.02901936367464
Mo	-0.08134414755850	-0.87393134646001	2.21698474648664
Mo	-1.29165930095582	-1.67721962085574	-0.22521579147074
Fe	-2.29619630278360	0.35887804559993	1.24639939231134
S	0.98593924850382	-1.27386638324621	0.17236557798806
S	-0.62014208087290	1.42566288569146	2.16208505121172
S	-2.09481427548913	0.42586905721907	-0.92868883411406
S	-2.26269582796295	-1.73054905220119	1.91769275222700
C	1.12282685711732	2.96042215604245	-0.06447689920145
C	1.69665176781029	1.36127035017441	-1.64628163041788
C	2.08289987723397	1.94999382783291	-0.38835464525570
C	0.11648092493858	2.96383870423400	-1.08302783553715
C	0.49377999035498	1.98933009889027	-2.07703904967157
C	0.13763235637545	-0.79854690012918	4.56034382102115
C	1.40028320066452	-0.36263680206142	4.01348619221460
C	1.22199260323330	3.92878044243975	1.07427726250682
H	0.23421141771853	4.27014557970889	1.39420746715724
H	1.80182066317220	4.80904132604131	0.76430057719784
H	1.72141446343831	3.48020563915294	1.93680384917504
C	3.36432932178243	1.67295001163565	0.33904627537564
H	3.27382498366416	1.90620100116657	1.40282729707803
H	4.18320962317461	2.28301354043811	-0.06779402767843
H	3.65183473488954	0.62265933197517	0.24381691635150
C	-0.03685999113627	-2.17597986044343	4.21120999078209
C	1.96334463222548	-1.44699140326454	3.28601600593671
C	1.06372204350975	-2.57151375763180	3.39112094853246
C	-2.18289873248307	-2.43956933829927	-2.30363192870051
C	2.52447658534746	0.38210117962609	-2.42081418113035
H	2.96200721367910	-0.37370580266713	-1.76211399982731
H	3.34607852608717	0.90279379351833	-2.93134045870031
H	1.93023255788616	-0.13100987791482	-3.17932576987306
C	-0.82752461101864	-2.87207154370223	-2.20613802646948
C	-2.42089111796028	-4.84168982667100	0.59022024172891
H	-1.57452803680955	-5.07428461067884	1.24181756223785
H	-2.78940515882293	-5.78559997978419	0.16589271226615
H	-3.21450249257902	-4.41267948976747	1.20683225916499
C	-2.02512706115877	-3.90419631534106	-0.50952854143949
C	2.03294393140735	0.97170230520479	4.26418530552360
H	2.78291984927339	1.20454098904931	3.50419386261581
H	2.52990770003458	0.98362299999628	5.24369919783479
H	1.28381977934210	1.76934536271890	4.25627307880693
C	-0.73370737200093	-3.79458924809716	-1.09909864623381
C	-2.92249440178214	-3.03527666203636	-1.22850481066478
C	-0.20451619470970	1.77135626565795	-3.38471886780203
H	-0.04045207684178	0.75854389925772	-3.76102037584274
H	0.17025818152997	2.47665499830128	-4.13897400456539

H	-1.28223167284820	1.92419438350108	-3.28406709750435
C	-2.76085035532019	-1.59910239450803	-3.39968375335938
H	-3.61305894561119	-1.01401061451197	-3.04479181717662
H	-3.10861581435839	-2.24198815164962	-4.21996590478547
H	-2.02004872227245	-0.90510588119736	-3.80489626275079
C	-1.13133159702746	-3.07783428430551	4.69406852010880
H	-2.04400033789422	-2.51697825758161	4.91097016060325
H	-0.81761844640976	-3.58794658416584	5.61503631893566
H	-1.37309967326153	-3.84048862823567	3.94902531895825
C	0.47926584184131	-4.60443237478056	-0.75536212071887
H	1.39080095515131	-4.00562721797962	-0.84105539601005
H	0.57268808807965	-5.46131977085846	-1.43657785523882
H	0.42096402340257	-4.99030885215854	0.26444601704679
C	1.34089261775011	-3.95233978482792	2.87777550433130
H	0.41310187557736	-4.50552096329948	2.70757244578960
H	1.94315656124048	-4.52508633919194	3.59732910429247
H	1.89309044105040	-3.91795466544363	1.93480981207884
C	3.32371117102813	-1.49277616886883	2.65963096558207
H	3.31458651145868	-2.06884136172419	1.73007563491460
H	4.03937846891034	-1.96766699326357	3.34459472124310
H	3.69252477604439	-0.48991542096962	2.43362553634634
C	0.27587610018674	-2.58318264049835	-3.17798965275282
H	0.11209407899913	-1.63403820693308	-3.69482176434611
H	0.33779329311168	-3.37255900469988	-3.94010617288475
H	1.24247187592809	-2.53202249294407	-2.66978383781848
C	-1.04569318262473	3.90750231066511	-1.17380641192029
H	-0.77186704178336	4.81983644116758	-1.72183644558213
H	-1.88767461761052	3.44240928807309	-1.69475217235330
H	-1.38699579827111	4.20390582340739	-0.17774218381789
C	-4.39929494882709	-2.90867750453703	-0.99768734559992
H	-4.95432755220531	-3.67123183352668	-1.56200962980158
H	-4.64430940373278	-3.03199109453081	0.06126392518983
H	-4.76346773921799	-1.92721304409849	-1.31549583533246
C	-0.74499259483104	0.00982959575046	5.46470954860633
H	-1.78114783320119	-0.33713165634614	5.41669261358373
H	-0.41376709984507	-0.06357915882530	6.51002440983479
H	-0.72908627603121	1.06617987022509	5.18025253879906
C	-5.32208800126661	0.45470324548016	1.48801894200164
O	-4.06107170110201	1.19154969645802	1.67949890853215
C	-4.28036220973603	2.62128261128522	1.43476387445867
C	-5.78595733181427	2.80083575593861	1.55218150240447
C	-6.30995946354466	1.48486971442629	0.95229818196503
H	-5.11490385077947	-0.36846160604057	0.80348601104368
H	-5.61067614437469	0.06104705444268	2.46761566702722
H	-3.68946198766437	3.15900342632203	2.17797589680193
H	-3.91237596996362	2.85071927482656	0.42949752150236
H	-6.08113463121669	2.89084104296174	2.60290905272809
H	-6.13599375907590	3.68322097796489	1.01060348713518
H	-7.33659842232764	1.25837305674431	1.25013196217963
H	-6.26185043561384	1.52396648268450	-0.14085707973304

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E = -4465,766336 AU

Mo	-0.07222870650047	0.91114933161561	0.22709847819359
Mo	0.00207928174209	-0.94265516500470	2.38790725857396
Mo	-1.37652106048674	-1.63917601904170	-0.02877875170002
Fe	-2.21968806295324	0.41278608538315	1.73927376015494
S	0.90690589127412	-1.22556863865228	0.23893244089121
S	-0.39933531861630	1.37967974892120	2.52264191604593
S	-2.30529240325566	0.55066820693827	-0.49101052624040
S	-2.23177096707657	-1.77132150542433	2.23843253073190
C	0.95413647644224	3.04327901580035	0.17778577077009
C	1.52067195745094	1.47106286085250	-1.43516184515871
C	1.93047278308990	2.05647878835716	-0.18492784371777
C	-0.08537176263665	3.02599852150184	-0.80126117533115
C	0.28166302922488	2.06295532098500	-1.81215818026592
C	0.43736456220410	-1.01441775056169	4.69721754794855
C	1.65572207161327	-0.58381312767178	4.05224452246357
C	1.06966309923579	4.00676798328553	1.31865138194663
H	0.08575730659029	4.31614298421013	1.68040400265854
H	1.61019017254572	4.90504463590836	0.99080522207763
H	1.61705147816203	3.56826348457528	2.15680952847450
C	3.23663224383214	1.80556923658284	0.50652063286961
H	3.16360441813329	2.02607604097739	1.57414969791657
H	4.03069699866894	2.43893928501667	0.08704717984711
H	3.54550240896706	0.76309958366811	0.39439131579916
C	0.17829283411732	-2.35599593445819	4.28069157769878
C	2.11387876504505	-1.63703195709170	3.21414460001766
C	1.18346900702197	-2.73264692674343	3.33100698420591
C	-2.55912534727914	-2.33690572631828	-1.94749450612447
C	2.34342196178672	0.52454259927227	-2.25408420750772
H	2.90802976420534	-0.16129749420463	-1.61700717613859
H	3.06044029644400	1.08555784177819	-2.86871619450618
H	1.72024244443244	-0.07073955708632	-2.92461852382430
C	-1.18296021598483	-2.66846137231621	-2.12978096241806
C	-2.10068735517439	-4.89330612793897	0.78845192313834
H	-1.12216306442299	-5.25905799852130	1.10881707823759
H	-2.68508728387006	-5.75523640464186	0.43868804011890
H	-2.60780681547748	-4.47280800597504	1.66362222032620
C	-1.96589620947611	-3.87043993398776	-0.29688977218288
C	2.37179524789374	0.70156833412987	4.33339976267493
H	3.06460421663638	0.95469056234317	3.52772832117682
H	2.95243146826388	0.61121480673420	5.26122307712813
H	1.67014620992050	1.53144622129780	4.45349850755102
C	-0.82035962949161	-3.62647223965650	-1.11446512922421
C	-3.04371852191306	-3.04281899269259	-0.79778131868426
C	-0.46060190794851	1.84328871629456	-3.09447043103908
H	-0.17414489272931	0.89857652853576	-3.56115432298045
H	-0.23426232323712	2.65147810987252	-3.80295706133973
H	-1.54154880512283	1.83040972985148	-2.92794308494708
C	-3.37846120127251	-1.47656288434962	-2.85945738596097

H	-4.19174701660094	-0.98520440592030	-2.31905105497971
H	-3.81910202255842	-2.08978716943989	-3.65746366206768
H	-2.76730944825333	-0.70032340490502	-3.32671060174733
C	-0.88430924186940	-3.25740085541518	4.82910356476132
H	-1.76055149913680	-2.68972074956402	5.15145461429376
H	-0.49201079200457	-3.80289373762312	5.69834770170744
H	-1.20801239824059	-3.98899601033135	4.08498692508986
C	0.48850886826135	-4.35496904889701	-1.05487171166053
H	1.32489612242011	-3.68808797481828	-1.28290131809718
H	0.50092895985332	-5.17472995261390	-1.78615198949439
H	0.66054784567030	-4.78464027484911	-0.06577253904248
C	1.36611176805886	-4.09163969225457	2.72742747743008
H	0.40552544313197	-4.59169133864558	2.58328000069732
H	1.98138826910738	-4.72746561960839	3.37937434933172
H	1.86540742294578	-4.02531024341860	1.75768844773046
C	3.41124833229574	-1.68302457113796	2.46690553222805
H	3.30772564274037	-2.22727638548520	1.52429204627257
H	4.17561862680021	-2.19140157040355	3.07009109086246
H	3.77578368938265	-0.67861631969521	2.24036116709500
C	-0.30976872150873	-2.24654998124163	-3.27262678590785
H	-0.60184846512105	-1.26461005797264	-3.65261510415584
H	-0.38349545792474	-2.96177619506483	-4.10433527207614
H	0.73913887475460	-2.19817526754321	-2.96850931682479
C	-1.27128972753916	3.94173451151732	-0.86250519300680
H	-1.06492689905568	4.80757634136560	-1.50672248138859
H	-2.14479313675553	3.42082672254816	-1.26560178930824
H	-1.53055472881491	4.31734950890179	0.13134599793063
C	-4.45636627126897	-3.05075122502319	-0.29252637911010
H	-5.05376443211881	-3.82300795572483	-0.79819943970899
H	-4.48403026352757	-3.25307453126786	0.78203159146649
H	-4.94400083603179	-2.08642599217545	-0.46373608865813
C	-0.32475018612980	-0.23914001337345	5.73011951873345
H	-1.37528625463013	-0.54237684776235	5.75294391463205
H	0.09529121821354	-0.40110991155113	6.73240008589892
H	-0.28631073803965	0.83323781779358	5.51787162464332
C	-5.26114443477053	0.50278392827343	2.23439066600587
O	-4.02248059897269	1.23775177925177	2.48177068933553
C	-4.25964734623410	2.59549078746041	1.98286664852743
C	-5.24450266189440	2.45534555368560	0.80745504422341
C	-5.70777665915663	0.97715581478900	0.85649094027844
H	-5.01041476196597	-0.55648865225911	2.29914928555976
H	-5.97722381507484	0.77600351460906	3.01936192824233
H	-4.68043147109248	3.18063145609990	2.80759990623853
H	-3.28375703130407	2.99676848587249	1.70312930835088
H	-6.08446917327940	3.14334265720301	0.93345291335794
H	-4.75461957244195	2.67645092186933	-0.14334537252875
H	-6.78720943494898	0.87145481003103	0.72029174257059
H	-5.19443518538782	0.39709141236426	0.08572544592178

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E = -4465.742105 AU

Mo	-0.12132221446695	0.95257293877412	0.23883195936848
Mo	-0.03315627863455	-0.89352870807710	2.41663015624964
Mo	-1.34624977853383	-1.68416085875207	-0.07883711743059
Fe	-2.19362892842482	0.41669225749660	1.76181172516659
S	0.90790526732102	-1.16539944255602	0.27486763433327
S	-0.41041502339955	1.49913688054285	2.59167966689907
S	-2.34489021781385	0.48422685256381	-0.50468723833152
S	-2.23006634298134	-1.81062728807275	2.17072629318616
C	0.91221295975022	3.05701529604878	0.11197367729371
C	1.45124042288816	1.45128194404793	-1.47628456685589
C	1.88083781000797	2.06437457341862	-0.24587247796261
C	-0.14829223958177	3.00950833493589	-0.84830743405800
C	0.20345966483149	2.02559863639797	-1.84781371238388
C	0.38403252867770	-1.03739286466959	4.71098853719151
C	1.60512032370241	-0.60122279807183	4.07600280505537
C	1.05392852362340	4.05540148813989	1.21965501224254
H	0.07882355692211	4.38878644195685	1.58315256714998
H	1.60154255059268	4.93477225710357	0.85398717308481
H	1.60589013068463	3.63707385839923	2.06459561986940
C	3.19209315225862	1.82062837494961	0.43890591342718
H	3.12231566670008	2.03992002012754	1.50722196586918
H	3.97985713555201	2.45940461336466	0.01575133281458
H	3.50606148790161	0.78006715852368	0.32354819420648
C	0.11680714932642	-2.37203670285073	4.27235674403118
C	2.05386709278251	-1.64641130857613	3.21908067797330
C	1.11948173714354	-2.74113192233955	3.32223244807003
C	-2.40721152111501	-2.39094270920356	-2.04548089022221
C	2.27436064463665	0.49834689841544	-2.28623365742265
H	2.78966158777502	-0.22505494022093	-1.64840349750514
H	3.03539636249981	1.05344656846733	-2.85077864800208
H	1.66189270542126	-0.05256586372969	-3.00154979610206
C	-1.02316426751675	-2.72994791666176	-2.15016339392625
C	-2.10836673903735	-4.95182983126804	0.70865465294346
H	-1.15244170983761	-5.27520764496633	1.12597424655982
H	-2.61975254266295	-5.83823369737179	0.31010898903499
H	-2.71553434340775	-4.54836872461292	1.52479431408505
C	-1.91303840586520	-3.93341586715876	-0.37217295974737
C	2.33338345451683	0.67190275219093	4.37809740808865
H	3.01836094767300	0.93694140025493	3.56914444540712
H	2.92317643292902	0.55889114177416	5.29765327251534
H	1.63669194463380	1.50270070738804	4.51831449704159
C	-0.72022587217524	-3.68801987362368	-1.11820928750679
C	-2.95726015496817	-3.10891744300408	-0.93039978691778
C	-0.55340494634909	1.78911409498865	-3.11777611106291
H	-0.30352972992402	0.82086735308790	-3.55642320801785
H	-0.31007597084982	2.56595810460074	-3.85525847294395
H	-1.63280323100191	1.81365539647655	-2.94241535061909
C	-3.17324085294284	-1.53342643402097	-3.00493150376046

H	-4.03864181471707	-1.07234623423832	-2.52220717027354
H	-3.53503317561659	-2.14151479721914	-3.84531166124728
H	-2.54697853243553	-0.73414548466945	-3.40877463870353
C	-0.96042914678018	-3.26867390935238	4.79848997563790
H	-1.83644122034566	-2.69668259781583	5.11422098621535
H	-0.58445373538441	-3.82370674609879	5.66869747216568
H	-1.27924996143599	-3.99193066641966	4.04424412011973
C	0.58585022185630	-4.41109556949986	-0.98765108333679
H	1.43145826174949	-3.72767349604690	-1.10882203490638
H	0.66675627985121	-5.18750618029936	-1.76049145548640
H	0.67767952050133	-4.89615249753467	-0.01430028856130
C	1.30704693099016	-4.09449183162581	2.71124897186682
H	0.35091095285531	-4.60692114578508	2.58309286989972
H	1.94109968033975	-4.72397156625501	3.35119407155532
H	1.79026334337897	-4.02009209462379	1.73429357980979
C	3.35443938135702	-1.69003041772001	2.47743517845366
H	3.25760815598901	-2.23928773707768	1.53702129179990
H	4.11768068656584	-2.19257064397389	3.08694806844367
H	3.71591710181761	-0.68503296589947	2.24756864043851
C	-0.08960279150338	-2.32563160727341	-3.24989427215661
H	-0.36186838686151	-1.35233603588770	-3.66369360096530
H	-0.12294006422594	-3.05751250288205	-4.06922716017944
H	0.94186069306865	-2.27206971568044	-2.89312177838935
C	-1.33660420777275	3.92215453720137	-0.91136824660563
H	-1.14195475326144	4.77224814379958	-1.57999312377228
H	-2.21624480158230	3.39140248811549	-1.28785834027845
H	-1.57912190329512	4.32205017875034	0.07707145825878
C	-4.39257602926744	-3.10755819160942	-0.49412929550586
H	-4.96244557652633	-3.88599162896477	-1.02070338834257
H	-4.47205031510206	-3.29955449524810	0.57952342228546
H	-4.86869721407944	-2.14501156984221	-0.70162426404258
C	-0.38153237829292	-0.27166210884436	5.74864515977661
H	-1.43400076147439	-0.56864454939040	5.76043495784248
H	0.03146336693760	-0.45131402032199	6.75083576515692
H	-0.33525088395965	0.80301842862409	5.55083048252272
C	-5.18821851738695	0.67128126092465	2.49651570502610
O	-3.94061049379645	1.41976653112900	2.62288551611492
C	-4.14246556653298	2.73713128028022	2.00200972325174
C	-5.41861241309319	2.62720157460896	1.14847321116393
C	-5.75035408529703	1.12141461028767	1.15723922357170
H	-4.91928401083113	-0.38595053389243	2.55005017697827
H	-5.84353931861221	0.94003599162271	3.33453329302788
H	-4.22852447436732	3.47755093720033	2.80263517280553
H	-3.24355931435041	2.93598284284410	1.41262467585873
H	-6.23099507900256	3.20036903224978	1.60445559530049
H	-5.25591680577000	3.00549503204763	0.13622960235050
H	-6.82187464449596	0.92572160872322	1.06314095790365
H	-5.21667718906339	0.60812642895529	0.35137060877116

I3 ([Cp*₃Mo₃S₄Fe(CO₂)])

S = 1/2

E = -4421,906436 AU

Mo	0.03186813015006	0.74089247312946	-0.13800987649460
Mo	-0.15783971576381	-0.88540409299068	2.17247586346771
Mo	-1.24358626539546	-1.80081868151211	-0.29013648213461
Fe	-2.38314857202268	0.27593922074797	1.06434004482988
S	1.00442347110990	-1.36186905348278	0.19608889223506
S	-0.68293588176151	1.38040701195315	1.98969508674184
S	-2.03358931719560	0.24374980877678	-1.11312022988529
S	-2.27869593364775	-1.80014866625076	1.80939893934776
C	1.14351255372445	2.82843638871430	-0.16576190525315
C	1.71232250964924	1.20548443298946	-1.72711487665646
C	2.08850070057330	1.79717978354207	-0.46545745588100
C	0.14896070540474	2.83842430631889	-1.19548328087532
C	0.52679141445647	1.85384314705132	-2.17781949942670
C	-0.18959239800030	-0.91943754611869	4.51996309686598
C	1.04154110901311	-0.28928524122862	4.12371120111844
C	1.24068365374386	3.79801389521221	0.97141118247203
H	0.25737758724274	4.17929839312879	1.25666213064537
H	1.86274473093246	4.65166499282288	0.67158362012699
H	1.69834569096106	3.33817044137451	1.85111925861922
C	3.35056313468487	1.50622458666861	0.28852461084741
H	3.24403342470709	1.75657851716231	1.34688048141077
H	4.18300649368700	2.09832823084175	-0.11518000164660
H	3.62156593526890	0.45024100619597	0.21367025650385
C	-0.13543307175169	-2.28814483130144	4.08988593222999
C	1.81688406356887	-1.24050464734848	3.39813373589854
C	1.07992954632039	-2.48159541368599	3.36652631893801
C	-2.30483972928513	-2.74521198040154	-2.17894890341663
C	2.53373422520058	0.20828669299617	-2.48442848073904
H	2.96723731223222	-0.53802858117420	-1.81292626396259
H	3.35831956280071	0.71760254966105	-3.00058701249052
H	1.93727277362114	-0.31095290748459	-3.23662895364153
C	-0.89107082569671	-2.98285979737370	-2.27359815813877
C	-1.78545703452570	-5.05677282066986	0.74528929685506
H	-0.82075333597780	-5.18160877258060	1.24167415076575
H	-2.11819682268228	-6.04516153650326	0.40186698794442
H	-2.50795449185014	-4.69645439607338	1.48253032250560
C	-1.68263243614479	-4.11968719273848	-0.41809174550346
C	1.47089305141908	1.09775748504298	4.49317008388992
H	2.13309345811609	1.52581880352135	3.73621138025270
H	2.01400366574119	1.07607330254854	5.44702859146745
H	0.61043686104619	1.76090345357967	4.60849019344193
C	-0.51694739079880	-3.85823951818631	-1.19383920859723
C	-2.79183829437180	-3.41759497601591	-1.01786002340998
C	-0.15769258194706	1.64275555061830	-3.49327561383036
H	-0.00465908676442	0.62778735837310	-3.86551676022845
H	0.24598187416095	2.34127633796833	-4.23783110988654

H	-1.23276670576193	1.81969732557120	-3.41123749982492
C	-3.13942360605498	-2.02358019530746	-3.19110023180895
H	-4.01540937849192	-1.55943167946793	-2.73104191191715
H	-3.49095474711838	-2.73441740713860	-3.95070839308745
H	-2.56573603602166	-1.24380177355351	-3.69828225343074
C	-1.12912567911458	-3.35315487765604	4.43595787518716
H	-2.13260869704142	-2.93898962006050	4.55766007310618
H	-0.83996041717328	-3.82851280957720	5.38251295092828
H	-1.16837298796664	-4.12745399791568	3.66647321552610
C	0.82770117137773	-4.49350225453447	-1.01553502183259
H	1.62847338876498	-3.83078208905417	-1.35281666958262
H	0.88164748817430	-5.41854601809491	-1.60454329416588
H	1.01264039300787	-4.74777871507355	0.03018601493207
C	1.60865464276573	-3.77595909892989	2.82846772395397
H	0.79890449698525	-4.47110996452312	2.59563293674582
H	2.26241801769911	-4.25755787608608	3.56802110135854
H	2.19364613039073	-3.61195721081909	1.91974713391403
C	3.22517339332424	-1.06771880142243	2.91803693182804
H	3.37496931985766	-1.52715379097133	1.93676678710752
H	3.91999192805573	-1.54393154692400	3.62242507886952
H	3.49196528389619	-0.01190885828183	2.84608550955599
C	0.00205679410906	-2.55644628445152	-3.39902176499065
H	-0.30781038388576	-1.59099746130258	-3.80570477037761
H	-0.03125188579214	-3.29043907545463	-4.21546323909845
H	1.03887019585747	-2.47266648251057	-3.06547270173914
C	-4.27361776383080	0.34690788727911	0.94151466769615
O	-5.32041925110773	-0.10206964047135	0.50931903899294
O	-3.93634816037708	1.33622333699087	1.69330016840783
C	-1.00284714829713	3.79255831273449	-1.30376165605754
H	-0.70418692270001	4.70212160503323	-1.84178373800854
H	-1.83796622893701	3.34042088599861	-1.84578582331887
H	-1.36068171867161	4.08854607260320	-0.31398438734103
C	-4.22066170669651	-3.51175433610996	-0.57672030630061
H	-4.70541936617089	-4.38264698271752	-1.03787357079321
H	-4.28768502282657	-3.62470079368279	0.50878054626301
H	-4.78273932806755	-2.61901110855797	-0.85916195761747
C	-1.27255051219543	-0.29703175053883	5.35047104259986
H	-2.24168363432275	-0.75642771628657	5.13805230588702
H	-1.06484646394890	-0.42479034593262	6.42117837705701
H	-1.35397634564655	0.77432961937959	5.14818189405347

$S = 3/2$

E = -4421,876698 AU

Mo	-0.01592060223755	0.75584777657199	-0.16476978174223
Mo	-0.11438935499810	-0.98519392239445	2.16933352963465
Mo	-1.30999678582177	-1.78742799652950	-0.29932112391054
Fe	-2.54713591007053	0.28009887576525	0.76024945463493
S	0.97572363087385	-1.36112946752680	0.14465613886255
S	-0.84434116797762	1.30293703141285	1.94982694218462
S	-1.93917698856707	0.20188531779763	-1.36347464682522
S	-2.37001442521427	-1.68842613135168	1.80911473901084
C	1.10740426943917	2.83808815070510	-0.06763811587704
C	1.71454937581576	1.26869848473086	-1.67072267134783
C	2.05781426362136	1.81627005345114	-0.37964989840227
C	0.14651884245604	2.89251077328824	-1.12816304414261
C	0.55026057757406	1.94627651851552	-2.13555619525444
C	-0.10029762663787	-0.95305409938507	4.48311503371132
C	1.12311915566692	-0.31844968342113	4.05762882194199
C	1.16511218839378	3.76384059613851	1.10702420950818
H	0.16661246707107	4.09485445804606	1.40213139662707
H	1.75468160084379	4.65204448630416	0.84384096500932
H	1.63634716117085	3.28671884771064	1.96942066868032
C	3.30969095246405	1.50827135404834	0.38175134882348
H	3.19112062855593	1.72915547426216	1.44432181650050
H	4.14035100000053	2.11840607960516	0.00208698186383
H	3.59017076078587	0.45793982219264	0.27694142212700
C	-0.04854649725566	-2.32949324476369	4.07177018520685
C	1.90144136921973	-1.28625595143622	3.35937305628485
C	1.17214255617702	-2.52917014646078	3.35394410424803
C	-2.36880556591451	-2.81803009708442	-2.13214590756079
C	2.54452475577096	0.28939599677928	-2.44223607336561
H	2.97846485175937	-0.46587776380958	-1.78132136461352
H	3.36786978328462	0.81036147030190	-2.94866366043962
H	1.95128450984571	-0.22154331732540	-3.20371360503138
C	-0.95080564236341	-3.03975881739591	-2.23265268164700
C	-1.79413905240779	-5.01735727778308	0.86590320048696
H	-0.81888621615712	-5.13731176179827	1.34192407873044
H	-2.14740698756023	-6.01230687585975	0.56482327404770
H	-2.49329301384028	-4.62119722712450	1.60720479444047
C	-1.70999765677056	-4.12113493392770	-0.32993327146527
C	1.52899634778450	1.08300209407118	4.39516351318039
H	2.27323422071915	1.46573333033438	3.69267218398576
H	1.96489184938611	1.11664291394309	5.40223960316972
H	0.66838010040729	1.75737274410788	4.37764367971489
C	-0.55866258003979	-3.87943949839710	-1.13268413408376
C	-2.83360697270180	-3.45308143002399	-0.94176567504308
C	-0.07640951058657	1.79581477294480	-3.48716449338083
H	0.03366494053273	0.77822662200437	-3.86893626457453
H	0.41124524864931	2.47884162434325	-4.19494487715127
H	-1.14072696289296	2.03991150204337	-3.46014157669872
C	-3.22880554165799	-2.15181653537323	-3.16060784076599

H	-4.09118079651916	-1.65864513365332	-2.70468966950469
H	-3.60250921710199	-2.90603761910591	-3.86564910597254
H	-2.66779744727238	-1.40615913439380	-3.72916096769655
C	-1.04553522621270	-3.38703136398887	4.43417945976951
H	-2.05704169844167	-2.97667930584246	4.48875559787992
H	-0.79785713172849	-3.81168967913143	5.41603681602956
H	-1.04543825693531	-4.20031702789302	3.70515095741073
C	0.79288649465964	-4.49582770457932	-0.94669251486597
H	1.58196663652422	-3.85153763177310	-1.34136503162240
H	0.83566443346427	-5.45303869505507	-1.48277508048751
H	1.00216999167575	-4.68935973413935	0.10721483129665
C	1.70779590678020	-3.82987735699510	2.83728302090389
H	0.90297536545126	-4.53308122369519	2.61091439220671
H	2.35949153132252	-4.29799686044342	3.58771862499815
H	2.29888418799663	-3.67830314976627	1.93023888853906
C	3.30491580220424	-1.12564368044819	2.86086300357844
H	3.43134918021413	-1.55455182091765	1.86237179531499
H	3.99896148239734	-1.64238220609509	3.53684799264553
H	3.59587691165496	-0.07508505720937	2.82244556117527
C	-0.06866926169517	-2.60607664375573	-3.36458996021914
H	-0.40802334708986	-1.65520110327436	-3.78313529561703
H	-0.07611114257107	-3.35183133125851	-4.17067884744887
H	0.96394281611004	-2.48309236195474	-3.02887787953322
C	-4.41186867469089	0.51367391924074	0.37696767094193
O	-5.41506500639169	-0.02077949039041	-0.05822489482959
O	-4.08151356254197	1.63778307232666	0.87721871728300
C	-1.00079244549595	3.85283492038637	-1.23009697386900
H	-0.68332796521393	4.78049706281921	-1.72445786518340
H	-1.82236398970086	3.42548542168750	-1.81077641721208
H	-1.38315533922562	4.11220615508490	-0.23946704846740
C	-4.25548153978474	-3.54128308878252	-0.47865385058650
H	-4.73935013628190	-4.42941119360890	-0.90636317835235
H	-4.30652320746731	-3.62087294695877	0.61075604299830
H	-4.82610024962872	-2.66036327265667	-0.78108484318048
C	-1.17204718130854	-0.32360657862693	5.32277374962480
H	-2.14410230118151	-0.78548863334730	5.12934858022255
H	-0.94763556036983	-0.44327141795999	6.39150418649575
H	-1.25641540219997	0.74628290390806	5.11373929604078

$S = 5/2$

E = -4421,845259 AU

Mo	-0.04790266463227	0.73535814700177	-0.14108425866794
Mo	-0.04636697703589	-0.94984137092486	2.16428944954869
Mo	-1.18235115252090	-1.81654651531203	-0.35147139086965
Fe	-2.55779235671980	0.54065217980803	0.91615844000155
S	1.06513572644470	-1.35547346240097	0.14926824366416
S	-0.73207078614718	1.34969109879587	2.02076715005022
S	-2.06707794948604	0.22301900999499	-1.24237887381521
S	-2.34266077264280	-1.56177373665933	1.75954528284148
C	1.05614897050254	2.84325562107681	-0.09714983631016
C	1.63227195083804	1.26183328360509	-1.69627075555833
C	2.00514536094192	1.82481910457826	-0.41837179200596
C	0.05935804701044	2.87027710867322	-1.12596352967276
C	0.44763644319360	1.91900238795946	-2.13558298263904
C	-0.10329521065099	-0.98533499759172	4.47902207615224
C	1.13931342611816	-0.36268730938362	4.09408159087054
C	1.14201923647332	3.78857421349092	1.05927652427290
H	0.15203923403008	4.12907924975580	1.37149206687423
H	1.72658063084947	4.66944534070058	0.76243291454659
H	1.63421750644716	3.32722823894759	1.91878096501515
C	3.26773966363800	1.52010201328108	0.32712612096725
H	3.16631977300264	1.76338845358766	1.38708715409514
H	4.10122425447170	2.10983945029196	-0.07723923792061
H	3.53036705102807	0.46286281110715	0.24150793332061
C	-0.06084628877257	-2.35583027364555	4.04651342847296
C	1.92012427535900	-1.33188638137625	3.39590401613766
C	1.17505763512643	-2.56338893934679	3.36017971927440
C	-2.24698050879887	-2.82613242879074	-2.19668126476240
C	2.45288896739159	0.28724300202314	-2.48332576272221
H	2.93063022079720	-0.44736728671977	-1.82969085369939
H	3.24293720885356	0.82126119010442	-3.02757041488696
H	1.84318481922230	-0.24801274703313	-3.21413401160760
C	-0.84382895325446	-3.10216867891351	-2.26956769084373
C	-1.81414493932432	-4.96728348687427	0.87127705687801
H	-0.85010895663414	-5.13677563512722	1.35480782334124
H	-2.22633973739447	-5.94446472128676	0.58631409255204
H	-2.49102471344220	-4.51581867800182	1.60210875357453
C	-1.66920328526125	-4.09409485857961	-0.33508713736047
C	1.56729289143315	1.02485984786801	4.46121637643450
H	2.29557736812333	1.42009578616504	3.74869248511852
H	2.03185303747880	1.02282040498322	5.45583675050197
H	0.71378242333873	1.70710325069440	4.48806871018789
C	-0.49190734282420	-3.90255059646875	-1.12493132977729
C	-2.75701437844947	-3.40826659234184	-0.99366877138328
C	-0.22109504988340	1.73743413788890	-3.46271242869517
H	-0.11323231866318	0.71332046672586	-3.82694542582749
H	0.23588489570176	2.41194972901469	-4.19858378328241
H	-1.28622490792833	1.97063895072593	-3.40260727315806
C	-3.06040281638204	-2.14223661273357	-3.25139360172855

H	-3.93708594683255	-1.65121169750202	-2.82197836349163
H	-3.40855548782721	-2.88477111360072	-3.98139009929813
H	-2.47445950839309	-1.39110916227331	-3.78697479268448
C	-1.08750761913781	-3.39692340289419	4.36720422987257
H	-2.09705457057516	-2.97824206456704	4.34125834173280
H	-0.91056645899568	-3.79351221811328	5.37560475509351
H	-1.04339747361999	-4.23027623803146	3.66366939016642
C	0.84009702968967	-4.55101284549194	-0.90139522326924
H	1.65541896769292	-3.91982696884327	-1.26351331647745
H	0.88295260747084	-5.50455960029327	-1.44389681062927
H	1.01171317296662	-4.75631734606517	0.15674330097851
C	1.70422580889189	-3.86174121427718	2.83293089694279
H	0.89698944559658	-4.55568723462059	2.58925417282912
H	2.34184723468481	-4.34166218737880	3.58753085285417
H	2.30897847542481	-3.70511778969093	1.93612936999634
C	3.32719766390441	-1.16759206270485	2.90821398865260
H	3.46549052327432	-1.61977772727538	1.92156443947617
H	4.02271628693738	-1.65706930148385	3.60261634709995
H	3.60396421051362	-0.11381455173701	2.84348138483300
C	0.06894824460231	-2.73894305860926	-3.40198760379125
H	-0.23285805573679	-1.79566821969688	-3.86424169130812
H	0.04614880923156	-3.51587519952295	-4.17829989877752
H	1.10149789161704	-2.63893718317595	-3.05842423135731
C	-4.48608689322058	0.79001855972458	0.67062135912926
O	-5.51830005277436	0.23131150055938	0.34769344836068
O	-4.12454792337236	1.94402357690768	1.06199741606094
C	-1.10202339051745	3.81526587636647	-1.20477474001211
H	-0.81078353266920	4.74283652442976	-1.71492027745706
H	-1.93295368136671	3.37148527230694	-1.75929841922908
H	-1.46177571161084	4.07642890401355	-0.20614067377929
C	-4.19242006907413	-3.43059650584089	-0.56225825049628
H	-4.70368838762259	-4.30550566551407	-0.98576886198406
H	-4.27163242514212	-3.48501401151394	0.52649602672502
H	-4.72011449556081	-2.53423224216806	-0.89700144002815
C	-1.18913604228762	-0.35993120134924	5.30280593995050
H	-2.16365183657374	-0.78983370393786	5.05507055590792
H	-1.00740639366441	-0.52657431720008	6.37313064427307
H	-1.23981236689041	0.71867865172747	5.13239311563515

I3 ([Cp*₃Mo₃S₄Fe(CO₂), CO₂ binding in the end-on fashion)

S = 1/2

E = -4421.856115 AU

Mo	-0.05360221851283	0.74056868492558	-0.11424279030428
Mo	-0.15526607577116	-0.90287286772735	2.19904292173032
Mo	-1.26740423148996	-1.82769563559238	-0.29412946574004
Fe	-2.38361386994676	0.17360953017865	1.12677495644712
S	0.97811044162275	-1.33819267303430	0.18895871883756
S	-0.78278355037217	1.35837691062253	2.04584805004873
S	-2.15250137692624	0.21698980431884	-1.05551552152480
S	-2.25683086097776	-1.89819478261132	1.84160358113631
C	1.04215811885088	2.85595653209793	-0.13130980554223
C	1.62763936299638	1.25804622720167	-1.70919800038929
C	2.00368087119177	1.85129975239058	-0.44643692981749
C	0.03526635704852	2.84954317686656	-1.15189980428102
C	0.42838381154586	1.88365876295609	-2.14816554820302
C	-0.13250147440017	-0.95597727234211	4.54468472792407
C	1.08605266710795	-0.31695438677296	4.11845554497545
C	1.12471119133278	3.81528553862206	1.01566120072187
H	0.13439969365743	4.17342855926958	1.30780807535528
H	1.73035051506251	4.68605628652911	0.72999354024583
H	1.58897419990632	3.35276146142819	1.89092936593230
C	3.27763595174752	1.57607446121916	0.29374908124684
H	3.18038943381685	1.82782393568558	1.35301483654657
H	4.10372115624846	2.17261658318581	-0.11790352075660
H	3.55714049480572	0.52182134830964	0.21995913475160
C	-0.08054791209164	-2.32352719290741	4.11357159483990
C	1.85131404045427	-1.26540798458615	3.38060192419426
C	1.11776684834333	-2.50865414948005	3.36187840998325
C	-2.27008854267036	-2.78380845408249	-2.20068713182238
C	2.46352934069110	0.27974987067722	-2.47630619748115
H	2.91016902069335	-0.46485048834610	-1.81094516597867
H	3.27941985124707	0.80180554883549	-2.99442165708051
H	1.87213008269870	-0.24643361032883	-3.22833400259186
C	-0.85858996851454	-3.03386166934664	-2.25211607873305
C	-1.86102426590631	-5.09965171927819	0.74118069590644
H	-0.92061337687459	-5.20852828540024	1.28685263444212
H	-2.16208216926971	-6.09527367122177	0.38801377100580
H	-2.62199584660070	-4.74653757291985	1.44255065891147
C	-1.71587677842898	-4.16100595239243	-0.41676502737640
C	1.51563890107785	1.07089372264488	4.48627363784688
H	2.18301356818955	1.49511398499955	3.73160753667561
H	2.05208337682268	1.05712301904330	5.44462680594552
H	0.65448917834644	1.73567444305653	4.58809155820408
C	-0.52530807371763	-3.90499052735602	-1.15486412765833
C	-2.79814663187378	-3.44743960103995	-1.04980251410253
C	-0.26921955470530	1.65570552958235	-3.45411020979757
H	-0.07397855400785	0.65208304345970	-3.83994240764373
H	0.07836259970197	2.37959958340724	-4.20329560805524

H	-1.35101919338640	1.77199001096574	-3.34604363211768
C	-3.06630868894054	-2.06026238739783	-3.24278252919706
H	-3.96046456094256	-1.60022755647258	-2.81434619671715
H	-3.38649116553632	-2.76575641614960	-4.02155497092108
H	-2.47519180108941	-1.27420425596579	-3.71936287416880
C	-1.05997967997649	-3.39469235043823	4.48101764674267
H	-2.06435540961000	-2.98659866749923	4.61838574666951
H	-0.75404241301261	-3.86916064319748	5.42325225323265
H	-1.11015294673834	-4.16956764476632	3.71214987447658
C	0.81187917704511	-4.54521561229902	-0.93784192937186
H	1.62512636602154	-3.85331746723962	-1.17224086942937
H	0.91647577943310	-5.42475132074652	-1.58721889385470
H	0.93329846522454	-4.87410914971290	0.09620547555060
C	1.63583255688850	-3.79896348564454	2.80350983660291
H	0.82070917066100	-4.49058052278736	2.57651891855911
H	2.30240862351056	-4.29230240044462	3.52439050871857
H	2.20411656871898	-3.62601968613380	1.88574646775493
C	3.24768348353838	-1.08673562901899	2.86824789099723
H	3.37256933400113	-1.53625924385787	1.87858684556850
H	3.96309022825231	-1.56762112579879	3.54906813884820
H	3.51154707882167	-0.02972920122947	2.79796649907718
C	0.07568006950525	-2.61459478225773	-3.34728689861793
H	-0.21238113353709	-1.64562183630905	-3.76330625731911
H	0.07067613794484	-3.34662676462036	-4.16687474900341
H	1.10022304450772	-2.53459223423711	-2.97571301099818
C	-5.05475687168845	1.73478162397490	1.70015290414287
O	-5.88636670151000	2.55499219109444	1.74482990913774
O	-4.22830272455612	0.90272929409623	1.66274123399310
C	-1.13162517203031	3.78728574981052	-1.24969083358462
H	-0.85623560202724	4.70671574742819	-1.78485168399038
H	-1.96307089144568	3.32288829720724	-1.78797332659868
H	-1.48921643665258	4.07295537318733	-0.25610753400374
C	-4.24008281167949	-3.51004077055292	-0.64330042223999
H	-4.73863247829638	-4.37439286529232	-1.10302742815752
H	-4.33434493667412	-3.60526697356778	0.44214979064527
H	-4.77598849055902	-2.60865247319933	-0.95346384495890
C	-1.19051566008625	-0.34084171200867	5.41257396503004
H	-2.16363283724875	-0.80755913426041	5.23554226078067
H	-0.94689087506710	-0.46243065042661	6.47702666590551
H	-1.28720261393294	0.72961102102108	5.21020063384123



$S = 1/2$

E = -5883.903808 AU

Mo	8.48710965655356	13.36991681130513	2.89215244719909
Mo	8.52745456435628	11.54291502753980	5.07046486739065
Mo	7.45558928171030	10.72599391187714	2.56381346895621
Fe	6.18326259704054	12.58696133030135	4.14707114250087
S	9.65874503794088	11.34757506200290	3.03071233180973
S	7.81727526398418	13.76111839115267	5.08146947200522
S	6.44118770119329	12.73511526554659	1.94499100593861
S	6.48027495409802	10.46626438559553	4.67913375265093
Si	7.10627642892879	16.85258196559378	2.63734419226944
Si	7.57081653374104	12.52910890329692	8.54138279926759
C	9.70732372068934	15.38079928999620	3.06389676240438
C	9.85906034094793	14.12350182073288	1.12356005446505
C	10.51792491059572	14.44176551745737	2.36511044210565
C	8.50433855870240	15.63025808087246	2.29250233076183
C	8.64832968075485	14.87174109621698	1.06900820707493
C	8.76306813036211	11.62147415909641	7.39235020995767
C	10.02073728091882	12.05732143385498	6.80653968928486
C	10.12506476084782	16.06624326012943	4.33049024540357
H	9.31306387205426	16.12887143777293	5.05515123552287
H	10.45440650800184	17.08731471585097	4.10065822662171
H	10.95995367371522	15.54103016460711	4.79900623511504
C	11.88871248895449	13.97372920899586	2.75132708180244
H	12.02075772140689	13.97250165429940	3.83552365152613
H	12.64975910845234	14.63591968587595	2.31805080005161
H	12.07270016340411	12.96100200937123	2.38416745463134
C	8.61146763774872	10.23496498232168	7.03552986304403
C	10.59343053461828	10.96864157611936	6.08863832101600
C	9.70951648995120	9.84211919387429	6.20783716375899
C	6.95733998527345	9.94732374422874	0.38628195020152
C	10.45092608331737	13.30591161750896	0.01832117266699
H	11.00333421184025	12.44954477978038	0.41212495945787
H	11.14913484601103	13.91666113953321	-0.56970833458353
H	9.67658171779689	12.93769403588408	-0.65761404568846
C	8.30067241614044	9.57462232626373	0.66800663504666
C	6.48838204542807	7.47379600290051	3.20104217965801
H	7.27909628870977	7.29013916071536	3.93273807297400
H	6.24264862185447	6.51673219284579	2.72357621064791
H	5.60753204263612	7.82279645257617	3.73953867354942
C	6.93143908618507	8.46106765752545	2.16252951268087
C	10.68487469857026	13.38902114345849	6.99605627414200
H	11.50817429057748	13.51431377767128	6.28884038990629
H	11.09609227748026	13.46076810154683	8.01049794206077
H	9.98730595561761	14.21586334419740	6.85509032453860
C	8.28551511264742	8.65041878919781	1.77045729155907
C	6.07471595899999	9.28182285564706	1.32607243991436
C	7.75769832255001	14.94550566262671	-0.13465160632991

H	7.68599512987048	13.97935119062582	-0.64015206042044
H	8.17400666923144	15.66954575084729	-0.84719670003633
H	6.74997213755904	15.27123944683288	0.12518463306060
C	7.17513826193344	17.50008137492168	4.41412126594495
H	7.22447080481354	16.64218433075330	5.09794290006205
H	8.09977220098474	18.07076953881802	4.56496211233758
C	6.56304571112331	10.81681445538408	-0.77007692349677
H	5.70094611156547	11.43917698269937	-0.53327192207783
H	6.31169208362935	10.19336297884825	-1.63725528805466
H	7.38648529631995	11.47604572988395	-1.05643562557000
C	5.80088450160906	12.44526474425058	7.86759241953367
H	5.62675660199805	13.36252398524003	7.29048184519794
H	5.74197870622992	11.63689402222250	7.12880109845400
C	7.56098670465511	9.28933678324887	7.53727006964896
H	6.63170127870888	9.80433039817642	7.78657358341422
H	7.92656823639523	8.79191411499191	8.44482105510749
H	7.33565102537700	8.51869799803172	6.79576795922565
C	7.38816183972824	18.29681237836994	1.44082811235052
H	7.18839989300760	17.95138911979663	0.41712023151610
H	6.64371908630236	19.07870263788799	1.64612591444725
C	9.48608523865696	7.88785283847239	2.23878167836330
H	10.34800778655833	8.54586104295959	2.38390987647343
H	9.76102700037159	7.14108940706271	1.48213093356109
H	9.29057393211788	7.36042008426043	3.17297703923718
C	5.39824463900239	16.08407746275585	2.35195173508971
H	5.49307575233000	15.20400238023309	1.70726901807242
H	5.05589255494648	15.68865541983355	3.31661195238801
C	9.99763489625017	8.45414275668788	5.72619972232739
H	9.07528478769303	7.90119465072407	5.53270383879730
H	10.56672547011688	7.90043685109098	6.48519452563283
H	10.58839951274496	8.46930720208652	4.80864773065201
C	8.80778172411295	18.88764349511769	1.52292729381395
H	8.94458593755842	19.71664664847139	0.81818324801971
H	9.56246318767191	18.12617934185665	1.29393705203644
H	9.02150480381058	19.26921658455014	2.52805481447111
C	11.94360699705110	10.93408180157764	5.44128481049269
H	11.96079097202265	10.23587171524160	4.60089402499668
H	12.69481688400670	10.60519041865476	6.17137645134620
H	12.23962097355299	11.91790645658937	5.07256118222019
C	5.96196960495966	18.37641920962756	4.78271536889247
H	5.86929557252153	19.23786779638409	4.11127074591062
H	6.04832916678733	18.76120571337495	5.80567918258704
H	5.02916020900306	17.80611352433235	4.72114025910427
C	8.05935873679816	14.34092152637168	8.78212510101297
H	9.06124473339484	14.39783288323876	9.22610860889728
H	8.12487335328605	14.82445813941544	7.79945992148265
C	7.68798525012820	11.64904252045174	10.21751630843834
H	7.07039913800357	12.19610993844866	10.94329431374042
H	7.23765925682230	10.65143242808342	10.13257002069406
C	9.13016617628220	11.52583441975478	10.74310365812296

H	9.75308460014012	10.95323184683699	10.04606925323527
H	9.16596418747647	11.02062687683435	11.71574233437184
H	9.59502399601408	12.51113013537447	10.86424958058717
C	9.51859106153716	9.89215581332544	-0.14184448667678
H	9.36818503997384	10.77457185465742	-0.76387885691921
H	9.74948239114085	9.04693155145917	-0.80396243517295
H	10.38859907014266	10.06322477658318	0.49795777550366
C	4.34210350290397	17.03903389223241	1.76405092876501
H	4.63144732949018	17.38171210485714	0.76440419110352
H	4.20589183799027	17.92835768819805	2.38846491767552
H	3.36845718559860	16.54194054417344	1.67715343578271
C	4.69090011795339	12.26498783266886	8.91949242578497
H	3.70081291959613	12.25482304409088	8.44822856008367
H	4.69824946162773	13.07266868738555	9.65934012127649
H	4.81089239755477	11.32123683461060	9.46300717287181
C	3.29528843116571	8.96811069948155	2.79121368800582
H	3.65629328386971	8.12367476693446	3.39071050358272
H	3.53157345329255	9.87919551233932	3.35218325372111
C	4.91281210836803	7.12717769598596	-0.95476382948672
H	5.97822543478716	7.29201869046985	-0.75705038401554
H	4.60515052725027	7.85175430847976	-1.71740688284795
H	4.80438575375128	6.12502807798446	-1.38693527237140
C	7.05454236909833	15.11234310623849	9.66113256563927
H	6.06180090400680	15.13331526412053	9.19859243427311
H	7.37284152140909	16.15088293309035	9.80959520390018
H	6.94876004026382	14.65310432786845	10.65048058332942
C	4.08471837948777	7.28561890412958	0.33371566401847
H	4.39275533468025	6.52753425639319	1.06697687686812
H	3.02344461306171	7.08990802995641	0.12297109156357
C	3.35268100945835	10.21346667194400	-0.02404923602945
H	3.85725294570160	10.20339774245955	-0.99796286179395
H	2.36662966361459	9.75873897402058	-0.20475492207723
C	1.76608505349689	8.84691035058963	2.62790147357902
H	1.49013054630114	7.94531748064246	2.06830209603557
H	1.35257951322983	9.70766688915946	2.09217803869996
H	1.26907477202291	8.79684340723258	3.60391304205794
C	3.15894689568043	11.65833840860362	0.46556357811313
H	4.11794827630350	12.15871090869149	0.63575409997395
H	2.61975986788759	11.68594840284980	1.41676963683907
H	2.59557115045940	12.25354628849784	-0.26333597457714
Si	4.21531420890440	8.99882943563019	1.14306146981003
C	4.27536994919252	12.61306569614309	4.20306870634908
O	3.18778286886336	12.11775198355613	3.96937877632492
O	4.67949093233532	13.67504855791088	4.80415206778310

$S = 3/2$

E = -5883,879258 AU

Mo	8.43866967858595	13.40481608275810	2.89517657274029
Mo	8.47320234844736	11.60191020265148	5.05359716706869
Mo	7.57429016189957	10.67230620683869	2.46883329051869
Fe	6.19933447741334	12.83923772607291	4.27856160896125
S	9.69511801843040	11.41305737231822	3.04631698489480
S	7.93825709576515	13.87790107856411	5.13021001317144
S	6.38821509598252	12.69448845487622	2.00218846626271
S	6.41300918438480	10.58010629542843	4.56765839271501
Si	7.10046049435037	16.91311054990373	2.67478908811103
Si	7.47465619243637	12.45975197435502	8.56328964377704
C	9.69698231939448	15.39455001508962	2.97815527152946
C	9.71491912086224	14.13188865983822	1.03697547414576
C	10.45228412431619	14.44397574132362	2.23587400294640
C	8.45427713218568	15.65853419436607	2.27780802247216
C	8.51352599390625	14.89680898529947	1.05173323188861
C	8.66074870277900	11.58470213065844	7.38282614802270
C	9.93926742366624	12.01152720262565	6.84214957876719
C	10.20233923403294	16.07540955509512	4.21460276957451
H	9.42018165628807	16.21229854931248	4.96106846918026
H	10.59484900669228	17.06523815375308	3.94874940734608
H	11.01349380079503	15.50220177122215	4.66915420078930
C	11.83786266036853	13.96628416492478	2.54814837758712
H	12.00367530372579	13.89834331819116	3.62612642995183
H	12.57836351921738	14.66305642898565	2.13409079371719
H	12.01969785143449	12.98016724945816	2.11437160933606
C	8.48522384558535	10.21541919923542	6.97301214735218
C	10.50272970226539	10.93840500328374	6.09579458309170
C	9.59140621083164	9.82777264961847	6.15624006479977
C	7.11600924845877	9.91142258575994	0.30306988433885
C	10.23462155322274	13.31551682707418	-0.10360787978343
H	10.83489765670527	12.47563973929519	0.25153107533736
H	10.87168397039650	13.93679951522895	-0.74736622221018
H	9.41974346861663	12.92644304845582	-0.71672730079878
C	8.45930956439878	9.53422601250087	0.59010717413608
C	6.63431390095970	7.42925596441541	3.11525606520363
H	7.39663300827227	7.27840435007807	3.88343115068990
H	6.44032498578037	6.45869563484499	2.64117764090432
H	5.71827551407987	7.75454311146161	3.60957868241940
C	7.08759989552106	8.41929584275544	2.08389611129989
C	10.63548858196822	13.31724508875513	7.08820124932378
H	11.36491619580931	13.52421052345884	6.30102509790414
H	11.17181644717765	13.27792733008621	8.04496594833933
H	9.93365368368741	14.15017520192616	7.12845772780816
C	8.44189036575177	8.61113048408919	1.69138399990297
C	6.23393762838001	9.23770759765816	1.23945594931224
C	7.55038343764332	14.97254614215648	-0.09342977779248
H	7.46528340460280	14.01140378058528	-0.60617156261369
H	7.91084071860111	15.71361906780150	-0.81874277130509

H	6.55372871614360	15.27495937392721	0.23011558526424
C	7.26030569410108	17.59037786241109	4.43310254698547
H	7.29987652642924	16.74652118602341	5.13500989592634
H	8.20902000012226	18.12994926007978	4.54242054434071
C	6.71157628633283	10.78868881453006	-0.84370144982934
H	5.87808994071811	11.43885196619135	-0.57680207197542
H	6.40632614526464	10.17453981804303	-1.70023554984234
H	7.54323918675861	11.42169359429061	-1.16241117920631
C	5.70325033996079	12.41088096653217	7.89204817145164
H	5.49615387693760	13.39297594109142	7.44876633786517
H	5.65350910812650	11.70828708077890	7.05082286609961
C	7.39844214943147	9.28070544965521	7.40959600413090
H	6.48205745586417	9.81200422717271	7.67236314423214
H	7.73346518519946	8.72367088547783	8.29406522814392
H	7.16047813149899	8.55878398597147	6.62424930874475
C	7.36245844403846	18.33136611473415	1.44442305746082
H	7.11982318984404	17.97432709295092	0.43429852765351
H	6.64010722427517	19.13000078248863	1.66321501318885
C	9.64287753613604	7.84741758437560	2.15882527166087
H	10.49780121745327	8.50599260619698	2.33889764909865
H	9.93839435343275	7.12653588875628	1.38478675945805
H	9.43565027592856	7.28882259619932	3.07224076413291
C	5.36695993605289	16.17077487815716	2.48515197123217
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H	5.01993763510585	15.90621855417666	3.49190473770918
C	9.86045861608265	8.44950405199592	5.64072483685101
H	8.93472774516705	7.94683062462083	5.35292321033898
H	10.34256513539127	7.84292206017188	6.41911472437329
H	10.52420517487328	8.47456437621753	4.77521042559617
C	8.79468105048216	18.89673235512042	1.46625483975621
H	8.92017751731690	19.71137424486337	0.74305074721587
H	9.52716086319534	18.11814142104038	1.22317946385450
H	9.05161368644408	19.29032964462330	2.45647088948150
C	11.87001539368912	10.90086512590437	5.48685579121373
H	11.90331672937152	10.22877063701707	4.62605457335028
H	12.59313809174741	10.53882474270214	6.22952797534325
H	12.19170129177922	11.89146813427017	5.15838868727316
C	6.09106391530846	18.51958776826055	4.81595262951017
H	6.02340683043907	19.37970538914848	4.13991610002491
H	6.21077513626276	18.90721531592584	5.83437714889692
H	5.13334070290866	17.98973681119596	4.77380458340836
C	7.95837699584537	14.26240906141997	8.86941854469423
H	8.96411318761574	14.31347520503145	9.30490904777889
H	8.00793018233907	14.78556703960239	7.90580637178438
C	7.60086714764509	11.51974641630908	10.20479918278658
H	6.96221687642752	12.02151231596652	10.94486430430325
H	7.17901710290277	10.51418254291401	10.07799914131474
C	9.04141074811640	11.41532982151625	10.73903930697640
H	9.68741800412503	10.89076975902289	10.02535378308520
H	9.08214354138951	10.87010483547964	11.68953605123043

H	9.47650446170053	12.40718937144040	10.90712077942672
C	9.68810472932014	9.84618281972919	-0.20719978673924
H	9.52326687215854	10.67011538601304	-0.90140696699467
H	9.97511646052627	8.96359320625946	-0.79439647165099
H	10.53176131938281	10.10070663931096	0.44094164906379
C	4.33511124970668	17.08765111413815	1.80166160800337
H	4.62440475532230	17.30996376801760	0.76847007808768
H	4.23377994979641	18.04413268632116	2.32621886796892
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C	3.53080380912703	9.37993268692339	2.83931851463948
H	4.00902077117075	8.77786069321371	3.62080351373415
H	3.71478713659648	10.42513764757464	3.11316205156304
C	4.86272795149520	6.82808001258172	-0.59495722359908
H	5.94069889222708	6.90185267263372	-0.41130837079645
H	4.63225293861097	7.47407591599286	-1.45023421960096
H	4.64324255913061	5.79491720981742	-0.89019926836216
C	6.95528500644162	14.98512638677908	9.79132357309856
H	5.94995813750922	14.98987911064096	9.35595258694295
H	7.24949176060168	16.02805095015266	9.95705693036939
H	6.88891779748859	14.49957889749333	10.77141407096411
C	4.06555511643671	7.24831391228039	0.65390039547288
H	4.31241730070027	6.58320925083912	1.49206709750320
H	2.98903248096829	7.11920157057309	0.47210692553617
C	3.51021263824962	10.12839533125855	-0.13280720495614
H	4.04868976305478	10.04850958992664	-1.08492260114377
H	2.54088309894040	9.63610488453429	-0.30530332226333
C	2.01364966203356	9.10609380978825	2.83785475870933
H	1.79431843773447	8.05288318106098	2.62858030587955
H	1.49844022810160	9.70681878730943	2.07994637483415
H	1.56896563779115	9.35289426132357	3.80925798016809
C	3.26004464659178	11.60543705309292	0.21881361627743
H	4.19545417158962	12.14839421870739	0.38931583598999
H	2.66893184497706	11.69942846043739	1.13488138071675
H	2.71748118683294	12.11770157271501	-0.58498036126022
Si	4.35504349142287	9.05044593823464	1.17750030225597
C	4.26982015921561	12.96457487507042	4.29513240777116
O	3.18005153369577	12.56019756467732	3.93277578911764
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E = -5883.845462 AU

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Mo	7.56582414287753	10.64792662449344	2.54176713171092
Fe	5.96497607248938	12.69387117468439	4.28199826537950
S	9.74677897690071	11.32575266954972	3.03298325843604
S	7.77097727205516	13.92472683818428	4.88558405147021
S	6.39022920290698	12.67397299796647	2.03905071994711
S	6.45136290380158	10.51199875234934	4.66518051173907
Si	7.45622026824205	16.89462517912443	2.75331228398914
Si	7.12050808296715	12.12373876571209	8.52402069102247
C	9.97635051067274	15.19702938698450	2.74609321816855
C	9.71653891630642	14.05043253355557	0.74355894353130
C	10.58966209467679	14.25089540483053	1.86859382613054
C	8.69570034865194	15.58966899625685	2.17548940326497
C	8.57003366510928	14.87988598415902	0.92603596330871
C	8.50980851550514	11.62467687702216	7.34555383107463
C	9.66207814977803	12.40027035384666	6.92537091698628
C	10.60745330606001	15.75358062314068	3.98670061918162
H	9.89242169807150	15.80861509395720	4.80989716411936
H	10.98424337415531	16.76708524238854	3.80002366533465
H	11.44864068964930	15.13524243743661	4.30866074642578
C	11.96668892975122	13.67249757835081	1.99546926982100
H	12.28455874426428	13.61512677297434	3.03815562893852
H	12.68585613088508	14.30255706980994	1.45572514940989
H	12.01488973023374	12.66649182654042	1.57050555832524
C	8.74432464732904	10.27400218141981	6.88028620584571
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C	9.95221217084584	10.24390286506332	6.12887146322797
C	7.12444839672056	9.86049231108981	0.38144024086309
C	10.05523866138673	13.27090508164645	-0.48841163473467
H	10.69508970971621	12.41713483247183	-0.25720285061521
H	10.59746521537186	13.91236453881747	-1.19668778239861
H	9.15700096936221	12.90821271733750	-0.99285429829522
C	8.43229542781169	9.40593388413781	0.71899503355515
C	6.41639524685706	7.49834842582452	3.25188185044657
H	7.11710096310118	7.39760814552363	4.08531303833068
H	6.25715852458155	6.50147999036202	2.82185335254192
H	5.46559979818212	7.85242713428128	3.65296484983990
C	6.95212440624574	8.42334501274047	2.19994511272615
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H	10.77637829749365	14.21527121909948	6.67019991872626
H	10.35825733350992	13.82520169005526	8.34597319473516
H	9.12621464329111	14.46956563274660	7.24978044652037
C	8.32618206268708	8.51907815464592	1.84487754452583
C	6.17537981822195	9.27136717753529	1.31244395255527
C	7.47679822581928	15.04563573694739	-0.08681199113624
H	7.29341203152067	14.11367081693677	-0.62755389854758
H	7.76681250197466	15.81146158668246	-0.81764256804032

H	6.53991787778030	15.35849603913205	0.37776880857707
C	7.92220673036223	17.62940972313949	4.43337505738762
H	8.00639823247298	16.81025117594832	5.15854023799760
H	8.90981982967805	18.10431581684408	4.38114016379913
C	6.79818462465467	10.71519617068792	-0.80571672256165
H	6.04351555016561	11.46440852811245	-0.56265963245714
H	6.41381947154165	10.09498674055216	-1.62491280888210
H	7.68704336545016	11.23578525232314	-1.16768657715635
C	5.42598437357282	11.49539677533017	7.95249025980787
H	4.93910749816934	12.32379081662232	7.42408238080025
H	5.54812714127822	10.71513764862850	7.19380960802359
C	7.94356549123160	9.05332118892372	7.22101265486738
H	6.91843168802887	9.30011854251718	7.49615459024550
H	8.41166753793150	8.54644008015535	8.07496518451960
H	7.91530011345139	8.35067697032085	6.38437828594677
C	7.52647423775868	18.27253540458688	1.45220780333648
H	7.04676444171865	17.92463702479533	0.52805495973214
H	6.91944971994079	19.11778076723916	1.80508063584474
C	9.46156868951397	7.72830786853778	2.41572732180272
H	10.37399877469076	8.32766133913110	2.47505940747668
H	9.67090938149538	6.86184327361128	1.77399097483430
H	9.22701092424507	7.35635620844177	3.41463611414536
C	5.71067204558049	16.16683165721512	2.87496722663147
H	5.69897905821750	15.20734871221336	2.34483541391222
H	5.54135839043699	15.90968696875766	3.92938608967354
C	10.62336482395408	9.03076334052881	5.56667861844101
H	9.90376395506169	8.23209865943708	5.37880085438976
H	11.37026377926610	8.65403967205788	6.27804862600851
H	11.13719381152468	9.25949163605139	4.62925251510577
C	8.95980417135913	18.74635031502388	1.14751931131134
H	8.97089553978354	19.55721897287495	0.40936830782145
H	9.56589376593323	17.92389874790754	0.75049681815447
H	9.45919688317713	19.11368633612346	2.05173644864107
C	11.87344008083505	11.92480480759877	5.61705762725769
H	12.08374678393172	11.37778915927092	4.69435902304957
H	12.64976587939210	11.66618221430566	6.34903956838658
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C	6.88078125048249	18.64789137826612	4.93896955580162
H	6.77643323852837	19.49377694204188	4.25012363063261
H	7.16456330753604	19.05110389833973	5.91822166311372
H	5.89384105610131	18.18455642914710	5.04575084274340
C	7.01028874138162	14.00171023064282	8.71282411730394
H	7.92738529027537	14.38684636898723	9.17442663703054
H	6.95406489949941	14.44835868267209	7.71066384228527
C	7.57417245172910	11.34575245506958	10.19180999139393
H	6.82034738275050	11.64372930213760	10.93379352659169
H	7.49218586986523	10.25377993011848	10.10019307456262
C	8.98169680250154	11.72210280178993	10.68952399473266
H	9.74848715571074	11.41028878058543	9.97089333984938
H	9.21240381127264	11.24752574120680	11.65079819218135

H	9.07953398217497	12.80556093869769	10.82326618890705
C	9.70173947855523	9.64104207684361	-0.04022428133141
H	9.60221246820697	10.46156226228517	-0.75108782336406
H	9.96223531701841	8.73605847534054	-0.60456437479871
H	10.53538002450298	9.86521701692917	0.63167529469037
C	4.56536542713843	17.05850044124891	2.36390787224689
H	4.68084623735244	17.27697165877504	1.29639442653428
H	4.53009606322262	18.01695361187292	2.89331402320939
H	3.59507001374964	16.56623067836452	2.50002685349688
C	4.50881138805399	10.97934883204359	9.07744367189644
H	3.52981114222113	10.68433936926365	8.68106566828790
H	4.33901761021803	11.74137705979553	9.84590210465305
H	4.94401438084026	10.10496553890582	9.57397141547133
C	3.49538787753689	9.79125532123417	2.85169143911375
H	3.92049478108522	9.22953475730033	3.69232069446347
H	3.78994413482289	10.83436010889722	3.01843584920730
C	4.60266246026146	6.81799410952808	-0.31532783531052
H	5.68421322524823	6.82528339135497	-0.13755137958883
H	4.41827800092898	7.39479801399272	-1.22916860015930
H	4.30221744504111	5.78145702599866	-0.51008671823327
C	5.79092699511780	14.44665617210180	9.54453084105899
H	4.85298706526532	14.13528332581614	9.07271829710305
H	5.76218050930414	15.53740541568165	9.65062792833644
H	5.81457906541177	14.01568308848598	10.55208730744482
C	3.84528586247448	7.41671030915672	0.88498833578566
H	4.03237569628803	6.81057596069962	1.78089512007635
H	2.76202573105403	7.36478022725202	0.70483026366146
C	3.54415922042480	10.23364820221269	-0.18814117903151
H	4.11011437763971	10.04686689792227	-1.10875864917581
H	2.55831699512296	9.77304072241041	-0.35488404890487
C	1.96052545606094	9.66344320442616	2.86892184303784
H	1.64678184529653	8.61982067513657	2.75276187335756
H	1.50120638489276	10.23776428205245	2.05691617736492
H	1.54251982138172	10.03463786325082	3.81219242594023
C	3.35358205826141	11.74498534130100	0.02699984282615
H	4.30584181963800	12.25641137636685	0.19771144523657
H	2.72910134135815	11.94352456727087	0.90322087598060
H	2.87186593503808	12.21069709284724	-0.84129704677881
Si	4.28839713489734	9.22913590932930	1.23658113514346
C	4.05790503708809	13.24119594471831	4.13797788787100
O	3.07745508876407	13.37297399815153	3.43305269918415
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[Cp^{XL}₃Mo₃S₄Fe]

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E = -5695.161756 AU

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Mo	7.54734842117062	10.64229510262657	2.46357022339284
Fe	6.24233649773909	12.40546195390627	3.93859290624776
S	9.71906766337191	11.36218846071144	2.99454518540357
S	7.68246005874748	13.73903748158414	4.96691893663887
S	6.45067405833643	12.61077945898475	1.76973480707906
S	6.53986973014126	10.32926493083587	4.57583207672788
Si	7.21683184270013	16.80266416471890	2.97333730536521
Si	7.38918446788221	12.53532550173800	8.37259357099490
C	9.82446493698822	15.25791598835771	2.93738208776395
C	9.66591442464808	14.16954592021756	0.89700592692771
C	10.49762552792673	14.36796783786631	2.05429251622510
C	8.54702575738220	15.62479277032492	2.34492171305984
C	8.49188367143977	14.96474019669526	1.06377542157167
C	8.68619298948146	11.64509056267947	7.33456298575779
C	9.94814651854574	12.12814100066175	6.79347996821133
C	10.40926554106257	15.79972615099724	4.20697900722946
H	9.69445022151017	15.75542132636225	5.03036376228225
H	10.70742702680889	16.84683575274580	4.07070384053439
H	11.29617209293329	15.23248778136215	4.49674729080591
C	11.88804525365584	13.83196938483491	2.21341452474467
H	12.16486849506209	13.73653035638544	3.26590540442955
H	12.60848956083971	14.50875479512738	1.73486135172182
H	11.98831293569856	12.84835583293326	1.74736800251023
C	8.61360246716980	10.24622172383852	6.99900358313620
C	10.59385154061646	11.05609150666824	6.11420714398700
C	9.75950740427476	9.89007163494732	6.22402086440850
C	7.16882398191225	9.82828683278776	0.27734576923079
C	10.06088640084176	13.42160880559485	-0.33848845504063
H	10.70331260272118	12.57145523187821	-0.09838337337310
H	10.61674846191465	14.07795162064389	-1.02249556994105
H	9.18467124008841	13.05061793440782	-0.87596392951611
C	8.49342266959864	9.45545548314657	0.63450480266787
C	6.53382134121953	7.39554551955762	3.09281618250554
H	7.21913853653669	7.30885531303216	3.94013994691348
H	6.43777450260153	6.40410126655013	2.63156071350421
H	5.55584985355883	7.68674683156690	3.47904503052746
C	7.04200183432895	8.37447592834554	2.07630848757302
C	10.55075403151498	13.48359442348984	7.01205400509869
H	11.41759117395735	13.63044145832371	6.36406081861736
H	10.88462011653570	13.58420743947556	8.05252313302308
H	9.83499136145981	14.28169936986974	6.80887305534124
C	8.41705604375726	8.55690259720183	1.75807083455761
C	6.23664404963201	9.18885737363084	1.18827160406598
C	7.44415540212832	15.16021072240343	0.00896599339343

H	7.31633851828240	14.25817622378837	-0.59502792704061
H	7.74346591303052	15.97848732590955	-0.65913195607121
H	6.47614352953315	15.41699352794410	0.44443696212040
C	7.60650219391339	17.45140048122287	4.70855285706357
H	7.72678535389589	16.58807992357201	5.37522246622136
H	8.56811618742219	17.97947994305528	4.70637326672545
C	6.82375722308894	10.66095286160605	-0.92094469027406
H	5.96531853960967	11.30454062301981	-0.73174300532105
H	6.58390115026934	10.00820413196728	-1.77021145133658
H	7.66370554126251	11.29563031796943	-1.21215348595481
C	5.65996751607980	12.35045574167919	7.60688920224115
H	5.48463360928901	13.24055449948743	6.98611103166027
H	5.67764269710639	11.51120157158411	6.90097377626515
C	7.59138107401245	9.26105645832465	7.48238296821522
H	6.63224297093174	9.73648744221920	7.69654773525264
H	7.94897328431384	8.79116957238645	8.40816124961774
H	7.42207065074803	8.47100367416400	6.74604864178603
C	7.17908057175647	18.27416107263274	1.77645910787907
H	6.79834709549342	17.93671860484342	0.80341128826294
H	6.44981602653686	19.00829330616615	2.14630905670434
C	9.58511340750955	7.81238296161036	2.32666643201248
H	10.44466624632730	8.47280481459107	2.47510129077633
H	9.89226177983048	7.01297961525374	1.63878236919459
H	9.33568595867789	7.35355583688873	3.28406745365845
C	5.51540373455517	15.95892794888205	3.01540105789633
H	5.55717110468948	15.05378077270275	2.39757631578636
H	5.36514854667084	15.59496082524049	4.04209418696851
C	10.12236657902307	8.50198449209724	5.79264624499474
H	9.23801507694372	7.93694276051594	5.48696479544214
H	10.59576289697716	7.95664769307692	6.62091135357914
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C	8.55326157876449	18.94388023921153	1.59177591823625
H	8.50151318176030	19.79498134599861	0.90205890240971
H	9.28372783787352	18.23209040967856	1.18986288126246
H	8.94749798170840	19.31365791674545	2.54547490467908
C	11.96071933909679	11.08265595279746	5.50156266254201
H	12.02752624854273	10.38960560866642	4.65907064037377
H	12.71389635217476	10.78879568229286	6.24475523346571
H	12.21624409658562	12.08072336069558	5.13843455435374
C	6.50667400374701	18.37564377175088	5.26688843672647
H	6.36315809064719	19.25912651504642	4.63458564308109
H	6.75790959943131	18.72678800701228	6.27491030576533
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C	7.77615906557880	14.37711733585598	8.58323666066070
H	8.72499740929892	14.49457404533853	9.12235447855707
H	7.92383764831306	14.81928379078860	7.59039425861059
C	7.42348062634400	11.72189887112647	10.08716265626216
H	6.73238831921226	12.26235445317388	10.74898088622395
H	7.02651033777785	10.70120359575228	10.00841493562418
C	8.82950983803248	11.68424301380750	10.71404020554595

H	9.52668246874475	11.12757485686104	10.07697605072718
H	8.82259701574416	11.20560552880747	11.70078313347248
H	9.23629490269509	12.69444788376398	10.83900343605785
C	9.75712622005677	9.75998746928005	-0.10949891299862
H	9.62951542025182	10.60051800171532	-0.79276931433908
H	10.05944562832120	8.88615356807303	-0.70204622634183
H	10.57508289729785	9.99657834219995	0.57763203819513
C	4.32155254895026	16.82979034410084	2.58390048785687
H	4.42361176023823	17.15021322315149	1.54108005058612
H	4.23533509876719	17.73375478082275	3.19663439686755
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C	4.50474228202434	12.16643191813517	8.60799393946400
H	3.53902097607669	12.10168471329360	8.09197222778045
H	4.44682212657555	12.99874838316657	9.31769230977046
H	4.63182979715639	11.24746260784041	9.19080879891651
C	3.53976058491074	9.63141944652850	2.73479785801541
H	3.99095765918096	9.08688251705522	3.57326786927889
H	3.79496595075664	10.68661966766156	2.90955867548079
C	4.70494692585420	6.72422720900956	-0.47214706804515
H	5.78691944277962	6.75626224377177	-0.29977934324947
H	4.50140729752338	7.30890151978799	-1.37693983037918
H	4.42918984566738	5.68339495208383	-0.68031874871807
C	6.66066561727616	15.14446846037816	9.31969716830245
H	5.72116478039830	15.11088347839249	8.75706934966434
H	6.92705544905468	16.19973121864043	9.45363260341444
H	6.46635594898607	14.72342703685788	10.31279626211462
C	3.94002746768115	7.28713308094347	0.74081932173969
H	4.14476596845097	6.67081466224690	1.62585179150166
H	2.85731199291547	7.21543257255100	0.56447599293964
C	3.57733878940119	10.11182692157467	-0.29135873540246
H	4.14717149906630	9.96295960411077	-1.21642248777906
H	2.60419834320164	9.62868605468149	-0.46740480404307
C	2.01189539527484	9.43447925167709	2.75013261782168
H	1.74510170668452	8.37808085653632	2.63219195752089
H	1.52729218345762	9.98704359485054	1.93726127377600
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C	3.34700133611536	11.61274311635943	-0.04159401866896
H	4.28678527992098	12.14606506659655	0.13440135689595
H	2.72028605757811	11.77362983761011	0.84212975046120
H	2.84647825017862	12.08550455583551	-0.89533497897047
Si	4.35395584910633	9.10234373356682	1.11487875292504

$S = 3/2$

E = -5695,171870 AU

Mo	8.39959395659364	13.28867257876662	2.83225293215293
Mo	8.49864459768705	11.47212745288651	5.01232195081604
Mo	7.55696729694259	10.59735922170657	2.47013278530707
Fe	6.17445843315572	12.32873137084537	3.98983260024339
S	9.69827656435051	11.35251406473884	3.01065092811417
S	7.56408363595713	13.67137136947252	5.02620528789405
S	6.36714407507401	12.55511535987573	1.82137270826584
S	6.50019582769273	10.24646877968348	4.58593875085062
Si	7.03831300858151	16.75053994545091	2.95959548201448
Si	7.55919301121183	12.64269654436072	8.43073058497602
C	9.66668038791597	15.25667888121092	3.04969955514982
C	9.63096513955081	14.15200440447372	1.01372002319949
C	10.40473932129331	14.38161123321526	2.20596015625933
C	8.40449522371793	15.57970976197239	2.40242873760029
C	8.42715428669560	14.91288767679482	1.12449243926322
C	8.73357773321467	11.66336929063994	7.32818340773913
C	9.99404953759062	12.04906428609806	6.70976782896736
C	10.18496570325098	15.84337297178229	4.32741698609045
H	9.46350273475947	15.74154678352770	5.14118304346673
H	10.39204623459252	16.91174890107165	4.19022273825050
H	11.11318128597639	15.35461818082584	4.62797650596024
C	11.79878731655579	13.88518184598689	2.44097823555137
H	11.99730424674878	13.74583957485178	3.50665823138017
H	12.52862983289958	14.60620833716687	2.04971779210355
H	11.96442826173089	12.92855890495761	1.93923772581429
C	8.55412154196757	10.26911873676998	7.04376234872656
C	10.55127042911002	10.90771161936448	6.06043494942575
C	9.64667118725479	9.80884256716557	6.23832869284778
C	7.26193671513230	9.83678734700238	0.26097194107379
C	10.10318451949457	13.40795473426105	-0.19734533645980
H	10.74985679618151	12.57156504796572	0.07783800711779
H	10.67879092905854	14.07440496476205	-0.85452058121326
H	9.26261301744023	13.01811039535031	-0.77629340288518
C	8.55970845177956	9.42224653229894	0.66554854785550
C	6.45288482867948	7.36943390100065	3.00496821294192
H	7.10901465540628	7.25249956100121	3.87138988946324
H	6.34637833191795	6.38799945068263	2.52505506090691
H	5.47128658136495	7.67975933843408	3.36707535885972
C	7.02157167577971	8.35027690123236	2.02281686585633
C	10.67810807481407	13.37507820525022	6.84392077459085
H	11.47822935186982	13.47747823313397	6.10642809661193
H	11.12398569472710	13.47420504251345	7.84230991634619
H	9.98054497520321	14.20153074754493	6.70439661762656
C	8.41442650381373	8.50750621001425	1.76779208857804
C	6.27490911320132	9.19743305412908	1.11605838215085
C	7.42417965122048	15.07007553624647	0.02091279998322
H	7.33568415286537	14.15498146512004	-0.57008862638109
H	7.74425500745507	15.87860814901451	-0.64955389605581

H	6.43438523782411	15.32298623276195	0.40561695689362
C	7.31820161609984	17.39154737917184	4.71872393389465
H	7.41958694554030	16.52949908195616	5.39048672421367
H	8.26630689515424	17.94025797345154	4.77385145045063
C	6.98444181326431	10.69944213162301	-0.93302280850457
H	6.15279467321889	11.38089696027883	-0.75299327207275
H	6.73236382276019	10.07146281409021	-1.79717240429940
H	7.86023777686264	11.29622810362816	-1.19782872142109
C	5.76878680688990	12.52717532612870	7.79769020921659
H	5.51676331257263	13.50162009887283	7.35823861338142
H	5.73958312657657	11.82308609506001	6.95541558825397
C	7.48459708120451	9.37683963357690	7.59862410532849
H	6.56873298578646	9.92969576496685	7.81685683131384
H	7.83750354302535	8.92304762492786	8.53403302795566
H	7.23753533623134	8.57046843853617	6.90364573860112
C	7.08857661285536	18.22554307732925	1.76701393630903
H	6.79924014156676	17.88181720696566	0.76483324467725
H	6.32452888620641	18.95578322014566	2.06740918569913
C	9.54131254032678	7.72596274870898	2.36978005538358
H	10.41476344169758	8.36036264434100	2.54747877937208
H	9.84710486687342	6.92127484570845	1.68726567629038
H	9.24907297721296	7.26957487580185	3.31599452212606
C	5.33933786395346	15.90692439382374	2.89546160488641
H	5.41940841043846	14.99964267000532	2.28545438737140
H	5.12319234963589	15.54277235027821	3.91010935983571
C	9.89182801402917	8.38455365701254	5.84586817051277
H	8.96007639367301	7.88558096767655	5.56582352384690
H	10.32937429901973	7.82681628589662	6.68534494486419
H	10.58302781961907	8.31795977177424	5.00382159439774
C	8.47036750642819	18.90282688389791	1.70495078122138
H	8.48823352733987	19.72712217101184	0.98187780826608
H	9.24494700360505	18.18399951102139	1.41274406210426
H	8.75549484325450	19.31179076104511	2.68114977769391
C	11.90370004616117	10.81912701506177	5.42216093735131
H	11.91696649500195	10.07461133042889	4.62238286124283
H	12.64989193669062	10.52522256462131	6.17237913481494
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C	6.16851975635938	18.29217999900650	5.21162840554439
H	6.04330722883910	19.17173720819394	4.56987338734789
H	6.35388496707693	18.64975885702307	6.23154449551572
H	5.21633367294744	17.75047670282345	5.21998149970991
C	8.04313243610055	14.46660351818334	8.57517459882542
H	9.05977732737166	14.55415271157336	8.97833989410113
H	8.06743170323539	14.90251768463151	7.56841749498367
C	7.69052915316286	11.86060884414592	10.15542243224843
H	7.05586135843497	12.42785155699362	10.85040991245173
H	7.26695174533859	10.84838778272831	10.12128590666454
C	9.13320136403160	11.80000713691179	10.69026609022121
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H	9.17943203355684	11.33567644923354	11.68273298206121

H	9.57002426287449	12.80198726143809	10.77270847029501
C	9.85896396776531	9.70816791308753	-0.02273483872889
H	9.77497774882043	10.55516405034872	-0.70507778094695
H	10.16697827237727	8.83218828386537	-0.60904739908369
H	10.65436832726867	9.92503717804610	0.69636294994918
C	4.17534969967248	16.77666886507105	2.38622032021905
H	4.34719411307907	17.09867316568434	1.35308333539833
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H	3.22840543009233	16.22352187650958	2.40857034882381
C	4.70927729978125	12.14030963396914	8.84490173686687
H	3.70515583969935	12.12134845862471	8.40396283688485
H	4.69145123283545	12.84745486583130	9.68179163463319
H	4.90678918295484	11.14630819136201	9.26175793885173
C	3.56299486345611	9.77667514796457	2.55411151120247
H	4.00514888924882	9.26063068168019	3.41514293893071
H	3.82810392199501	10.83541785637103	2.68908737971160
C	4.68942264698461	6.75515679931976	-0.56063580851797
H	5.76846398016085	6.75533800314220	-0.36788877445006
H	4.52252979630315	7.32779821978434	-1.48047848394143
H	4.38341028797953	5.71989642717030	-0.75376764178297
C	7.06301547379913	15.26504150121482	9.45747397553168
H	6.04149213007874	15.21251692710320	9.06403184967025
H	7.34380758651943	16.32384318039963	9.50580938642904
H	7.04173343305177	14.88050660443970	10.48338790613318
C	3.92061874986083	7.36814955376389	0.62540077962349
H	4.08283910240002	6.76118095178601	1.52520562364059
H	2.84013983421017	7.33462064970590	0.42575840389509
C	3.70692066444902	10.16814946905121	-0.49343960559701
H	4.33366199383605	10.00613487089078	-1.37860918939419
H	2.74695199254982	9.68145366141768	-0.72361921769920
C	2.03311379889026	9.60004847716252	2.56635869450672
H	1.75565403342743	8.54250496494102	2.49201664789847
H	1.56120868166154	10.12191927501225	1.72608497749010
H	1.59283334151447	9.99500392284271	3.48985309250944
C	3.46048544164561	11.67254419266125	-0.28308835027529
H	4.38227517475625	12.20484037997534	-0.02824680021186
H	2.75680564031895	11.84474160588896	0.53843189390681
H	3.03998746998877	12.13587617419098	-1.18384880978449
Si	4.39600923848483	9.17440682467031	0.97051352452052

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E = -5695.146411 AU

Mo	8.43765332374071	13.31883667859707	2.85243341130279
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Mo	7.47125763582341	10.55251954461713	2.52931241000992
Fe	6.18603430755652	12.17861390110078	4.11111627793265
S	9.63688079745097	11.31121025985152	3.06141519141440
S	7.57703141042153	13.64793470656191	5.07426149122044
S	6.35376577038495	12.55050713960033	1.91167019959273
S	6.51289378748195	10.05819453756403	4.69873951792891
Si	7.02881782290568	16.73051852712952	2.84255218648501
Si	7.57251810248009	12.58416133769816	8.49586289098829
C	9.66675662865121	15.28027612920615	3.06227784284685
C	9.72140756148334	14.12325800712200	1.04966862552871
C	10.44196769162221	14.38538550092902	2.26668035831795
C	8.42607619985890	15.56263259026529	2.35855604917291
C	8.49989826287833	14.85576236368499	1.09647892247997
C	8.77170084360222	11.65218500459574	7.37794431203092
C	9.99916623248536	12.09389219576709	6.73155844054908
C	10.14074037824185	15.92521971322163	4.32886901204003
H	9.40115252316626	15.84303955525058	5.12839365827941
H	10.33476717198462	16.99133562828678	4.15680494614489
H	11.06861291738234	15.46520247449401	4.67390168843418
C	11.83198478758396	13.90626575606006	2.55672107706142
H	12.03233960356362	13.88458085101766	3.63053518795662
H	12.56785335031353	14.57411506319614	2.08921524869989
H	11.99146652281161	12.89960724273314	2.16148569111189
C	8.64858267557892	10.24558219478646	7.09962686998015
C	10.58847356119732	10.97649646126036	6.07104959700705
C	9.74308346712592	9.83652074943758	6.27068678552400
C	7.21343831006598	9.89330120073603	0.27352706402633
C	10.25490059342509	13.35626073115484	-0.12044347954930
H	10.88644198848620	12.52644392539161	0.20480646602493
H	10.86480859949455	14.01283459900818	-0.75638041532687
H	9.44690387235343	12.95629452007880	-0.73697840191426
C	8.50564404380717	9.45712372940270	0.66902276509380
C	6.38939983490642	7.32382889304343	2.92429799863392
H	7.03645255523696	7.18311001492279	3.79377016054731
H	6.30113924716384	6.36036573787807	2.40570774992415
H	5.39975925879289	7.60778521329981	3.28599798427730
C	6.96014027609764	8.34848927808072	1.98931172223115
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H	11.43771060231226	13.56345860019577	6.12429324506030
H	11.06639289968965	13.57298953293948	7.85571824578364
H	9.90971156142620	14.24435176815768	6.69353348236150
C	8.35555158066451	8.51469386599482	1.74527646379364
C	6.22175855079497	9.22903253814892	1.10503168481215
C	7.53382419049478	14.96323658832408	-0.04469837948252
H	7.48111588803831	14.02915781755197	-0.60999758520652
H	7.85801823004938	15.75763145188129	-0.72997929242206

H	6.52676153431425	15.20509979996001	0.29930959312051
C	7.22454161926477	17.38443335924864	4.60841414342781
H	7.32164984126909	16.52697523788751	5.28695327639484
H	8.15656483343901	17.95593421553667	4.69625167441738
C	6.94017151708531	10.79621515234749	-0.89065159417773
H	6.08179443207298	11.44091201197372	-0.70310590749497
H	6.73262262139956	10.20053870373406	-1.78916335502830
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C	5.78700315067010	12.40733636443862	7.86803562141012
H	5.52011086752206	13.35370016108492	7.37852974534834
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C	7.14216047392749	18.19239612184991	1.63765058038167
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C	5.32937642054952	15.89725860473252	2.70363051974852
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C	10.04146717938103	8.43103874711626	5.84906552800006
H	9.12170766807459	7.87124219409180	5.65979748324080
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C	8.53919906124164	18.83990905105682	1.60688636225434
H	8.58953480466313	19.66654638215784	0.88797001419951
H	9.30375524058944	18.10559568319805	1.32757282100287
H	8.81364073598299	19.23857010498232	2.59047465948261
C	11.92232621717618	10.94735073504522	5.39111449518951
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H	12.70329557086524	10.69716091369080	6.12146436376872
H	12.17117219327852	11.91388530383140	4.94857630023099
C	6.03923072549369	18.26080070406256	5.05886312654792
H	5.90748532077299	19.12833857158355	4.40208996527466
H	6.19001339699410	18.63689474097619	6.07784323237098
H	5.10147207979332	17.69484544375119	5.05148178254567
C	7.99640552391434	14.42106060592990	8.64850109221035
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C	7.74312980116275	11.79523744761092	10.21384837886682
H	7.11139928683456	12.35137758081405	10.92040219470436
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H	10.13445857148236	8.87305621242479	-0.57277055147908
H	10.59334282092982	9.99124515160837	0.71977873585938
C	4.18156611542897	16.80254439599488	2.21880672831794
H	4.37607231511806	17.17551824204623	1.20714659782103
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C	4.73359255111774	12.05614589756844	8.93381852979326
H	3.72894964455751	12.00474109016018	8.49663909993053
H	4.70885583485390	12.80161993067516	9.73660661469384
H	4.94427076473259	11.08498165312708	9.39552034423989
C	3.53129655455139	9.78446273176479	2.58454484939857
H	3.97929333120093	9.23581479183736	3.42217120725716
H	3.80766117252741	10.83593664790595	2.75071592640154
C	4.60564765088653	6.85062441630691	-0.63138979327005
H	5.68604776753218	6.83686849566887	-0.44703992174707
H	4.43648412666777	7.44811308713345	-1.53484914463217
H	4.28941644122821	5.82329355642153	-0.84872514238625
C	6.99315203493668	15.18023275064465	9.53955114800845
H	5.97271208023913	15.09543753994559	9.14880762672214
H	7.23842742695353	16.24749997489455	9.59397538785625
H	6.98772012846153	14.78865088081676	10.56298809808293
C	3.85033903245925	7.43731752595301	0.57636918379850
H	4.01382910688240	6.80407357948657	1.45743343543728
H	2.76826089369439	7.41793576607960	0.38363123418567
C	3.65009937245052	10.27212082769302	-0.45617666613183
H	4.26856292062033	10.12797652084823	-1.35044367167789
H	2.68330208905522	9.80213986245573	-0.69247354612821
C	2.00027316787888	9.62035998921586	2.60921435409882
H	1.71263853873652	8.56854808502355	2.50059680675710
H	1.52306351419246	10.17616236296326	1.79408251434385
H	1.57450776170947	9.98532281749618	3.55167623044598
C	3.42114520183419	11.77228347270708	-0.20069711360158
H	4.34972712013702	12.28657795961268	0.06644015669686
H	2.72357320876977	11.92729057814033	0.62943251627544
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Si	4.34068071809656	9.22903397472029	0.97154917753998

CO

E = -113.375708 AU

C	0.37961355627083	-1.22279127000000	0.00000000000000
O	-0.75453085627083	-1.22279127000000	0.00000000000000

CO₂

E = -188.697898 AU

C	0.44174134995639	-1.22279127717667	0.00000000722564
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O	-0.72685522576255	-1.22279126641167	-0.00000000361282
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THF

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C	1.16708884175051	1.62552056442853	0.09255148052516
C	0.00731913852447	2.63793094791755	0.02482640452196
C	-1.26403866911401	1.74842774857673	0.11937005114772
H	-0.62900385176636	-0.10678774074305	-0.85014240532649
H	-1.26141024477127	-0.36590127726135	0.80291365776492
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H	1.52098997904137	1.36709710232913	-0.91747720242913
H	0.05214680558099	3.33854825451541	0.86275639230374
H	0.04041407331009	3.21634156314975	-0.90246707425376
H	-1.82015678428103	1.96816848826604	1.03479377837000
H	-1.93760412348796	1.89019602518207	-0.73021945175599

Cl⁻

E = -460.393529 AU

Cl	-4.27632050147754	1.14162902464356	1.56115513546799
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[Cp*₃Mo₃S₄Fe]⁻

S = 0

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Mo	12.17160368317212	2.97955787136967	11.19308217099196
Mo	11.67463150477581	2.24882041151743	8.47565825065060
Fe	13.94650597359485	3.60445600198196	9.19643645792294
S	10.18106801826818	3.25513459084405	9.97859006117973
S	13.47895306126088	1.58984133242811	9.82292839849998
S	13.36927375090813	4.95653436097039	10.77991587055181
S	12.75817717427317	4.06524552167741	7.45174301815024
C	10.89512394855780	2.94123700664920	13.17992706518827
O	16.78713928714364	3.84687543301287	8.58902223980846
C	11.77247557665068	7.18558618255727	8.45141892532285
C	10.69784732989381	6.56318499799960	7.71846258651463
C	9.99554905138342	1.55384849905407	6.97591529743625
C	12.11209917500362	3.61732998612897	13.47438244717642
C	11.32719466708186	-0.04794798812072	7.99942518230647
C	12.08016119250586	0.54106021693860	6.91959017830446
C	11.36387889759218	7.28797963678312	9.82363880188267
C	11.21434769810925	1.57942379818082	12.81956024637314
C	10.05276877381826	0.58347707102903	8.04378938290166
C	9.66608440888384	6.23509035764846	8.64175143544411
C	15.62259993531289	3.74935260881400	8.83979041729742
C	11.77945793352491	-1.19752125252309	8.84812230681025
H	11.23050515063405	-1.23178943573959	9.79284938879046
H	11.61191555140717	-2.15018567246481	8.32655424848435
H	12.84555630953800	-1.12059845816491	9.07965040488226
C	13.44708560843560	0.11468124560558	6.47164116345810
H	14.04867362713630	-0.22182367627006	7.32122215474039
H	13.38826533087801	-0.71356192558042	5.75100104935219
H	13.97963254877290	0.93997249797034	5.99016304833709
C	10.64429679473267	6.38924240385888	6.23074792877142
H	10.01296295357291	5.54089431748008	5.95170452848564
H	10.23367645409594	7.28907766345710	5.75182337465884
H	11.64216640003665	6.21191838236532	5.82138919307235
C	13.19789049877458	2.68744669815159	13.28084391119403
C	8.30907707190879	5.69043966988352	8.31256822356161
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H	7.56733411903515	6.50105865142205	8.28826496080146
H	8.30413853283636	5.20306566018039	7.33516970161507
C	11.23431412656018	1.49818051340443	6.26793663764312
C	8.90182133690843	0.20675746039284	8.92738737218558
H	8.32632062094964	1.08788674804301	9.22541612965306
H	8.22304040719389	-0.47992681961365	8.40254705039904
H	9.24826939942892	-0.29229716197049	9.83518054845277
C	13.02930389262290	7.74938461000064	7.85600532694684
H	13.34691562598937	7.16100525881683	6.99025925368105
H	12.88304425642756	8.78715042022887	7.52401041038217
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C	12.63062122682154	1.42160642726981	12.91961807202603
C	10.08329896401926	6.67322911423347	9.95366402358565
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H	8.83180747074454	3.09556923871987	12.59353168041945
H	9.10911222471355	3.18040619492450	14.34297876049706
H	9.49441233893030	4.56921621907790	13.31239518078669
C	10.21063844656653	0.49607784539986	12.55954619662736
H	10.63600844467940	-0.29637239052540	11.93751534685244
H	9.87139254685627	0.03766094973107	13.49978879399969
H	9.33096301909121	0.89326831046904	12.04562758648616
C	9.22810522882838	6.63265807884709	11.18452470058871
H	9.83645867868534	6.67989150867378	12.09177928305409
H	8.52982685470912	7.48178822007373	11.20539076434537
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H	13.14817845136627	5.49595159903273	13.59679274011822
C	13.38063769463452	0.13193433236793	12.78249325272692
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H	12.88575353997466	-0.54300309406654	12.07935470847918
C	11.55114066709792	2.23209200530269	5.00064637082465
H	12.62447769077961	2.41474828736205	4.90515895536198
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C	14.64660575393577	2.96273306350875	13.55652682239371
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Mo	11.66100031470660	2.28327405415618	8.43953987631381
Fe	13.97450087038036	3.74640884602972	8.89865834789552
S	10.15002611576098	3.28103763507567	9.95171268945234
S	13.49504346516288	1.72637887665939	9.76892700879850
S	13.47262406037509	4.97355003895599	10.67925377269304
S	12.58874955554147	4.11673496073503	7.27622385885781
C	10.86354450159430	2.93654812745631	13.15868912766109
O	16.73592000989767	3.61962138070189	7.94729962304993
C	11.77526804647571	7.22964957911666	8.51808342318949
C	10.69755068909412	6.63851405563162	7.76523219936626
C	10.03032793602593	1.50585927721844	6.95602803349116
C	12.08048507408257	3.63041441148409	13.46053903746306
C	11.32794149422604	-0.04326981336071	8.09419056189669
C	12.11137635030968	0.48528352556050	7.00426688641635
C	11.36810281894584	7.27651198086269	9.89513279993665
C	11.19447753907570	1.57785309176850	12.79818224531160
C	10.05143184913296	0.58717288135846	8.06533194598866
C	9.67327532996067	6.26289223040169	8.67675286817367
C	15.61441871832016	3.67175915792161	8.35371889396582
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H	11.15825229187577	-1.18174929587994	9.91231719073038
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H	12.80918371148903	-1.03567469172337	9.29044126348755
C	13.48786787615682	0.02955540434764	6.62206310132032
H	14.07998492609040	-0.20127579969269	7.51242566060145
H	13.44442797115094	-0.87404500094215	5.99787995783129
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C	10.62139243789663	6.53925623557160	6.27219018257959
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C	13.17017038179454	2.70591343838315	13.25508712730714
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