

Supporting Information for

MAPPING FREE ENERGY REGIMES IN ELECTROCATALYTIC REDUCTIONS TO
SCREEN TRANSITION METAL-BASED CATALYSTS

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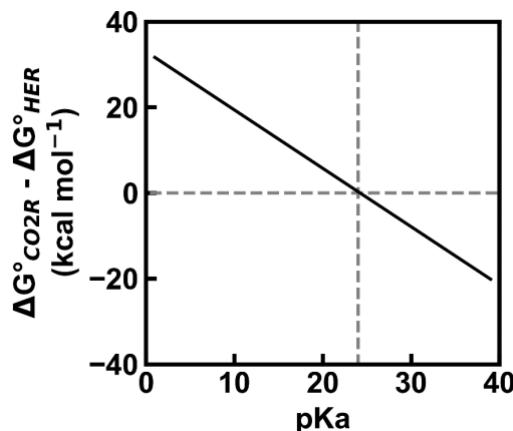
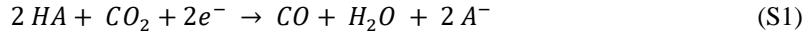


Figure S1. Relative driving forces for CO₂ reduction to formate versus proton reduction to H₂ in acetonitrile at standard state as a function of the pKa of the proton source (equations 5 and 6). Ferrocene is the stoichiometric electron donor. Dashed lines show the crossing point ($\Delta G^{\circ}_{\text{CO}2\text{R}} = \Delta G^{\circ}_{\text{HER}}$) at a pKa of ca. 24.

Table S1. Thermochemical cycle for the redox-potential calculation of the two-electron reduction of CO₂ to formate in acetonitrile with a generic proton source HA and ferrocene as the electron donor at standard state.

| Equation | Std. State Free Energy (kcal/mol) |
|---|---|
| $H^- + CO_2 \rightleftharpoons HCO_2^-$ | $-\Delta G^{\circ}_{H^-(HCO_2^-)} = -43^1$ |
| $H_2 \rightleftharpoons H^+ + H^-$ | $\Delta G^{\circ}_{H^-(H_2)} = 76^2$ |
| $2H^+ + 2e^- \rightleftharpoons H_2$ | $\Delta G^{\circ}_{H^+/H_2} = -2FE^{\circ}_{H^+/H_2} = 1.3^3$ |
| $HA \rightleftharpoons H^+ + A^-$ | $2.303 RT \text{ pKa}_{(\text{HA})}$ |
| $HA + CO_2 + 2e^- \rightleftharpoons HCO_2^- + A^-$ | $34.3 + 2.303 RT \text{ pKa}_{(\text{HA})}$ |

Table S2. Thermochemical cycle for CO production.



The two-proton reduction of CO_2 to CO and water (equation S1), can be deconvoluted into H_2 evolution and the reverse water-gas shift reaction:

| | |
|--|--------------------------------|
| $\text{CO}_2 + \text{H}_2 \rightleftharpoons \text{CO} + \text{H}_2\text{O}$ | $\Delta G_{\text{RWGS}}^\circ$ |
| $2 \text{HA} + 2e^- \rightleftharpoons \text{H}_2 + 2A^-$ | $\Delta G_{\text{HER}}^\circ$ |
| $2 \text{HA} + \text{CO}_2 + 2e^- \rightleftharpoons \text{CO} + \text{H}_2\text{O} \text{ (1 mM)} + 2A^-$ | $\Delta G_{\text{CO}}^\circ$ |

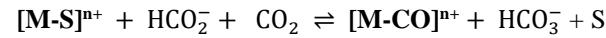
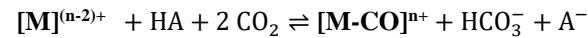
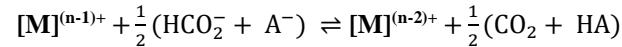
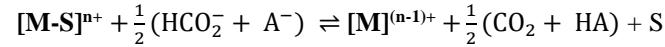
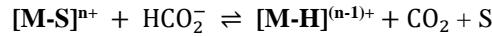
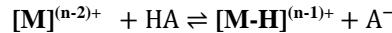
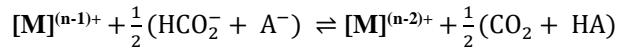
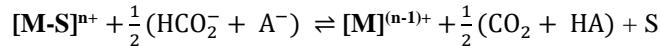
At 298 K and 1 atm of H_2O , the $\Delta G_{\text{RWGS}}^\circ$ (reverse water-gas shift reaction) is ca. 6.8 kcal/mol.⁴ However, note that unlike HER, CO production (equation S1) is favored by producing an additional species, water, that is present at very low concentration in the nominally dry acetonitrile used in this work. Assuming approximately 1 mM water, the modified free energy of the reaction with all other species still at standard state, ΔG_{RWGS}^* is reduced to $6.8 \text{ kcal/mol} + 0.593 \text{ kcal/mol} * \ln[\frac{(p_{\text{CO}}/1 \text{ atm})}{(p_{\text{H}_2}/1 \text{ atm})}] * \frac{(1 \text{ mM}/40 \text{ mM})}{(p_{\text{CO}_2}/1 \text{ atm})}] = 4.8 \text{ kcal/mol}$.

$$\text{Therefore, from table S2: } \Delta G_{\text{CO}}^* = \Delta G_{\text{HER}}^\circ + 4.8 \text{ (in kcal/mol)} \quad (\text{S2})$$

$$\text{With phenol as the proton donor, } \Delta G_{\text{CO}}^* = 6.7 + 4.8 = 11.5 \text{ kcal/mol}$$

Subtracting equation 3 from equation S1 yields the proton-transfer equilibrium for converting the proton donor HA and HCO_3^- to CO_2 , H_2O and the conjugate base, A^- . Under weakly acidic conditions, it is probable that the one-proton CO production pathway (equation 3) might be thermodynamically more favorable than equation S1. We use the free energy of the dehydration pathway (equation S1) as an upper bound for the free energy of CO production.

Table S3. Thermochemical cycles for the calculation of ΔG_{M-H}° and ΔG_{M-CO}° relative to HCO_3^- for a proton donor HA.



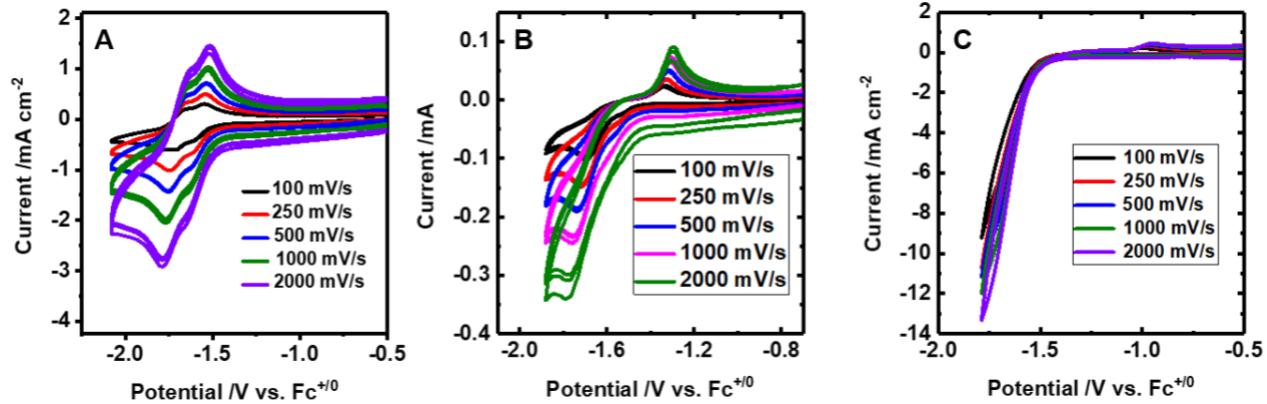


Figure S2. Scan-rate dependence of the CV of (A) 2 mM $[\text{Fe}(\text{bpy}2\text{PYMe})(\text{CH}_3\text{CN})]^{2+}$, (B) 2 mM $[\text{Fe}(\text{bpy}2\text{PYMe})(\text{CH}_3\text{CN})]^{2+}$ in the presence of ca. 0.28 M CO_2 and 0.3 M phenol, and (C) 2 mM $[\text{Fe}(\text{bpy}2\text{PYMe})(\text{CH}_3\text{CN})]^{2+}$ in the presence of ca. 0.28 M CO_2 and 0.5 M acetic acid, all in acetonitrile.

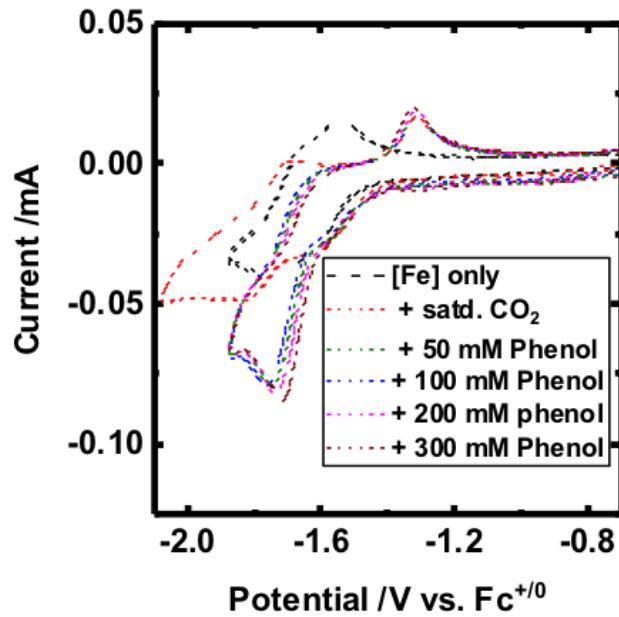


Figure S3. CV of (A) 2 mM $[\text{Fe}(\text{bpy}2\text{PYMe})(\text{CH}_3\text{CN})]^{2+}$, with the addition of ca. 0.28 M CO_2 and then incremental addition of phenol; scan rate = 100 mV/s.

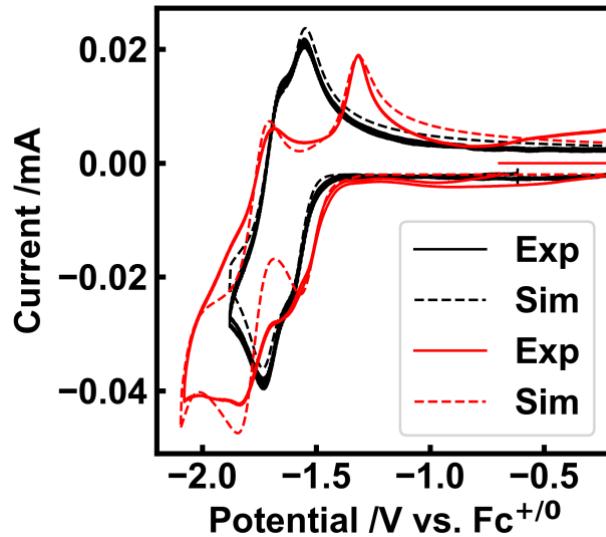


Figure S4. Experimental and simulated cyclic voltammograms (scan rate = 100 mV/s) of 2 mM $[\text{Fe}(\text{bpy}2\text{PYMe})(\text{CH}_3\text{CN})]^{2+}$ (in black), with the addition of ca. 0.28 M CO_2 (in red).

Simulation Parameters

All voltammograms were simulated with a planar semi-infinite 1D diffusion model in DigielchTM, with the following input parameters: area of the electrode = 0.07 cm²; R_u = 100 Ω ; C_{dl} = 20 μF (to model large background charging current); temperature = 298 K; α (transfer coefficient) = 0.5; k_0 = 0.01 cm/s; $[\text{Fe}(\text{bpy}2\text{PYMe})(\text{CH}_3\text{CN})]$ abbr. as $[\text{Fe}]$. $c_{[\text{Fe}]} = 2 \text{ mM}$; $c_{[\text{CO}_2]} = 0.28 \text{ M}$. Diffusion coefficients for the Fe-species: $D = 4 \times 10^{-6} \text{ cm}^2\text{s}^{-1}$, and for all other species $D = 1 \times 10^{-5} \text{ cm}^2\text{s}^{-1}$.

The experimental current was corrected by subtracting a background of 7 $\mu\text{A/V}$.

Table S4. Redox potentials employed in the DigielchTM simulations.

| | $E^\circ([\text{Fe}]^{2+/+})$ V vs. $\text{Fc}^{+/0}$ | $E^\circ([\text{Fe}]^{+/0})$ V vs. $\text{Fc}^{+/0}$ | $E^\circ([\text{Fe}]^{0/-1})$ V vs. $\text{Fc}^{+/0}$ |
|---|--|---|--|
| $[\text{Fe}(\text{bpy}2\text{PYMe})(\text{CH}_3\text{CN})]$ | -1.58 | -1.70 | - |
| $[\text{Fe}(\text{bpy}2\text{PYMe})(\text{CO}_2)]$ | -1.35 | -1.78 | -2.10 |
| $[\text{Fe}(\text{bpy}2\text{PYMe})(\text{CO})]$ | -1.35 | -1.75 | - |

Table S5. Equilibrium constants and rate constants for CO_2 binding and deoxygenation to CO, employed in the DigielchTM simulations.

| | $[\text{Fe}]^{n+} + \text{CO}_2 \rightleftharpoons [\text{Fe}-\text{CO}_2]^{n+}$ | | $[\text{Fe}-\text{CO}_2]^{(n-2)+} + \text{CO}_2 \rightleftharpoons [\text{Fe}-\text{CO}]^{n+} + \text{CO}_3^{2-}$ | | $[\text{Fe}]^{n+} + \text{CO} \rightleftharpoons [\text{Fe}-\text{CO}]^{n+}$ | |
|---------|--|------------------------------------|---|------------------------------------|--|------------------------------------|
| | K_{eq} / M^{-1} | $k_f / \text{M}^{-1}\text{s}^{-1}$ | K_{eq} | $k_f / \text{M}^{-1}\text{s}^{-1}$ | K_{eq} / M^{-1} | $k_f / \text{M}^{-1}\text{s}^{-1}$ |
| $n = 2$ | 0.1 | 0.1 | 10.0 | 3.0 | 0.1 | 0.01 |
| $n = 1$ | 1000 | 3000 | 4.7 | 30.0 | 771 | 100 |
| $n = 0$ | 44.5 | 3000 | - | - | - | - |

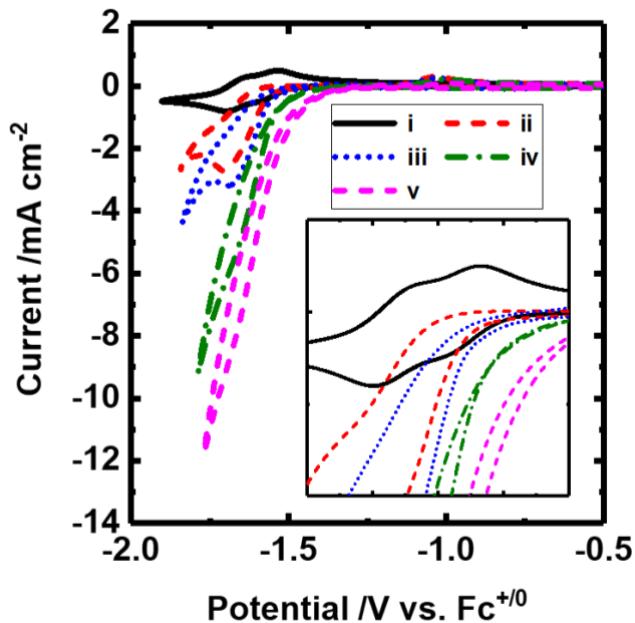


Figure S5. CV of (i) 2 mM $[\text{Fe}(\text{bpy})_2\text{PYMe}](\text{CH}_3\text{CN})^{2+}$ in acetonitrile at a scan rate of 100 mV/s, with the incremental addition of (ii) 0.1 M, (iii) 0.3 M, (iv) 0.5 M acetic acid, and (v) ca. 0.28 M CO_2 . Inset is a magnification of the region where the positive shift of the onset potentials is clearly seen.

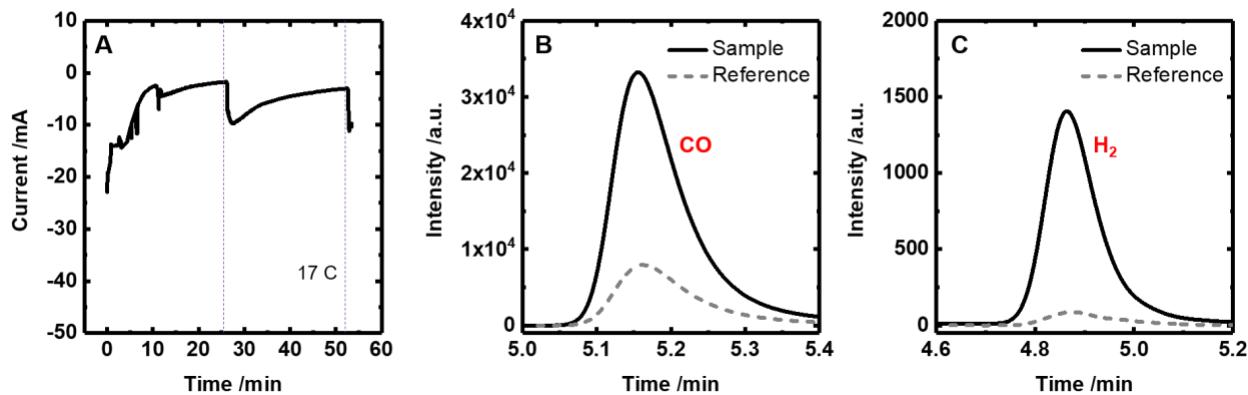


Figure S6. (A) Current vs. time plot of the bulk electrolysis experiment. Gas chromatographs of the headspace after 52 min of electrolysis for (B) CO and (C) H_2 production, based on comparison with a 1% reference gas standard.

References

- 1 J. T. Muckerman, P. Achord, C. Creutz, D. E. Polyansky and E. Fujita, *Proc. Natl. Acad. Sci.*, 2012, **109**, 15657–15662.
- 2 A. D. Wilson, A. J. M. Miller, D. L. Dubois, J. A. Labinger and J. E. Bercaw, *Inorg. Chem.*, 2010, **49**, 3918–3926.
- 3 J. A. S. Roberts and R. M. Bullock, *Inorg. Chem.*, 2013, **52**, 3823–3835.
- 4 E. Demirel and N. Azcan, *Proc. World Congr. Eng. Comput. Sci.*, 2012, **II**, 24–27.

Cartesian Coordinates of Intermediates

1. Cyclopentadienyl Systems: $[CpM(L-L)]^{n+}$

L-L = bis CO

M = Mn

[Mn-S]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.25365200 | -1.48287500 | -1.16537200 |
| C | -0.66259500 | -2.06420700 | 0.00031100 |
| C | -1.25424000 | -1.48246800 | 1.16547200 |
| C | -2.22303400 | -0.51095100 | 0.71570800 |
| C | -2.22267200 | -0.51121400 | -0.71642900 |
| H | -1.01172600 | -1.72228000 | -2.20155300 |
| H | 0.14759900 | -2.79596900 | 0.00065100 |
| H | -1.01281400 | -1.72148800 | 2.20185900 |
| H | -2.85148100 | 0.11170500 | 1.35435400 |
| H | -2.85079100 | 0.11122500 | -1.35561200 |
| Mn | -0.30060100 | 0.10541800 | 0.00000000 |
| C | -0.19079400 | 1.33358700 | -1.26507000 |
| C | -0.19081200 | 1.33342500 | 1.26523400 |
| O | -0.16627100 | 2.14731900 | -2.11854200 |
| O | -0.16632100 | 2.14704300 | 2.11881500 |
| N | 1.55865800 | -0.22458500 | -0.00002800 |
| C | 2.71609600 | -0.44092500 | -0.00005000 |
| C | 4.15328000 | -0.69494600 | -0.00005500 |
| H | 4.45212000 | -1.26861900 | 0.89626600 |
| H | 4.45208200 | -1.26875000 | -0.89630500 |
| H | 4.71071500 | 0.25936000 | -0.00013700 |

[Mn-H]⁻¹

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.68348400 | 1.16339500 | -0.18061800 |
| C | -1.88462900 | -0.00010100 | -0.99312800 |
| C | -1.68345200 | -1.16344400 | -0.18041400 |
| C | -1.31614900 | -0.71658200 | 1.14423700 |
| C | -1.31616600 | 0.71677100 | 1.14410900 |
| H | -1.74172200 | 2.19993400 | -0.51792600 |
| H | -2.12669600 | -0.00019900 | -2.05719500 |
| H | -1.74165100 | -2.20004500 | -0.51754100 |
| H | -1.08008500 | -1.35911800 | 1.99494600 |
| H | -1.08011300 | 1.35946200 | 1.99470400 |
| Mn | 0.15422500 | 0.00000200 | -0.24148600 |
| H | 0.51690200 | 0.00000100 | -1.75713900 |
| C | 1.34887800 | 1.25100700 | -0.03884500 |
| C | 1.34886900 | -1.25101300 | -0.03884800 |
| O | 2.15717900 | 2.12363900 | 0.10989900 |
| O | 2.15713900 | -2.12367500 | 0.10989500 |

[Mn-CO]⁰

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -1.72663000 | 1.16193800 | -0.39535600 |
| C | -1.72464700 | -0.00726200 | -1.22544400 |
| C | -1.72657400 | -1.16631000 | -0.38129100 |
| C | -1.73589500 | -0.70856600 | 0.98544200 |
| C | -1.73582000 | 0.72072300 | 0.97683400 |
| H | -1.72301500 | 2.19657900 | -0.73981700 |
| H | -1.70459300 | -0.01385700 | -2.31646800 |

| | | | |
|----|-------------|-------------|-------------|
| H | -1.72301300 | -2.20507200 | -0.71310500 |
| H | -1.72892900 | -1.34259400 | 1.87324300 |
| H | -1.72874000 | 1.36535100 | 1.85696500 |
| Mn | 0.06316900 | 0.00018400 | 0.00142900 |
| C | 1.04274200 | 1.28989200 | 0.73553200 |
| C | 1.04278500 | -1.28020600 | 0.75173600 |
| O | 1.66162700 | 2.15671900 | 1.22758900 |
| O | 1.66005300 | -2.14226100 | 1.25409800 |
| C | 1.05774100 | -0.00906700 | -1.47231100 |
| O | 1.68667800 | -0.01594100 | -2.46261200 |

L-L = bis CO

M = Fe

[Fe-S]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 1.27065000 | -1.43230800 | 1.16582000 |
| C | 0.70112100 | -2.03684800 | -0.00046300 |
| C | 1.27128100 | -1.43173500 | -1.16611400 |
| C | 2.22744400 | -0.44380400 | -0.71613200 |
| C | 2.22708000 | -0.44419600 | 0.71684500 |
| H | 1.03826800 | -1.68061600 | 2.20236600 |
| H | -0.08730400 | -2.79155300 | -0.00086900 |
| H | 1.03944500 | -1.67952400 | -2.20290600 |
| H | 2.84583100 | 0.19095900 | -1.35369700 |
| H | 2.84512800 | 0.19024600 | 1.35505800 |
| Fe | 0.31078700 | 0.09403500 | -0.00001000 |
| C | 0.16944200 | 1.30346500 | 1.29212200 |
| C | 0.16955400 | 1.30361800 | -1.29202200 |
| O | 0.09915100 | 2.09187300 | 2.13901700 |
| O | 0.09933500 | 2.09213700 | -2.13881700 |
| N | -1.55430800 | -0.26411100 | -0.00007700 |
| C | -2.70927700 | -0.45617600 | -0.00008800 |
| C | -4.14541800 | -0.69868800 | -0.00006900 |
| H | -4.43621900 | -1.27047000 | -0.89888600 |
| H | -4.43619500 | -1.27034200 | 0.89884400 |
| H | -4.68839400 | 0.26311800 | -0.00009300 |

[Fe-H]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.61824200 | 1.16030800 | -0.21747100 |
| C | -1.80008500 | -0.00019100 | -1.03876500 |
| C | -1.61818500 | -1.16042400 | -0.21711300 |
| C | -1.34297300 | -0.71260600 | 1.13195200 |
| C | -1.34301000 | 0.71291000 | 1.13173100 |
| H | -1.67320000 | 2.19707000 | -0.55140000 |
| H | -1.99802500 | -0.00036200 | -2.11083500 |
| H | -1.67308400 | -2.19729200 | -0.55072500 |
| H | -1.15057700 | -1.35475800 | 1.99249000 |
| H | -1.15063300 | 1.35533500 | 1.99206900 |
| Fe | 0.15363900 | -0.00000300 | -0.20317600 |
| H | 0.57953600 | -0.00002100 | -1.64393900 |
| C | 1.31973900 | 1.27458000 | -0.01338900 |
| C | 1.31975300 | -1.27457400 | -0.01338200 |
| O | 2.09807600 | 2.14384300 | 0.09834700 |

O 2.09809800 -2.14383200 0.09834400

[Fe-CO]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 1.68690400 | 1.16511600 | 0.38960800 |
| C | 1.69938200 | 0.00165000 | 1.23089500 |
| C | 1.68407800 | -1.16609300 | 0.39357100 |
| C | 1.70725500 | -0.71833500 | -0.98061300 |
| C | 1.70649700 | 0.71235400 | -0.98383700 |
| H | 1.69150600 | 2.20330000 | 0.72653300 |
| H | 1.68972400 | 0.00386300 | 2.32312400 |
| H | 1.68814200 | -2.20300100 | 0.73421600 |
| H | 1.71170700 | -1.35954200 | -1.86452100 |
| H | 1.71225300 | 1.35003600 | -1.87022500 |
| Fe | -0.06010200 | 0.00003900 | -0.00203100 |
| C | -1.02144900 | 1.32169900 | -0.72635300 |
| C | -1.02335800 | -1.28723900 | -0.78332800 |
| O | -1.62654700 | 2.18543700 | -1.19772300 |
| O | -1.62997200 | -2.12845100 | -1.29199000 |
| C | -1.03986200 | -0.03253600 | 1.49172900 |
| O | -1.65940000 | -0.05390600 | 2.46642000 |

| | | | |
|----|-------------|-------------|-------------|
| H | -1.93722000 | -0.00034000 | -2.15269500 |
| H | -1.63469300 | -2.19715500 | -0.57585500 |
| H | -1.25018300 | -1.35485600 | 1.99816700 |
| H | -1.25024800 | 1.35543600 | 1.99776300 |
| Co | 0.15646500 | 0.00000300 | -0.18425900 |
| H | 0.58605600 | -0.00011000 | -1.60775400 |
| C | 1.32139800 | 1.33275200 | 0.00948500 |
| C | 1.32138200 | -1.33275100 | 0.00951300 |
| O | 2.08023000 | 2.19429100 | 0.10143300 |
| O | 2.08017300 | -2.19433000 | 0.10143100 |

[Co-CO]²⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 1.69057700 | 1.17007300 | 0.38608100 |
| C | 1.72423200 | 0.00195800 | 1.23240300 |
| C | 1.69063100 | -1.16878000 | 0.38972600 |
| C | 1.72054800 | -0.71973600 | -0.99166900 |
| C | 1.72053000 | 0.71671500 | -0.99390200 |
| H | 1.70322500 | 2.21133000 | 0.72452800 |
| H | 1.74064000 | 0.00366300 | 2.32793500 |
| H | 1.70332200 | -2.20897700 | 0.73141600 |
| H | 1.74152700 | -1.36244500 | -1.87842100 |
| H | 1.74148400 | 1.35665400 | -1.88265500 |
| Co | -0.05444700 | -0.00000200 | -0.00270400 |
| C | -1.03600700 | 1.35341200 | -0.78323500 |
| C | -1.03595800 | -1.35613400 | -0.77857300 |
| O | -1.65412500 | 2.18603800 | -1.26161100 |
| O | -1.65393400 | -2.19047900 | -1.25412900 |
| C | -1.03862800 | 0.00266800 | 1.55467100 |
| O | -1.66389800 | 0.00428800 | 2.51038900 |

L-L = bpy

M = Mn

[Mn-S]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -2.81499800 | -1.17270200 | -0.58109200 |
| C | -3.16492400 | 0.00047500 | 0.16495300 |
| C | -2.81465900 | 1.17297200 | -0.58195000 |
| C | -2.19891900 | 0.71901800 | -1.80189700 |
| C | -2.19911600 | -0.71980800 | -1.80135300 |
| H | -2.99923700 | -2.20607400 | -0.28010100 |
| H | -3.59253800 | 0.00091500 | 1.17060300 |
| H | -2.99859400 | 2.20661500 | -0.28170300 |
| H | -1.78607800 | 1.35304300 | -2.59057800 |
| H | -1.78645900 | -1.35452600 | -2.58957500 |
| Mn | -1.02686100 | -0.00000800 | -0.18701100 |
| N | 0.42266900 | 1.26162400 | -0.38401200 |
| C | 0.32501800 | 2.62005000 | -0.51423400 |
| C | 1.70321400 | 0.72547500 | -0.27530000 |
| C | 1.42485900 | 3.47424200 | -0.51375900 |
| H | -0.69473700 | 3.00648100 | -0.59272700 |
| C | 2.84952300 | 1.54955200 | -0.22905300 |
| C | 2.72337500 | 2.93423800 | -0.34947200 |
| H | 1.26630200 | 4.55279800 | -0.61851100 |
| H | 3.83762700 | 1.09371700 | -0.10331100 |
| H | 3.60511300 | 3.58282300 | -0.31655100 |
| N | 0.42264600 | -1.26165000 | -0.38397200 |
| C | 1.70320000 | -0.72552400 | -0.27528200 |

[Co-H]⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -1.58471500 | 1.15788700 | -0.24451900 |
| C | -1.75509500 | -0.00017400 | -1.07688300 |
| C | -1.58466000 | -1.15798200 | -0.24416700 |
| C | -1.39136800 | -0.70905800 | 1.12913900 |
| C | -1.39139200 | 0.70937400 | 1.12892400 |
| H | -1.63479200 | 2.19696100 | -0.57651100 |

| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | 0.32495400 | -2.62008600 | -0.51408200 | H | 1.74522700 | 1.34962200 | -2.38770900 |
| C | 2.84949100 | -1.54962600 | -0.22900900 | Mn | 1.04276400 | -0.00006000 | 0.10073500 |
| C | 1.42477300 | -3.47430400 | -0.51355600 | N | -0.42835600 | -1.26564300 | -0.09775900 |
| H | -0.69481400 | -3.00649900 | -0.59250500 | C | -0.32079500 | -2.62318100 | -0.19040200 |
| C | 2.72330700 | -2.93431600 | -0.34934200 | C | -1.70541400 | -0.72763600 | -0.08370100 |
| H | 3.83760600 | -1.09380900 | -0.10330500 | C | -1.42102100 | -3.47743500 | -0.24407700 |
| H | 1.26618900 | -4.55286600 | -0.61821300 | H | 0.70170200 | -3.00905400 | -0.19089300 |
| H | 3.60503200 | -3.58292000 | -0.31640000 | C | -2.85470100 | -1.54569900 | -0.09837800 |
| N | -0.76931500 | -0.00002800 | 1.65055000 | C | -2.72265800 | -2.93316600 | -0.17987700 |
| C | -0.58030800 | 0.00005600 | 2.82031200 | H | -1.25827600 | -4.55794100 | -0.31208900 |
| C | -0.39564000 | 0.00027000 | 4.26805200 | H | -3.84758400 | -1.08712100 | -0.04781400 |
| H | -0.85349500 | 0.89534900 | 4.73185900 | H | -3.60623400 | -3.57970300 | -0.19075800 |
| H | -0.85172000 | -0.89570000 | 4.73189500 | N | -0.42823500 | 1.26565300 | -0.09779900 |
| H | 0.68041500 | 0.00134000 | 4.52282000 | C | -1.70534200 | 0.72777600 | -0.08371900 |

[Mn-H]¹

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -2.88603700 | 1.17401500 | -0.20127300 |
| C | -3.07236300 | -0.00003100 | -1.00710700 |
| C | -2.88603100 | -1.17403900 | -0.20122200 |
| C | -2.51208900 | -0.72449100 | 1.11634100 |
| C | -2.51209400 | 0.72452600 | 1.11631000 |
| H | -2.98964600 | 2.20867300 | -0.53920700 |
| H | -3.30490500 | -0.00005600 | -2.07467700 |
| H | -2.98963100 | -2.20871300 | -0.53911100 |
| H | -2.26778000 | -1.36662500 | 1.96864700 |
| H | -2.26779000 | 1.36669800 | 1.96858800 |
| Mn | -1.06458100 | -0.00000200 | -0.20294800 |
| H | -0.85855600 | -0.00000500 | -1.76115800 |
| N | 0.34116100 | -1.24331700 | -0.03608100 |
| C | 0.24724300 | -2.61770700 | 0.06125100 |
| C | 1.65674000 | -0.71654600 | -0.04944800 |
| C | 1.33617900 | -3.47693400 | 0.10211600 |
| H | -0.77735200 | -3.00283300 | 0.07840600 |
| C | 2.79230700 | -1.55850300 | -0.04277100 |
| C | 2.65972900 | -2.94629100 | 0.03246200 |
| H | 1.16042100 | -4.55794100 | 0.17078900 |
| H | 3.78934600 | -1.10225200 | -0.09846800 |
| H | 3.53871400 | -3.60164400 | 0.03633100 |
| N | 0.34115500 | 1.24331600 | -0.03608000 |
| C | 1.65673700 | 0.71655200 | -0.04944800 |
| C | 0.24723100 | 2.61770600 | 0.06125500 |
| C | 2.79230000 | 1.55851400 | -0.04277300 |
| C | 1.33616300 | 3.47693800 | 0.10211700 |
| H | -0.77736500 | 3.00282700 | 0.07841200 |
| C | 2.65971600 | 2.94630100 | 0.03246100 |
| H | 3.78934000 | 1.10226700 | -0.09847100 |
| H | 1.16040100 | 4.55794400 | 0.17079000 |
| H | 3.53869700 | 3.60165800 | 0.03632700 |

[Mn-CO]⁰

| | x | y | z |
|---|------------|-------------|-------------|
| C | 2.79541600 | 1.17233700 | -0.39589300 |
| C | 3.15832000 | -0.00051300 | 0.35449000 |
| C | 2.79497500 | -1.17281700 | -0.39649800 |
| C | 2.17902500 | -0.71658700 | -1.61033500 |
| C | 2.17928400 | 0.71696200 | -1.60994300 |
| H | 2.98845200 | 2.20604700 | -0.10339500 |
| H | 3.64486900 | -0.00086500 | 1.33204300 |
| H | 2.98767000 | -2.20674600 | -0.10455000 |
| H | 1.74475000 | -1.34867600 | -2.38844100 |

| | | | |
|----|-------------|-------------|-------------|
| Mn | 1.04276400 | -0.00006000 | 0.10073500 |
| N | -0.42835600 | -1.26564300 | -0.09775900 |
| C | -0.32079500 | -2.62318100 | -0.19040200 |
| C | -1.70541400 | -0.72763600 | -0.08370100 |
| C | -1.42102100 | -3.47743500 | -0.24407700 |
| H | 0.70170200 | -3.00905400 | -0.19089300 |
| C | -2.85470100 | -1.54569900 | -0.09837800 |
| C | -2.72265800 | -2.93316600 | -0.17987700 |
| H | -1.25827600 | -4.55794100 | -0.31208900 |
| H | -3.84758400 | -1.08712100 | -0.04781400 |
| H | -3.60623400 | -3.57970300 | -0.19075800 |
| N | -0.42823500 | 1.26565300 | -0.09779900 |
| C | -1.70534200 | 0.72777600 | -0.08371900 |
| C | -0.32051900 | 2.62317700 | -0.19043500 |
| C | -2.85454100 | 1.54596500 | -0.09840100 |
| C | -1.42065200 | 3.47755000 | -0.24410900 |
| H | 0.70202400 | 3.00893100 | -0.19091600 |
| C | -2.72234700 | 2.93341700 | -0.17991100 |
| H | -3.84747500 | 1.08749700 | -0.04782600 |
| H | -1.25779400 | 4.55804400 | -0.31211600 |
| H | -3.60585300 | 3.58004800 | -0.19079700 |
| C | 0.91886200 | 0.00003700 | 1.85832700 |
| O | 0.87102400 | 0.00002900 | 3.04287100 |

L-L = bpy

M = Fe

[Fe-S]¹⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 2.56265800 | 1.16824900 | -1.06947400 |
| C | 3.09159900 | -0.00082000 | -0.43058500 |
| C | 2.56190600 | -1.16919400 | -1.07004800 |
| C | 1.69409200 | -0.71490800 | -2.12913300 |
| C | 1.69459600 | 0.71502600 | -2.12878600 |
| H | 2.80856800 | 2.20129400 | -0.81922600 |
| H | 3.74702200 | -0.00125200 | 0.44253000 |
| H | 2.80713000 | -2.20251800 | -0.82028000 |
| H | 1.10669100 | -1.34794800 | -2.79706700 |
| H | 1.10757900 | 1.34877600 | -2.79638700 |
| Fe | 0.97524000 | -0.00013700 | -0.28399400 |
| N | -0.49241400 | -1.27639500 | -0.21038600 |
| C | -0.36986500 | -2.62905100 | -0.20214200 |
| C | -1.75233400 | -0.73360200 | -0.13661900 |
| C | -1.47257900 | -3.48752100 | -0.14791600 |
| H | 0.65152200 | -3.01458700 | -0.23700200 |
| C | -2.90020900 | -1.54469800 | -0.06802100 |
| C | -2.76447300 | -2.93741800 | -0.08044200 |
| H | -1.31268100 | -4.56989700 | -0.15302900 |
| H | -3.89235500 | -1.08820500 | -0.00701700 |
| H | -3.64797900 | -3.58176100 | -0.03335600 |
| N | -0.49211800 | 1.27642500 | -0.21055300 |
| C | -1.75216100 | 0.73394500 | -0.13669300 |
| C | -0.36921900 | 2.62905000 | -0.20242200 |
| C | -2.89983200 | 1.54533600 | -0.06812700 |
| C | -1.47171400 | 3.48780000 | -0.14822500 |
| H | 0.65227200 | 3.01431400 | -0.23733500 |
| C | -2.76374400 | 2.93802100 | -0.08066700 |
| H | -3.89209000 | 1.08910100 | -0.00704300 |
| H | -1.31154900 | 4.57013600 | -0.15342000 |
| H | -3.64708700 | 3.58258900 | -0.03359800 |

| | | | |
|---|------------|-------------|------------|
| N | 1.11853700 | -0.00000100 | 1.58287000 |
| C | 1.22757300 | 0.00007700 | 2.75305200 |
| C | 1.38956600 | 0.00016700 | 4.20314200 |
| H | 1.94580300 | -0.89622900 | 4.53079100 |
| H | 1.94460000 | 0.89729200 | 4.53082900 |
| H | 0.40311800 | -0.00051400 | 4.69956500 |

[Fe-H]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -2.82295600 | 1.16563000 | -0.17069400 |
| C | -3.02092500 | -0.00038100 | -0.98353300 |
| C | -2.82284400 | -1.16597000 | -0.17014400 |
| C | -2.48121500 | -0.71738700 | 1.15619700 |
| C | -2.48127900 | 0.71769100 | 1.15585100 |
| H | -2.91571000 | 2.19943200 | -0.50881200 |
| H | -3.26447700 | -0.00064800 | -2.04682700 |
| H | -2.91549000 | -2.19994200 | -0.50777200 |
| H | -2.24068700 | -1.35580200 | 2.00922600 |
| H | -2.24079100 | 1.35652400 | 2.00858100 |
| Fe | -1.04809800 | -0.00004600 | -0.21126200 |
| H | -0.79158600 | -0.00002200 | -1.70659600 |
| N | 0.34837700 | -1.24994200 | -0.05684300 |
| C | 0.23242200 | -2.61462000 | -0.01675700 |
| C | 1.63549200 | -0.72414500 | -0.02851100 |
| C | 1.32454500 | -3.47423500 | 0.04739000 |
| H | -0.78983700 | -2.99750600 | -0.05102200 |
| C | 2.77609400 | -1.55240900 | 0.01375100 |
| C | 2.63424800 | -2.93979400 | 0.05453700 |
| H | 1.15174900 | -4.55504900 | 0.07956000 |
| H | 3.77198200 | -1.09708500 | 0.01669500 |
| H | 3.51176500 | -3.59346100 | 0.08962600 |
| N | 0.34827300 | 1.24994500 | -0.05681900 |
| C | 1.63543200 | 0.72425700 | -0.02851000 |
| C | 0.23219500 | 2.61461200 | -0.01671600 |
| C | 2.77596200 | 1.55262100 | 0.01372200 |
| C | 1.32424600 | 3.47432100 | 0.04740200 |
| H | -0.79010000 | 2.99740900 | -0.05094500 |
| C | 2.63399600 | 2.93999300 | 0.05450700 |
| H | 3.77189100 | 1.09738400 | 0.01663900 |
| H | 1.15135800 | 4.55512000 | 0.07957900 |
| H | 3.51145700 | 3.59373700 | 0.08956700 |

[Fe-CO]¹⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 2.66805100 | 1.16576300 | -0.60346900 |
| C | 3.14577000 | -0.00189100 | 0.08601500 |
| C | 2.66632700 | -1.16772400 | -0.60521500 |
| C | 1.92302200 | -0.71157700 | -1.75217000 |
| C | 1.92415900 | 0.71241500 | -1.75110200 |
| H | 2.88777900 | 2.19978300 | -0.33388500 |
| H | 3.75695700 | -0.00303400 | 0.99072400 |
| H | 2.88448600 | -2.20247200 | -0.33715600 |
| H | 1.40584200 | -1.34589100 | -2.47461000 |
| H | 1.40785900 | 1.34860000 | -2.47253200 |
| Fe | 1.03894300 | -0.00031900 | 0.09489800 |
| N | -0.43842900 | -1.28006300 | 0.02162100 |
| C | -0.31920700 | -2.62888700 | 0.10050000 |
| C | -1.68843400 | -0.73397900 | -0.12497100 |
| C | -1.41978400 | -3.48708100 | 0.00378000 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.69187400 | -3.01224700 | 0.25314600 |
| C | -2.83368400 | -1.54466600 | -0.22554900 |
| C | -2.70069100 | -2.93685600 | -0.16852200 |
| H | -1.26613100 | -4.56810400 | 0.07075300 |
| H | -3.82111300 | -1.08952100 | -0.34261300 |
| H | -3.58217300 | -3.58099000 | -0.24608600 |
| N | -0.43769600 | 1.28020400 | 0.02157600 |
| C | -1.68801400 | 0.73484200 | -0.12496800 |
| C | -0.31765300 | 2.62895900 | 0.10040800 |
| C | -2.83279300 | 1.54620600 | -0.22547800 |
| C | -1.41773100 | 3.48779700 | 0.00376700 |
| H | 0.69368800 | 3.01169300 | 0.25293600 |
| C | -2.69897400 | 2.93831500 | -0.16843900 |
| H | -3.82049800 | 1.09164700 | -0.34248400 |
| H | -1.26344500 | 4.56873000 | 0.07072400 |
| H | -3.58008400 | 3.58296700 | -0.24592800 |
| C | 1.11323800 | -0.00028600 | 1.84285000 |
| O | 1.19796500 | -0.00024400 | 3.00783100 |

L-L = bpy

M = Co

[Co-S]²⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 2.45139400 | 1.16353600 | -1.24511900 |
| C | 3.05628100 | -0.00334400 | -0.67182600 |
| C | 2.44787400 | -1.16649700 | -1.24853200 |
| C | 1.48613000 | -0.71423100 | -2.22619000 |
| C | 1.48860500 | 0.71709000 | -2.22427400 |
| H | 2.71089200 | 2.19681900 | -1.00868200 |
| H | 3.80311700 | -0.00567700 | 0.12497800 |
| H | 2.70411700 | -2.20127300 | -1.01511100 |
| H | 0.84360200 | -1.34787100 | -2.84110000 |
| H | 0.84803100 | 1.35449700 | -2.83733300 |
| Co | 0.94186900 | -0.00043700 | -0.31631800 |
| N | -0.51222600 | -1.29480100 | -0.14650400 |
| C | -0.37268300 | -2.64005200 | -0.06981700 |
| C | -1.76242300 | -0.73506200 | -0.10754500 |
| C | -1.47903800 | -3.49493700 | 0.01616000 |
| H | 0.64707000 | -3.03102700 | -0.07355100 |
| C | -2.90886400 | -1.54515600 | -0.02737600 |
| C | -2.76813200 | -2.93878200 | 0.02543100 |
| H | -1.32023400 | -4.57611600 | 0.07056100 |
| H | -3.90365700 | -1.09188100 | -0.00091100 |
| H | -3.65326800 | -3.58047300 | 0.08283100 |
| N | -0.51107400 | 1.29505800 | -0.14636700 |
| C | -1.76176300 | 0.73643600 | -0.10748000 |
| C | -0.37026000 | 2.64017700 | -0.06966000 |
| C | -2.90745400 | 1.54759200 | -0.02727300 |
| C | -1.47582600 | 3.49606900 | 0.01636100 |
| H | 0.64987400 | 3.03017400 | -0.07348800 |
| C | -2.76543000 | 2.94108200 | 0.02561200 |
| H | -3.90266500 | 1.09523700 | -0.00085500 |
| H | -1.31604100 | 4.57710300 | 0.07077600 |
| H | -3.64997800 | 3.58358300 | 0.08303600 |
| N | 1.24896500 | -0.00067900 | 1.56228000 |
| C | 1.45284900 | -0.00074400 | 2.71487600 |
| C | 1.71718600 | -0.00081400 | 4.14592200 |
| H | 2.29522400 | -0.89988400 | 4.42524600 |
| H | 2.29700800 | 0.89718000 | 4.42499800 |
| H | 0.76611800 | 0.00018900 | 4.70770700 |

[Co-H]¹⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -2.78821300 | 1.15624800 | -0.10421500 |
| C | -3.02951800 | -0.00107300 | -0.91786700 |
| C | -2.78768700 | -1.15736100 | -0.10293600 |
| C | -2.46936900 | -0.70833300 | 1.23770400 |
| C | -2.46968800 | 0.70878500 | 1.23690700 |
| H | -2.88696200 | 2.19134000 | -0.43534800 |
| H | -3.31479100 | -0.00172300 | -1.97024400 |
| H | -2.88591800 | -2.19286100 | -0.43294700 |
| H | -2.23180100 | -1.34948600 | 2.08857500 |
| H | -2.23233600 | 1.35096700 | 2.08706400 |
| Co | -1.04697600 | -0.00016100 | -0.24420700 |
| N | 0.36849700 | -1.27890800 | -0.10562600 |
| C | 0.24704900 | -2.63005400 | -0.15432400 |
| C | 1.62223500 | -0.73276700 | 0.02203400 |
| C | 1.34718900 | -3.48685900 | -0.05322000 |
| H | -0.76400700 | -3.01973500 | -0.28195400 |
| C | 2.76666900 | -1.54425000 | 0.12234400 |
| C | 2.63189800 | -2.93640900 | 0.08947700 |
| H | 1.18973200 | -4.56864000 | -0.09309700 |
| H | 3.75541800 | -1.08802700 | 0.22208000 |
| H | 3.51319900 | -3.58060400 | 0.16772000 |
| N | 0.36810800 | 1.27895300 | -0.10558800 |
| C | 1.62201200 | 0.73320300 | 0.02204200 |
| C | 0.24620800 | 2.63005700 | -0.15429000 |
| C | 2.76618600 | 1.54505700 | 0.12232000 |
| C | 1.34607300 | 3.48721600 | -0.05322500 |
| H | -0.76498800 | 3.01938700 | -0.28190000 |
| C | 2.63096200 | 2.93717300 | 0.08944200 |
| H | 3.75508700 | 1.08915900 | 0.22202800 |
| H | 1.18827400 | 4.56894700 | -0.09311300 |
| H | 3.51205900 | 3.58165100 | 0.16764900 |
| H | -0.81287900 | -0.00012500 | -1.70758600 |

[Co-CO]²⁺

| | x | y | z |
|----|-------------|--------------|-------------|
| C | 2.65732200 | 1.16309400 | -0.61122400 |
| C | 3.16144100 | -0.00305900 | 0.06448400 |
| C | 2.65468800 | -1.16623300 | -0.61412000 |
| C | 1.89545900 | -0.71277500 | -1.75610100 |
| C | 1.89729300 | 0.71419100 | -1.75440700 |
| H | 2.87247500 | 2.19788700 | -0.33702200 |
| H | 3.79378900 | -0.00491200 | 0.95658400 |
| H | 2.86732700 | -2.202220100 | -0.34242700 |
| H | 1.38121200 | -1.34952600 | -2.47948900 |
| H | 1.38449500 | 1.35392900 | -2.47619000 |
| Co | 1.02699000 | -0.00047800 | 0.08759600 |
| N | -0.43784300 | -1.29761100 | 0.02975300 |
| C | -0.31287700 | -2.64282400 | 0.14617900 |
| C | -1.67483300 | -0.73449700 | -0.15654900 |
| C | -1.41865700 | -3.49570000 | 0.04178700 |
| H | 0.68900300 | -3.03502500 | 0.33295200 |
| C | -2.81629000 | -1.54660500 | -0.27491400 |
| C | -2.68805200 | -2.93977300 | -0.18375700 |
| H | -1.27308600 | -4.57578000 | 0.13997800 |
| H | -3.79997400 | -1.09401800 | -0.42771100 |
| H | -3.57070100 | -3.58124300 | -0.27410500 |
| N | -0.43668300 | 1.29784200 | 0.02964400 |
| C | -1.67417900 | 0.73582500 | -0.15655300 |

| | | | |
|---|-------------|-------------|-------------|
| C | -0.31045400 | 2.64294600 | 0.14599200 |
| C | -2.81491100 | 1.54897500 | -0.27479900 |
| C | -1.41547200 | 3.49681600 | 0.04172900 |
| H | 0.69183300 | 3.03421300 | 0.33256000 |
| C | -2.68540100 | 2.94202200 | -0.18363900 |
| H | -3.79902300 | 1.09728400 | -0.42748600 |
| H | -1.26891600 | 4.57676700 | 0.13987500 |
| H | -3.56748400 | 3.58428900 | -0.27386000 |
| C | 1.08198700 | -0.00038600 | 1.87944100 |
| O | 1.09620300 | -0.00031000 | 3.02927000 |

L-L = dppe

M = Mn

[Mn-S]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.33595200 | 0.23622500 | 2.78729600 |
| C | -0.52992600 | -0.87382000 | 3.18799900 |
| C | 0.85442900 | -0.47254300 | 3.15378200 |
| C | 0.89029200 | 0.89630500 | 2.72020000 |
| C | -0.45715100 | 1.34409000 | 2.49985800 |
| H | -2.42563000 | 0.25403000 | 2.72813400 |
| H | -0.89771700 | -1.87169000 | 3.43728900 |
| H | 1.71464000 | -1.09810900 | 3.39840600 |
| H | 1.79061000 | 1.50341000 | 2.60201500 |
| H | -0.77515400 | 2.34508500 | 2.20390300 |
| Mn | 0.00290600 | -0.30031000 | 1.19054200 |
| C | 0.74373200 | -0.17946000 | -2.04270600 |
| H | 1.37817800 | 0.19509800 | -2.86777500 |
| H | 0.64865200 | -1.27689900 | -2.14431000 |
| C | -0.64856100 | 0.46662000 | -2.05316500 |
| H | -1.24427800 | 0.12860900 | -2.91943100 |
| H | -0.55834000 | 1.56574900 | -2.12479600 |
| P | 1.51601800 | 0.15583200 | -0.34640500 |
| P | -1.49360600 | 0.06471700 | -0.39417500 |
| C | 3.07480500 | -0.87425100 | -0.38712100 |
| C | 3.38387900 | -1.80076600 | -1.40640800 |
| C | 3.96080300 | -0.76944800 | 0.71070100 |
| C | 4.54349500 | -2.59723300 | -1.33235400 |
| H | 2.72822700 | -1.90540200 | -2.27761800 |
| C | 5.12254900 | -1.55234200 | 0.78164000 |
| H | 3.73535200 | -0.06339600 | 1.51927100 |
| C | 5.41723800 | -2.47559300 | -0.24026000 |
| H | 4.76421100 | -3.30883700 | -2.13768800 |
| H | 5.79897900 | -1.44581300 | 1.63832400 |
| H | 6.32218200 | -3.09193200 | -0.18410000 |
| C | 2.25585700 | 1.85528700 | -0.62353900 |
| C | 1.68393100 | 2.97955300 | 0.00696500 |
| C | 3.35522000 | 2.05363200 | -1.48978800 |
| C | 2.19199200 | 4.27172100 | -0.22089500 |
| H | 0.83795500 | 2.83018300 | 0.68624300 |
| C | 3.86081600 | 3.34315900 | -1.72447300 |
| H | 3.82847400 | 1.19153500 | -1.97550900 |
| C | 3.28038500 | 4.45687200 | -1.08997400 |
| H | 1.73862200 | 5.13252300 | 0.28549300 |
| H | 4.71473100 | 3.47820300 | -2.39939400 |
| H | 3.67930900 | 5.46238000 | -1.26871600 |
| C | -2.69789100 | 1.48485000 | -0.21401000 |
| C | -2.24690300 | 2.81729400 | -0.35546000 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -4.04269900 | 1.27327700 | 0.16370300 | C | 1.96558700 | 2.64588900 | 0.13495600 |
| C | -3.11457300 | 3.90215200 | -0.14507700 | C | 3.20038300 | 1.76072900 | -1.75145700 |
| H | -1.20396400 | 3.01643200 | -0.62871100 | C | 2.47372400 | 3.93149400 | -0.12985700 |
| C | -4.91001100 | 2.35834000 | 0.38544300 | H | 1.26629900 | 2.47446600 | 0.96385300 |
| H | -4.42288900 | 0.25181100 | 0.27793800 | C | 3.69555600 | 3.04687100 | -2.03639100 |
| C | -4.45135700 | 3.67697900 | 0.22910200 | H | 3.51340500 | 0.91323100 | -2.37532900 |
| H | -2.74278900 | 4.92622400 | -0.27172700 | C | 3.33472700 | 4.13810500 | -1.22434600 |
| H | -5.94971600 | 2.16807900 | 0.67826600 | H | 2.19082800 | 4.77471700 | 0.51410600 |
| H | -5.12852300 | 4.52257600 | 0.39721000 | H | 4.36777800 | 3.19731400 | -2.89211200 |
| C | -2.68814900 | -1.30720100 | -0.86822500 | H | 3.72135800 | 5.14175200 | -1.44420300 |
| C | -3.39039700 | -1.34584700 | -2.09387300 | C | -2.62602900 | 1.33882700 | -0.17201000 |
| C | -2.92624200 | -2.33012100 | 0.07405000 | C | -2.14185700 | 2.65483700 | -0.36557200 |
| C | -4.29193900 | -2.38644800 | -2.37630600 | C | -3.94983200 | 1.19312500 | 0.30694300 |
| H | -3.25543700 | -0.54714600 | -2.83322200 | C | -2.95591900 | 3.77612000 | -0.13404600 |
| C | -3.83528800 | -3.36814100 | -0.20037800 | H | -1.10209900 | 2.80556000 | -0.68209000 |
| H | -2.38568800 | -2.29918600 | 1.02693800 | C | -4.76251000 | 2.31399100 | 0.56289000 |
| C | -4.51572300 | -3.40287300 | -1.42951400 | H | -4.35451100 | 0.18834300 | 0.47750700 |
| H | -4.82861900 | -2.39747900 | -3.33286700 | C | -4.27479400 | 3.61204900 | 0.33505900 |
| H | -4.01075300 | -4.15139900 | 0.54739400 | H | -2.55539700 | 4.78328000 | -0.30975300 |
| H | -5.22135900 | -4.21324200 | -1.64823200 | H | -5.78392700 | 2.16833000 | 0.93962800 |
| N | 0.21714300 | -2.08973800 | 0.74361700 | H | -4.90902400 | 4.48676300 | 0.52801100 |
| C | 0.37775500 | -3.24568500 | 0.52356400 | C | -2.69788800 | -1.46213200 | -0.78967700 |
| C | 0.63874000 | -4.65793900 | 0.26168800 | C | -3.62733000 | -1.32503100 | -1.84577200 |
| H | 1.72067100 | -4.84734300 | 0.11884300 | C | -2.66717400 | -2.68050300 | -0.08265400 |
| H | 0.29276100 | -5.28882200 | 1.10273800 | C | -4.49813500 | -2.37558000 | -2.18722900 |
| H | 0.10953100 | -4.99743800 | -0.64927300 | H | -3.68334200 | -0.37949900 | -2.40196100 |

[Mn-H]⁻¹

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.20556200 | -0.21090800 | 2.95826800 |
| C | -0.40942100 | -1.40051100 | 3.06670200 |
| C | 0.98227000 | -1.01708300 | 3.02824600 |
| C | 1.02756100 | 0.41947000 | 2.87638600 |
| C | -0.31990300 | 0.92167900 | 2.85025700 |
| H | -2.29741600 | -0.16975700 | 2.94554800 |
| H | -0.79137100 | -2.41931600 | 3.16106500 |
| H | 1.84110400 | -1.68860700 | 3.08027100 |
| H | 1.93766800 | 1.02342100 | 2.82957700 |
| H | -0.62577300 | 1.96694700 | 2.76121900 |
| Mn | 0.03299500 | -0.45132200 | 1.22394300 |
| H | 0.10345300 | -1.91072500 | 0.63282700 |
| C | 0.74100100 | -0.46133100 | -2.02311200 |
| H | 1.38150300 | -0.06806400 | -2.83546800 |
| H | 0.66500200 | -1.55718300 | -2.14174500 |
| C | -0.65283600 | 0.17910800 | -2.02898500 |
| H | -1.29105900 | -0.22536800 | -2.83750200 |
| H | -0.56714700 | 1.27099000 | -2.18049100 |
| P | 1.49415100 | -0.13036500 | -0.29972400 |
| P | -1.43701400 | -0.11804400 | -0.30076900 |
| C | 3.02287900 | -1.22741500 | -0.34569500 |
| C | 2.88522200 | -2.60277300 | -0.65386200 |
| C | 4.29148400 | -0.78109200 | 0.09639200 |
| C | 3.97318800 | -3.48517300 | -0.56378200 |
| H | 1.89951900 | -2.99127300 | -0.93683000 |
| C | 5.38044100 | -1.66534800 | 0.20729100 |
| H | 4.43171500 | 0.27475300 | 0.35802500 |
| C | 5.23207200 | -3.02188300 | -0.13049600 |
| H | 3.83600700 | -4.54409600 | -0.82049400 |
| H | 6.35096700 | -1.28856800 | 0.55763100 |
| H | 6.08133200 | -3.71230000 | -0.04915200 |
| C | 2.32074000 | 1.54072700 | -0.66562400 |

[Mn-CO]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -0.80746100 | -1.11386100 | 3.06998300 |
| C | 0.63338700 | -1.16792400 | 3.10814300 |
| C | 1.13032000 | 0.13362000 | 2.78154200 |
| C | 0.00730600 | 1.00333300 | 2.54657500 |
| C | -1.18701900 | 0.22105900 | 2.71933600 |
| H | -1.48502800 | -1.94483800 | 3.27290000 |
| H | 1.23548800 | -2.04687500 | 3.34480100 |
| H | 2.18114200 | 0.42288900 | 2.74786500 |
| H | 0.05133800 | 2.06331800 | 2.29510600 |
| H | -2.20889300 | 0.58847400 | 2.61116600 |
| Mn | -0.01270100 | -0.63068800 | 1.12328700 |
| C | 0.74110900 | -0.37098900 | -2.09090800 |
| H | 1.36276300 | 0.07476200 | -2.88947500 |
| H | 0.74013500 | -1.46496200 | -2.24727600 |
| C | -0.69645800 | 0.17461900 | -2.10994400 |
| H | -1.29497100 | -0.32767900 | -2.88986200 |
| H | -0.71535000 | 1.25668400 | -2.33083000 |
| P | 1.51935000 | -0.14090500 | -0.38519600 |
| P | -1.51222600 | -0.06305500 | -0.39734600 |
| C | 3.06898400 | -1.17265900 | -0.54781400 |
| C | 3.29978200 | -2.23271100 | 0.35066700 |
| C | 4.02302300 | -0.91598900 | -1.55927700 |
| C | 4.45463400 | -3.02801800 | 0.24049900 |
| H | 2.56051300 | -2.43439000 | 1.13281800 |
| C | 5.17253800 | -1.71391200 | -1.67581400 |
| H | 3.87548700 | -0.08009900 | -2.25421200 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 5.39149600 | -2.77238400 | -0.77417200 | H | -0.51146500 | 1.60912800 | -2.07154300 |
| H | 4.61772000 | -3.85076500 | 0.94666000 | P | 1.55819600 | 0.17471300 | -0.37917200 |
| H | 5.90215400 | -1.50557600 | -2.46756600 | P | -1.52360000 | 0.09107700 | -0.42765900 |
| H | 6.29097400 | -3.39290100 | -0.86368800 | C | 3.07358500 | -0.88449000 | -0.34898800 |
| C | 2.29560300 | 1.55791200 | -0.47068300 | C | 3.37658400 | -1.81966500 | -1.36205400 |
| C | 3.31216200 | 1.89684600 | 0.45296600 | C | 3.95407600 | -0.76135800 | 0.75077700 |
| C | 1.89308700 | 2.53950500 | -1.40323000 | C | 4.53566900 | -2.61381400 | -1.27665800 |
| C | 3.89245300 | 3.17519900 | 0.45638000 | H | 2.72671500 | -1.92737200 | -2.23697100 |
| H | 3.67756300 | 1.14174600 | 1.15880700 | C | 5.11075800 | -1.55104000 | 0.83274900 |
| C | 2.47578800 | 3.82040600 | -1.40573700 | H | 3.74397400 | -0.03194300 | 1.54202300 |
| H | 1.12851600 | 2.30927600 | -2.15308900 | C | 5.40310600 | -2.48338000 | -0.18008300 |
| C | 3.47251000 | 4.14568700 | -0.47125400 | H | 4.76346200 | -3.32656100 | -2.07759400 |
| H | 4.68242500 | 3.41040000 | 1.17953100 | H | 5.78744800 | -1.43635700 | 1.68696000 |
| H | 2.15120700 | 4.56124900 | -2.14638500 | H | 6.30770900 | -3.09810300 | -0.11713700 |
| H | 3.92699400 | 5.14312300 | -0.47202900 | C | 2.25674000 | 1.87589700 | -0.61296400 |
| C | -2.41716600 | 1.55809400 | -0.16599300 | C | 1.59265300 | 3.00700400 | -0.09257500 |
| C | -1.67467000 | 2.76141600 | -0.17808000 | C | 3.43474700 | 2.06408400 | -1.37305500 |
| C | -3.79977500 | 1.62672100 | 0.11354500 | C | 2.09091500 | 4.30094700 | -0.32629500 |
| C | -2.29924100 | 3.99768600 | 0.05368400 | H | 0.68682300 | 2.87483100 | 0.50707600 |
| H | -0.59348700 | 2.73552500 | -0.35955600 | C | 3.92868100 | 3.35718500 | -1.60857100 |
| C | -4.42392500 | 2.86416600 | 0.35775900 | H | 3.97574300 | 1.19961300 | -1.77457000 |
| H | -4.40024100 | 0.71093300 | 0.13563700 | C | 3.25898000 | 4.47816400 | -1.08593400 |
| C | -3.67868900 | 4.05407200 | 0.32354200 | H | 1.56873800 | 5.16888200 | 0.09212400 |
| H | -1.70350700 | 4.91815200 | 0.03146300 | H | 4.84351600 | 3.48791300 | -2.19732000 |
| H | -5.49892600 | 2.89330400 | 0.57257400 | H | 3.65100000 | 5.48528900 | -1.26527200 |
| H | -4.16636400 | 5.01806400 | 0.50962600 | C | -2.73952500 | 1.47447200 | -0.20591300 |
| C | -2.94155300 | -1.20092700 | -0.78579100 | C | -2.34068900 | 2.81928900 | -0.38334000 |
| C | -3.73118100 | -1.04608100 | -1.94879500 | C | -4.06678000 | 1.20705800 | 0.19861900 |
| C | -3.26988500 | -2.22981200 | 0.11977000 | C | -3.25100100 | 3.86874200 | -0.17559700 |
| C | -4.81028700 | -1.90802200 | -2.20406200 | H | -1.31751500 | 3.06148800 | -0.69277200 |
| H | -3.51932900 | -0.23576800 | -2.65706300 | C | -4.97252900 | 2.26000300 | 0.41487500 |
| C | -4.35425400 | -3.09001300 | -0.12963100 | H | -4.40508500 | 0.17347700 | 0.33049700 |
| H | -2.65738000 | -2.36003700 | 1.01828200 | C | -4.56918800 | 3.59244300 | 0.22731200 |
| C | -5.12383600 | -2.93451600 | -1.29417900 | H | -2.92846000 | 4.90431700 | -0.33225200 |
| H | -5.40937100 | -1.77539600 | -3.11296200 | H | -5.99934100 | 2.03350900 | 0.72325800 |
| H | -4.58901200 | -3.88897700 | 0.58344000 | H | -5.27846700 | 4.41143800 | 0.38899800 |
| H | -5.96456200 | -3.60898200 | -1.49477700 | C | -2.63022200 | -1.33947900 | -0.84877600 |
| C | -0.01584400 | -2.29181600 | 0.57197000 | C | -3.27136700 | -1.44975700 | -2.10343300 |
| O | -0.02062100 | -3.44353500 | 0.26850900 | C | -2.90782500 | -2.30403000 | 0.14441100 |
| | | | | C | -4.15220800 | -2.51272100 | -2.36391700 |
| | | | | H | -3.10764500 | -0.69770600 | -2.88340500 |
| | | | | C | -3.79927500 | -3.36050100 | -0.11216800 |
| | | | | H | -2.42318900 | -2.22087200 | 1.12320000 |
| | | | | C | -4.41762900 | -3.47079500 | -1.36942500 |
| | | | | H | -4.64007100 | -2.58470500 | -3.34243300 |
| | | | | H | -4.01309200 | -4.09564200 | 0.67231300 |
| | | | | H | -5.11021100 | -4.29523600 | -1.57211300 |
| | | | | N | 0.21831400 | -2.06617000 | 0.69996500 |
| | | | | C | 0.38829500 | -3.20917600 | 0.47575600 |
| | | | | C | 0.59107300 | -4.62801000 | 0.20453200 |
| | | | | H | 1.59549200 | -4.80077900 | -0.22170500 |
| | | | | H | 0.50472000 | -5.21387100 | 1.13715100 |
| | | | | H | -0.16684800 | -4.99726700 | -0.50954300 |

L-L = dppe
M = Fe

[Fe-S]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.31420100 | 0.24641500 | 2.73911800 |
| C | -0.47743800 | -0.83068000 | 3.15481600 |
| C | 0.89775800 | -0.40100500 | 3.08241600 |
| C | 0.89740100 | 0.95744600 | 2.62426400 |
| C | -0.46165200 | 1.36163800 | 2.39544300 |
| H | -2.40418100 | 0.23862600 | 2.69344800 |
| H | -0.81698800 | -1.82914700 | 3.43683100 |
| H | 1.77381300 | -1.00218400 | 3.32871500 |
| H | 1.78020900 | 1.57997600 | 2.46707900 |
| H | -0.80672400 | 2.34521900 | 2.07509000 |
| Fe | 0.00911200 | -0.27684600 | 1.15824900 |
| C | 0.74136100 | -0.17496100 | -2.03384000 |
| H | 1.37118800 | 0.17873800 | -2.86993000 |
| H | 0.62053800 | -1.26955800 | -2.12712300 |
| C | -0.63217600 | 0.51186400 | -2.03306500 |
| H | -1.22794100 | 0.22246000 | -2.91544000 |

[Fe-H]⁰

| | x | y | z |
|---|-------------|-------------|------------|
| C | -1.18372400 | -0.26996100 | 2.87023200 |
| C | -0.37810000 | -1.45396800 | 2.95906200 |
| C | 1.00642400 | -1.05838200 | 2.91939400 |
| C | 1.04066500 | 0.37960900 | 2.80834900 |
| C | -0.30622200 | 0.87328300 | 2.78656100 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | -2.27506200 | -0.23664700 | 2.86930600 | | x | y | z |
| H | -0.74941600 | -2.47727700 | 3.03378200 | C | -0.85522500 | -0.85172800 | 3.02752300 |
| H | 1.87106700 | -1.72224600 | 2.94898600 | C | 0.56755500 | -1.08991600 | 3.07604500 |
| H | 1.94666100 | 0.98788900 | 2.76119100 | C | 1.23137300 | 0.11270000 | 2.67950600 |
| H | -0.61971600 | 1.91716900 | 2.72862600 | C | 0.22715800 | 1.10342900 | 2.37620700 |
| Fe | 0.03953800 | -0.46279200 | 1.16559500 | C | -1.05526300 | 0.50177800 | 2.60701900 |
| H | 0.11210400 | -1.83609200 | 0.51045000 | H | -1.63539700 | -1.56878300 | 3.28619100 |
| C | 0.72077500 | -0.45663300 | -2.01760100 | H | 1.04901800 | -2.02555900 | 3.36547200 |
| H | 1.35414400 | -0.09946600 | -2.84978500 | H | 2.31101600 | 0.25658300 | 2.63553700 |
| H | 0.60437800 | -1.55025800 | -2.11673500 | H | 0.41222700 | 2.12723500 | 2.05154600 |
| C | -0.64933400 | 0.23751800 | -2.00340500 | H | -2.02009000 | 0.99047400 | 2.46529200 |
| H | -1.29177500 | -0.09867700 | -2.83697200 | Fe | 0.00301200 | -0.57407900 | 1.08753100 |
| H | -0.51831200 | 1.33061800 | -2.09771900 | C | 0.71733000 | -0.37702500 | -2.10283500 |
| P | 1.51793500 | -0.11636600 | -0.34199200 | H | 1.32698000 | 0.03991500 | -2.92458300 |
| P | -1.46674800 | -0.09993900 | -0.32464800 | H | 0.69347100 | -1.47344300 | -2.23903200 |
| C | 3.02781000 | -1.20583500 | -0.32515700 | C | -0.70746100 | 0.20096600 | -2.10791000 |
| C | 2.89229500 | -2.58153000 | -0.62085900 | H | -1.31268000 | -0.27417100 | -2.89867700 |
| C | 4.28942700 | -0.73004700 | 0.09562600 | H | -0.70816400 | 1.28557500 | -2.31058800 |
| C | 3.99262300 | -3.44886600 | -0.53149700 | P | 1.55489600 | -0.11634700 | -0.44766200 |
| H | 1.91309900 | -2.98466400 | -0.90456100 | P | -1.55666100 | -0.03954900 | -0.43486000 |
| C | 5.38872000 | -1.60130300 | 0.19975700 | C | 3.05064900 | -1.19667200 | -0.51665500 |
| H | 4.42092100 | 0.32965500 | 0.34213400 | C | 3.28523200 | -2.18026600 | 0.46510300 |
| C | 5.24660400 | -2.96197500 | -0.11905000 | C | 3.98241300 | -1.03198900 | -1.56865600 |
| H | 3.86765100 | -4.51058400 | -0.77581300 | C | 4.42582600 | -2.99883700 | 0.39284900 |
| H | 6.35873600 | -1.21117200 | 0.53082500 | H | 2.57437400 | -2.30961700 | 1.28727600 |
| H | 6.10438200 | -3.64031000 | -0.04232000 | C | 5.11504000 | -1.85656000 | -1.64305500 |
| C | 2.26785600 | 1.56995800 | -0.65968300 | H | 3.83308700 | -0.25300300 | -2.32571800 |
| C | 1.87997800 | 2.66048800 | 0.14489700 | C | 5.33851800 | -2.84111700 | -0.66254400 |
| C | 3.16731200 | 1.80256600 | -1.72601600 | H | 4.59759900 | -3.76066400 | 1.16116500 |
| C | 2.37957800 | 3.95284700 | -0.10130000 | H | 5.82762000 | -1.72597200 | -2.46491000 |
| H | 1.17473200 | 2.48434200 | 0.96525600 | H | 6.22573300 | -3.48094000 | -0.72158300 |
| C | 3.66105900 | 3.09287300 | -1.98025200 | C | 2.30174900 | 1.57700500 | -0.50569900 |
| H | 3.49706400 | 0.96754400 | -2.35653700 | C | 3.36416800 | 1.88537100 | 0.37615800 |
| C | 3.26876900 | 4.17229400 | -1.16675100 | C | 1.85551000 | 2.57257500 | -1.40307400 |
| H | 2.07060500 | 4.78794500 | 0.53896800 | C | 3.94894000 | 3.16128100 | 0.37360800 |
| H | 4.35602400 | 3.25574700 | -2.81286200 | H | 3.76827800 | 1.11409100 | 1.04209800 |
| H | 3.65637000 | 5.17870800 | -1.36404900 | C | 2.44810900 | 3.84798900 | -1.40979800 |
| C | -2.63597700 | 1.34063100 | -0.12507300 | H | 1.06177100 | 2.36034400 | -2.12634200 |
| C | -2.15023600 | 2.65971900 | -0.27805100 | C | 3.48849100 | 4.14873900 | -0.51563900 |
| C | -3.97185300 | 1.16428300 | 0.29941500 | H | 4.77655900 | 3.37875700 | 1.05780100 |
| C | -2.98342700 | 3.76689200 | -0.04923900 | H | 2.09914800 | 4.60231600 | -2.12392100 |
| H | -1.10731700 | 2.82940700 | -0.57164000 | H | 3.94997400 | 5.14209400 | -0.52193000 |
| C | -4.80283000 | 2.27270000 | 0.54306400 | C | -2.47490700 | 1.54824900 | -0.17069500 |
| H | -4.37371400 | 0.15373300 | 0.43369000 | C | -1.76573700 | 2.77207400 | -0.17854200 |
| C | -4.31475000 | 3.57765500 | 0.36407700 | C | -3.86148700 | 1.56074600 | 0.09744000 |
| H | -2.58866700 | 4.78054100 | -0.18845400 | C | -2.43545200 | 3.98381600 | 0.05341100 |
| H | -5.83683400 | 2.11135100 | 0.87101100 | H | -0.68434500 | 2.78769500 | -0.36058900 |
| H | -4.96448400 | 4.44135800 | 0.54745700 | C | -4.52652900 | 2.77705500 | 0.33566300 |
| C | -2.65730300 | -1.47497700 | -0.77328700 | H | -4.43050700 | 0.62550800 | 0.11254800 |
| C | -3.58117800 | -1.35116900 | -1.83652600 | C | -3.81840500 | 3.98946100 | 0.31146100 |
| C | -2.61181200 | -2.68526900 | -0.05379200 | H | -1.87466700 | 4.92509800 | 0.03573600 |
| C | -4.43288200 | -2.41624000 | -2.17332700 | H | -5.60354200 | 2.77155500 | 0.53670600 |
| H | -3.64782200 | -0.41242500 | -2.40085000 | H | -4.33950100 | 4.93556600 | 0.49375800 |
| C | -3.46718400 | -3.75188200 | -0.38536700 | C | -2.90447800 | -1.26424000 | -0.74935300 |
| H | -1.88049900 | -2.78040800 | 0.75728000 | C | -3.67330700 | -1.20179800 | -1.93571700 |
| C | -4.37774000 | -3.62086300 | -1.44721000 | C | -3.22453500 | -2.23531900 | 0.22195200 |
| H | -5.14193000 | -2.30558700 | -3.00270800 | C | -4.72243200 | -2.10949100 | -2.14968300 |
| H | -3.41779400 | -4.68741300 | 0.18489600 | H | -3.47400300 | -0.43493300 | -2.69326300 |
| H | -5.04244200 | -4.45212700 | -1.71068700 | C | -4.27968700 | -3.13879100 | 0.00910600 |
| | | | | H | -2.64187100 | -2.29034000 | 1.14661300 |
| | | | | C | -5.02554800 | -3.08172800 | -1.17937000 |
| | | | | H | -5.30609700 | -2.05335600 | -3.07514600 |

[Fe-CO]⁺

| | | | |
|---|-------------|-------------|-------------|
| H | -4.51167700 | -3.89172900 | 0.77021400 |
| H | -5.84311600 | -3.79042300 | -1.35049200 |
| C | -0.01578800 | -2.23970400 | 0.59005900 |
| O | -0.02299600 | -3.37921000 | 0.31094200 |

L-L = dppe
M = Co

[Co-S]²⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.28380200 | 0.47351000 | 2.69349000 |
| C | -0.49243200 | -0.60276700 | 3.18145200 |
| C | 0.90337000 | -0.23500900 | 3.07526100 |
| C | 0.96506300 | 1.08445800 | 2.53260300 |
| C | -0.38200500 | 1.51584000 | 2.25209400 |
| H | -2.37327300 | 0.51322100 | 2.65011900 |
| H | -0.86932900 | -1.56140800 | 3.54339100 |
| H | 1.75218300 | -0.85791700 | 3.36131800 |
| H | 1.86838800 | 1.66621800 | 2.34180600 |
| H | -0.68465800 | 2.49136600 | 1.87045600 |
| Co | 0.01463800 | -0.19060800 | 1.12358300 |
| C | 0.71330000 | -0.13778800 | -2.05337200 |
| H | 1.33399100 | 0.19697000 | -2.90384600 |
| H | 0.56198300 | -1.22846300 | -2.14037100 |
| C | -0.63587300 | 0.59433100 | -2.02846600 |
| H | -1.23499000 | 0.36815200 | -2.92708500 |
| H | -0.48691000 | 1.68815100 | -2.01854800 |
| P | 1.60822400 | 0.20581300 | -0.44950100 |
| P | -1.57969300 | 0.14097200 | -0.48120800 |
| C | 3.03543700 | -0.93450700 | -0.34722700 |
| C | 3.28976000 | -1.90647400 | -1.34189500 |
| C | 3.91949700 | -0.81804500 | 0.75259300 |
| C | 4.41564500 | -2.74261900 | -1.23749300 |
| H | 2.64055700 | -2.00202100 | -2.21845500 |
| C | 5.03752900 | -1.65896300 | 0.85329000 |
| H | 3.75229700 | -0.05372200 | 1.52057100 |
| C | 5.28623300 | -2.62448400 | -0.14050700 |
| H | 4.61870800 | -3.47637700 | -2.02520300 |
| H | 5.72164200 | -1.55413100 | 1.70218600 |
| H | 6.16478500 | -3.27396300 | -0.06499800 |
| C | 2.32278100 | 1.88911400 | -0.62102400 |
| C | 1.55329400 | 3.03880400 | -0.33069000 |
| C | 3.63296600 | 2.04332800 | -1.13579200 |
| C | 2.07919300 | 4.32121300 | -0.55346900 |
| H | 0.54466900 | 2.93420000 | 0.08116100 |
| C | 4.15225000 | 3.32975500 | -1.35607900 |
| H | 4.24935200 | 1.16806100 | -1.36405500 |
| C | 3.38043900 | 4.46804200 | -1.06618700 |
| H | 1.47715800 | 5.20598800 | -0.31983100 |
| H | 5.16730800 | 3.43893600 | -1.75259500 |
| H | 3.79362600 | 5.46826400 | -1.23343600 |
| C | -2.83860800 | 1.45732900 | -0.23446000 |
| C | -2.51733100 | 2.82050400 | -0.44439500 |
| C | -4.14609700 | 1.11153800 | 0.18322000 |
| C | -3.49102100 | 3.81368700 | -0.25478100 |
| H | -1.51893400 | 3.12233200 | -0.78031300 |
| C | -5.11171000 | 2.11259600 | 0.37836300 |
| H | -4.42431900 | 0.06266400 | 0.32946300 |
| C | -4.78811900 | 3.46286400 | 0.16122100 |
| H | -3.23756200 | 4.86292700 | -0.44068300 |
| H | -6.12375000 | 1.83168400 | 0.68884400 |

| | | | |
|---|-------------|-------------|-------------|
| H | -5.54597100 | 4.23982200 | 0.30644100 |
| C | -2.54019400 | -1.38806100 | -0.83358300 |
| C | -2.98548100 | -1.68874200 | -2.14162400 |
| C | -2.94261000 | -2.21682500 | 0.24001000 |
| C | -3.80631400 | -2.80658400 | -2.36880900 |
| H | -2.72151400 | -1.05275900 | -2.99274700 |
| C | -3.77409500 | -3.32485300 | 0.00886600 |
| H | -2.61248300 | -1.99414200 | 1.26102100 |
| C | -4.20291000 | -3.62445900 | -1.29692100 |
| H | -4.14544800 | -3.02781200 | -3.38644900 |
| H | -4.09327200 | -3.95048900 | 0.84979800 |
| H | -4.85166200 | -4.48824300 | -1.47717300 |
| N | 0.19245100 | -2.02076300 | 0.74164300 |
| C | 0.33388200 | -3.17277500 | 0.58316800 |
| C | 0.49846300 | -4.60544700 | 0.38519700 |
| H | 1.49107300 | -4.81740200 | -0.04977500 |
| H | 0.41688600 | -5.13420700 | 1.35158700 |
| H | -0.28388000 | -4.98701000 | -0.29454100 |

[Co-H]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.16360400 | -0.44638400 | 2.82589900 |
| C | -0.22344000 | -1.52798200 | 2.90435600 |
| C | 1.09944400 | -0.97259500 | 2.84814500 |
| C | 0.96830500 | 0.46455600 | 2.76781300 |
| C | -0.42232100 | 0.79296000 | 2.75069500 |
| H | -2.25073400 | -0.53972300 | 2.84097400 |
| H | -0.46808200 | -2.58863800 | 2.97355300 |
| H | 2.03470100 | -1.53311600 | 2.86378800 |
| H | 1.79794100 | 1.17223700 | 2.72573900 |
| H | -0.85631500 | 1.79260000 | 2.69915500 |
| Co | 0.04937600 | -0.47508200 | 1.10125300 |
| H | 0.11499500 | -1.79838700 | 0.42977800 |
| C | 0.71816800 | -0.45622800 | -2.04358300 |
| H | 1.34654300 | -0.12152200 | -2.88788400 |
| H | 0.57615600 | -1.54755400 | -2.13119500 |
| C | -0.63359700 | 0.27457900 | -2.01957600 |
| H | -1.27582500 | -0.02891200 | -2.86466700 |
| H | -0.48044400 | 1.36611400 | -2.08986200 |
| P | 1.56638100 | -0.10058700 | -0.41363400 |
| P | -1.50249300 | -0.08774300 | -0.39128700 |
| C | 3.05101700 | -1.18264700 | -0.31811900 |
| C | 2.94843500 | -2.54758500 | -0.67088600 |
| C | 4.27348700 | -0.69154500 | 0.19308900 |
| C | 4.05826900 | -3.39743200 | -0.54337700 |
| H | 2.00212900 | -2.95786400 | -1.04189100 |
| C | 5.37828900 | -1.54928600 | 0.32867200 |
| H | 4.37208500 | 0.36194400 | 0.47734200 |
| C | 5.27499500 | -2.90056300 | -0.04232600 |
| H | 3.97073500 | -4.45035400 | -0.83315600 |
| H | 6.32221600 | -1.15638000 | 0.72244300 |
| H | 6.13924300 | -3.56593300 | 0.05920000 |
| C | 2.22324600 | 1.60871100 | -0.66439400 |
| C | 1.71300800 | 2.69295000 | 0.07875500 |
| C | 3.19898300 | 1.85259600 | -1.66048600 |
| C | 2.17382400 | 4.00039000 | -0.15920500 |
| H | 0.95106900 | 2.51037500 | 0.84376200 |
| C | 3.65476000 | 3.15881600 | -1.89781600 |
| H | 3.61536100 | 1.02294000 | -2.24410500 |
| C | 3.14470500 | 4.23415200 | -1.14679900 |
| H | 1.77485200 | 4.83429400 | 0.42918700 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 4.41310100 | 3.33648800 | -2.66836400 | H | 4.28660100 | 0.86445000 | 0.32346700 |
| H | 3.50634200 | 5.25150900 | -1.33200000 | C | 2.52832200 | 3.99109700 | -1.23637300 |
| C | -2.63967600 | 1.33557700 | -0.09932100 | H | 0.81240600 | 2.72615800 | -1.54790900 |
| C | -2.18000700 | 2.66164100 | -0.27210100 | C | 3.84364000 | 4.08819800 | -0.74531400 |
| C | -3.95254300 | 1.11987100 | 0.37730900 | H | 5.49318800 | 3.02970000 | 0.19467100 |
| C | -3.02772400 | 3.74777800 | -0.00164500 | H | 2.04680700 | 4.86138900 | -1.69510400 |
| H | -1.15920300 | 2.85725300 | -0.62096200 | H | 4.38476600 | 5.03770100 | -0.81429000 |
| C | -4.79335100 | 2.21067100 | 0.65655400 | C | -2.86026400 | 1.39254700 | -0.36932200 |
| H | -4.32894900 | 0.10049700 | 0.51668600 | C | -2.39853000 | 2.73161300 | -0.31915100 |
| C | -4.33572900 | 3.52519900 | 0.46482000 | C | -4.25097700 | 1.13390600 | -0.39399300 |
| H | -2.66494000 | 4.77003400 | -0.15661000 | C | -3.31411000 | 3.79292100 | -0.30066800 |
| H | -5.81136200 | 2.02878800 | 1.01849600 | H | -1.32429400 | 2.95233700 | -0.30068900 |
| H | -4.99567200 | 4.37373600 | 0.67551000 | C | -5.16061200 | 2.20534800 | -0.37329600 |
| C | -2.62471800 | -1.50055600 | -0.78611500 | H | -4.62894100 | 0.10879400 | -0.44953800 |
| C | -3.55660900 | -1.38961300 | -1.84548100 | C | -4.69780500 | 3.53042300 | -0.32389800 |
| C | -2.55629200 | -2.70148600 | -0.05140800 | H | -2.95056200 | 4.82561100 | -0.27002700 |
| C | -4.39390500 | -2.46958300 | -2.16504400 | H | -6.23541100 | 1.99749400 | -0.40306100 |
| H | -3.64210200 | -0.45736200 | -2.41682200 | H | -5.41168100 | 4.36062300 | -0.30704900 |
| C | -3.39959700 | -3.78014600 | -0.37118200 | C | -2.56995200 | -1.53508000 | -0.65136900 |
| H | -1.83248000 | -2.78985600 | 0.76538400 | C | -2.53995200 | -2.31155100 | -1.83233100 |
| C | -4.31649000 | -3.66669900 | -1.42891700 | C | -3.32932400 | -1.98135200 | 0.45925400 |
| H | -5.10991100 | -2.37504100 | -2.98894700 | C | -3.27195800 | -3.50910100 | -1.90216100 |
| H | -3.33708900 | -4.70911000 | 0.20642700 | H | -1.96296200 | -1.99652200 | -2.70777100 |
| H | -4.97183100 | -4.50761800 | -1.68093500 | C | -4.06246400 | -3.17336200 | 0.37804700 |

[Co-CO]²⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -0.78183900 | -0.17199200 | 3.13726900 |
| C | 0.66602300 | -0.24979200 | 3.17159700 |
| C | 1.18798800 | 0.91659800 | 2.53396800 |
| C | 0.07434700 | 1.71002400 | 2.07449000 |
| C | -1.13944400 | 1.04624800 | 2.48458200 |
| H | -1.47031400 | -0.91058800 | 3.55214700 |
| H | 1.24732900 | -1.05866800 | 3.61897200 |
| H | 2.24301800 | 1.16522000 | 2.40707200 |
| H | 0.14836400 | 2.67747300 | 1.57781800 |
| H | -2.15348400 | 1.40758700 | 2.30713700 |
| Co | -0.01220400 | -0.17489200 | 1.13031300 |
| C | 0.67907400 | -0.27094300 | -2.08950200 |
| H | 1.28098300 | 0.12575200 | -2.92665500 |
| H | 0.62489400 | -1.36883800 | -2.20593700 |
| C | -0.71922700 | 0.35672400 | -2.08359900 |
| H | -1.32939600 | 0.00303300 | -2.93445300 |
| H | -0.67479000 | 1.45445500 | -2.18260900 |
| P | 1.59164200 | 0.02160700 | -0.48074700 |
| P | -1.64016200 | 0.02966100 | -0.49344900 |
| C | 2.90400300 | -1.25105900 | -0.41644300 |
| C | 3.28622400 | -1.86088200 | 0.79896600 |
| C | 3.59358000 | -1.57724900 | -1.61032300 |
| C | 4.33454600 | -2.79529100 | 0.82086000 |
| H | 2.76772700 | -1.61360900 | 1.73116800 |
| C | 4.63586600 | -2.51661600 | -1.58034500 |
| H | 3.33557000 | -1.09961900 | -2.56184800 |
| C | 5.00674800 | -3.12626800 | -0.36811300 |
| H | 4.62360500 | -3.26623000 | 1.76629900 |
| H | 5.16112000 | -2.76827700 | -2.50778500 |
| H | 5.82085300 | -3.85841800 | -0.35111900 |
| C | 2.45455000 | 1.63637500 | -0.58643400 |
| C | 3.77852400 | 1.74039500 | -0.09424000 |
| C | 1.83072800 | 2.77675100 | -1.14874000 |
| C | 4.46487800 | 2.96306500 | -0.17621400 |

| | | | |
|---|-------------|-------------|-------------|
| H | 4.28660100 | 0.86445000 | 0.32346700 |
| C | 2.52832200 | 3.99109700 | -1.23637300 |
| H | 0.81240600 | 2.72615800 | -1.54790900 |
| C | 3.84364000 | 4.08819800 | -0.74531400 |
| H | 5.49318800 | 3.02970000 | 0.19467100 |
| H | 2.04680700 | 4.86138900 | -1.69510400 |
| H | 4.38476600 | 5.03770100 | -0.81429000 |
| C | -2.86026400 | 1.39254700 | -0.36932200 |
| C | -2.39853000 | 2.73161300 | -0.31915100 |
| C | -4.25097700 | 1.13390600 | -0.39399300 |
| C | -3.31411000 | 3.79292100 | -0.30066800 |
| H | -1.32429400 | 2.95233700 | -0.30068900 |
| C | -5.16061200 | 2.20534800 | -0.37329600 |
| H | -4.62894100 | 0.10879400 | -0.44953800 |
| C | -4.69780500 | 3.53042300 | -0.32389800 |
| H | -2.95056200 | 4.82561100 | -0.27002700 |
| H | -6.23541100 | 1.99749400 | -0.40306100 |
| H | -5.41168100 | 4.36062300 | -0.30704900 |
| C | -2.56995200 | -1.53508000 | -0.65136900 |
| C | -2.53995200 | -2.31155100 | -1.83233100 |
| C | -3.32932400 | -1.98135200 | 0.45925400 |
| C | -3.27195800 | -3.50910100 | -1.90216100 |
| H | -1.96296200 | -1.99652200 | -2.70777100 |
| C | -4.06246400 | -3.17336200 | 0.37804700 |
| H | -3.36085300 | -1.39246200 | 1.38400200 |
| C | -4.03258700 | -3.94019700 | -0.80221500 |
| H | -3.24851600 | -4.10207100 | -2.82246500 |
| H | -4.65768700 | -3.50518900 | 1.23533700 |
| H | -4.60271600 | -4.87308600 | -0.86304800 |
| C | -0.00993100 | -1.93071000 | 0.96361800 |
| O | 0.00141400 | -3.08698200 | 0.91701700 |

L-L = en

M = Mn

[Mn-S]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 1.97187600 | 0.72504800 | -1.16760300 |
| C | 1.36322300 | 1.87106700 | -0.55042700 |
| C | 1.48045400 | 1.73350900 | 0.88024100 |
| C | 2.14538200 | 0.49006500 | 1.13507200 |
| C | 2.48506700 | -0.13647700 | -0.11423100 |
| H | 2.08144000 | 0.56698600 | -2.24534700 |
| H | 0.86301800 | 2.68828000 | -1.07515100 |
| H | 1.10491700 | 2.43045100 | 1.63231600 |
| H | 2.36130000 | 0.08404500 | 2.12929700 |
| H | 3.06304700 | -1.05638000 | -0.23989400 |
| Mn | 0.36983600 | 0.10297500 | 0.00028600 |
| C | -1.17054700 | -2.31704300 | 0.70261300 |
| H | -1.33108400 | -3.22235300 | 1.32235800 |
| H | -2.15508300 | -1.86621100 | 0.48377500 |
| C | -0.46418500 | -2.66708800 | -0.60753700 |
| H | -1.07456700 | -3.37432900 | -1.20619800 |
| H | 0.51284400 | -3.14135000 | -0.39983500 |
| N | -0.35414700 | -1.27640900 | 1.38883900 |
| N | -0.19468600 | -1.38450200 | -1.31466700 |
| H | -0.92610200 | -0.76616800 | 2.07279300 |
| H | 0.49344600 | -1.52345700 | -2.06523400 |
| H | -1.06039200 | -1.03175800 | -1.75772600 |
| H | 0.41940800 | -1.71238500 | 1.90867900 |
| N | -1.27219300 | 0.79367700 | -0.17030800 |

| | | | |
|---|-------------|------------|-------------|
| C | -2.38383500 | 1.19180700 | -0.46993300 |
| C | -3.60160700 | 1.83851700 | 0.09166300 |
| H | -3.48744000 | 2.07051600 | 1.17369400 |
| H | -3.82854500 | 2.78368300 | -0.43653000 |
| H | -4.48987900 | 1.19026400 | -0.03034800 |

[Mn-H]⁻¹

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.69108800 | 1.23514700 | 0.32161000 |
| C | -2.11865900 | 0.47357400 | -0.83765900 |
| C | -2.06495300 | -0.93678900 | -0.48402600 |
| C | -1.57523200 | -1.00221900 | 0.87612800 |
| C | -1.40586800 | 0.32511300 | 1.41763600 |
| H | -1.63134800 | 2.33236900 | 0.37382700 |
| H | -2.44644600 | 0.88858400 | -1.79580500 |
| H | -2.34669600 | -1.78483600 | -1.11665400 |
| H | -1.37178000 | -1.93464900 | 1.42488100 |
| H | -1.16381700 | 0.58948100 | 2.45444200 |
| Mn | -0.19742100 | -0.01530200 | -0.32737100 |
| H | 0.28161000 | -0.19134100 | -1.91489400 |
| C | 2.62824900 | -0.71444200 | -0.10840300 |
| H | 3.45809400 | -1.25190600 | 0.40953300 |
| H | 2.84572500 | -0.69095900 | -1.19265600 |
| C | 2.52649200 | 0.72181300 | 0.41714000 |
| H | 3.48797200 | 1.26359700 | 0.23231600 |
| H | 2.33645100 | 0.71207200 | 1.50829900 |
| N | 1.30872000 | -1.36779800 | 0.06266300 |
| N | 1.35012200 | 1.35598300 | -0.23347900 |
| H | 1.16483800 | -2.09164800 | -0.65086700 |
| H | 1.10620900 | 2.23280800 | 0.25050900 |
| H | 1.56922800 | 1.58527600 | -1.21448700 |
| H | 1.23993600 | -1.80677700 | 0.99699000 |

[Mn-CO]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 1.71946300 | -0.74164000 | -1.18733000 |
| C | 2.23528300 | 0.38662100 | -0.46075500 |
| C | 2.14253800 | 0.10560500 | 0.95429100 |
| C | 1.56268100 | -1.19617800 | 1.08534100 |
| C | 1.32015500 | -1.74565600 | -0.21691000 |
| H | 1.71494700 | -0.84980100 | -2.27568400 |
| H | 2.62990400 | 1.30283300 | -0.90426500 |
| H | 2.45805500 | 0.76098900 | 1.76779100 |
| H | 1.33230900 | -1.68916600 | 2.03562200 |
| H | 0.93136200 | -2.74471200 | -0.43116200 |
| Mn | 0.20589400 | 0.09720100 | -0.00812400 |
| C | -2.64262300 | -0.18569800 | 0.69737600 |
| H | -3.45681500 | -0.61252200 | 1.31768800 |
| H | -2.87697400 | 0.87454800 | 0.49745800 |
| C | -2.50288700 | -0.95147500 | -0.61861900 |
| H | -3.43679400 | -0.89115000 | -1.21306500 |
| H | -2.29835500 | -2.01862400 | -0.41176600 |
| N | -1.31543400 | -0.22418100 | 1.37423400 |
| N | -1.31728700 | -0.40089800 | -1.33738400 |
| H | -1.25983600 | 0.50327600 | 2.09594000 |
| H | -0.97440000 | -1.07649800 | -2.03209900 |
| H | -1.57459600 | 0.44741800 | -1.85539100 |
| H | -1.18994800 | -1.12751400 | 1.85244800 |
| C | -0.06530700 | 1.82029700 | -0.10363500 |
| O | -0.16662100 | 3.01439900 | -0.17461300 |

L-L = en

M = Fe

[Fe-S]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 1.72214600 | 1.18856800 | -1.17704100 |
| C | 0.79499600 | 2.10108400 | -0.59215800 |
| C | 0.89820300 | 1.98780200 | 0.84749500 |
| C | 1.89916700 | 1.00532500 | 1.12588200 |
| C | 2.41368200 | 0.48955000 | -0.11497900 |
| H | 1.86954600 | 1.03976700 | -2.24956300 |
| H | 0.10388900 | 2.74548200 | -1.13794100 |
| H | 0.31934700 | 2.54623400 | 1.58453100 |
| H | 2.19625200 | 0.67587100 | 2.12530300 |
| H | 3.21908000 | -0.23838400 | -0.23069100 |
| Fe | 0.35603900 | 0.13649900 | 0.00420200 |
| C | -0.45932600 | -2.56988900 | 0.68695800 |
| H | -0.34006500 | -3.48217800 | 1.29973600 |
| H | -1.53848500 | -2.39208600 | 0.53989800 |
| C | 0.24647400 | -2.70548700 | -0.65855200 |
| H | -0.19126000 | -3.52107000 | -1.26328100 |
| H | 1.31829700 | -2.92572200 | -0.51097500 |
| N | 0.10702700 | -1.35970100 | 1.35861700 |
| N | 0.15117000 | -1.37824100 | -1.34359200 |
| H | -0.50868700 | -1.05418300 | 2.12436500 |
| H | 0.84665100 | -1.32094800 | -2.09884000 |
| H | -0.76876100 | -1.28233400 | -1.79795100 |
| H | 1.01106100 | -1.59352500 | 1.79205300 |
| N | -1.48491100 | 0.43541900 | -0.01993300 |
| C | -2.63427100 | 0.70444300 | -0.04618100 |
| C | -4.04117300 | 1.09435300 | -0.07333100 |
| H | -4.27957700 | 1.74051400 | 0.79091100 |
| H | -4.27190500 | 1.65174200 | -0.99925000 |
| H | -4.69478300 | 0.20500400 | -0.03176700 |

[Fe-H]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.68390100 | 1.22200800 | 0.37185300 |
| C | -2.05672200 | 0.55922300 | -0.84946700 |
| C | -2.02801500 | -0.86750700 | -0.59598600 |
| C | -1.63497000 | -1.04618300 | 0.77922700 |
| C | -1.45393400 | 0.23867000 | 1.40687800 |
| H | -1.59083000 | 2.30691700 | 0.49188000 |
| H | -2.30434100 | 1.04464800 | -1.79489800 |
| H | -2.25935200 | -1.65933600 | -1.31060800 |
| H | -1.49691100 | -2.01634300 | 1.26923600 |
| H | -1.24104900 | 0.43113800 | 2.46132400 |
| Fe | -0.17857200 | -0.03091300 | -0.27839100 |
| H | 0.24392200 | -0.20832800 | -1.77293600 |
| C | 2.62428600 | -0.70197100 | -0.15115100 |
| H | 3.46950600 | -1.24903200 | 0.31368000 |
| H | 2.76940500 | -0.69128800 | -1.24526500 |
| C | 2.54602900 | 0.73239600 | 0.37605000 |
| H | 3.46737800 | 1.29608600 | 0.12233500 |
| H | 2.43977500 | 0.72571600 | 1.47658600 |
| N | 1.30629200 | -1.34428800 | 0.10745700 |
| N | 1.31182800 | 1.34683900 | -0.18693400 |
| H | 1.17345900 | -2.14825500 | -0.51657100 |
| H | 1.04107200 | 2.17688900 | 0.35550000 |
| H | 1.46786000 | 1.65123400 | -1.15550100 |
| H | 1.25949700 | -1.69399300 | 1.07531100 |

| [Fe-CO] ⁺ | | | |
|----------------------|-------------|-------------|-------------|
| | x | y | z |
| C | 1.68013100 | -0.96989700 | -1.10320000 |
| C | 2.18287800 | 0.29859300 | -0.68431900 |
| C | 2.14346300 | 0.33236000 | 0.76535900 |
| C | 1.62529700 | -0.92241700 | 1.21121700 |
| C | 1.32624000 | -1.73772600 | 0.06527000 |
| H | 1.57965400 | -1.29412400 | -2.14174000 |
| H | 2.53304200 | 1.09907900 | -1.33790700 |
| H | 2.46604400 | 1.15923400 | 1.39984300 |
| H | 1.46254100 | -1.19897100 | 2.25594400 |
| H | 0.96118400 | -2.76635100 | 0.07891400 |
| Fe | 0.18538400 | 0.06525400 | -0.00859500 |
| C | -2.61902600 | -0.16547700 | 0.68657100 |
| H | -3.41475400 | -0.58125800 | 1.33076500 |
| H | -2.85337500 | 0.89460400 | 0.48904500 |
| C | -2.48789200 | -0.94795600 | -0.61518500 |
| H | -3.39971000 | -0.86489900 | -1.23319200 |
| H | -2.31311500 | -2.01791600 | -0.40535900 |
| N | -1.27981700 | -0.21712000 | 1.35500100 |
| N | -1.27942500 | -0.42424400 | -1.33307400 |
| H | -1.23122200 | 0.47793000 | 2.11221800 |
| H | -0.94813500 | -1.12115600 | -2.01317700 |
| H | -1.53240300 | 0.40416600 | -1.88841000 |
| H | -1.15406100 | -1.13580800 | 1.80394900 |
| C | -0.08906200 | 1.79346000 | -0.12352400 |
| O | -0.20414600 | 2.95659900 | -0.19925700 |

| L-L = en | | | |
|-----------------------|-------------|-------------|-------------|
| M = Co | | | |
| [Co-H] ⁺ | | | |
| | x | y | z |
| H | 4.34196100 | -1.67852400 | 0.76906500 |
| H | 4.34588400 | -1.52029700 | -1.02214600 |
| H | 4.71911500 | -0.09539200 | 0.00757900 |
| [Co-S] ²⁺ | | | |
| | x | y | z |
| C | -1.72342500 | -1.23406700 | -1.17305600 |
| C | -0.74852500 | -2.11195100 | -0.62056400 |
| C | -0.82188800 | -2.01438400 | 0.82693100 |
| C | -1.85901300 | -1.08729100 | 1.14658000 |
| C | -2.39172100 | -0.55347700 | -0.08280800 |
| H | -1.90737800 | -1.08030300 | -2.23932400 |
| H | -0.05014100 | -2.73083700 | -1.18769300 |
| H | -0.20261100 | -2.56033200 | 1.54159700 |
| H | -2.15849300 | -0.79383300 | 2.15631800 |
| H | -3.21132900 | 0.16317700 | -0.17323400 |
| Co | -0.35813300 | -0.11567400 | 0.00397700 |
| C | 0.40013000 | 2.56977100 | 0.68313800 |
| H | 0.26111500 | 3.46485900 | 1.31485100 |
| H | 1.48190300 | 2.41050200 | 0.54300400 |
| C | -0.31781800 | 2.70336800 | -0.65228900 |
| H | 0.11677500 | 3.50600700 | -1.27393600 |
| H | -1.38925400 | 2.92456300 | -0.50878900 |
| N | -0.15966200 | 1.34777800 | 1.35604400 |
| N | -0.21489700 | 1.37136200 | -1.34456300 |
| H | 0.45250300 | 1.04430300 | 2.12852300 |
| H | -0.90686900 | 1.31603900 | -2.10585900 |
| H | 0.70695800 | 1.27467200 | -1.79757700 |
| H | -1.06919300 | 1.57638800 | 1.78501200 |
| N | 1.54492700 | -0.39254300 | -0.02356900 |
| C | 2.68683900 | -0.66242200 | -0.04654200 |
| C | 4.09976600 | -1.00688100 | -0.07474800 |
| [Co-CO] ²⁺ | | | |
| | x | y | z |
| C | 1.72782500 | -0.93627600 | -1.10679200 |
| C | 2.17350900 | 0.35574000 | -0.68876500 |
| C | 2.12715900 | 0.39153200 | 0.76710400 |
| C | 1.66888600 | -0.88781300 | 1.21811300 |
| C | 1.38285300 | -1.70420700 | 0.06703500 |
| H | 1.65095100 | -1.27255200 | -2.14451200 |
| H | 2.50608300 | 1.16574300 | -1.34370700 |
| H | 2.42650900 | 1.23056200 | 1.40092800 |
| H | 1.52987100 | -1.17656100 | 2.26393100 |
| H | 1.04801400 | -2.74467800 | 0.08111600 |
| Co | 0.17283300 | 0.04824200 | -0.00657900 |
| C | -2.60912100 | -0.19988200 | 0.68103500 |
| H | -3.38798400 | -0.61951400 | 1.34259800 |
| H | -2.86175300 | 0.85563800 | 0.48278400 |
| C | -2.46800100 | -1.00062000 | -0.60486500 |
| H | -3.36768400 | -0.92103400 | -1.24029000 |
| H | -2.29243400 | -2.06913100 | -0.39257700 |
| N | -1.26548700 | -0.23967100 | 1.36046100 |
| N | -1.25783800 | -0.47204700 | -1.33459100 |
| H | -1.22416300 | 0.44964000 | 2.12789300 |
| H | -0.92494400 | -1.17350700 | -2.01282100 |
| H | -1.51752100 | 0.34860100 | -1.90385700 |
| H | -1.13221800 | -1.16165600 | 1.80490200 |
| C | -0.14583100 | 1.82778500 | -0.13262000 |
| O | -0.32495200 | 2.96129800 | -0.20891200 |

2. Pincer Systems: [(PCP)M(L-L)]ⁿ⁺

L-L = bis CO

M = Mn

[Mn-S]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.19575100 | 2.00790000 | -0.11460800 |
| C | 0.00000800 | 1.27024300 | -0.15718100 |
| C | 1.19578700 | 2.00785200 | -0.11441000 |
| C | 1.22693100 | 3.41133600 | -0.02451400 |
| C | 0.00004800 | 4.09995200 | 0.01820000 |
| C | -1.22685600 | 3.41138500 | -0.02471900 |
| H | 2.18302700 | 3.94426800 | 0.00474900 |
| H | 0.00006400 | 5.19431500 | 0.08289100 |
| H | -2.18293600 | 3.94435300 | 0.00439100 |
| O | -2.41220800 | 1.31388000 | -0.16104100 |
| O | 2.41222600 | 1.31378800 | -0.16064900 |
| P | -2.19820100 | -0.37884600 | -0.24011300 |
| P | 2.19817200 | -0.37890100 | -0.24035100 |
| Mn | -0.00002300 | -0.78492900 | -0.24538400 |
| C | -3.26531300 | -0.77812400 | -1.69203300 |
| H | -3.36912500 | -1.87430400 | -1.77961000 |
| H | -4.26388700 | -0.32236300 | -1.57482800 |
| H | -2.79695100 | -0.39607900 | -2.61343100 |
| C | -3.29413600 | -0.89910800 | 1.15828800 |
| H | -4.28513400 | -0.42069700 | 1.06951000 |
| H | -3.41246000 | -1.99704700 | 1.14203400 |
| H | -2.83781100 | -0.60607400 | 2.11731200 |
| C | 3.29432500 | -0.89970300 | 1.15767300 |
| H | 3.41265900 | -1.99763300 | 1.14095700 |
| H | 4.28530400 | -0.42124200 | 1.06894200 |
| H | 2.83813000 | -0.60706800 | 2.11688000 |
| C | 3.26503900 | -0.77766700 | -1.69259600 |
| H | 4.26369800 | -0.32211600 | -1.57529900 |
| H | 3.36866600 | -1.87382200 | -1.78071000 |
| H | 2.79661600 | -0.39511300 | -2.61375300 |
| C | -0.00013700 | -0.69379700 | -2.01080000 |
| O | -0.00025700 | -0.62639900 | -3.18936300 |
| C | -0.00006400 | -2.58105000 | -0.27674300 |
| O | -0.00012300 | -3.76141300 | -0.31750800 |
| N | 0.00012200 | -0.73934000 | 1.72499800 |
| C | 0.00011900 | -0.67161100 | 2.89732000 |
| C | 0.00033300 | -0.57018700 | 4.35367800 |
| H | 0.89781500 | -1.05504100 | 4.77813200 |
| H | -0.00440500 | 0.49043300 | 4.66260500 |
| H | -0.89221800 | -1.06334600 | 4.77896300 |

[Mn-H]⁻¹

| | x | y | z |
|---|-------------|------------|-------------|
| C | 1.19227500 | 1.95942600 | -0.02707000 |
| C | 0.00004800 | 1.20960900 | -0.01715300 |
| C | -1.19212300 | 1.95951500 | -0.02712200 |
| C | -1.22470200 | 3.36791400 | -0.00270500 |
| C | 0.00015300 | 4.06435100 | 0.01738400 |
| C | 1.22495800 | 3.36782300 | -0.00265100 |
| H | -2.18379300 | 3.89940400 | -0.00383000 |
| H | 0.00019400 | 5.16203800 | 0.03802000 |
| H | 2.18408900 | 3.89924200 | -0.00373700 |

| | | | |
|----|-------------|-------------|-------------|
| O | 2.40235200 | 1.26141900 | -0.07585600 |
| O | -2.40225000 | 1.26159900 | -0.07595600 |
| P | 2.12398200 | -0.43870100 | -0.21609100 |
| P | -2.12401100 | -0.43855000 | -0.21608500 |
| Mn | -0.00002800 | -0.84406900 | -0.03121400 |
| C | 3.39622200 | -1.00617900 | 1.01779200 |
| H | 3.53243200 | -2.09885900 | 0.92096500 |
| H | 4.36557200 | -0.49785900 | 0.86065700 |
| H | 3.02640100 | -0.79094900 | 2.03408900 |
| C | 3.05810800 | -0.75433800 | -1.79439400 |
| H | 4.08874000 | -0.35526000 | -1.75143100 |
| H | 3.08681100 | -1.84333600 | -1.98220400 |
| H | 2.50546500 | -0.27589900 | -2.61969700 |
| C | -3.05819000 | -0.75422000 | -1.79434900 |
| H | -3.08697100 | -1.84322800 | -1.98208900 |
| H | -4.08879400 | -0.35506900 | -1.75139000 |
| H | -2.50553100 | -0.27587100 | -2.61969500 |
| C | -3.39627100 | -1.00585800 | 1.01785800 |
| H | -4.36558700 | -0.49748000 | 0.86070500 |
| H | -3.53255900 | -2.09853500 | 0.92110800 |
| H | -3.02641700 | -0.79058500 | 2.03413400 |
| C | -0.00002200 | -1.03814000 | 1.73489500 |
| O | -0.00006000 | -1.19913500 | 2.91697500 |
| C | -0.00009400 | -2.57016800 | -0.45119200 |
| O | -0.00017600 | -3.71729400 | -0.77703600 |
| H | -0.00002900 | -0.62839300 | -1.62539700 |

[Mn-CO]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.19772200 | 1.98486800 | -0.00011500 |
| C | 0.00000000 | 1.25364300 | 0.00009000 |
| C | 1.19772700 | 1.98486000 | 0.00010300 |
| C | 1.22754400 | 3.39010400 | -0.00025300 |
| C | 0.00001000 | 4.07850300 | -0.00054800 |
| C | -1.22752900 | 3.39011300 | -0.00047700 |
| H | 2.18323800 | 3.92377700 | -0.00024400 |
| H | 0.00001400 | 5.17437200 | -0.00080400 |
| H | -2.18321900 | 3.92379300 | -0.00063900 |
| O | -2.40940400 | 1.28163900 | 0.00024900 |
| O | 2.40940400 | 1.28162100 | 0.00069900 |
| P | -2.20557900 | -0.40742500 | -0.00045200 |
| P | 2.20556700 | -0.40744100 | -0.00057200 |
| Mn | -0.00000900 | -0.81268900 | 0.00065500 |
| C | -3.27140700 | -0.87976300 | -1.43025700 |
| H | -3.36022300 | -1.97985600 | -1.47279600 |
| H | -4.27592400 | -0.43534000 | -1.32099000 |
| H | -2.81891600 | -0.52558400 | -2.37042900 |
| C | -3.27307200 | -0.88133400 | 1.42756500 |
| H | -4.27748600 | -0.43675700 | 1.31794100 |
| H | -3.36195200 | -1.98149100 | 1.46846200 |
| H | -2.82150200 | -0.52849200 | 2.36869000 |
| C | 3.27324300 | -0.88182800 | 1.42714200 |
| H | 3.36223200 | -1.98199400 | 1.46756700 |
| H | 4.27760400 | -0.43711200 | 1.31759700 |
| H | 2.82173900 | -0.52942100 | 2.36846200 |
| C | 3.27120400 | -0.87931500 | -1.43068000 |
| H | 4.27578400 | -0.43505500 | -1.32133200 |
| H | 3.35988600 | -1.97940100 | -1.47369700 |
| H | 2.81865600 | -0.52468500 | -2.37065500 |

| | | | |
|---|-------------|-------------|-------------|
| C | -0.00009500 | -0.71410400 | -1.81311300 |
| O | -0.00015100 | -0.63380300 | -2.98279600 |
| C | -0.00001300 | -2.60819400 | 0.00229500 |
| O | -0.00005200 | -3.78576100 | 0.00364200 |
| C | 0.00005400 | -0.71055800 | 1.81441800 |
| O | 0.00030300 | -0.62725600 | 2.98381200 |

L-L = bis CO

M = Fe

[Fe-S]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.20138800 | 1.98777100 | -0.03313800 |
| C | -0.00038200 | 1.26475900 | -0.10888700 |
| C | 1.20028700 | 1.98831200 | -0.03292200 |
| C | 1.22777800 | 3.38203600 | 0.12539000 |
| C | -0.00104300 | 4.06340000 | 0.19972300 |
| C | -1.22954200 | 3.38148300 | 0.12516200 |
| H | 2.18199400 | 3.91400200 | 0.18220300 |
| H | -0.00129900 | 5.15210800 | 0.31654800 |
| H | -2.18401000 | 3.91301600 | 0.18180800 |
| O | -2.41457100 | 1.28773700 | -0.11301700 |
| O | 2.41381300 | 1.28884200 | -0.11254600 |
| P | -2.23265000 | -0.37726700 | -0.25459400 |
| P | 2.23271900 | -0.37616900 | -0.25509600 |
| Fe | 0.00011400 | -0.73553400 | -0.27421400 |
| C | -3.24509000 | -0.76800700 | -1.73374300 |
| H | -3.30275300 | -1.86274100 | -1.86757200 |
| H | -4.26409500 | -0.36590700 | -1.59902900 |
| H | -2.80048600 | -0.31975000 | -2.63650200 |
| C | -3.25173700 | -1.01471100 | 1.13455600 |
| H | -4.27081600 | -0.59745000 | 1.05940800 |
| H | -3.30469300 | -2.11624600 | 1.08249400 |
| H | -2.81341300 | -0.71752600 | 2.09925400 |
| C | 3.25265500 | -1.01386600 | 1.13330200 |
| H | 3.30649700 | -2.11531500 | 1.08034500 |
| H | 4.27137600 | -0.59572100 | 1.05820400 |
| H | 2.81435700 | -0.71781800 | 2.09836100 |
| C | 3.24483100 | -0.76556200 | -1.73483700 |
| H | 4.26377100 | -0.36329900 | -1.60012700 |
| H | 3.30273600 | -1.86017900 | -1.86951300 |
| H | 2.79984200 | -0.31674100 | -2.63712600 |
| C | -0.00019600 | -0.44491700 | -1.99502600 |
| O | -0.00049500 | -0.22984000 | -3.14081200 |
| C | 0.00049100 | -2.52817500 | -0.41337900 |
| O | 0.00137300 | -3.68754000 | -0.52165800 |
| N | 0.00040900 | -0.79569700 | 1.68699700 |
| C | 0.00068200 | -0.78586000 | 2.85722100 |
| C | 0.00099000 | -0.75674000 | 4.31518100 |
| H | 0.89652800 | -1.26879400 | 4.70897900 |
| H | 0.00155900 | 0.28840200 | 4.67154900 |
| H | -0.89492300 | -1.26788900 | 4.70931800 |

[Fe-H]⁰

| | x | y | z |
|---|-------------|------------|-------------|
| C | 1.19383100 | 1.93704700 | -0.04427200 |
| C | -0.00001300 | 1.19948400 | -0.03088500 |
| C | -1.19385800 | 1.93703900 | -0.04468000 |
| C | -1.22581300 | 3.34146600 | -0.04233800 |

| | | | |
|----|-------------|-------------|-------------|
| C | -0.00001900 | 4.03254500 | -0.03183400 |
| C | 1.22578400 | 3.34147300 | -0.04192500 |
| H | -2.18261100 | 3.87303300 | -0.04953700 |
| H | -0.00002300 | 5.12833200 | -0.02820600 |
| H | 2.18258200 | 3.87304300 | -0.04881500 |
| O | 2.40164600 | 1.22625800 | -0.07240400 |
| O | -2.40165800 | 1.22625700 | -0.07321500 |
| P | 2.14349800 | -0.44186100 | -0.22742400 |
| P | -2.14353700 | -0.44194900 | -0.22738000 |
| Fe | -0.00000500 | -0.80772700 | -0.00423000 |
| C | 3.36310400 | -1.08269300 | 0.99635200 |
| H | 3.42686300 | -2.18179800 | 0.90871900 |
| H | 4.36002500 | -0.64322400 | 0.81698700 |
| H | 3.03044500 | -0.82850600 | 2.01583800 |
| C | 2.96357400 | -0.80772700 | -1.83670700 |
| H | 4.00744800 | -0.44816200 | -1.83670200 |
| H | 2.94837700 | -1.89752000 | -2.01582000 |
| H | 2.40016300 | -0.31155200 | -2.64338100 |
| C | -2.96390600 | -0.80861800 | -1.83632500 |
| H | -2.94893500 | -1.89852100 | -2.01479300 |
| H | -4.00772100 | -0.44887900 | -1.83635300 |
| H | -2.40055400 | -0.31301500 | -2.64338900 |
| C | -3.36297100 | -1.08216100 | 0.99690700 |
| H | -4.35994000 | -0.64285400 | 0.81741300 |
| H | -3.42667100 | -2.18132000 | 0.90991400 |
| H | -3.03020200 | -0.82737100 | 2.01620700 |
| C | 0.00003200 | -0.86857900 | 1.76910100 |
| O | 0.00004500 | -0.90485200 | 2.94133000 |
| C | 0.00002000 | -2.53395100 | -0.36273900 |
| O | 0.00034000 | -3.67261300 | -0.65165400 |
| H | -0.00010100 | -0.62598500 | -1.53241500 |

[Fe-CO]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.20496700 | 1.95394200 | 0.00009700 |
| C | 0.00011900 | 1.23699100 | 0.00027800 |
| C | 1.20530100 | 1.95377900 | 0.00027900 |
| C | 1.23079900 | 3.35546900 | 0.00049700 |
| C | 0.00030800 | 4.03867200 | 0.00055800 |
| C | -1.23027600 | 3.35563600 | 0.00031100 |
| H | 2.18402000 | 3.89185500 | 0.00056000 |
| H | 0.00038100 | 5.13338900 | 0.00075100 |
| H | -2.18342400 | 3.89215000 | 0.00023100 |
| O | -2.41145500 | 1.23949200 | -0.00050000 |
| O | 2.41168700 | 1.23916400 | -0.00010100 |
| P | -2.24423100 | -0.42889400 | -0.00017000 |
| P | 2.24422600 | -0.42920000 | -0.00037100 |
| Fe | -0.00002500 | -0.78424700 | 0.00027800 |
| C | -3.24196000 | -0.95692900 | -1.44416200 |
| H | -3.27630700 | -2.05994100 | -1.48781300 |
| H | -4.26940800 | -0.56792900 | -1.33587000 |
| H | -2.81000600 | -0.57141200 | -2.38116400 |
| C | -3.24269900 | -0.95633800 | 1.44351900 |
| H | -4.27029400 | -0.56806500 | 1.33402600 |
| H | -3.27636800 | -2.05931800 | 1.48826800 |
| H | -2.81167900 | -0.56954900 | 2.38043600 |
| C | 3.24284700 | -0.95725800 | 1.44298000 |
| H | 3.27650200 | -2.06025600 | 1.48725800 |
| H | 4.27043600 | -0.56895700 | 1.33352400 |
| H | 2.81194800 | -0.57085500 | 2.38011100 |
| C | 3.24166400 | -0.95688900 | -1.44469700 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|------------|-------------|
| H | 4.26922300 | -0.56819500 | -1.33636200 | C | -1.20045500 | 1.91841100 | -0.06323700 |
| H | 3.27572500 | -2.05989100 | -1.48881400 | C | -1.22723200 | 3.31968000 | -0.07761100 |
| H | 2.80969900 | -0.57087000 | -2.38148500 | C | 0.00037000 | 4.00603300 | -0.07718400 |
| C | -0.00007800 | -0.58568300 | -1.78682200 | C | 1.22784800 | 3.31945600 | -0.07720900 |
| O | -0.00074100 | -0.41535200 | -2.93471400 | H | -2.18234700 | 3.85250300 | -0.08869000 |
| C | -0.00011700 | -2.57845400 | -0.00000300 | H | 0.00047100 | 5.10057900 | -0.08745100 |
| O | -0.00038100 | -3.74043300 | -0.00029500 | H | 2.18306400 | 3.85210300 | -0.08799300 |
| C | 0.00013100 | -0.58701300 | 1.78788800 | O | 2.40646800 | 1.20251700 | -0.06468900 |
| O | 0.00012000 | -0.41735300 | 2.93597400 | O | -2.40625200 | 1.20297700 | -0.06549000 |

L-L = bis CO

M = Co

[Co-S]²⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.24310300 | 1.96045300 | 0.45151800 |
| C | -0.00005800 | 1.36935500 | 0.02284200 |
| C | 1.24292500 | 1.96053400 | 0.45158500 |
| C | 1.24615000 | 3.16480500 | 1.14938500 |
| C | -0.00018100 | 3.75034100 | 1.47009300 |
| C | -1.24645700 | 3.16473900 | 1.14928800 |
| H | 2.18785300 | 3.63164400 | 1.45192900 |
| H | -0.00022700 | 4.69571500 | 2.02398000 |
| H | -2.18821200 | 3.63152700 | 1.45174800 |
| O | -2.40826300 | 1.32931700 | 0.10519600 |
| O | 2.40815200 | 1.32948100 | 0.10534200 |
| P | -2.27753800 | -0.31496800 | -0.33923300 |
| P | 2.27758300 | -0.31481600 | -0.33909800 |
| Co | 0.00004100 | -0.60686300 | -0.37469600 |
| C | -3.23561300 | -0.39089600 | -1.88618700 |
| H | -3.37192700 | -1.44697200 | -2.18135300 |
| H | -4.22845200 | 0.06579800 | -1.72329700 |
| H | -2.71438500 | 0.14558700 | -2.69581500 |
| C | -3.26214000 | -1.16401500 | 0.94311900 |
| H | -4.29295500 | -0.76735600 | 0.92077500 |
| H | -3.28626000 | -2.24703200 | 0.72730300 |
| H | -2.82483500 | -0.99423600 | 1.93892400 |
| C | 3.26212800 | -1.16381000 | 0.94332700 |
| H | 3.28630200 | -2.24682900 | 0.72752700 |
| H | 4.29292900 | -0.76711100 | 0.92107200 |
| H | 2.82472400 | -0.99403200 | 1.93909100 |
| C | 3.23574200 | -0.39065300 | -1.88602000 |
| H | 4.22853800 | 0.06611500 | -1.72306500 |
| H | 3.37215000 | -1.44671300 | -2.18118200 |
| H | 2.71449900 | 0.14580200 | -2.69564000 |
| C | 0.00001200 | 0.82584700 | -1.45895600 |
| O | 0.00004300 | 1.31755800 | -2.54203500 |
| C | 0.00016500 | -2.03229000 | -1.46148400 |
| O | 0.00034300 | -2.91365700 | -2.20766500 |
| N | 0.00001400 | -1.54394300 | 1.41570600 |
| C | -0.00003500 | -2.14932500 | 2.41919000 |
| C | -0.00011400 | -2.90686900 | 3.66367000 |
| H | 0.89797200 | -3.54782300 | 3.71919300 |
| H | -0.00406000 | -2.22170700 | 4.53007300 |
| H | -0.89426100 | -3.55361200 | 3.71551900 |

[Co-H]⁺

| | x | y | z |
|---|------------|------------|-------------|
| C | 1.20080300 | 1.91819400 | -0.06284000 |
| C | 0.00010400 | 1.19449900 | -0.04233200 |

| | | | |
|----|-------------|-------------|-------------|
| C | -1.20045500 | 1.91841100 | -0.06323700 |
| C | -1.22723200 | 3.31968000 | -0.07761100 |
| C | 0.00037000 | 4.00603300 | -0.07718400 |
| C | 1.22784800 | 3.31945600 | -0.07720900 |
| H | -2.18234700 | 3.85250300 | -0.08869000 |
| H | 0.00047100 | 5.10057900 | -0.08745100 |
| H | 2.18306400 | 3.85210300 | -0.08799300 |
| O | 2.40646800 | 1.20251700 | -0.06468900 |
| O | -2.40625200 | 1.20297700 | -0.06549000 |
| P | 2.19580900 | -0.44481800 | -0.24234100 |
| P | -2.19592300 | -0.44449700 | -0.24226400 |
| Co | -0.00007900 | -0.78237200 | 0.01487900 |
| C | 3.36749600 | -1.13721300 | 0.98055000 |
| H | 3.39153300 | -2.23763500 | 0.89341700 |
| H | 4.37864600 | -0.73769700 | 0.78656800 |
| H | 3.06102400 | -0.86115100 | 2.00222000 |
| C | 2.91866300 | -0.83208100 | -1.87934400 |
| H | 3.96766200 | -0.48937100 | -1.91141500 |
| H | 2.88707600 | -1.92174600 | -2.05604800 |
| H | 2.34176600 | -0.32294400 | -2.66824200 |
| C | -2.91915600 | -0.83244900 | -1.87893100 |
| H | -2.88801500 | -1.92223000 | -2.05499700 |
| H | -3.96803300 | -0.48936800 | -1.91103300 |
| H | -2.34220400 | -0.32398900 | -2.66822400 |
| C | -3.36754500 | -1.13606600 | 0.98117000 |
| H | -4.37866800 | -0.73651400 | 0.78711700 |
| H | -3.39174400 | -2.23653100 | 0.89464300 |
| H | -3.06088900 | -0.85948900 | 2.00264500 |
| C | -0.00000700 | -0.73144300 | 1.82805000 |
| O | 0.00007500 | -0.64645800 | 2.98116500 |
| C | -0.00019400 | -2.54836800 | -0.29242700 |
| O | -0.00023300 | -3.67953300 | -0.54281400 |
| H | -0.00013700 | -0.59069400 | -1.46248500 |

[Co-CO]²⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.21670200 | 1.93000600 | 0.00002500 |
| C | -0.00000500 | 1.22717100 | 0.00005300 |
| C | 1.21668900 | 1.93001000 | 0.00002400 |
| C | 1.23353900 | 3.32935400 | 0.00009800 |
| C | 0.00001000 | 4.00899900 | 0.00015200 |
| C | -1.23355600 | 3.32935000 | 0.00009700 |
| H | 2.18560700 | 3.86865200 | 0.00006800 |
| H | -0.00001100 | 5.10360700 | 0.00020400 |
| H | -2.18562600 | 3.86864400 | 0.00006800 |
| O | -2.41934700 | 1.21420900 | -0.00023800 |
| O | 2.41933800 | 1.21421800 | -0.00023400 |
| P | -2.32302600 | -0.44119400 | -0.00006000 |
| P | 2.32302500 | -0.44118500 | -0.00013700 |
| Co | -0.00000200 | -0.76457200 | 0.00001000 |
| C | -3.26277000 | -0.99463500 | -1.46218400 |
| H | -3.28431400 | -2.09855400 | -1.50233100 |
| H | -4.29936800 | -0.62268700 | -1.35833700 |
| H | -2.83504800 | -0.59643800 | -2.39592300 |
| C | -3.26222100 | -0.99438800 | 1.46255400 |
| H | -4.29952400 | -0.62462400 | 1.35804200 |
| H | -3.28162300 | -2.09827700 | 1.50446500 |
| H | -2.83538400 | -0.59387900 | 2.39571900 |
| C | 3.26226900 | -0.99444100 | 1.46242300 |
| H | 3.28166700 | -2.09833200 | 1.50429100 |
| H | 4.29957000 | -0.62467800 | 1.35789200 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 2.83546200 | -0.59396500 | 2.39561800 | C | -3.80157900 | 2.40571000 | 0.00203000 |
| C | 3.26272300 | -0.99456000 | -1.46231700 | H | -1.69166000 | 2.91690700 | 0.00277200 |
| H | 4.29932600 | -0.62262500 | -1.35848000 | H | -5.81580200 | 1.53803800 | 0.00099500 |
| H | 3.28425700 | -2.09847600 | -1.50252100 | H | -4.12838100 | 3.45150300 | 0.00328600 |
| H | 2.83497700 | -0.59631100 | -2.39602200 | N | -1.92734400 | 0.84709900 | 0.00013900 |
| C | -0.00003800 | -0.48564800 | -1.78410600 | N | -0.83675200 | -1.45641100 | -0.00354500 |
| O | -0.00015700 | -0.27043000 | -2.91577200 | N | 0.58793300 | 2.11258800 | 0.00322900 |
| C | 0.00000600 | -2.60207300 | -0.00013000 | C | 0.98416300 | 3.23410700 | 0.00488600 |
| O | 0.00000300 | -3.75106700 | -0.00022100 | C | 1.65009500 | 4.53509300 | 0.00643100 |
| C | 0.00002800 | -0.48595900 | 1.78413600 | H | 1.36993500 | 5.13142300 | -0.88290900 |
| O | 0.00021200 | -0.27093400 | 2.91583600 | H | 1.37636300 | 5.12597400 | 0.90138500 |
| | | | | H | 2.75193300 | 4.41721200 | 0.00210300 |

L-L = bpy

M = Mn

[Mn-H]⁻¹

[Mn-S]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 2.62879700 | -0.61443900 | -1.18676200 |
| C | 1.90305000 | -0.36821300 | 0.00094500 |
| C | 2.62485300 | -0.62266700 | 1.18930200 |
| C | 3.94797700 | -1.09828100 | 1.22469600 |
| C | 4.60520800 | -1.33227800 | 0.00210300 |
| C | 3.95204000 | -1.08983200 | -1.22102100 |
| H | 4.44445000 | -1.27757700 | 2.18459800 |
| H | 5.63668900 | -1.70397000 | 0.00253400 |
| H | 4.45167500 | -1.26260800 | -2.18047900 |
| O | 1.99019300 | -0.37748900 | -2.41350600 |
| O | 1.98209500 | -0.39417000 | 2.41549200 |
| P | 0.41278400 | 0.23978600 | -2.19298600 |
| P | 0.40832400 | 0.23182700 | 2.19369300 |
| Mn | -0.01140000 | 0.35452000 | 0.00015700 |
| C | -0.52734500 | -0.90538000 | -3.30744800 |
| H | -1.55751700 | -0.52739900 | -3.43839200 |
| H | -0.03773800 | -0.98161300 | -4.29444100 |
| H | -0.57821300 | -1.90780000 | -2.85151600 |
| C | 0.52468800 | 1.74275600 | -3.27384500 |
| H | 0.93208700 | 1.48236000 | -4.26662100 |
| H | -0.47966500 | 2.18759600 | -3.39396900 |
| H | 1.18380800 | 2.48670600 | -2.79765400 |
| C | 0.52570900 | 1.73225100 | 3.27756700 |
| H | -0.47658300 | 2.18196300 | 3.39683500 |
| H | 0.93020200 | 1.46804000 | 4.27051700 |
| H | 1.18931500 | 2.47369400 | 2.80366900 |
| C | -0.53910400 | -0.91110200 | 3.30411600 |
| H | -0.05172800 | -0.99151500 | 4.29188400 |
| H | -1.56769500 | -0.52845500 | 3.43389400 |
| H | -0.59383900 | -1.91241500 | 2.84619400 |
| C | -0.17143000 | -2.65382100 | -0.00591400 |
| C | -2.22371000 | -1.50685900 | -0.00330400 |
| C | -0.81235200 | -3.89144700 | -0.00762700 |
| H | 0.91935200 | -2.56968700 | -0.00631800 |
| C | -2.92255600 | -2.73309500 | -0.00496000 |
| C | -2.22356500 | -3.94194200 | -0.00704800 |
| H | -0.20847400 | -4.80497700 | -0.00932100 |
| H | -4.01738100 | -2.73098400 | -0.00455300 |
| H | -2.75759500 | -4.89802600 | -0.00824100 |
| C | -2.85008800 | -0.19288100 | -0.00127000 |
| C | -4.24143200 | 0.04033400 | -0.00091100 |
| C | -2.44006700 | 2.11939100 | 0.00171600 |
| C | -4.73807000 | 1.34565000 | 0.00074100 |
| H | -4.93204200 | -0.80956800 | -0.00196800 |

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 2.67083400 | -1.19080700 | 0.17463000 |
| C | 1.92273900 | -0.00037700 | -0.02730000 |
| C | 2.67157700 | 1.18923800 | 0.17670700 |
| C | 4.00511000 | 1.22144300 | 0.62593300 |
| C | 4.66560300 | -0.00201100 | 0.86548200 |
| C | 4.00435000 | -1.22463000 | 0.62377600 |
| H | 4.51193200 | 2.18285200 | 0.77513400 |
| H | 5.70426800 | -0.00264400 | 1.22098700 |
| H | 4.51057600 | -2.18661600 | 0.77126700 |
| O | 2.02603100 | -2.39894900 | -0.10449900 |
| O | 2.02749600 | 2.39825000 | -0.10027900 |
| P | 0.52384000 | -2.04186700 | -0.90147800 |
| P | 0.52521500 | 2.04339700 | -0.89815300 |
| Mn | -0.06970800 | 0.00069000 | -0.52155600 |
| C | -0.42479300 | -3.51503300 | -0.25357600 |
| H | -1.39060600 | -3.58500800 | -0.78632200 |
| H | 0.14080300 | -4.45640400 | -0.38846400 |
| H | -0.62897800 | -3.36354000 | 0.81982700 |
| C | 0.95997200 | -2.68072900 | -2.59880100 |
| H | 1.40081600 | -3.69451800 | -2.55447700 |
| H | 0.05131200 | -2.69331400 | -3.22836300 |
| H | 1.68199000 | -1.97905300 | -3.04908600 |
| C | 0.96215100 | 2.68452800 | -2.59441800 |
| H | 0.05369100 | 2.69840700 | -3.22423600 |
| H | 1.40343700 | 3.69805500 | -2.54850400 |
| H | 1.68400300 | 1.98318200 | -3.04549300 |
| C | -0.42247300 | 3.51630400 | -0.24823300 |
| H | 0.14401600 | 4.45740300 | -0.38126000 |
| H | -1.38793600 | 3.58801600 | -0.78138600 |
| H | -0.62736500 | 3.36318900 | 0.82479300 |
| H | 0.03359600 | 0.00197000 | -2.11856200 |
| C | 0.18745200 | -0.00145600 | 2.48499500 |
| C | -2.00483100 | -0.00109400 | 1.62240500 |
| C | -0.28027500 | -0.00261400 | 3.79167700 |
| H | 1.25880100 | -0.00114400 | 2.26586100 |
| C | -2.52885700 | -0.00229900 | 2.93729800 |
| C | -1.68059500 | -0.00308500 | 4.04288300 |
| H | 0.44495100 | -0.00315300 | 4.61429000 |
| H | -3.61659500 | -0.00259700 | 3.07770200 |
| H | -2.07932100 | -0.00402600 | 5.06408200 |
| C | -2.79770500 | -0.00007000 | 0.41853700 |
| C | -4.21207200 | -0.00019700 | 0.36603100 |
| C | -2.70605100 | 0.00230500 | -1.93742800 |
| C | -4.88209700 | 0.00092800 | -0.85673000 |
| H | -4.78097000 | -0.00123600 | 1.30357400 |
| C | -4.09082500 | 0.00224300 | -2.04003200 |

| | | | |
|---|-------------|-------------|-------------|
| H | -2.06145200 | 0.00327400 | -2.82152300 |
| H | -5.97739900 | 0.00080900 | -0.90199500 |
| H | -4.55407400 | 0.00323200 | -3.03417000 |
| N | -2.01459400 | 0.00111600 | -0.74558200 |
| N | -0.62199600 | -0.00072500 | 1.36770900 |

[Mn-CO]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 2.71700900 | 0.96990300 | -0.69170800 |
| C | 1.97422500 | 0.01599300 | 0.03630800 |
| C | 2.70727600 | -1.11637700 | 0.45120400 |
| C | 4.06843000 | -1.31992900 | 0.16206700 |
| C | 4.74584100 | -0.33369000 | -0.57840000 |
| C | 4.07851300 | 0.82612100 | -1.01341700 |
| H | 4.57822700 | -2.22306800 | 0.51386000 |
| H | 5.80780500 | -0.46806400 | -0.81482900 |
| H | 4.59597800 | 1.60493900 | -1.58350100 |
| O | 2.05928800 | 2.12800200 | -1.12644500 |
| O | 2.04002600 | -2.10107600 | 1.19180500 |
| P | 0.43024600 | 2.16094300 | -0.62274800 |
| P | 0.41563300 | -1.67836600 | 1.49107000 |
| Mn | -0.00999700 | 0.26951900 | 0.48270500 |
| C | -0.38228200 | 2.55423100 | -2.24304200 |
| H | -1.44898300 | 2.78867000 | -2.07535900 |
| H | 0.10906000 | 3.41944000 | -2.72236600 |
| H | -0.31450400 | 1.68359300 | -2.91576500 |
| C | 0.38452800 | 3.81618300 | 0.19910900 |
| H | 0.82186700 | 4.58717400 | -0.45934800 |
| H | -0.66117500 | 4.08577900 | 0.43317600 |
| H | 0.95328400 | 3.77444100 | 1.14208200 |
| C | 0.37115300 | -1.86554000 | 3.32984000 |
| H | -0.67340000 | -1.80433600 | 3.68523400 |
| H | 0.80262300 | -2.83634200 | 3.63093400 |
| H | 0.94639700 | -1.04949100 | 3.79631800 |
| C | -0.41293000 | -3.25033400 | 0.96203800 |
| H | 0.07151700 | -4.12231000 | 1.43585000 |
| H | -1.47811800 | -3.22151700 | 1.25442500 |
| H | -0.35110400 | -3.35433800 | -0.13358600 |
| C | 0.22206600 | -1.21144200 | -2.19733000 |
| C | -1.95890000 | -0.78976600 | -1.43758000 |
| C | -0.24897100 | -1.85267200 | -3.34411200 |
| H | 1.29243200 | -1.09932100 | -1.99831900 |
| C | -2.49493100 | -1.42716800 | -2.57913100 |
| C | -1.64040300 | -1.96551700 | -3.54305500 |
| H | 0.46720000 | -2.25612700 | -4.06711200 |
| H | -3.57957900 | -1.49862500 | -2.70562800 |
| H | -2.04558200 | -2.46279500 | -4.43089300 |
| C | -2.75152300 | -0.19656000 | -0.36772300 |
| C | -4.16250500 | -0.17845200 | -0.33973100 |
| C | -2.67482300 | 0.93630400 | 1.68604700 |
| C | -4.83955000 | 0.41247000 | 0.72744400 |
| H | -4.72497100 | -0.63201900 | -1.16206500 |
| C | -4.06303800 | 0.98157700 | 1.76214100 |
| H | -2.05618200 | 1.36962500 | 2.47580400 |
| H | -5.93355700 | 0.43214000 | 0.75934300 |
| H | -4.53230400 | 1.46054600 | 2.62801300 |
| N | -1.98318400 | 0.36185800 | 0.64647500 |
| N | -0.59739100 | -0.68219000 | -1.24515300 |
| C | 0.33040400 | 1.09424300 | 1.98445800 |
| O | 0.54585100 | 1.65935400 | 3.01207000 |

L-L = bpy

M = Fe

[Fe-S]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -2.57698800 | 0.64835600 | -1.18971300 |
| C | -1.86548100 | 0.40743900 | 0.00253400 |
| C | -2.57274800 | 0.65529300 | 1.19589000 |
| C | -3.89039800 | 1.13981400 | 1.22940600 |
| C | -4.54050200 | 1.37739500 | 0.00450100 |
| C | -3.89477200 | 1.13267700 | -1.22130800 |
| H | -4.38877600 | 1.32161800 | 2.18666200 |
| H | -5.56852200 | 1.75532400 | 0.00523200 |
| H | -4.39652000 | 1.30908200 | -2.17781700 |
| O | -1.93279400 | 0.39645400 | -2.41296300 |
| O | -1.92391400 | 0.41074200 | 2.41816100 |
| P | -0.36223300 | -0.19280400 | -2.20911600 |
| P | -0.35836200 | -0.19061300 | 2.21119000 |
| Fe | -0.02055300 | -0.32771000 | 0.00136400 |
| C | 0.60291000 | 0.97534600 | -3.26067500 |
| H | 1.63991400 | 0.61076400 | -3.37036100 |
| H | 0.14027300 | 1.05005900 | -4.26002900 |
| H | 0.62429800 | 1.97724900 | -2.80257600 |
| C | -0.40378700 | -1.70273400 | -3.26655700 |
| H | -0.75780500 | -1.44949400 | -4.28070800 |
| H | 0.60953000 | -2.13731300 | -3.33314100 |
| H | -1.08390100 | -2.44990200 | -2.82805900 |
| C | -0.40855600 | -1.70190400 | 3.26639700 |
| H | 0.60075500 | -2.14676800 | 3.32578700 |
| H | -0.75383500 | -1.44738600 | 4.28322800 |
| H | -1.09874900 | -2.44129000 | 2.83038700 |
| C | 0.61684500 | 0.96977000 | 3.26176100 |
| H | 0.15511500 | 1.04931200 | 4.26117000 |
| H | 1.65058800 | 0.59607700 | 3.37153600 |
| H | 0.64690500 | 1.97105800 | 2.80279900 |
| C | 0.22484000 | 2.63931400 | -0.00331400 |
| C | 2.23134700 | 1.41620700 | -0.00393200 |
| C | 0.91591100 | 3.85449000 | -0.00638700 |
| H | -0.86791900 | 2.59458700 | -0.00164300 |
| C | 2.97908200 | 2.61004900 | -0.00725000 |
| C | 2.32179700 | 3.84478200 | -0.00855500 |
| H | 0.35037500 | 4.79134000 | -0.00699900 |
| H | 4.07212600 | 2.57050900 | -0.00868300 |
| H | 2.89295600 | 4.77859900 | -0.01107900 |
| C | 2.81521600 | 0.06906700 | -0.00155400 |
| C | 4.19654800 | -0.20783800 | -0.00184100 |
| C | 2.32035400 | -2.22182400 | 0.00461500 |
| C | 4.63821300 | -1.53527300 | 0.00115800 |
| H | 4.92198400 | 0.61092700 | -0.00428300 |
| C | 3.67576100 | -2.56129600 | 0.00457300 |
| H | 1.54051300 | -2.98815000 | 0.00726900 |
| H | 5.70818000 | -1.76559800 | 0.00099000 |
| H | 3.96855800 | -3.61588900 | 0.00718000 |
| N | 1.87558300 | -0.93668300 | 0.00147100 |
| N | 0.85360000 | 1.43119800 | -0.00230200 |
| N | -0.75902800 | -2.04037000 | -0.00004400 |
| C | -1.30121700 | -3.08580600 | -0.00307600 |
| C | -2.01435100 | -4.35976100 | -0.00829400 |
| H | -1.74994300 | -4.95460500 | -0.90094400 |
| H | -1.76528000 | -4.95337900 | 0.88954700 |
| H | -3.10509600 | -4.18298800 | -0.01775700 |

[Fe-H]⁰

| | x | y | z | | x | y | z |
|----|-------------|--------------|-------------|----|-------------|-------------|-------------|
| C | -2.69884300 | 1.18990300 | 0.01966100 | H | 4.55799300 | 2.18696300 | 0.56353400 |
| C | -1.95334300 | -0.00015000 | -0.12856900 | H | 5.77499200 | 0.00643600 | 0.87566200 |
| C | -2.69836500 | -1.19027900 | 0.02155000 | H | 4.55991900 | -2.17819600 | 0.58567700 |
| C | -4.06398300 | -1.22440700 | 0.35314200 | O | 2.00364800 | -2.41292700 | -0.04074400 |
| C | -4.73782300 | -0.00019900 | 0.52672900 | O | 2.00141200 | 2.41304400 | -0.06483800 |
| C | -4.06447700 | 1.22400200 | 0.35120300 | P | 0.37789600 | -2.22105600 | -0.44123100 |
| H | -4.58187200 | -2.18333100 | 0.46222500 | P | 0.37663500 | 2.21584600 | -0.46675400 |
| H | -5.80283300 | -0.00020900 | 0.78654000 | Fe | 0.02634100 | -0.00319600 | -0.52947300 |
| H | -4.58273500 | 2.18289200 | 0.45882100 | C | -0.45027800 | -3.25123900 | 0.84262700 |
| O | -2.02459000 | 2.40147800 | -0.18283200 | H | -1.52639300 | -3.34185100 | 0.61096800 |
| O | -2.02358300 | -2.40186800 | -0.17915800 | H | 0.00029800 | -4.25887600 | 0.85648200 |
| P | -0.44522000 | 2.10734600 | -0.76095600 | H | -0.33394700 | -2.79335000 | 1.83786900 |
| P | -0.44522400 | -2.10756500 | -0.76003300 | C | 0.24042200 | -3.27193300 | -1.94446600 |
| Fe | -0.00354100 | -0.00005300 | -0.51912600 | H | 0.64280900 | -4.27788600 | -1.73364500 |
| C | 0.45640300 | 3.41916300 | 0.19089400 | H | -0.81803500 | -3.36386800 | -2.24669000 |
| H | 1.49146300 | 3.50353800 | -0.18629500 | H | 0.81081500 | -2.82462800 | -2.77427900 |
| H | -0.04788900 | 4.39676900 | 0.08972400 | C | 0.24169600 | 3.24956000 | -1.98216000 |
| H | 0.49162400 | 3.13908500 | 1.25684500 | H | -0.81620500 | 3.33717500 | -2.28763800 |
| C | -0.55009600 | 2.88684900 | -2.43591900 | H | 0.64256900 | 4.25822000 | -1.78161000 |
| H | -0.92896700 | 3.92258100 | -2.37317900 | H | 0.81440900 | 2.79376300 | -2.80574300 |
| H | 0.44992500 | 2.88886900 | -2.90654000 | C | -0.45448900 | 3.26059200 | 0.80330800 |
| H | -1.22760600 | 2.28042400 | -3.05899200 | H | -0.00477400 | 4.26870400 | 0.80578800 |
| C | -0.55294900 | -2.88676700 | -2.43496900 | H | -1.53024700 | 3.34745700 | 0.56866400 |
| H | 0.44620600 | -2.88840400 | -2.90742800 | H | -0.33947400 | 2.81494200 | 1.80424700 |
| H | -0.93148100 | -3.92259500 | -2.37178000 | C | 0.24187800 | 0.01473300 | 2.49923100 |
| H | -1.23172700 | -2.28032500 | -3.05664800 | C | -1.92735700 | 0.00897300 | 1.60094100 |
| C | 0.45805900 | -3.41942600 | 0.19010300 | C | -0.25165800 | 0.02200500 | 3.80860800 |
| H | -0.04617300 | -4.39711300 | 0.08942100 | H | 1.31537200 | 0.01367300 | 2.28624100 |
| H | 1.49255400 | -3.50346000 | -0.18870100 | C | -2.48440300 | 0.01620100 | 2.89555000 |
| H | 0.49485100 | -3.13966000 | 1.25608000 | C | -1.64186100 | 0.02276700 | 4.01282800 |
| H | -0.26663100 | -0.00023700 | -2.03307800 | H | 0.45040700 | 0.02693900 | 4.64785600 |
| C | -0.23935300 | 0.00086400 | 2.47250600 | H | -3.56982300 | 0.01663100 | 3.02830200 |
| C | 1.93140200 | 0.00034800 | 1.57674600 | H | -2.06237300 | 0.02831800 | 5.02359600 |
| C | 0.25439500 | 0.00122300 | 3.77708200 | C | -2.71441300 | 0.00158800 | 0.35843000 |
| H | -1.31334400 | 0.00088800 | 2.26211800 | C | -4.12241400 | 0.00119700 | 0.31164900 |
| C | 2.48703300 | 0.00071100 | 2.87355600 | C | -2.60530100 | -0.01174800 | -1.98330800 |
| C | 1.64899900 | 0.00114600 | 3.99149000 | C | -4.77754000 | -0.00573300 | -0.92438600 |
| H | -0.44999200 | 0.00155500 | 4.61560300 | H | -4.70339200 | 0.00651200 | 1.23819600 |
| H | 3.57451100 | 0.00066400 | 3.00047200 | C | -3.99845200 | -0.01230000 | -2.09422200 |
| H | 2.06660700 | 0.00142900 | 5.00382900 | H | -1.97150100 | -0.01670500 | -2.87382000 |
| C | 2.70666600 | 0.00000700 | 0.33842100 | H | -5.87086300 | -0.00597400 | -0.97453200 |
| C | 4.11558900 | -0.00019200 | 0.26402100 | H | -4.45824300 | -0.01788100 | -3.08715900 |
| C | 2.55891000 | -0.00056700 | -2.00795000 | N | -1.95383400 | -0.00494000 | -0.78782200 |
| C | 4.75156900 | -0.00057200 | -0.97991300 | N | -0.56822600 | 0.00813600 | 1.40934000 |
| H | 4.70831400 | -0.000008700 | 1.18446300 | C | 0.49596600 | -0.01315200 | -2.19313500 |
| C | 3.94647900 | -0.00075300 | -2.13988400 | O | 0.83083000 | -0.02036800 | -3.31904400 |
| H | 1.89269200 | -0.00073800 | -2.87483800 | | | | |
| H | 5.84431400 | -0.00075500 | -1.04967800 | | | | |
| H | 4.39088200 | -0.00105000 | -3.14076500 | | | | |
| N | 1.91757100 | -0.00019200 | -0.79946800 | | | | |
| N | 0.56297100 | 0.00042400 | 1.36667100 | | | | |

[Fe-CO]⁺

| | x | y | z |
|---|------------|-------------|-------------|
| C | 2.67992800 | -1.19438800 | 0.12131500 |
| C | 1.95556400 | 0.00006800 | -0.05268300 |
| C | 2.67886800 | 1.19680700 | 0.10924100 |
| C | 4.04096100 | 1.22987600 | 0.44587100 |
| C | 4.71086900 | 0.00466200 | 0.61718100 |
| C | 4.04204000 | -1.22280800 | 0.45832700 |

L-L = bpy

M = Co

[Co-S]²⁺

| | x | y | z |
|---|-------------|------------|-------------|
| C | -2.53809000 | 0.66297000 | -1.20216000 |
| C | -1.84720000 | 0.42581100 | -0.00013900 |
| C | -2.53926500 | 0.65983300 | 1.20182800 |
| C | -3.85056300 | 1.15673000 | 1.22738300 |
| C | -4.49111800 | 1.40501000 | -0.00015500 |
| C | -3.84936800 | 1.15990800 | -1.22771000 |
| H | -4.35189900 | 1.33846200 | 2.18278500 |
| H | -5.51504300 | 1.79209000 | -0.00015400 |
| H | -4.34979100 | 1.34406800 | -2.18312400 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| O | -1.89476400 | 0.39558000 | -2.42106000 | P | -0.42437400 | -2.16176600 | -0.70548000 |
| O | -1.89717700 | 0.38909800 | 2.42063500 | Co | -0.05781500 | 0.00037300 | -0.51692000 |
| P | -0.33013900 | -0.17211600 | -2.26032400 | C | 0.46856000 | 3.36960200 | 0.36282600 |
| P | -0.33133800 | -0.17535500 | 2.25997500 | H | 1.52263700 | 3.44648200 | 0.04269500 |
| Co | -0.04027200 | -0.31325300 | -0.00018800 | H | -0.00408000 | 4.36420600 | 0.28284100 |
| C | 0.65830700 | 1.01681500 | -3.24703400 | H | 0.43494300 | 3.03975300 | 1.41396200 |
| H | 1.69964200 | 0.66098200 | -3.33874000 | C | -0.39657200 | 2.95286000 | -2.36206900 |
| H | 0.21863200 | 1.09269700 | -4.25739300 | H | -0.74444100 | 3.99852600 | -2.29737900 |
| H | 0.65287200 | 2.01583200 | -2.78338100 | H | 0.63004000 | 2.93784500 | -2.76956700 |
| C | -0.32569800 | -1.69345500 | -3.28290900 | H | -1.05711900 | 2.38844600 | -3.04016100 |
| H | -0.68180300 | -1.44884000 | -4.29920600 | C | -0.39768200 | -2.94945500 | -2.36623700 |
| H | 0.69933500 | -2.09843900 | -3.35018900 | H | 0.62885600 | -2.93458600 | -2.77392300 |
| H | -0.98991400 | -2.45595300 | -2.84835800 | H | -0.74626800 | -3.99496900 | -2.30292700 |
| C | -0.32476500 | -1.69750000 | 3.28130100 | H | -1.05798100 | -2.38362400 | -3.04338900 |
| H | 0.70121900 | -2.09978000 | 3.35025400 | C | 0.46861600 | -3.37011400 | 0.35775200 |
| H | -0.68341200 | -1.45455400 | 4.29710900 | H | -0.00406000 | -4.36460300 | 0.27658100 |
| H | -0.98611700 | -2.46148300 | 2.84499200 | H | 1.52257400 | -3.44655500 | 0.03712700 |
| C | 0.65455400 | 1.01447500 | 3.24822300 | H | 0.43540700 | -3.04169900 | 1.40935500 |
| H | 0.21463800 | 1.08824800 | 4.25862900 | H | -0.41907600 | 0.00148000 | -1.95420300 |
| H | 1.69665000 | 0.66078400 | 3.33957800 | C | -0.24336900 | -0.00204600 | 2.49605000 |
| H | 0.64703300 | 2.01400800 | 2.78571400 | C | 1.90800200 | -0.00122900 | 1.55418800 |
| C | 0.22797900 | 2.62960900 | 0.00171500 | C | 0.27827500 | -0.00310200 | 3.79563200 |
| C | 2.22286900 | 1.37133300 | 0.00136800 | H | -1.32121100 | -0.00193400 | 2.30248100 |
| C | 0.93934500 | 3.83517000 | 0.00261000 | C | 2.49408900 | -0.00225900 | 2.83503200 |
| H | -0.86490200 | 2.60399300 | 0.00150100 | C | 1.67247200 | -0.00319500 | 3.96925000 |
| C | 2.98465700 | 2.55503200 | 0.00229300 | H | -0.40344900 | -0.00382800 | 4.65157800 |
| C | 2.34300000 | 3.80006400 | 0.00291900 | H | 3.58207600 | -0.00232900 | 2.94723800 |
| H | 0.38876000 | 4.78077700 | 0.00306000 | H | 2.11370400 | -0.00399700 | 4.97117300 |
| H | 4.07684100 | 2.50307400 | 0.00249800 | C | 2.66683500 | -0.00023200 | 0.28888700 |
| H | 2.92914900 | 4.72467600 | 0.00362600 | C | 4.07302200 | -0.00014200 | 0.20087200 |
| C | 2.79564700 | 0.01391200 | 0.00048900 | C | 2.49100600 | 0.00149100 | -2.05516500 |
| C | 4.17361000 | -0.27573800 | 0.00052300 | C | 4.68944400 | 0.00077800 | -1.05589500 |
| C | 2.27498800 | -2.27543100 | -0.00146100 | H | 4.68219300 | -0.00080000 | 1.10915700 |
| C | 4.59661700 | -1.61157600 | -0.00045800 | C | 3.88148400 | 0.00160300 | -2.20620900 |
| H | 4.91226900 | 0.53058000 | 0.00128000 | H | 1.81778200 | 0.00211200 | -2.91673700 |
| C | 3.62960700 | -2.63026200 | -0.00149700 | H | 5.78112000 | 0.00084500 | -1.13682300 |
| H | 1.48734200 | -3.03376700 | -0.00232000 | H | 4.31680900 | 0.00232700 | -3.21007800 |
| H | 5.66446400 | -1.85253100 | -0.00044300 | N | 1.88397200 | 0.00060000 | -0.84002400 |
| H | 3.91454300 | -3.68668900 | -0.00232000 | N | 0.54535300 | -0.00110900 | 1.39386900 |
| N | 1.85881800 | -0.98656100 | -0.00046100 | | | | |
| N | 0.84774000 | 1.42022500 | 0.00109100 | | | | |
| N | -0.85535400 | -2.00946300 | -0.00141600 | | | | |
| C | -1.46260400 | -3.01211900 | -0.00181400 | | | | |
| C | -2.23433200 | -4.24805600 | -0.00200500 | | | | |
| H | -1.56448100 | -5.12578100 | 0.02059400 | | | | |
| H | -2.89571400 | -4.28178300 | 0.88238500 | | | | |
| H | -2.86277100 | -4.30283200 | -0.90902000 | | | | |

[Co-H]⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -2.69942600 | 1.19651900 | -0.03320800 |
| C | -1.96886200 | 0.00022600 | -0.16528300 |
| C | -2.69948000 | -1.19618100 | -0.03454300 |
| C | -4.07109200 | -1.22613700 | 0.26043700 |
| C | -4.74396600 | -0.00003400 | 0.41281500 |
| C | -4.07103600 | 1.22620700 | 0.26180500 |
| H | -4.59315600 | -2.18277400 | 0.35834900 |
| H | -5.81504500 | -0.00013500 | 0.64065900 |
| H | -4.59305200 | 2.18275900 | 0.36079500 |
| O | -2.01421600 | 2.40772700 | -0.20249000 |
| O | -2.01431800 | -2.40722600 | -0.20521800 |
| P | -0.42410200 | 2.16280400 | -0.70244300 |

[Co-CO]²⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -2.66010800 | -1.20672900 | -0.11271800 |
| C | -1.95287600 | 0.00011100 | 0.04560700 |
| C | -2.65927500 | 1.20808800 | -0.10758400 |
| C | -4.02049300 | 1.23168700 | -0.43849800 |
| C | -4.68619600 | 0.00242800 | -0.60127700 |
| C | -4.02133100 | -1.22796500 | -0.44379400 |
| H | -4.54160900 | 2.18618700 | -0.55800200 |
| H | -5.75149900 | 0.00332700 | -0.85280200 |
| H | -4.54307900 | -2.18159600 | -0.56742500 |
| O | -1.98005800 | -2.41906300 | 0.05884400 |
| O | -1.97843800 | 2.41928300 | 0.06902100 |
| P | -0.35645300 | -2.27612600 | 0.41775800 |
| P | -0.35508600 | 2.27397400 | 0.42821900 |
| Co | -0.04294500 | -0.00132800 | 0.48831500 |
| C | 0.48138800 | -3.23950300 | -0.89475800 |
| H | 1.56177600 | -3.31020100 | -0.67848100 |
| H | 0.05333300 | -4.25800700 | -0.90769100 |
| H | 0.33106300 | -2.77580300 | -1.88194500 |
| C | -0.16449600 | -3.28586800 | 1.93176600 |
| H | -0.55040900 | -4.30153600 | 1.73142500 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 0.90148100 | -3.35998200 | 2.21044000 | H | -2.83173200 | 2.03892700 | 1.93398600 |
| H | -0.73311300 | -2.85208900 | 2.76998900 | H | -4.00831000 | 0.69883300 | 1.65107800 |
| C | -0.16334300 | 3.27721900 | 1.94658800 | H | -2.44316100 | 0.38036900 | 2.47826300 |
| H | 0.90256600 | 3.35008200 | 2.22584000 | C | -3.38415900 | 1.35135100 | -1.08619900 |
| H | -0.54897800 | 4.29379900 | 1.75034500 | H | -4.38849600 | 0.93754800 | -0.88331500 |
| H | -0.73229000 | 2.84010300 | 2.78284300 | H | -3.41686800 | 2.44895900 | -0.95162600 |
| C | 0.48404900 | 3.24244100 | -0.87974600 | H | -3.13372600 | 1.13491300 | -2.14023200 |
| H | 0.05679300 | 4.26131800 | -0.88847300 | N | 0.46134100 | 2.66469000 | -0.58063600 |
| H | 1.56438000 | 3.31124400 | -0.66257900 | N | 0.04724500 | 0.50463400 | -2.23806100 |
| H | 0.33386900 | 2.78309700 | -1.86900900 | H | 1.18370900 | 3.02684100 | 0.05516300 |
| C | -0.22010400 | 0.00596400 | -2.50778700 | H | -0.75857000 | -0.06358200 | -2.53073000 |
| C | 1.93889200 | 0.00357500 | -1.56065000 | H | 0.87024600 | -0.00195500 | -2.59015600 |
| C | 0.30316700 | 0.00911100 | -3.80704600 | H | -0.38144800 | 3.22324100 | -0.39595200 |
| H | -1.29810400 | 0.00551100 | -2.32072200 | C | -0.01062900 | 1.86649800 | -2.83736000 |
| C | 2.51903400 | 0.00662900 | -2.84354900 | H | -1.06040100 | 2.20811000 | -2.79611000 |
| C | 1.69705700 | 0.00947500 | -3.97863400 | H | 0.30467900 | 1.88193600 | -3.90021000 |
| H | -0.37982300 | 0.01123500 | -4.66195400 | C | 0.86778200 | 2.80324500 | -2.00112400 |
| H | 3.60649600 | 0.00681700 | -2.95751700 | H | 1.92550200 | 2.49444100 | -2.07680300 |
| H | 2.13922600 | 0.01188900 | -4.98021800 | H | 0.78844600 | 3.84385500 | -2.37822400 |
| C | 2.70350800 | 0.00034400 | -0.29969300 | N | 0.21419200 | 1.01390500 | 1.65801200 |
| C | 4.10912100 | 0.00011100 | -0.22094600 | C | 0.33116500 | 1.48070800 | 2.76323000 |
| C | 2.54230700 | -0.00569200 | 2.04714400 | C | 0.33476700 | 1.34190600 | 4.23379400 |
| C | 4.73363400 | -0.00300900 | 1.03363700 | H | -0.47976200 | 1.93301900 | 4.69406500 |
| H | 4.71509300 | 0.00238300 | -1.13110900 | H | 0.20342100 | 0.28262600 | 4.54006300 |
| C | 3.93496100 | -0.00599100 | 2.18860000 | H | 1.28235500 | 1.70855100 | 4.67123700 |
| H | 1.89100800 | -0.00810400 | 2.92560500 | | | | |
| H | 5.82590800 | -0.00312800 | 1.10706200 | | | | |
| H | 4.37579000 | -0.00856500 | 3.19007600 | | | | |
| N | 1.93079000 | -0.00253000 | 0.83469300 | | | | |
| N | 0.57420700 | 0.00321000 | -1.40775500 | | | | |
| C | -0.66224200 | -0.00457000 | 2.12154600 | | | | |
| O | -1.07927900 | -0.00668700 | 3.20367900 | | | | |

L-L = en
M = Mn

[Mn-S]⁰

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 0.77193200 | -2.34638300 | -0.11579100 |
| C | -0.26262100 | -1.38127400 | -0.08506900 |
| C | -1.56829400 | -1.92078600 | -0.15316600 |
| C | -1.85341500 | -3.29731600 | -0.21762300 |
| C | -0.77465000 | -4.20131400 | -0.22774500 |
| C | 0.55256100 | -3.73515500 | -0.17870600 |
| H | -2.89171900 | -3.64492300 | -0.25655500 |
| H | -0.96973600 | -5.27938000 | -0.27577800 |
| H | 1.40198300 | -4.42716400 | -0.19084600 |
| O | 2.09474900 | -1.89690800 | -0.09229000 |
| O | -2.64753200 | -1.02865700 | -0.16180700 |
| P | 2.17463700 | -0.17415400 | -0.00337400 |
| P | -2.11086400 | 0.59428100 | 0.06336400 |
| Mn | 0.10297500 | 0.61461600 | -0.10368300 |
| C | 3.54549200 | 0.00394900 | -1.27403800 |
| H | 4.01276000 | 1.00312500 | -1.19201900 |
| H | 4.32078000 | -0.76713300 | -1.11520400 |
| H | 3.15766700 | -0.11449500 | -2.30252400 |
| C | 3.20773100 | -0.02004500 | 1.53436100 |
| H | 4.11080100 | -0.65073800 | 1.45972800 |
| H | 3.50422000 | 1.03319300 | 1.69357500 |
| H | 2.60948400 | -0.34529100 | 2.40034400 |
| C | -2.93770900 | 0.96641500 | 1.68686500 |

[Mn-H]⁻¹

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 0.93509600 | 2.07870300 | 0.37283000 |
| C | -0.15839100 | 1.19528700 | 0.12717300 |
| C | -1.43854600 | 1.77619200 | 0.36766400 |
| C | -1.63672600 | 3.09685000 | 0.81937900 |
| C | -0.50754500 | 3.91166800 | 1.05436100 |
| C | 0.79128300 | 3.40577300 | 0.82477100 |
| H | -2.65526400 | 3.47721000 | 0.97249000 |
| H | -0.63938300 | 4.94323200 | 1.40848300 |
| H | 1.68070000 | 4.02971200 | 0.98395400 |
| O | 2.21469600 | 1.58950100 | 0.12991900 |
| O | -2.55422500 | 0.98111300 | 0.11273500 |
| P | 2.06419100 | -0.01623800 | -0.61596900 |
| P | -1.99717300 | -0.52811500 | -0.62864800 |
| Mn | 0.09441400 | -0.75668900 | -0.27679700 |
| C | 3.78570100 | -0.54251500 | 0.02773600 |
| H | 4.11265100 | -1.46372800 | -0.49381300 |
| H | 4.54705600 | 0.24765000 | -0.12927600 |
| H | 3.72848700 | -0.75882500 | 1.11131900 |
| C | 2.63724800 | 0.45446900 | -2.34123200 |
| H | 3.54334200 | 1.09072900 | -2.31711800 |
| H | 2.83827500 | -0.46171100 | -2.92859900 |
| H | 1.80913700 | 0.99618900 | -2.82737600 |
| C | -2.66234300 | -0.22095100 | -2.35903100 |
| H | -2.62051200 | -1.16123100 | -2.94117000 |
| H | -3.70067700 | 0.16385000 | -2.34278900 |
| H | -1.99696400 | 0.51079600 | -2.84627000 |
| C | -3.52678700 | -1.49060000 | -0.00422400 |
| H | -4.46927700 | -0.93505500 | -0.18222900 |
| H | -3.58826300 | -2.46944900 | -0.52067400 |
| H | -3.43138700 | -1.67551300 | 1.08210300 |
| H | 0.11808100 | -0.88316100 | -1.88484000 |
| N | 0.35425700 | -2.87800200 | -0.14011700 |
| N | 0.12542300 | -0.99016800 | 1.86792600 |

| | | | |
|---|-------------|-------------|-------------|
| H | 1.04438500 | -3.12039200 | -0.85672800 |
| H | -0.63749300 | -0.41461100 | 2.24380500 |
| H | 0.99688500 | -0.59532100 | 2.24290800 |
| H | -0.52216000 | -3.35316900 | -0.38149100 |
| C | -0.01653900 | -2.41636900 | 2.22492600 |
| H | -1.08707500 | -2.67817400 | 2.12110100 |
| H | 0.29757000 | -2.65584300 | 3.26610200 |
| C | 0.80410700 | -3.24081600 | 1.22258500 |
| H | 1.87051600 | -2.95650600 | 1.30014500 |
| H | 0.71487700 | -4.32802900 | 1.45161200 |

[Fe-S]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 1.07279100 | -2.06003100 | -0.70424600 |
| C | -0.06422100 | -1.29515700 | -0.37713400 |
| C | -1.28442700 | -1.99893000 | -0.36121700 |
| C | -1.39357600 | -3.36903500 | -0.64765800 |
| C | -0.22020900 | -4.07575000 | -0.96826900 |
| C | 1.03000900 | -3.43064500 | -1.00224000 |
| H | -2.37016800 | -3.86269200 | -0.62565900 |
| H | -0.28092000 | -5.14526100 | -1.19615900 |
| H | 1.94860300 | -3.97482400 | -1.24285700 |
| O | 2.31740700 | -1.39987500 | -0.72043800 |
| O | -2.45271300 | -1.28156400 | -0.05355600 |
| P | 2.21695800 | 0.07676800 | 0.10831400 |
| P | -2.18798900 | 0.38810000 | -0.11099600 |
| Fe | 0.04846200 | 0.64291100 | 0.01281100 |
| C | 3.62663900 | 0.93094600 | -0.73843300 |
| H | 3.90726200 | 1.84324400 | -0.18213100 |
| H | 4.49986200 | 0.25620800 | -0.77571400 |
| H | 3.37323100 | 1.21438900 | -1.77456700 |
| C | 2.98018800 | -0.34526400 | 1.73707900 |
| H | 3.98472000 | -0.77493500 | 1.58350200 |
| H | 3.06203800 | 0.55366000 | 2.37396800 |
| H | 2.34773800 | -1.08892500 | 2.24880900 |
| C | -3.33236800 | 0.92714700 | 1.23139100 |
| H | -3.49233800 | 2.01938100 | 1.18366800 |
| H | -4.30683600 | 0.42045500 | 1.12226500 |
| H | -2.90639500 | 0.67236800 | 2.21441800 |
| C | -3.19303100 | 0.82570800 | -1.61303300 |
| H | -4.18711500 | 0.35167700 | -1.53579300 |
| H | -3.33039800 | 1.91915500 | -1.69467000 |
| H | -2.71719300 | 0.45379100 | -2.53756000 |
| N | 0.18903900 | 2.74617200 | 0.16281800 |
| N | 0.22110400 | 1.04037300 | -1.98971000 |
| H | 0.82523100 | 3.03844300 | 0.91578600 |
| H | -0.44313500 | 0.46245800 | -2.52306800 |
| H | 1.14424000 | 0.75669500 | -2.34775500 |
| H | -0.72438200 | 3.15040900 | 0.40774400 |
| C | -0.00318100 | 2.49348300 | -2.26449600 |
| H | -1.09270600 | 2.66663600 | -2.27149500 |
| H | 0.39071500 | 2.79453800 | -3.25334200 |
| C | 0.65283600 | 3.30088500 | -1.14431200 |
| H | 1.74976400 | 3.18798300 | -1.18469200 |
| H | 0.42214700 | 4.37751700 | -1.25361000 |
| N | -0.09717000 | 0.42024000 | 1.84469400 |
| C | -0.18650200 | 0.26258400 | 3.01038100 |
| C | -0.29267800 | 0.02515400 | 4.44738800 |
| H | -0.77964600 | 0.87705100 | 4.95517100 |
| H | -0.88909600 | -0.88444100 | 4.64298900 |
| H | 0.70824400 | -0.11623000 | 4.89401900 |

[Fe-H]⁰

| | x | y | z |
|---|-------------|------------|------------|
| C | 0.99478600 | 2.06799600 | 0.35677600 |
| C | -0.12195900 | 1.23651300 | 0.10696400 |
| C | -1.37980800 | 1.85955400 | 0.27756300 |
| C | -1.54225300 | 3.19820100 | 0.67733600 |
| C | -0.38807700 | 3.96760800 | 0.92082500 |

L-L = en
M = Fe

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 0.89599500 | 3.41145100 | 0.75945100 | H | -2.41858000 | 0.99852900 | 2.46005900 |
| H | -2.54599100 | 3.62275500 | 0.78924100 | C | 3.25464300 | -0.82495200 | 1.65360400 |
| H | -0.49008400 | 5.01379900 | 1.23271100 | H | 3.36501000 | -1.92226300 | 1.72290700 |
| H | 1.80107200 | 4.00390700 | 0.93312600 | H | 4.25642700 | -0.37462300 | 1.54467500 |
| O | 2.26405500 | 1.50225200 | 0.18475800 | H | 2.79514500 | -0.45486200 | 2.58380800 |
| O | -2.51967700 | 1.08520200 | 0.03400300 | C | 3.29325200 | -0.92937700 | -1.20037800 |
| P | 2.09647100 | -0.04814900 | -0.55500700 | H | 4.28575300 | -0.45699800 | -1.09637300 |
| P | -2.05879900 | -0.46717800 | -0.55296800 | H | 3.42309400 | -2.02659900 | -1.18644900 |
| Fe | 0.06227600 | -0.68986500 | -0.26139100 | H | 2.87700500 | -0.62709600 | -2.17646200 |
| C | 3.68164400 | -0.75498100 | 0.15141500 | N | -0.16095100 | -2.73874700 | 0.23249600 |
| H | 3.93929200 | -1.69872100 | -0.36469200 | N | -0.13606300 | -0.95532400 | -1.84812300 |
| H | 4.51823200 | -0.04364300 | 0.02653900 | H | -0.80530300 | -3.08340300 | 0.95585200 |
| H | 3.56480900 | -0.96565300 | 1.22956700 | H | 0.54400000 | -0.35096300 | -2.32947300 |
| C | 2.68447800 | 0.34604700 | -2.27069700 | H | -1.04855000 | -0.65083700 | -2.21550200 |
| H | 3.65672300 | 0.87048200 | -2.25533900 | H | 0.75365800 | -3.14057400 | 0.47668900 |
| H | 2.77216700 | -0.58562000 | -2.85910100 | C | 0.09591900 | -2.39471200 | -2.17841500 |
| H | 1.92375100 | 0.98266600 | -2.75150700 | H | 1.18508000 | -2.56900200 | -2.16576000 |
| C | -2.75988200 | -0.37805400 | -2.26961800 | H | -0.27364500 | -2.65545000 | -3.18748400 |
| H | -2.69450900 | -1.37036700 | -2.75287400 | C | -0.58693200 | -3.24526500 | -1.10917300 |
| H | -3.81192100 | -0.04069300 | -2.25959500 | H | -1.68306300 | -3.14000800 | -1.17444400 |
| H | -2.14707400 | 0.32770900 | -2.85360600 | H | -0.34482200 | -4.31594100 | -1.24446200 |
| C | -3.44866800 | -1.40828300 | 0.28354900 | C | 0.04090600 | -0.42957200 | 1.93055500 |
| H | -4.42225400 | -0.91637400 | 0.10562400 | O | 0.09214900 | -0.29521300 | 3.09743000 |
| H | -3.50006700 | -2.44315900 | -0.10483100 | | | | |
| H | -3.27615000 | -1.45019200 | 1.37362300 | | | | |
| H | 0.05071200 | -0.61713300 | -1.79557500 | | | | |
| N | 0.26790300 | -2.77238900 | -0.29493000 | | | | |
| N | 0.10663000 | -1.01541300 | 1.82489200 | | | | |
| H | 0.93263900 | -3.05026700 | -1.02578300 | | | | |
| H | -0.63183800 | -0.45826200 | 2.27251900 | | | | |
| H | 0.99051500 | -0.66121100 | 2.21255100 | | | | |
| H | -0.62389100 | -3.21898500 | -0.54107900 | | | | |
| C | -0.05190300 | -2.46372300 | 2.10973000 | | | | |
| H | -1.12887400 | -2.70217800 | 2.03846100 | | | | |
| H | 0.29147900 | -2.75154200 | 3.12427500 | | | | |
| C | 0.71814900 | -3.24808200 | 1.04246000 | | | | |
| H | 1.79842300 | -3.03194900 | 1.12394100 | | | | |
| H | 0.57681200 | -4.33948200 | 1.18326700 | | | | |

[Fe-CO]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.06965000 | 2.05000100 | -0.50746600 |
| C | 0.07218100 | 1.30191400 | -0.16625500 |
| C | 1.29395900 | 1.99905800 | -0.17239600 |
| C | 1.39955900 | 3.36077500 | -0.49540600 |
| C | 0.22361600 | 4.05672900 | -0.82750700 |
| C | -1.02680800 | 3.41160100 | -0.84139200 |
| H | 2.37525700 | 3.85593100 | -0.48809100 |
| H | 0.28226100 | 5.12043300 | -1.08061100 |
| H | -1.94594000 | 3.94902400 | -1.09376000 |
| O | -2.31075800 | 1.38531500 | -0.51737200 |
| O | 2.46194800 | 1.29047400 | 0.14854000 |
| P | -2.22486400 | -0.09990300 | 0.28512000 |
| P | 2.21464400 | -0.37497500 | 0.20413400 |
| Fe | -0.03506400 | -0.63953300 | 0.22026200 |
| C | -3.58019800 | -0.97793200 | -0.61582500 |
| H | -3.83980900 | -1.91410400 | -0.09032400 |
| H | -4.47445000 | -0.33069600 | -0.64439300 |
| H | -3.29928600 | -1.21762100 | -1.65536700 |
| C | -3.02348000 | 0.26327800 | 1.90460100 |
| H | -4.03250600 | 0.67765900 | 1.73898000 |
| H | -3.10118000 | -0.65490600 | 2.51367400 |

L-L = en

M = Co

[Co-S]²⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -0.98538900 | 2.07684300 | -0.42542100 |
| C | 0.12740000 | 1.21879600 | -0.45879600 |
| C | 1.35606400 | 1.77099200 | -0.85876900 |
| C | 1.49371100 | 3.11501500 | -1.23188000 |
| C | 0.34994000 | 3.93392100 | -1.18834700 |
| C | -0.90018200 | 3.42961300 | -0.78415400 |
| H | 2.47018700 | 3.50933400 | -1.52919600 |
| H | 0.43474300 | 4.98702400 | -1.47440200 |
| H | -1.79180800 | 4.06359300 | -0.76068700 |
| O | -2.22436900 | 1.53466300 | -0.03508600 |
| O | 2.48383000 | 0.92090900 | -0.85492400 |
| P | -2.24655800 | -0.12084500 | -0.26463400 |
| P | 2.26026000 | -0.32117000 | 0.25142900 |
| Co | -0.02302800 | -0.66592000 | 0.04775600 |
| C | -2.98820800 | -0.30163700 | -1.94503100 |
| H | -3.09049100 | -1.36149000 | -2.23966500 |
| H | -3.99571000 | 0.15155600 | -1.93576200 |
| H | -2.39052000 | 0.24269600 | -2.69799900 |
| C | -3.58016400 | -0.64232200 | 0.87580100 |
| H | -4.44961300 | 0.02604800 | 0.74161900 |
| H | -3.89424100 | -1.67588500 | 0.64575900 |
| H | -3.24909100 | -0.58789400 | 1.92449600 |
| C | 2.85480400 | 0.35834000 | 1.84946100 |
| H | 2.78318400 | -0.40653800 | 2.64256900 |
| H | 3.90932900 | 0.66638800 | 1.74122300 |
| H | 2.25139200 | 1.23671500 | 2.13001600 |
| C | 3.59677900 | -1.46509900 | -0.27480000 |
| H | 4.55579400 | -0.91637100 | -0.26320600 |
| H | 3.67346200 | -2.31788300 | 0.42253400 |
| H | 3.43380200 | -1.84370700 | -1.29691900 |
| N | -0.20667700 | -2.70768900 | 0.40472200 |
| N | 0.24058600 | -1.22612900 | -1.83888100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -0.97393700 | -2.93256100 | 1.05301400 |
| H | 1.01347400 | -0.70397600 | -2.28199100 |
| H | -0.59301600 | -0.96757100 | -2.38639700 |
| H | 0.64217300 | -3.07467800 | 0.85778300 |
| C | 0.46973300 | -2.71069800 | -1.93826500 |
| H | 1.53217500 | -2.90249400 | -1.71695200 |
| H | 0.26746700 | -3.07207800 | -2.96212100 |
| C | -0.41930500 | -3.39933600 | -0.90767700 |
| H | -1.48531000 | -3.29721000 | -1.17522300 |
| H | -0.19262800 | -4.47908900 | -0.84989200 |
| N | -0.28097600 | -0.22702200 | 1.86345600 |
| C | -0.45907700 | 0.09327500 | 2.97737200 |
| C | -0.67946700 | 0.50549000 | 4.35709800 |
| H | -1.22987400 | -0.27553500 | 4.91134000 |
| H | 0.28601400 | 0.68257300 | 4.86397600 |
| H | -1.26677100 | 1.44122500 | 4.38020600 |

[Co-H]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -1.30116300 | 1.93939100 | -0.22418000 |
| C | -0.07133200 | 1.26215600 | -0.12690100 |
| C | 1.08332800 | 2.02866600 | -0.37713700 |
| C | 1.04171400 | 3.38510900 | -0.73068400 |
| C | -0.21708700 | 4.00534200 | -0.83068100 |
| C | -1.40298900 | 3.29425400 | -0.57438900 |
| H | 1.96895500 | 3.93669100 | -0.91288600 |
| H | -0.27410300 | 5.06425000 | -1.10338200 |
| H | -2.38436500 | 3.77347100 | -0.64125800 |
| O | -2.47509800 | 1.21507900 | 0.02773800 |
| O | 2.32879600 | 1.38689600 | -0.26289600 |
| P | -2.14967700 | -0.36842700 | 0.50275800 |
| P | 2.15139900 | -0.09854800 | 0.51945800 |
| Co | 0.02899300 | -0.64297200 | 0.23066500 |
| C | -3.44455600 | -1.25670400 | -0.47519300 |
| H | -3.51640700 | -2.31319000 | -0.15929100 |
| H | -4.42502900 | -0.77551600 | -0.31122000 |
| H | -3.21714900 | -1.21766500 | -1.55387700 |
| C | -2.83865600 | -0.42845000 | 2.20766400 |
| H | -3.89346400 | -0.10342000 | 2.21098500 |
| H | -2.77523600 | -1.45610000 | 2.60902800 |
| H | -2.24617500 | 0.23685500 | 2.85634800 |
| C | 2.70424900 | 0.25635700 | 2.23806800 |
| H | 2.69382200 | -0.67194700 | 2.83712500 |
| H | 3.72163600 | 0.68400700 | 2.24097900 |
| H | 2.00070100 | 0.97168000 | 2.69468600 |
| C | 3.60793000 | -0.97940100 | -0.19781400 |
| H | 4.50819200 | -0.34882600 | -0.08980400 |
| H | 3.78103200 | -1.93127500 | 0.33536900 |
| H | 3.46047900 | -1.18884300 | -1.27057100 |
| H | -0.00341800 | -0.40273900 | 1.69259300 |
| N | 0.15843700 | -2.69392800 | 0.42329100 |
| N | 0.07338800 | -1.07145400 | -1.80507200 |
| H | -0.75106500 | -3.09439800 | 0.68841500 |
| H | 0.96802900 | -0.76409700 | -2.21064400 |
| H | -0.64137700 | -0.52905100 | -2.30813300 |
| H | 0.80152600 | -2.97546300 | 1.17447000 |
| C | -0.11973100 | -2.53675800 | -2.01137300 |
| H | 0.24720700 | -2.87769400 | -2.99748900 |
| H | -1.20380100 | -2.74266400 | -1.97133300 |
| C | 0.59731300 | -3.28054700 | -0.88334700 |
| H | 0.39635400 | -4.36694300 | -0.93835800 |

[Co-CO]²⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| H | 1.68852500 | -3.13686400 | -0.96340800 |
| C | -0.98341900 | 2.13907600 | -0.09093400 |
| C | 0.11228600 | 1.26625600 | -0.20578300 |
| C | 1.33700700 | 1.80181000 | -0.63941600 |
| C | 1.48130500 | 3.15314900 | -0.97719500 |
| C | 0.35634800 | 3.99147400 | -0.85452000 |
| C | -0.88510500 | 3.50024200 | -0.41193900 |
| H | 2.45081100 | 3.53942400 | -1.30633900 |
| H | 0.45141100 | 5.05215200 | -1.10720700 |
| H | -1.76077900 | 4.15057200 | -0.32509300 |
| O | -2.20870900 | 1.61036900 | 0.34790300 |
| O | 2.44279500 | 0.92984000 | -0.72799500 |
| P | -2.29635500 | -0.03836100 | 0.13000000 |
| P | 2.26730400 | -0.38247100 | 0.29084100 |
| Co | -0.04850800 | -0.64960000 | 0.21266400 |
| C | -3.19703300 | -0.22028300 | -1.46755300 |
| H | -3.33657500 | -1.27937900 | -1.74736000 |
| H | -4.19459800 | 0.23993200 | -1.34634500 |
| H | -2.68127700 | 0.32256100 | -2.27929800 |
| C | -3.49000900 | -0.54332900 | 1.41705200 |
| H | -4.38513300 | 0.10047800 | 1.34035000 |
| H | -3.79972000 | -1.59259900 | 1.26468000 |
| H | -3.05999400 | -0.42967300 | 2.42531800 |
| C | 3.00829000 | 0.12468200 | 1.88841600 |
| H | 2.93480300 | -0.69193800 | 2.62890000 |
| H | 4.07318300 | 0.36892000 | 1.72802300 |
| H | 2.49374300 | 1.01567200 | 2.28472900 |
| C | 3.47108400 | -1.55875500 | -0.43458200 |
| H | 4.45721600 | -1.06002600 | -0.47000800 |
| H | 3.56108600 | -2.45912000 | 0.19839200 |
| H | 3.19918600 | -1.85280100 | -1.46098000 |
| N | -0.23888200 | -2.70286300 | 0.43058300 |
| N | 0.04331400 | -1.10177400 | -1.76305100 |
| H | -0.91635300 | -2.98270300 | 1.15449100 |
| H | 0.81279200 | -0.59847600 | -2.23127200 |
| H | -0.80935300 | -0.75255000 | -2.22318600 |
| H | 0.65564900 | -3.11316200 | 0.73565900 |
| C | 0.16519800 | -2.58665700 | -1.97988500 |
| H | 1.23199000 | -2.85563000 | -1.91179700 |
| H | -0.18454900 | -2.87027400 | -2.98826000 |
| C | -0.63424100 | -3.29539800 | -0.89194100 |
| H | -1.71727200 | -3.13104800 | -1.02312300 |
| H | -0.45737600 | -4.38578500 | -0.91541600 |
| C | -0.12518900 | -0.24158000 | 1.91332700 |
| O | -0.18453000 | 0.03047600 | 3.03729300 |

3. Bis-Bipyridine Systems: [(bpy)₂M(L)]ⁿ⁺

L = CO

M = Mn

[Mn-S]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -0.71512700 | 3.90841400 | 0.48473600 |
| C | -0.11083200 | 2.65400500 | 0.61280600 |
| C | -2.12388500 | 1.54962700 | 0.14705900 |
| C | -2.78890100 | 2.78175900 | -0.00089900 |
| C | -2.08203100 | 3.97748200 | 0.16719600 |
| H | -0.11730200 | 4.81251600 | 0.63503300 |
| H | -3.85495400 | 2.80477400 | -0.24377500 |
| H | -2.58787400 | 4.94205100 | 0.05847900 |
| C | 2.56256700 | 0.47041000 | 1.90744900 |
| C | 3.89757400 | 0.87547700 | 1.95832300 |
| C | 2.58369800 | 0.43937800 | -0.43751400 |
| C | 4.60527000 | 1.07322600 | 0.75810200 |
| H | 4.37108400 | 1.03057900 | 2.93278500 |
| C | 3.93175100 | 0.84713900 | -0.44639300 |
| H | 5.65251400 | 1.39084300 | 0.76255800 |
| H | 4.45344500 | 0.98404000 | -1.39802900 |
| N | 1.88308100 | 0.25457400 | 0.74070500 |
| N | -0.78427100 | 1.48655200 | 0.44778300 |
| C | 1.80185800 | 0.17051200 | -1.65134500 |
| C | 2.29151900 | 0.30416200 | -2.96684600 |
| C | -0.27975200 | -0.53105400 | -2.46529200 |
| C | 1.45773900 | 0.00618600 | -4.04990000 |
| H | 3.31756700 | 0.63886500 | -3.14328100 |
| C | 0.14432400 | -0.42411700 | -3.79439000 |
| H | -1.29255400 | -0.86426500 | -2.22209000 |
| H | 1.82658400 | 0.10635300 | -5.07588400 |
| H | -0.54474400 | -0.67294600 | -4.60716500 |
| C | -2.76916200 | 0.23515400 | 0.02470500 |
| C | -4.13934400 | 0.03977800 | -0.23391100 |
| C | -2.42899300 | -2.08101200 | 0.14565900 |
| C | -4.65668600 | -1.25848400 | -0.30312300 |
| H | -4.79986900 | 0.90025900 | -0.37344100 |
| C | -3.77941500 | -2.33924100 | -0.10589900 |
| H | -1.71652000 | -2.89223700 | 0.31125500 |
| H | -5.72073600 | -1.42370900 | -0.49922500 |
| H | -4.13288800 | -3.37437000 | -0.14044900 |
| N | 0.51705600 | -0.24161000 | -1.40853700 |
| N | -1.91066800 | -0.82503700 | 0.20968000 |
| Mn | 0.00286700 | -0.35357800 | 0.58846700 |
| H | 1.99471200 | 0.30895100 | 2.82638000 |
| H | 0.94828200 | 2.56118300 | 0.86473100 |
| N | 0.61002400 | -2.17178900 | 0.59843400 |
| C | 1.05286200 | -3.26241300 | 0.62255700 |
| C | 1.60347200 | -4.61287700 | 0.68266000 |
| H | 2.70779500 | -4.57967700 | 0.69606300 |
| H | 1.26102500 | -5.12690900 | 1.59869600 |
| H | 1.28465700 | -5.20680300 | -0.19253200 |
| C | -0.28997900 | -0.40311800 | 2.34051900 |
| O | -0.49245300 | -0.44265300 | 3.50052700 |

[Mn-H]⁰

| | x | y | z |
|---|------------|-------------|-------------|
| C | 0.29503100 | -2.39620000 | -2.86944800 |

| | | | |
|----|-------------|-------------|-------------|
| C | -0.18772700 | -1.81306000 | -1.69766000 |
| C | 1.92490200 | -0.94151000 | -1.17065800 |
| C | 2.47174100 | -1.50782500 | -2.33993900 |
| C | 1.65688500 | -2.24480300 | -3.20431200 |
| H | -0.38920100 | -2.96148300 | -3.51092600 |
| H | 3.53260600 | -1.36706900 | -2.57037600 |
| H | 2.06803600 | -2.69024500 | -4.11620000 |
| C | -2.55999900 | -1.72735000 | 1.08707900 |
| C | -3.92343200 | -1.94649700 | 0.93491800 |
| C | -2.71540700 | 0.38213400 | 0.05934100 |
| C | -4.73316200 | -0.95895200 | 0.32399200 |
| H | -4.35110700 | -2.88707800 | 1.29838000 |
| C | -4.10501800 | 0.20767600 | -0.11135900 |
| H | -5.81092800 | -1.10243300 | 0.19777600 |
| H | -4.68922500 | 1.00070800 | -0.58974500 |
| N | -1.91194600 | -0.58256500 | 0.67234600 |
| N | 0.59317600 | -1.09550400 | -0.84094100 |
| C | -1.97736700 | 1.56085200 | -0.35745300 |
| C | -2.53399900 | 2.69367100 | -0.99312500 |
| C | 0.14666600 | 2.55823400 | -0.39283200 |
| C | -1.72033800 | 3.77738200 | -1.32626600 |
| H | -3.60383100 | 2.71774200 | -1.22283100 |
| C | -0.34520800 | 3.70572100 | -1.01543400 |
| H | 1.20607800 | 2.46835600 | -0.13726000 |
| H | -2.14251100 | 4.66064300 | -1.81754300 |
| H | 0.33851100 | 4.52689100 | -1.25401800 |
| C | 2.67420600 | -0.16130300 | -0.18651100 |
| C | 4.05632300 | 0.10849100 | -0.25271900 |
| C | 2.51257300 | 1.01717200 | 1.83998500 |
| C | 4.67195600 | 0.85578000 | 0.75557200 |
| H | 4.64473200 | -0.27225400 | -1.09356800 |
| C | 3.87491200 | 1.31834800 | 1.82309500 |
| H | 1.85436900 | 1.34383300 | 2.64913500 |
| H | 5.74508700 | 1.07016200 | 0.71609800 |
| H | 4.30391000 | 1.90559000 | 2.64155400 |
| N | -0.63168000 | 1.49317300 | -0.05771100 |
| N | 1.89418500 | 0.28960500 | 0.86247000 |
| Mn | -0.02654900 | -0.21068500 | 0.84085700 |
| H | -0.14317200 | 0.59448100 | 2.19763300 |
| H | -1.92472700 | -2.47737800 | 1.56340300 |
| H | -1.23670300 | -1.91265200 | -1.40417400 |
| C | 0.23778900 | -1.48362600 | 2.03881800 |
| O | 0.41596700 | -2.26370800 | 2.91345000 |

[Mn-CO]⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.14618600 | 3.10149600 | -2.24022200 |
| C | 0.28612700 | 2.23427500 | -1.23013600 |
| C | -1.84164900 | 1.28043600 | -1.02055100 |
| C | -2.34005400 | 2.11955900 | -2.03623900 |
| C | -1.48567100 | 3.03874000 | -2.65589500 |
| H | 0.55849800 | 3.81044800 | -2.68505400 |
| H | -3.38926200 | 2.05979800 | -2.33768200 |
| H | -1.86151800 | 3.69903700 | -3.44401600 |
| C | 2.66172300 | 1.28898400 | 1.44411200 |
| C | 4.03201200 | 1.51973900 | 1.28814900 |
| C | 2.65672900 | -0.30852700 | -0.27186700 |
| C | 4.73802400 | 0.80524700 | 0.30645800 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | 4.52953200 | 2.24797400 | 1.93568500 | H | 3.27589200 | 0.66756300 | -3.14214200 |
| C | 4.03665500 | -0.11812100 | -0.47670900 | C | 0.10469800 | -0.40169300 | -3.79085900 |
| H | 5.81167400 | 0.95811400 | 0.15875400 | H | -1.33077600 | -0.85469200 | -2.22045300 |
| H | 4.56276200 | -0.69606100 | -1.24149200 | H | 1.78055100 | 0.13809300 | -5.07211500 |
| N | 1.96471100 | 0.39906400 | 0.68467400 | H | -0.58419400 | -0.65079200 | -4.60345000 |
| N | -0.52989100 | 1.33546800 | -0.63062800 | C | -2.74945800 | 0.21066900 | 0.03640100 |
| C | 1.84168500 | -1.28040600 | -1.02053800 | C | -4.12076900 | 0.00620000 | -0.20198600 |
| C | 2.34009900 | -2.11942500 | -2.03630300 | C | -2.38448500 | -2.11059900 | 0.12329400 |
| C | -0.28598400 | -2.23453400 | -1.22993200 | C | -4.62365700 | -1.29955800 | -0.27668200 |
| C | 1.48578600 | -3.03872600 | -2.65587600 | H | -4.79471800 | 0.85896600 | -0.31991400 |
| H | 3.38925800 | -2.05949200 | -2.33788700 | C | -3.73940900 | -2.37691100 | -0.10920100 |
| C | 0.14635700 | -3.10169800 | -2.24005100 | H | -1.66211700 | -2.91687100 | 0.26523600 |
| H | -1.31917800 | -2.25553000 | -0.87374000 | H | -5.68986200 | -1.47151200 | -0.45533300 |
| H | 1.86164700 | -3.69894800 | -3.44405300 | H | -4.08679200 | -3.41352900 | -0.15003700 |
| H | -0.55825800 | -3.81076700 | -2.68480800 | N | 0.48160700 | -0.22442200 | -1.41078600 |
| C | -2.65673300 | 0.30857800 | -0.27188900 | N | -1.89144600 | -0.84934500 | 0.18760800 |
| C | -4.03665100 | 0.11818100 | -0.47676300 | Fe | -0.00204900 | -0.34264300 | 0.55172600 |
| C | -2.66175300 | -1.28906100 | 1.44397700 | H | 1.97061900 | 0.29744100 | 2.83406300 |
| C | -4.73803500 | -0.80525600 | 0.30631200 | H | 0.97777900 | 2.55643200 | 0.83441300 |
| H | -4.56274700 | 0.69616300 | -1.24152000 | N | 0.67095300 | -2.15213800 | 0.57518600 |
| C | -4.03203400 | -1.51982000 | 1.28795600 | C | 1.15147400 | -3.21907700 | 0.63283400 |
| H | -2.08749000 | -1.82473600 | 2.20326100 | C | 1.73902000 | -4.55032200 | 0.71210200 |
| H | -5.81168100 | -0.95811400 | 0.15857500 | H | 2.83753500 | -4.47608800 | 0.79955300 |
| H | -4.52955800 | -2.24811600 | 1.93542100 | H | 1.35023600 | -5.08505200 | 1.59697700 |
| N | 0.52996700 | -1.33560800 | -0.63049700 | H | 1.49518000 | -5.13326400 | -0.19361100 |
| N | -1.96472000 | -0.39906600 | 0.68463100 | C | -0.35787100 | -0.40265600 | 2.28718600 |
| Mn | -0.00003300 | -0.00002100 | 0.85764600 | O | -0.62202400 | -0.44962400 | 3.41683800 |
| H | 2.08741700 | 1.82464700 | 2.20336800 | | | | |
| H | 1.31935000 | 2.25517500 | -0.87401700 | | | | |
| C | 0.31499800 | -1.20855500 | 2.12758500 | | | | |
| O | 0.52916900 | -1.99576400 | 2.97253400 | | | | |
| C | -0.31515800 | 1.20873400 | 2.12735800 | | | | |
| O | -0.52939700 | 1.99612800 | 2.97211100 | | | | |

L = CO
M = Fe

[Fe-S]²⁺

| | x | y | z |
|---|-------------|-------------|--------------|
| C | -0.70158000 | 3.89571600 | 0.49685300 |
| C | -0.08549300 | 2.64252200 | 0.60207800 |
| C | -2.10715400 | 1.52977400 | 0.16268400 |
| C | -2.78015500 | 2.75865900 | 0.04090300 |
| C | -2.07305400 | 3.95644100 | 0.20799200 |
| H | -0.10731200 | 4.80212600 | 0.64544400 |
| H | -3.85085400 | 2.78148800 | -0.17876600 |
| H | -2.58693300 | 4.91895100 | 0.12056400 |
| C | 2.53826500 | 0.46449500 | 1.91559600 |
| C | 3.87803400 | 0.86739700 | 1.97084000 |
| C | 2.55662800 | 0.45551700 | -0.43455800 |
| C | 4.57472500 | 1.07298600 | 0.77003600 |
| H | 4.35583100 | 1.01377100 | 2.94417600 |
| C | 3.90405700 | 0.86124400 | -0.441179800 |
| H | 5.62265100 | 1.38948800 | 0.77494400 |
| H | 4.42990500 | 1.00819900 | -1.38898700 |
| N | 1.87751700 | 0.26821000 | 0.74472300 |
| N | -0.76300400 | 1.48159100 | 0.43477200 |
| C | 1.76416000 | 0.19162600 | -1.64978900 |
| C | 2.25140700 | 0.33080000 | -2.96255900 |
| C | -0.32024000 | -0.51554700 | -2.46051600 |
| C | 1.41377000 | 0.03360500 | -4.04596000 |

[Fe-H]⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | 0.37071200 | -2.44197100 | -2.88398400 |
| C | -0.15948100 | -1.84340300 | -1.73429100 |
| C | 1.92107600 | -0.94639300 | -1.14507700 |
| C | 2.51862800 | -1.51913200 | -2.28370500 |
| C | 1.73663100 | -2.27650800 | -3.16467600 |
| H | -0.27987900 | -3.02661900 | -3.54142000 |
| H | 3.58510200 | -1.37815300 | -2.48083500 |
| H | 2.18669900 | -2.73090000 | -4.05309200 |
| C | -2.56194600 | -1.72495700 | 1.09616300 |
| C | -3.93918100 | -1.92965500 | 0.97628400 |
| C | -2.70985400 | 0.37517500 | 0.06241600 |
| C | -4.73153300 | -0.93440400 | 0.38016600 |
| H | -4.37611800 | -2.85860300 | 1.35490300 |
| C | -4.10200500 | 0.22651900 | -0.08100200 |
| H | -5.81397700 | -1.05947600 | 0.27804100 |
| H | -4.69049100 | 1.01958600 | -0.55064900 |
| N | -1.93563900 | -0.59660600 | 0.65741000 |
| N | 0.58741800 | -1.11091600 | -0.87630100 |
| C | -1.95083300 | 1.54848600 | -0.38654100 |
| C | -2.51555300 | 2.67571300 | -1.01359700 |
| C | 0.18176100 | 2.50465500 | -0.50537200 |
| C | -1.69261000 | 3.74238700 | -1.39069300 |
| H | -3.59161600 | 2.72000200 | -1.20264400 |
| C | -0.31525800 | 3.65291100 | -1.13153000 |
| H | 1.24670000 | 2.40472400 | -0.28274700 |
| H | -2.11807400 | 4.62646400 | -1.87609300 |
| H | 0.37170900 | 4.45899300 | -1.40622300 |
| C | 2.64009500 | -0.14280300 | -0.13908800 |
| C | 4.01778300 | 0.14377000 | -0.17667700 |
| C | 2.41513800 | 1.05291500 | 1.87564500 |

| | | | | | | | |
|----|-------------|-------------|----------------------------|----------------------------|-------------|-------------|-------------|
| C | 4.59568000 | 0.90725700 | 0.84512100 | O | -0.69963500 | 2.00355400 | 2.84676200 |
| H | 4.63571100 | -0.23261600 | -0.99673800 | | | | |
| C | 3.77806400 | 1.36957700 | 1.88985400 | L = CO | | | |
| H | 1.73451000 | 1.37773800 | 2.66654400 | M = Co | | | |
| H | 5.66681400 | 1.13247300 | 0.82880700 | | | | |
| H | 4.18438300 | 1.96382000 | 2.71370500 | [Co-S]³⁺ | | | |
| N | -0.60609600 | 1.46682500 | -0.13293300 | | x | y | z |
| N | 1.84770800 | 0.31749400 | 0.88422400 | C | -0.67533800 | 3.89802600 | 0.44081600 |
| Fe | -0.03865900 | -0.20248400 | 0.82069600 | C | -0.05159000 | 2.64639500 | 0.53343800 |
| H | -0.33186700 | 0.57257100 | 2.09986700 | C | -2.10042900 | 1.52734000 | 0.14414900 |
| H | -1.92490800 | -2.47951700 | 1.56289100 | C | -2.76959200 | 2.75965100 | 0.04148400 |
| H | -1.21716900 | -1.95020200 | -1.47572000 | C | -2.05483800 | 3.95712700 | 0.19001600 |
| C | 0.27112800 | -1.44993700 | 1.99392800 | H | -0.07511800 | 4.80407400 | 0.57143800 |
| O | 0.48415100 | -2.22181100 | 2.84955600 | H | -3.84622500 | 2.78412100 | -0.15003800 |
| | | | H | -2.57047100 | 4.92069700 | 0.11647800 | |
| | | | C | 2.47778400 | 0.49614300 | 1.94575000 | |
| | | | C | 3.81941300 | 0.89161200 | 2.02237200 | |
| | | | C | 2.55415000 | 0.45270500 | -0.41977200 | |
| | | | C | 4.54379000 | 1.07289500 | 0.83251800 | |
| | | | H | 4.27565300 | 1.05055700 | 3.00486600 | |
| | | | C | 3.90400700 | 0.84912600 | -0.39582300 | |
| | | | H | 5.59443100 | 1.38178400 | 0.85904100 | |
| | | | H | 4.45540500 | 0.97940700 | -1.33148700 | |
| | | | N | 1.85828600 | 0.29284800 | 0.75363800 | |
| | | | N | -0.74662800 | 1.49239000 | 0.38393500 | |
| | | | C | 1.77726200 | 0.17479400 | -1.63695800 | |
| | | | C | 2.27149500 | 0.27862100 | -2.94920800 | |
| | | | C | -0.32493400 | -0.52761200 | -2.45419000 | |
| | | | C | 1.43629800 | -0.03021300 | -4.03329800 | |
| | | | H | 3.30252400 | 0.59757800 | -3.12711400 | |
| | | | C | 0.11912700 | -0.44338300 | -3.78166600 | |
| | | | H | -1.34144200 | -0.84986700 | -2.22106800 | |
| | | | H | 1.81233000 | 0.04831400 | -5.05902400 | |
| | | | H | -0.56750000 | -0.70020400 | -4.59448600 | |
| | | | C | -2.74057500 | 0.21017700 | 0.02850600 | |
| | | | C | -4.11290400 | -0.01133600 | -0.18464200 | |
| | | | C | -2.34681400 | -2.12400000 | 0.09915300 | |
| | | | C | -4.60162700 | -1.32499100 | -0.25413700 | |
| | | | H | -4.79942700 | 0.83406400 | -0.28720500 | |
| | | | C | -3.70527600 | -2.39703200 | -0.11019200 | |
| | | | H | -1.61593200 | -2.92540900 | 0.22056200 | |
| | | | H | -5.67018900 | -1.50737600 | -0.41171800 | |
| | | | H | -4.04339900 | -3.43742500 | -0.15080700 | |
| | | | N | 0.48262000 | -0.22308000 | -1.41196000 | |
| | | | N | -1.87845300 | -0.85179500 | 0.15552700 | |
| | | | Co | 0.00227500 | -0.31341800 | 0.49424800 | |
| | | | H | 1.89049700 | 0.34861800 | 2.85551600 | |
| | | | H | 1.01703700 | 2.56526000 | 0.73668300 | |
| | | | N | 0.69660800 | -2.12685800 | 0.57425800 | |
| | | | C | 1.19456500 | -3.18182000 | 0.67923400 | |
| | | | C | 1.79633700 | -4.49815700 | 0.80503000 | |
| | | | H | 2.89103000 | -4.40350100 | 0.92931400 | |
| | | | H | 1.38288900 | -5.02119900 | 1.68746000 | |
| | | | H | 1.59139100 | -5.10020000 | -0.09946000 | |
| | | | C | -0.45677100 | -0.39062400 | 2.28084200 | |
| | | | O | -0.79414800 | -0.46302700 | 3.37225300 | |
| | | | [Co-H]²⁺ | x | y | z | |
| | | | C | 0.41434300 | -2.49153800 | -2.86941000 | |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -0.14681500 | -1.86874600 | -1.74533400 | H | 4.60951900 | -0.63224200 | -1.09034700 |
| C | 1.92732500 | -0.96277700 | -1.11844600 | N | 1.93126000 | 0.47151000 | 0.69140300 |
| C | 2.55218600 | -1.56095300 | -2.22726700 | N | -0.52983300 | 1.28861300 | -0.66450300 |
| C | 1.78731600 | -2.33480100 | -3.11239800 | C | 1.86273700 | -1.22990600 | -0.99817400 |
| H | -0.21860500 | -3.08803800 | -3.53307100 | C | 2.37848600 | -2.07818200 | -1.99404400 |
| H | 3.62361600 | -1.43081300 | -2.40212100 | C | -0.29129300 | -2.17496700 | -1.27681400 |
| H | 2.26022600 | -2.80974800 | -3.97798000 | C | 1.53164700 | -2.99212300 | -2.63954800 |
| C | -2.53450800 | -1.74035000 | 1.12590400 | H | 3.43801600 | -2.03054200 | -2.26200100 |
| C | -3.91501000 | -1.95213500 | 1.03744000 | C | 0.17752300 | -3.04297900 | -2.27315100 |
| C | -2.71794400 | 0.36274000 | 0.07687400 | H | -1.33506200 | -2.19395400 | -0.95821500 |
| C | -4.71918200 | -0.96027900 | 0.45482100 | H | 1.92816100 | -3.66011400 | -3.41202200 |
| H | -4.34077600 | -2.87983200 | 1.43126600 | H | -0.51893400 | -3.74676500 | -2.74034000 |
| C | -4.11099300 | 0.20386800 | -0.03238400 | C | -2.65079600 | 0.25792100 | -0.22791800 |
| H | -5.80366500 | -1.08978500 | 0.38076200 | C | -4.03666200 | 0.05444400 | -0.35994100 |
| H | -4.71808800 | 0.98751900 | -0.49346800 | C | -2.55949200 | -1.37253800 | 1.49561400 |
| N | -1.94325300 | -0.60975300 | 0.65950100 | C | -4.68713100 | -0.88279600 | 0.45718400 |
| N | 0.58661100 | -1.12305100 | -0.89124300 | H | -4.60933100 | 0.63334200 | -1.09060400 |
| C | -1.96544300 | 1.52905500 | -0.40510400 | C | -3.93689400 | -1.60680700 | 1.39916100 |
| C | -2.53608200 | 2.64010800 | -1.05024500 | H | -1.95420500 | -1.91601700 | 2.22548000 |
| C | 0.17700000 | 2.47757700 | -0.58815200 | H | -5.76769200 | -1.03876700 | 0.36477600 |
| C | -1.71393700 | 3.69395100 | -1.47054300 | H | -4.40072400 | -2.34253900 | 2.06471500 |
| H | -3.61488100 | 2.68515300 | -1.22161700 | N | 0.53009900 | -1.28837600 | -0.66492200 |
| C | -0.33310200 | 3.60870000 | -1.23821600 | N | -1.93151400 | -0.47177300 | 0.69093900 |
| H | 1.24501400 | 2.38335700 | -0.38324500 | Co | -0.00002500 | -0.00021700 | 0.74204800 |
| H | -2.14636600 | 4.56677500 | -1.96998500 | H | 1.95348000 | 1.91520400 | 2.22646600 |
| H | 0.35003500 | 4.40520100 | -1.54758200 | H | 1.33545900 | 2.19406600 | -0.95747900 |
| C | 2.62229800 | -0.13187000 | -0.11450000 | C | 0.49387300 | -1.26185000 | 2.00238600 |
| C | 3.99892400 | 0.15925600 | -0.12262700 | O | 0.85387800 | -2.04022300 | 2.75863400 |
| C | 2.34821300 | 1.13821400 | 1.86790900 | C | -0.49423100 | 1.26068300 | 2.00303300 |
| C | 4.54882100 | 0.95642600 | 0.89108600 | O | -0.85447400 | 2.03853700 | 2.75970400 |
| H | 4.63995900 | -0.23962600 | -0.91347100 | | | | |
| C | 3.71086400 | 1.45590500 | 1.90166900 | | | | |
| H | 1.65400800 | 1.49281800 | 2.63399100 | | | | |
| H | 5.62057300 | 1.18008200 | 0.89384800 | | | | |
| H | 4.09837900 | 2.07693900 | 2.71476500 | | | | |
| N | -0.61475800 | 1.45867500 | -0.18011600 | | | | |
| N | 1.81929200 | 0.37083400 | 0.87985100 | | | | |
| Co | -0.04949100 | -0.16509500 | 0.78430100 | | | | |
| H | -0.41124500 | 0.59132300 | 2.00766000 | | | | |
| H | -1.88521800 | -2.49273900 | 1.57946900 | | | | |
| H | -1.21147500 | -1.96833200 | -1.51442900 | | | | |
| C | 0.33638300 | -1.41986600 | 1.97709700 | | | | |
| O | 0.60944600 | -2.17556500 | 2.80426400 | | | | |

[Co-CO]³⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.17688400 | 3.04351100 | -2.27233700 |
| C | 0.29171600 | 2.17520900 | -1.27614200 |
| C | -1.86244500 | 1.23034700 | -0.99795600 |
| C | -2.37798100 | 2.07891900 | -1.99368000 |
| C | -1.53096900 | 2.99291400 | -2.63888500 |
| H | 0.51972300 | 3.74729900 | -2.73929600 |
| H | -3.43747800 | 2.03146200 | -2.26179500 |
| H | -1.92732500 | 3.66111600 | -3.41125900 |
| C | 2.55894400 | 1.37215700 | 1.49643700 |
| C | 3.93630600 | 1.60680400 | 1.40020100 |
| C | 2.65084000 | -0.25765100 | -0.22769500 |
| C | 4.68681200 | 0.88332400 | 0.45804200 |
| H | 4.39987900 | 2.34241200 | 2.06606900 |
| C | 4.03665100 | -0.05377000 | -0.35949800 |
| H | 5.76734400 | 1.03958400 | 0.36578300 |

L = Cl
M = Mn

[Mn-S]⁰

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.96241600 | 3.90987400 | 0.10490100 |
| C | -0.27310500 | 2.70032900 | 0.20224500 |
| C | -2.25872100 | 1.46178900 | 0.01674800 |
| C | -3.01022400 | 2.65097400 | -0.08034400 |
| C | -2.36575000 | 3.88941100 | -0.03383000 |
| H | -0.40621800 | 4.85201200 | 0.14575600 |
| H | -4.09784700 | 2.59889000 | -0.19144600 |
| H | -2.93964300 | 4.81958300 | -0.10426100 |
| C | 2.32640200 | 0.83801100 | 1.92825400 |
| C | 3.65987100 | 1.21979400 | 2.09587200 |
| C | 2.66754200 | 0.41977900 | -0.36163200 |
| C | 4.53404400 | 1.19409800 | 0.98921500 |
| H | 4.00677800 | 1.52719700 | 3.08810700 |
| C | 4.02453900 | 0.78688000 | -0.24788500 |
| H | 5.58579600 | 1.48301800 | 1.09104300 |
| H | 4.67427100 | 0.75062300 | -1.12839900 |
| N | 1.81488200 | 0.43776400 | 0.72823500 |
| N | -0.88669600 | 1.48660200 | 0.16800100 |
| C | 2.00626000 | 0.01876300 | -1.59872100 |
| C | 2.61517500 | -0.01796100 | -2.86914300 |
| C | -0.05466200 | -0.60996600 | -2.54603100 |
| C | 1.86788400 | -0.35870800 | -3.99981700 |
| H | 3.67671500 | 0.23233500 | -2.96672400 |
| C | 0.49661300 | -0.65126600 | -3.82446900 |
| H | -1.10811800 | -0.84334900 | -2.37282100 |

| | | | | | | | |
|----|-------------|-------------|-------------|----------------------|-------------|-------------|-------------|
| H | 2.33192100 | -0.38882400 | -4.99101500 | H | 3.87184100 | 2.56168600 | 2.61893200 |
| H | -0.14227200 | -0.91493800 | -4.67404700 | N | -0.83863800 | 1.44216400 | -0.18073500 |
| C | -2.80275400 | 0.11286100 | -0.05678900 | N | 1.75473700 | 0.61134300 | 0.78950000 |
| C | -4.16765800 | -0.20149700 | -0.20433300 | Mn | -0.05182100 | -0.05790500 | 0.67274400 |
| C | -2.24726000 | -2.16847100 | -0.08255000 | H | -0.29928000 | 0.62741800 | 2.08138400 |
| C | -4.57740100 | -1.53457400 | -0.29146100 | H | -1.58151600 | -2.55481600 | 1.48228900 |
| H | -4.90684300 | 0.60541900 | -0.23876600 | H | -1.02758100 | -1.78280200 | -1.66413800 |
| C | -3.58270700 | -2.53570300 | -0.23056600 | Cl | 0.68446500 | -1.93064400 | 2.04650900 |
| H | -1.45762100 | -2.92030100 | -0.01824700 | | | | |
| H | -5.63631500 | -1.79135600 | -0.39798100 | | | | |
| H | -3.84176900 | -3.59839800 | -0.28807500 | | | | |
| N | 0.66565800 | -0.29780000 | -1.42479400 | [Mn-CO] ⁰ | | | |
| N | -1.82345400 | -0.87020700 | 0.00670300 | x | y | z | |
| Mn | -0.02002700 | -0.26529900 | 0.38556800 | C | -0.34349700 | 3.01388700 | -2.37083200 |
| H | 1.60587000 | 0.81625500 | 2.75367800 | C | 0.16142100 | 2.12029600 | -1.42147900 |
| H | 0.81235200 | 2.67588000 | 0.32714600 | C | -1.95464800 | 1.19156300 | -1.03441100 |
| N | 0.65618900 | -2.00626900 | 0.72765900 | C | -2.52978200 | 2.06641300 | -1.98225900 |
| C | 1.12780600 | -3.04742700 | 1.01643600 | C | -1.72209400 | 2.98457000 | -2.65732700 |
| C | 1.69068100 | -4.32220200 | 1.44897900 | H | 0.33007400 | 3.72011700 | -2.86634200 |
| H | 2.78342100 | -4.23938300 | 1.59570800 | H | -3.60486500 | 2.03008500 | -2.18163900 |
| H | 1.23736500 | -4.62849100 | 2.40972100 | H | -2.15846700 | 3.67099100 | -3.39108500 |
| H | 1.50255600 | -5.11882200 | 0.70558500 | C | 2.49993800 | 1.50380800 | 1.35642000 |
| Cl | -0.61475000 | -0.18024900 | 2.70145500 | C | 3.86331800 | 1.80452700 | 1.27891300 |
| | | | C | 2.72890200 | -0.23520000 | -0.20602600 | |
| | | | C | 4.68940000 | 1.05125000 | 0.42373800 | |
| | | | H | 4.26673300 | 2.61882700 | 1.88948200 | |
| | | | C | 4.10995900 | 0.02039700 | -0.32355100 | |
| | | | H | 5.76179700 | 1.25988000 | 0.34487200 | |
| | | | H | 4.72498700 | -0.58828500 | -0.99358400 | |
| C | 0.67910500 | -2.39055200 | -2.86871400 | N | 1.92505400 | 0.50369800 | 0.63420500 |
| C | 0.05516500 | -1.72197800 | -1.81728400 | N | -0.60950400 | 1.22257100 | -0.76428100 |
| C | 2.10431300 | -0.86477700 | -1.03693100 | C | 2.00630500 | -1.28197800 | -0.93108300 |
| C | 2.79205700 | -1.52964000 | -2.07536900 | C | 2.58745500 | -2.15761600 | -1.86862300 |
| C | 2.08823900 | -2.30382900 | -3.00191300 | C | -0.09121300 | -2.28530900 | -1.25462500 |
| H | 0.07586100 | -2.98258000 | -3.56688800 | C | 1.80196600 | -3.11861700 | -2.51213200 |
| H | 3.88116200 | -1.43222600 | -2.15227400 | H | 3.65583000 | -2.08058100 | -2.09316500 |
| H | 2.61402500 | -2.82760100 | -3.80878800 | C | 0.43001800 | -3.17475000 | -2.19403200 |
| C | -2.35760200 | -1.89439500 | 1.08112100 | H | -1.14774400 | -2.30623700 | -0.97680000 |
| C | -3.70521800 | -2.23925900 | 1.07196000 | H | 2.24347500 | -3.80515200 | -3.24170700 |
| C | -2.82958400 | 0.20517100 | 0.11200900 | H | -0.23530200 | -3.90470300 | -2.66659700 |
| C | -4.66934000 | -1.32642800 | 0.57076700 | C | -2.68588400 | 0.19142000 | -0.26269900 |
| H | -4.00254300 | -3.21989700 | 1.46270800 | C | -4.07358600 | -0.02840400 | -0.37249400 |
| C | -4.20795600 | -0.09807600 | 0.09108000 | C | -2.52582200 | -1.49744100 | 1.35983600 |
| H | -5.73792700 | -1.57130900 | 0.56054900 | C | -4.69857700 | -1.00635200 | 0.40323200 |
| H | -4.91323700 | 0.64409300 | -0.30155600 | H | -4.66244900 | 0.58031500 | -1.06588400 |
| N | -1.87907000 | -0.68722900 | 0.62206200 | C | -3.89264700 | -1.75245600 | 1.29066000 |
| N | 0.72708400 | -0.97397100 | -0.89550800 | H | -1.89004000 | -2.05692800 | 2.04906100 |
| C | -2.22801500 | 1.42732800 | -0.36660700 | H | -5.77682100 | -1.18012000 | 0.32974200 |
| C | -2.90565000 | 2.50290300 | -0.97708500 | H | -4.32099800 | -2.52587300 | 1.93663400 |
| C | -0.16754600 | 2.54374300 | -0.66512500 | N | 0.66329800 | -1.34760200 | -0.61114000 |
| C | -2.20485600 | 3.62124300 | -1.43718700 | N | -1.88645100 | -0.54937300 | 0.60115100 |
| H | -3.99410600 | 2.44603900 | -1.09649400 | Mn | -0.01021900 | -0.06775500 | 0.71286000 |
| C | -0.79379800 | 3.62168600 | -1.27834400 | H | 1.80403300 | 2.04641900 | 2.00640100 |
| H | 0.91614200 | 2.52014600 | -0.52620700 | H | 1.22226600 | 2.11926600 | -1.15529500 |
| H | -2.72625400 | 4.45945800 | -1.91305800 | Cl | -0.56723200 | 1.66091100 | 2.25098800 |
| H | -0.18213200 | 4.46039300 | -1.63174300 | C | 0.34395000 | -1.13041700 | 2.09329000 |
| C | 2.70001600 | 0.02628900 | -0.05742800 | O | 0.60123300 | -1.82778100 | 3.01012100 |
| C | 4.07518000 | 0.32433800 | 0.04346800 | | | | |
| C | 2.22921900 | 1.50675600 | 1.71497100 | | | | |
| C | 4.53394800 | 1.23900000 | 0.99569200 | | | | |
| H | 4.78339500 | -0.17835000 | -0.62556900 | | | | |
| C | 3.57432500 | 1.84408900 | 1.84536200 | | | | |
| H | 1.45920900 | 1.92198000 | 2.37054600 | | | | |
| H | 5.60175000 | 1.46912400 | 1.08716800 | | | | |

L = Cl

M = Fe

[Fe-S]⁺

x y z

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -0.77269200 | 3.89730500 | 0.39750500 | C | -3.71513900 | -2.17605500 | 1.11121200 |
| C | -0.12836500 | 2.65538600 | 0.40579000 | C | -2.79412600 | 0.22502600 | 0.10224200 |
| C | -2.15340600 | 1.51761100 | 0.10383600 | C | -4.64880000 | -1.26802700 | 0.57434400 |
| C | -2.86035500 | 2.73336200 | 0.08884400 | H | -4.03185600 | -3.13956300 | 1.52405300 |
| C | -2.16695900 | 3.93947300 | 0.23959000 | C | -4.17361800 | -0.05524700 | 0.06498600 |
| H | -0.18341200 | 4.81074900 | 0.52151900 | H | -5.71900200 | -1.50020600 | 0.55532500 |
| H | -3.94682500 | 2.73542900 | -0.03474600 | H | -4.86736000 | 0.67740400 | -0.35968800 |
| H | -2.70467800 | 4.89288900 | 0.23619000 | N | -1.88239100 | -0.66128100 | 0.64272700 |
| C | 2.34480700 | 0.55705700 | 1.97725200 | N | 0.68862400 | -1.01556500 | -0.90578900 |
| C | 3.68521400 | 0.92286900 | 2.15790500 | C | -2.16423200 | 1.43707900 | -0.40783100 |
| C | 2.63293300 | 0.41932400 | -0.35205200 | C | -2.83452700 | 2.50553700 | -1.03239400 |
| C | 4.52291700 | 1.03668400 | 1.03629400 | C | -0.10033800 | 2.51966800 | -0.70856500 |
| H | 4.05751800 | 1.11177000 | 3.16945400 | C | -2.11378400 | 3.60720900 | -1.50357100 |
| C | 3.98783400 | 0.78035300 | -0.23280800 | H | -3.92226500 | 2.46620100 | -1.14890500 |
| H | 5.57519800 | 1.31885500 | 1.14564800 | C | -0.71345800 | 3.60174500 | -1.33876600 |
| H | 4.61938600 | 0.85809400 | -1.12250300 | H | 0.98126800 | 2.48887000 | -0.56046700 |
| N | 1.82135900 | 0.31193800 | 0.75009200 | H | -2.62428200 | 4.44494100 | -1.98952200 |
| N | -0.79160900 | 1.48279400 | 0.26573700 | H | -0.09516800 | 4.43224100 | -1.69531100 |
| C | 1.94659400 | 0.13264600 | -1.62112700 | C | 2.65603200 | 0.02582900 | -0.07856600 |
| C | 2.54292300 | 0.21775700 | -2.89293700 | C | 4.03068000 | 0.32110100 | -0.00405600 |
| C | -0.09860200 | -0.49421200 | -2.58551700 | C | 2.22101300 | 1.43799600 | 1.74910200 |
| C | 1.78550600 | -0.06410500 | -4.03573500 | C | 4.50187700 | 1.20268600 | 0.97444800 |
| H | 3.59333900 | 0.50750800 | -2.98805200 | H | 4.72820400 | -0.14948700 | -0.70396500 |
| C | 0.43720200 | -0.42559900 | -3.87566100 | C | 3.57300800 | 1.77036900 | 1.86721500 |
| H | -1.14088000 | -0.77596100 | -2.41836900 | H | 1.46313700 | 1.82735700 | 2.43277700 |
| H | 2.23712500 | -0.00051500 | -5.03077400 | H | 5.56970300 | 1.43431700 | 1.04767100 |
| H | -0.19892900 | -0.65328700 | -4.73639400 | H | 3.88988800 | 2.45456600 | 2.66084700 |
| C | -2.76366300 | 0.19157800 | -0.05102900 | N | -0.79110600 | 1.44252400 | -0.22825900 |
| C | -4.14027300 | -0.04494700 | -0.21476400 | N | 1.74857500 | 0.58988300 | 0.79422500 |
| C | -2.31607100 | -2.10536000 | -0.16388900 | Fe | -0.05637400 | -0.04821300 | 0.68254600 |
| C | -4.60550800 | -1.35737300 | -0.35586200 | H | -0.38573300 | 0.65531200 | 1.99431300 |
| H | -4.84455800 | 0.79163400 | -0.22014900 | H | -1.59129000 | -2.49683100 | 1.55901700 |
| C | -3.67183100 | -2.40633800 | -0.33191800 | H | -1.05852100 | -1.89689800 | -1.60025800 |
| H | -1.56024200 | -2.89190100 | -0.12348000 | Cl | 0.65795800 | -1.80497700 | 2.06686900 |
| H | -5.67485700 | -1.55745300 | -0.47637000 | | | | |
| H | -3.98375500 | -3.45040000 | -0.43116100 | | | | |
| N | 0.62825300 | -0.22676700 | -1.47082600 | | | | |
| N | -1.85435700 | -0.83715600 | -0.03060000 | | | | |
| Fe | -0.01958000 | -0.30523700 | 0.37075500 | | | | |
| H | 1.63805500 | 0.44270800 | 2.80674600 | | | | |
| H | 0.95227500 | 2.58299300 | 0.54241800 | | | | |
| N | 0.61568100 | -2.08014400 | 0.59532500 | | | | |
| C | 1.05165700 | -3.13948100 | 0.84487700 | | | | |
| C | 1.56826100 | -4.45558700 | 1.20354700 | | | | |
| H | 2.65913200 | -4.40802200 | 1.36804400 | | | | |
| H | 1.08836000 | -4.80472100 | 2.13513300 | | | | |
| H | 1.36642000 | -5.18844300 | 0.40268500 | | | | |
| Cl | -0.64374200 | -0.35240200 | 2.61138700 | | | | |

[Fe-H]⁰

| | x | y | z |
|---|-------------|-------------|-------------|
| C | 0.64698700 | -2.50315700 | -2.81419600 |
| C | 0.01929700 | -1.81226900 | -1.77293300 |
| C | 2.04536000 | -0.87800400 | -1.06125600 |
| C | 2.74129900 | -1.54563200 | -2.08841900 |
| C | 2.03950500 | -2.36982800 | -2.97514600 |
| H | 0.05452500 | -3.13890300 | -3.48028300 |
| H | 3.82420500 | -1.42388300 | -2.19030800 |
| H | 2.56661200 | -2.89991200 | -3.77560500 |
| C | -2.35829300 | -1.84374600 | 1.12998200 |

[Fe-CO]⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.27508300 | 2.97366100 | -2.40746800 |
| C | 0.22226900 | 2.07857200 | -1.45220100 |
| C | -1.90212400 | 1.17342700 | -1.07359300 |
| C | -2.46803500 | 2.04392600 | -2.02345200 |
| C | -1.64754200 | 2.95535900 | -2.69864200 |
| H | 0.40596900 | 3.67199900 | -2.90275800 |
| H | -3.54142000 | 2.01703100 | -2.22898100 |
| H | -2.07483700 | 3.64282400 | -3.43565700 |
| C | 2.43805700 | 1.52139400 | 1.37744100 |
| C | 3.80317100 | 1.83185700 | 1.31659700 |
| C | 2.70339800 | -0.22409200 | -0.17801100 |
| C | 4.63931400 | 1.08124100 | 0.47560100 |
| H | 4.19429700 | 2.64917600 | 1.92982900 |
| C | 4.08116600 | 0.04104600 | -0.27947300 |
| H | 5.71083800 | 1.29644500 | 0.41087800 |
| H | 4.71377300 | -0.56240200 | -0.93636600 |
| N | 1.89526700 | 0.51951100 | 0.64372700 |
| N | -0.56305500 | 1.19471100 | -0.79859100 |
| C | 1.99666500 | -1.29087100 | -0.90666100 |
| C | 2.60282600 | -2.17106700 | -1.82180300 |
| C | -0.08169600 | -2.33071200 | -1.23169800 |
| C | 1.83206700 | -3.15501300 | -2.45237900 |
| H | 3.67126200 | -2.08794300 | -2.03917900 |
| C | 0.46336300 | -3.23492300 | -2.15022300 |

| | | | |
|----|-------------|-------------|-------------|
| H | -1.14047300 | -2.36190300 | -0.96412800 |
| H | 2.29230700 | -3.84726000 | -3.16445300 |
| H | -0.18150300 | -3.98727300 | -2.61398900 |
| C | -2.66337900 | 0.18714600 | -0.28998200 |
| C | -4.05356200 | -0.00011000 | -0.39448900 |
| C | -2.53255300 | -1.47558500 | 1.35819500 |
| C | -4.68994900 | -0.95506100 | 0.40650400 |
| H | -4.63784600 | 0.60628800 | -1.09179900 |
| C | -3.91112100 | -1.70670400 | 1.29958600 |
| H | -1.90352800 | -2.03610700 | 2.05307300 |
| H | -5.77224500 | -1.10387100 | 0.33927200 |
| H | -4.35676500 | -2.45960600 | 1.95631300 |
| N | 0.65784000 | -1.37595700 | -0.61692000 |
| N | -1.90411200 | -0.55632200 | 0.58048800 |
| Fe | -0.00862300 | -0.05667300 | 0.68670100 |
| H | 1.73065100 | 2.06039400 | 2.01667100 |
| H | 1.28177800 | 2.07166800 | -1.18574000 |
| Cl | -0.65705200 | 1.58826700 | 2.18624800 |
| C | 0.35263700 | -1.04316100 | 2.09781900 |
| O | 0.61761600 | -1.67150700 | 3.04320600 |

L = Cl

M = Co

[Co-S]²⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.70922900 | 3.87374700 | 0.56009000 |
| C | -0.07665600 | 2.62407500 | 0.54863100 |
| C | -2.11584000 | 1.52016900 | 0.15108900 |
| C | -2.80284400 | 2.74587500 | 0.15089100 |
| C | -2.09551500 | 3.93706300 | 0.35853100 |
| H | -0.11300200 | 4.77440900 | 0.73312900 |
| H | -3.88508200 | 2.76852200 | -0.00231500 |
| H | -2.62074100 | 4.89737600 | 0.36813900 |
| C | 2.38487900 | 0.45717500 | 1.95718100 |
| C | 3.72999300 | 0.82599000 | 2.10666100 |
| C | 2.58848100 | 0.44079900 | -0.39465100 |
| C | 4.51965900 | 1.00565400 | 0.96105200 |
| H | 4.13792800 | 0.96592200 | 3.11223100 |
| C | 3.94218700 | 0.80919600 | -0.30223300 |
| H | 5.57281200 | 1.29306200 | 1.04552700 |
| H | 4.54299600 | 0.94002000 | -1.20643900 |
| N | 1.83051400 | 0.27813400 | 0.73609100 |
| N | -0.75968400 | 1.47521600 | 0.34538100 |
| C | 1.86474200 | 0.19932700 | -1.65563500 |
| C | 2.42508900 | 0.32933900 | -2.93920000 |
| C | -0.20322000 | -0.42901000 | -2.58608200 |
| C | 1.63636500 | 0.06919600 | -4.06800000 |
| H | 3.46881000 | 0.63253900 | -3.05851900 |
| C | 0.29946100 | -0.31762500 | -3.88915400 |
| H | -1.23659600 | -0.73083800 | -2.40099200 |
| H | 2.06127400 | 0.16736100 | -5.07213800 |
| H | -0.35367800 | -0.53191000 | -4.74023000 |
| C | -2.74278400 | 0.20498400 | -0.02917300 |
| C | -4.11817900 | -0.01871600 | -0.21201000 |
| C | -2.31682800 | -2.10836300 | -0.11129600 |
| C | -4.59213300 | -1.33073700 | -0.34519100 |
| H | -4.81558900 | 0.82293200 | -0.23695400 |
| C | -3.67603200 | -2.39255400 | -0.29505800 |
| H | -1.57102100 | -2.90201700 | -0.05139200 |
| H | -5.66204200 | -1.52000700 | -0.47853000 |

| | | | |
|----|-------------|-------------|-------------|
| H | -4.00036700 | -3.43335400 | -0.38586400 |
| N | 0.55770600 | -0.17764900 | -1.49722300 |
| N | -1.85985000 | -0.84103900 | 0.00806000 |
| Co | -0.02095800 | -0.31329600 | 0.39095400 |
| H | 1.71556900 | 0.29943600 | 2.80889100 |
| H | 0.99712500 | 2.53662500 | 0.71706300 |
| N | 0.64812700 | -2.10904700 | 0.52331600 |
| C | 1.10743600 | -3.16132900 | 0.74243000 |
| C | 1.65811200 | -4.47604500 | 1.03745300 |
| H | 2.75543400 | -4.41182700 | 1.14419300 |
| H | 1.23050000 | -4.85442300 | 1.98330000 |
| H | 1.42175600 | -5.18523400 | 0.22474000 |
| Cl | -0.60239800 | -0.42930500 | 2.56782800 |

[Co-H]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 0.58043600 | -2.45348300 | -2.90253600 |
| C | -0.03694200 | -1.80867000 | -1.82145400 |
| C | 1.98342200 | -0.85551500 | -1.12824600 |
| C | 2.67015700 | -1.46738100 | -2.19340400 |
| C | 1.95993900 | -2.27671600 | -3.09035800 |
| H | -0.01130900 | -3.08189800 | -3.57485000 |
| H | 3.74662600 | -1.32353600 | -2.32093200 |
| H | 2.47911800 | -2.76538100 | -3.92117800 |
| C | -2.42883000 | -1.78472000 | 1.17238400 |
| C | -3.79780700 | -2.07752500 | 1.10859100 |
| C | -2.76004000 | 0.27039900 | 0.07860000 |
| C | -4.67084700 | -1.15616500 | 0.51072900 |
| H | -4.16227300 | -3.01742100 | 1.53377200 |
| C | -4.14258900 | 0.03210000 | -0.01038900 |
| H | -5.74587600 | -1.35505600 | 0.45315800 |
| H | -4.80057000 | 0.76973700 | -0.47822400 |
| N | -1.91577800 | -0.63704400 | 0.66658000 |
| N | 0.64077300 | -1.02865900 | -0.95619500 |
| C | -2.07913000 | 1.47269600 | -0.42083700 |
| C | -2.71414500 | 2.55082900 | -1.06336300 |
| C | 0.00504400 | 2.53233100 | -0.62375000 |
| C | -1.95475800 | 3.64559100 | -1.49233200 |
| H | -3.79552900 | 2.53374700 | -1.22446500 |
| C | -0.56881800 | 3.63354100 | -1.26878400 |
| H | 1.07821300 | 2.48838500 | -0.42598000 |
| H | -2.43649500 | 4.49283600 | -1.99053100 |
| H | 0.06846700 | 4.46470100 | -1.58488900 |
| C | 2.62122500 | -0.00153400 | -0.10398500 |
| C | 3.99635000 | 0.29196100 | -0.05597700 |
| C | 2.25813500 | 1.24771200 | 1.86060100 |
| C | 4.50070700 | 1.08682800 | 0.98098100 |
| H | 4.67088600 | -0.10897100 | -0.81735800 |
| C | 3.61663100 | 1.57141600 | 1.95744900 |
| H | 1.52955400 | 1.57591300 | 2.60500000 |
| H | 5.57028700 | 1.31479900 | 1.03086900 |
| H | 3.96636400 | 2.18218700 | 2.79482100 |
| N | -0.72488300 | 1.47104300 | -0.20356200 |
| N | 1.76736500 | 0.49302800 | 0.84775300 |
| Co | -0.05827900 | -0.09035400 | 0.72823000 |
| H | -0.41430400 | 0.57136000 | 1.99440500 |
| H | -1.69989600 | -2.45154800 | 1.64307900 |
| H | -1.10846500 | -1.92286900 | -1.62806200 |
| Cl | 0.59044500 | -1.80812900 | 2.04727000 |

[Co-CO]²⁺

| | x | y | z | C | 3.73385000 | 1.36284000 | 2.00471000 |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -0.25287800 | 2.99069000 | -2.39020300 | C | 2.61755100 | 0.41301300 | -0.34652700 |
| C | 0.24603100 | 2.09186900 | -1.43801200 | C | 4.55131100 | 1.26262000 | 0.86225700 |
| C | -1.89379800 | 1.19071900 | -1.06367500 | H | 4.12479300 | 1.74017600 | 2.95492200 |
| C | -2.45200500 | 2.06773600 | -2.00944600 | C | 3.97538300 | 0.78646700 | -0.32034800 |
| C | -1.62511900 | 2.97920700 | -2.68000400 | H | 5.60552500 | 1.55449900 | 0.89360000 |
| H | 0.43152100 | 3.68710100 | -2.88351200 | H | 4.57944600 | 0.70307400 | -1.22873600 |
| H | -3.52517900 | 2.04619300 | -2.21673400 | N | 1.81673600 | 0.48623800 | 0.78143400 |
| H | -2.04896000 | 3.67200400 | -3.41398600 | N | -0.90476400 | 1.49753100 | 0.27079400 |
| C | 2.44056400 | 1.52512500 | 1.34777400 | C | 1.90356700 | -0.04917700 | -1.53740400 |
| C | 3.81134500 | 1.81271900 | 1.28236100 | C | 2.46377900 | -0.14066200 | -2.82709500 |
| C | 2.67983800 | -0.24946200 | -0.19859400 | C | -0.18058500 | -0.74976500 | -2.36260700 |
| C | 4.63261800 | 1.03759700 | 0.44972400 | C | 1.67169000 | -0.54549100 | -3.90557700 |
| H | 4.21450200 | 2.63012300 | 1.88774200 | H | 3.51565500 | 0.11531600 | -2.98546800 |
| C | 4.06013100 | -0.00271200 | -0.29763800 | C | 0.31802800 | -0.84963100 | -3.66251400 |
| H | 5.70785000 | 1.23384000 | 0.38468600 | H | -1.22200200 | -0.98979200 | -2.13577600 |
| H | 4.68627500 | -0.62036100 | -0.94726100 | H | 2.09480100 | -0.61740800 | -4.91238500 |
| N | 1.89306900 | 0.52466900 | 0.61705700 | H | -0.34878500 | -1.16522400 | -4.47106400 |
| N | -0.55140400 | 1.21224400 | -0.79300600 | C | -2.82381800 | 0.10857400 | 0.10379800 |
| C | 1.95742000 | -1.31054400 | -0.91970000 | C | -4.18763800 | -0.21068200 | -0.04625900 |
| C | 2.54962800 | -2.21480500 | -1.81936000 | C | -2.28430700 | -2.17275900 | 0.28126600 |
| C | -0.14933900 | -2.31485000 | -1.25038400 | C | -4.60376900 | -1.54538500 | -0.03141900 |
| C | 1.75955700 | -3.18972700 | -2.44335400 | H | -4.92140100 | 0.59124900 | -0.17320400 |
| H | 3.62094900 | -2.16012000 | -2.03072000 | C | -3.62053700 | -2.54297000 | 0.13599400 |
| C | 0.38729200 | -3.24025800 | -2.15483500 | H | -1.50063300 | -2.92376200 | 0.40447700 |
| H | -1.21063600 | -2.32318000 | -0.99345500 | H | -5.66049300 | -1.80454900 | -0.14715000 |
| H | 2.21131500 | -3.90051000 | -3.14278000 | H | -3.88642500 | -3.60487900 | 0.15219400 |
| H | -0.26844700 | -3.98489300 | -2.61571300 | N | 0.58109500 | -0.36582800 | -1.29886500 |
| C | -2.65508400 | 0.20546200 | -0.28278200 | N | -1.85136400 | -0.87130700 | 0.27112600 |
| C | -4.04466700 | 0.01060800 | -0.37252000 | Mn | -0.01887500 | -0.24483200 | 0.56124400 |
| C | -2.50258200 | -1.46584000 | 1.37518400 | H | 1.74817900 | 1.04919300 | 2.79607900 |
| C | -4.66666000 | -0.94771800 | 0.43843600 | H | 0.79012600 | 2.70866700 | 0.36504300 |
| H | -4.63957100 | 0.61207100 | -1.06507000 | N | 0.67798600 | -1.97851300 | 0.90781500 |
| C | -3.88160700 | -1.70046600 | 1.32530200 | C | 1.18965100 | -3.02315500 | 1.11928900 |
| H | -1.86804900 | -2.02832700 | 2.06357200 | C | 1.81230900 | -4.32199300 | 1.35956600 |
| H | -5.74940200 | -1.09943000 | 0.38239000 | H | 2.87171800 | -4.20195500 | 1.65079300 |
| H | -4.32032600 | -2.45584200 | 1.98399100 | H | 1.29087900 | -4.86279800 | 2.17014200 |
| N | 0.61492300 | -1.37442600 | -0.64887000 | H | 1.77401800 | -4.94678900 | 0.44841100 |
| N | -1.90044600 | -0.54258500 | 0.58446200 | N | -0.46564300 | -0.10384800 | 2.62173300 |
| Co | -0.01401100 | -0.02269200 | 0.65027900 | H | -1.37401400 | -0.55800300 | 2.79761300 |
| H | 1.75150700 | 2.08617400 | 1.98597700 | H | 0.21425100 | -0.58635300 | 3.222558600 |
| H | 1.30561900 | 2.08098300 | -1.17665100 | H | -0.55690000 | 0.86072200 | 2.97126100 |
| Cl | -0.63609800 | 1.49865000 | 2.20323100 | | | | |
| C | 0.40361200 | -0.99850900 | 2.11379200 | | | | |
| O | 0.70927700 | -1.59256700 | 3.04939600 | | | | |

L = NH₃
M = Mn

[Mn-S]⁺

| | x | y | z |
|---|-------------|------------|-------------|
| C | -0.98454800 | 3.91415800 | 0.02733600 |
| C | -0.29443600 | 2.71787500 | 0.23013200 |
| C | -2.27466500 | 1.46163600 | 0.08355600 |
| C | -3.02360400 | 2.63758300 | -0.12273100 |
| C | -2.38193500 | 3.87922800 | -0.14961500 |
| H | -0.43082700 | 4.85795800 | 0.00544700 |
| H | -4.10620700 | 2.57596200 | -0.26851900 |
| H | -2.95348100 | 4.79856400 | -0.31109000 |
| C | 2.39694600 | 0.97051500 | 1.91893400 |

[Mn-H]⁰

| | x | y | z |
|---|-------------|-------------|-------------|
| C | 0.81070200 | -3.02934500 | -2.21229500 |
| C | 0.14885900 | -2.15048500 | -1.36069900 |
| C | 2.17668700 | -1.13319700 | -0.71428500 |
| C | 2.89747000 | -2.01166800 | -1.55260500 |
| C | 2.22386300 | -2.97268500 | -2.30912600 |
| H | 0.23052600 | -3.75122600 | -2.79736000 |
| H | 3.98783300 | -1.92666900 | -1.61557900 |
| H | 2.77309500 | -3.65481500 | -2.96642000 |
| C | -2.30585100 | -1.86665800 | 1.20980100 |
| C | -3.65155600 | -2.21502600 | 1.27987800 |
| C | -2.80831900 | 0.16606900 | 0.13524200 |
| C | -4.62853800 | -1.32395000 | 0.77642200 |
| H | -3.93275700 | -3.18010500 | 1.71573900 |
| C | -4.18303300 | -0.13593500 | 0.18843600 |
| H | -5.69554700 | -1.56338000 | 0.82548600 |
| H | -4.90342700 | 0.57127600 | -0.23673000 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| N | -1.84116900 | -0.67621200 | 0.69699000 | C | 4.07497100 | 0.25246700 | 0.21726500 |
| N | 0.79006200 | -1.21211600 | -0.59291800 | C | 2.60696800 | -1.73713000 | -0.98855800 |
| C | -2.22004900 | 1.32709800 | -0.49578800 | C | 4.74163500 | -0.90075300 | -0.20388200 |
| C | -2.92318800 | 2.33540400 | -1.18831900 | H | 4.63332100 | 1.06141200 | 0.69761400 |
| C | -0.17133600 | 2.36889500 | -1.02362300 | C | 3.97922600 | -1.91377000 | -0.82039300 |
| C | -2.23303500 | 3.37767900 | -1.80816000 | H | 2.00102800 | -2.51343900 | -1.46107400 |
| H | -4.01601100 | 2.28691200 | -1.24314800 | H | 5.82071100 | -1.00980200 | -0.05973200 |
| C | -0.81889300 | 3.37685800 | -1.72897700 | H | 4.44245100 | -2.84041100 | -1.17364800 |
| H | 0.91781000 | 2.34332400 | -0.94016900 | N | -0.55863000 | -1.04216600 | 0.94079100 |
| H | -2.76987600 | 4.16399700 | -2.34892600 | N | 1.92648100 | -0.61588900 | -0.57880500 |
| H | -0.22252900 | 4.15744200 | -2.21363100 | Mn | 0.00783600 | -0.28156300 | -0.80790700 |
| C | 2.74724300 | -0.04784900 | 0.06466600 | H | -2.04124600 | 1.07726400 | -2.74192300 |
| C | 4.11987200 | 0.27096300 | 0.14524500 | H | -1.29681700 | 2.38478200 | 0.22619800 |
| C | 2.22252400 | 1.78135700 | 1.46277000 | C | -0.30482900 | -1.79756800 | -1.66902200 |
| C | 4.54664300 | 1.36960200 | 0.89625200 | O | -0.52363100 | -2.79949200 | -2.25637200 |
| H | 4.84951100 | -0.35117500 | -0.38447300 | N | 0.44345600 | 0.73421100 | -2.60689100 |
| C | 3.56478900 | 2.14264900 | 1.56143300 | H | 0.21420700 | 1.73860300 | -2.58220100 |
| H | 1.43082500 | 2.34060400 | 1.96904100 | H | 1.45949500 | 0.68012600 | -2.76986600 |
| H | 5.60980900 | 1.62262000 | 0.96524200 | H | 0.00627800 | 0.34128000 | -3.45135900 |
| H | 3.84010700 | 3.01925900 | 2.15772200 | | | | |
| N | -0.83136100 | 1.35156700 | -0.38016200 | | | | |
| N | 1.77816300 | 0.69694200 | 0.74376700 | | | | |
| Mn | -0.03706900 | -0.00157700 | 0.70884800 | | | | |
| H | -0.34850400 | 0.94478100 | 1.97101200 | | | | |
| H | -1.53896000 | -2.56193600 | 1.56700500 | | | | |
| H | -0.94084200 | -2.16816700 | -1.25897300 | | | | |
| N | 0.49855800 | -1.25802000 | 2.29638400 | | | | |
| H | 1.28439100 | -0.81136300 | 2.78777400 | | | | |
| H | -0.27190600 | -1.32256700 | 2.97321200 | | | | |
| H | 0.79426200 | -2.21316900 | 2.04594100 | | | | |

[Mn-CO]⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | 0.22286000 | 3.64811500 | 1.13243700 |
| C | -0.23971800 | 2.49849800 | 0.48425800 |
| C | 1.90604500 | 1.55007300 | 0.44211700 |
| C | 2.43555500 | 2.68162000 | 1.09815600 |
| C | 1.59113200 | 3.74011100 | 1.44721500 |
| H | -0.47783400 | 4.44940700 | 1.38582700 |
| H | 3.50169400 | 2.73191100 | 1.33660800 |
| H | 1.99181300 | 4.62190500 | 1.95758600 |
| C | -2.62693800 | 0.80949000 | -1.85886800 |
| C | -3.99582000 | 1.08584000 | -1.81791000 |
| C | -2.67150600 | -0.16888400 | 0.26613200 |
| C | -4.72986700 | 0.71746000 | -0.67683500 |
| H | -4.47338300 | 1.57657600 | -2.67145000 |
| C | -4.05344400 | 0.08203400 | 0.36976400 |
| H | -5.80438700 | 0.91361300 | -0.60882100 |
| H | -4.59953800 | -0.22746700 | 1.26528500 |
| N | -1.94870000 | 0.19942400 | -0.84871000 |
| N | 0.56801200 | 1.46346700 | 0.13819800 |
| C | -1.87536000 | -0.85623600 | 1.29076700 |
| C | -2.38503200 | -1.31775800 | 2.51964900 |
| C | 0.24728100 | -1.69781200 | 1.81728000 |
| C | -1.54360000 | -1.98734400 | 3.41423000 |
| H | -3.43617400 | -1.15564100 | 2.77429500 |
| C | -0.20024000 | -2.18198500 | 3.04984500 |
| H | 1.28263400 | -1.83623500 | 1.49804600 |
| H | -1.92764900 | -2.35319400 | 4.37159200 |
| H | 0.49969400 | -2.70533900 | 3.70839600 |
| C | 2.68443100 | 0.38125400 | 0.02555200 |

L = NH₃

M = Fe

[Fe-S]²⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.76917400 | -3.91363500 | -0.25378800 |
| C | -0.13103800 | -2.67696400 | -0.40855200 |
| C | -2.15726400 | -1.51755500 | -0.17303000 |
| C | -2.85517900 | -2.72811400 | -0.01073000 |
| C | -2.15799400 | -3.94235300 | -0.05200300 |
| H | -0.17814900 | -4.83364300 | -0.29062200 |
| H | -3.93676300 | -2.72393900 | 0.14974500 |
| H | -2.68914100 | -4.89118400 | 0.07291600 |
| C | 2.49458500 | -0.68123000 | -1.93790500 |
| C | 3.83547700 | -1.07941600 | -1.98361800 |
| C | 2.56296500 | -0.41787100 | 0.38919900 |
| C | 4.56303900 | -1.14311100 | -0.78411600 |
| H | 4.29293600 | -1.33220300 | -2.94483200 |
| C | 3.91542700 | -0.80814800 | 0.41155700 |
| H | 5.61423800 | -1.44818100 | -0.77962500 |
| H | 4.46161300 | -0.84810700 | 1.35787200 |
| N | 1.85372900 | -0.35584800 | -0.78633600 |
| N | -0.79746900 | -1.49434800 | -0.37675700 |
| C | 1.78335000 | -0.05044100 | 1.58327700 |
| C | 2.28305200 | -0.07379100 | 2.89838400 |
| C | -0.30588900 | 0.68638900 | 2.35294500 |
| C | 1.45143400 | 0.29545800 | 3.96325900 |
| H | 3.31425000 | -0.38100000 | 3.09269300 |
| C | 0.13261000 | 0.68417400 | 3.68299700 |
| H | -1.32422400 | 0.98736400 | 2.09838000 |
| H | 1.82729900 | 0.27984900 | 4.99112400 |
| H | -0.55621500 | 0.98319800 | 4.47873700 |
| C | -2.77853800 | -0.18403100 | -0.13902500 |
| C | -4.15331500 | 0.05638400 | 0.04188100 |
| C | -2.35891500 | 2.12266300 | -0.27610800 |
| C | -4.63103300 | 1.37327200 | 0.06306300 |
| H | -4.84818300 | -0.77908600 | 0.16415800 |
| C | -3.71442900 | 2.42512400 | -0.09984400 |
| H | -1.61374800 | 2.91153600 | -0.39998900 |
| H | -5.69804300 | 1.57350200 | 0.20253600 |
| H | -4.03803200 | 3.47033900 | -0.09189000 |

| | | | |
|----|-------------|-------------|-------------|
| N | 0.49119600 | 0.32739700 | 1.31667800 |
| N | -1.88310100 | 0.84915800 | -0.29439500 |
| Fe | -0.01305000 | 0.29566700 | -0.58329600 |
| H | 1.90953000 | -0.62750800 | -2.85969400 |
| H | 0.94826500 | -2.61802400 | -0.56374300 |
| N | 0.65963800 | 2.07216900 | -0.80657600 |
| C | 1.15207200 | 3.13149900 | -0.93113400 |
| C | 1.75482500 | 4.45150900 | -1.08028100 |
| H | 2.83135900 | 4.35772800 | -1.30878700 |
| H | 1.26862000 | 5.00828500 | -1.90095600 |
| H | 1.64329800 | 5.03082800 | -0.14639100 |
| N | -0.43545300 | 0.23427900 | -2.59155700 |
| H | -0.40473700 | -0.71123200 | -3.00029200 |
| H | -1.38888600 | 0.58540700 | -2.76677400 |
| H | 0.18784400 | 0.83022200 | -3.15483600 |

$$[\text{Fe-H}]^+$$

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -0.65130600 | -3.00718500 | 2.27974700 |
| C | -0.02713200 | -2.17714300 | 1.34317100 |
| C | -2.06242300 | -1.16374600 | 0.76936500 |
| C | -2.75219000 | -1.97379900 | 1.69236500 |
| C | -2.04363700 | -2.90867200 | 2.45642900 |
| H | -0.05286000 | -3.71575500 | 2.86080600 |
| H | -3.83412100 | -1.87081000 | 1.81834200 |
| H | -2.56493200 | -3.54369700 | 3.17969000 |
| C | 2.46203800 | -1.70804000 | -1.28809400 |
| C | 3.83459100 | -1.96815700 | -1.28511700 |
| C | 2.75650200 | 0.28683500 | -0.09605700 |
| C | 4.70432900 | -1.04573400 | -0.67588000 |
| H | 4.20982400 | -2.88277100 | -1.75453700 |
| C | 4.14829500 | 0.08423200 | -0.06661100 |
| H | 5.78598500 | -1.21105400 | -0.66522900 |
| H | 4.79346000 | 0.81156700 | 0.43471400 |
| N | 1.90425300 | -0.59186000 | -0.73747000 |
| N | -0.70222200 | -1.27165000 | 0.58738700 |
| C | 2.05385700 | 1.39265700 | 0.55196100 |
| C | 2.66659300 | 2.41034600 | 1.30646800 |
| C | -0.06728000 | 2.28464700 | 1.00740800 |
| C | 1.88071100 | 3.38826300 | 1.92413000 |
| H | 3.75522200 | 2.43193000 | 1.41137800 |
| C | 0.48401100 | 3.31162200 | 1.77690400 |
| H | -1.14711700 | 2.20372700 | 0.86875900 |
| H | 2.34367000 | 4.18665300 | 2.51226300 |
| H | -0.17958600 | 4.04148700 | 2.25087500 |
| C | -2.68341200 | -0.12498000 | -0.06589300 |
| C | -4.05818500 | 0.17872400 | -0.08536200 |
| C | -2.25747600 | 1.57009100 | -1.64474300 |
| C | -4.53343600 | 1.20745000 | -0.90773200 |
| H | -4.75299600 | -0.38896100 | 0.54057100 |
| C | -3.61121500 | 1.91674700 | -1.69879600 |
| H | -1.50010800 | 2.08965900 | -2.23759400 |
| H | -5.60027900 | 1.45112100 | -0.93138000 |
| H | -3.93164400 | 2.73152000 | -2.35535600 |
| N | 0.68653600 | 1.33842600 | 0.38194800 |
| N | -1.78133500 | 0.56777200 | -0.85023900 |
| Fe | 0.05439700 | -0.03879300 | -0.79194300 |
| H | 0.41613900 | 0.92212900 | -1.93643100 |
| H | 1.77026700 | -2.42241300 | -1.74327600 |
| H | 1.05414500 | -2.22028200 | 1.17854700 |
| N | -0.39097200 | -1.29962000 | -2.33450700 |

$$[\text{Fe}-\text{CO}]^{2+}$$

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 0.20276000 | 3.61772800 | 1.20504600 |
| C | -0.26544200 | 2.48565300 | 0.52496200 |
| C | 1.87922200 | 1.53551900 | 0.46490500 |
| C | 2.41189300 | 2.64381100 | 1.14932400 |
| C | 1.56682200 | 3.69693200 | 1.52488400 |
| H | -0.49567500 | 4.41522900 | 1.47560100 |
| H | 3.47729500 | 2.68839600 | 1.39061700 |
| H | 1.96909500 | 4.56435100 | 2.05797600 |
| C | -2.61496300 | 0.87288300 | -1.82350800 |
| C | -3.99061800 | 1.12496900 | -1.77083200 |
| C | -2.64296100 | -0.18662300 | 0.27015000 |
| C | -4.71224500 | 0.69862600 | -0.64467000 |
| H | -4.47856800 | 1.63957600 | -2.60388800 |
| C | -4.02793900 | 0.03728800 | 0.38295300 |
| H | -5.79046500 | 0.87206300 | -0.57000100 |
| H | -4.57246400 | -0.31036400 | 1.26480800 |
| N | -1.94111200 | 0.23898300 | -0.83118200 |
| N | 0.54428200 | 1.46290900 | 0.15820300 |
| C | -1.82924200 | -0.88986700 | 1.27650900 |
| C | -2.33118300 | -1.40364000 | 2.48600800 |
| C | 0.31822200 | -1.68804800 | 1.78964600 |
| C | -1.47170900 | -2.07764200 | 3.36330600 |
| H | -3.38726800 | -1.28389800 | 2.74176300 |
| C | -0.12283600 | -2.22306400 | 3.00660900 |
| H | 1.35861900 | -1.79085700 | 1.47544800 |
| H | -1.85150300 | -2.48625600 | 4.30505600 |
| H | 0.58674100 | -2.74758800 | 3.65335700 |
| C | 2.67058000 | 0.37517500 | 0.01473900 |
| C | 4.06055500 | 0.24720300 | 0.19461400 |
| C | 2.59306000 | -1.71046100 | -1.06960200 |
| C | 4.72282700 | -0.89539400 | -0.27396200 |
| H | 4.62614900 | 1.03726200 | 0.69583700 |
| C | 3.97300300 | -1.89181600 | -0.91820500 |
| H | 1.98422100 | -2.47229100 | -1.56260000 |
| H | 5.80386900 | -1.00313900 | -0.13975200 |
| H | 4.44073600 | -2.80247700 | -1.30439200 |
| N | -0.50725900 | -1.03143200 | 0.93960900 |
| N | 1.93867800 | -0.60624000 | -0.61500000 |
| Fe | 0.00040200 | -0.23546000 | -0.80447800 |
| H | -2.03360700 | 1.18845000 | -2.69297100 |
| H | -1.32144400 | 2.38666400 | 0.26093700 |
| C | -0.39006000 | -1.74017200 | -1.64025100 |
| O | -0.67911400 | -2.72535400 | -2.18822800 |
| N | 0.45244400 | 0.72405100 | -2.56688200 |
| H | 0.27719000 | 1.73852100 | -2.51504000 |
| H | 1.45733000 | 0.62155900 | -2.77399800 |
| H | -0.03550100 | 0.37733400 | -3.40549200 |

$$\begin{array}{l} \mathbf{L = NH_3} \\ \mathbf{M = Co} \end{array}$$

$$[\text{Co-S}]^{3+}$$

x y z

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -0.71520000 | 3.90602300 | 0.27359900 | H | 2.48050200 | -3.47368800 | -3.28931600 |
| C | -0.08116000 | 2.66443500 | 0.41895600 | C | -2.54543800 | -1.60670900 | 1.36352100 |
| C | -2.13144500 | 1.51672300 | 0.18716600 | C | -3.92725000 | -1.82450500 | 1.31837700 |
| C | -2.81543100 | 2.73583700 | 0.03526200 | C | -2.72944000 | 0.34009600 | 0.06552600 |
| C | -2.10458600 | 3.94407100 | 0.07890300 | C | -4.73518000 | -0.90598000 | 0.62984600 |
| H | -0.11610600 | 4.82117700 | 0.31413800 | H | -4.35199900 | -2.69872700 | 1.82055400 |
| H | -3.89846300 | 2.74337600 | -0.11730400 | C | -4.12473200 | 0.18011600 | -0.00959600 |
| H | -2.62893700 | 4.89851700 | -0.03769300 | H | -5.82096400 | -1.03692400 | 0.58471300 |
| C | 2.49708300 | 0.64658100 | 1.93291400 | H | -4.73150800 | 0.90077100 | -0.56428700 |
| C | 3.84073300 | 1.04112800 | 1.96112300 | N | -1.94820000 | -0.54451800 | 0.76757300 |
| C | 2.53213900 | 0.42252600 | -0.41335100 | N | 0.65308200 | -1.30892500 | -0.60780000 |
| C | 4.54732200 | 1.12540300 | 0.74993300 | C | -1.97028400 | 1.41062000 | -0.59357600 |
| H | 4.31372400 | 1.27545700 | 2.92006500 | C | -2.53381000 | 2.41638200 | -1.39810200 |
| C | 3.88424500 | 0.81240300 | -0.44521000 | C | 0.18539300 | 2.26087800 | -0.97742500 |
| H | 5.59944000 | 1.42955600 | 0.73562100 | C | -1.70176600 | 3.36618600 | -2.00432700 |
| H | 4.41928600 | 0.86906500 | -1.39733600 | H | -3.61547600 | 2.45787500 | -1.55164000 |
| N | 1.85187600 | 0.34945600 | 0.77716300 | C | -0.31733500 | 3.28027300 | -1.79544400 |
| N | -0.77013400 | 1.49649800 | 0.38235900 | H | 1.25601900 | 2.17264000 | -0.78762200 |
| C | 1.73353500 | 0.06772700 | -1.59674200 | H | -2.12780600 | 4.15659200 | -2.63026200 |
| C | 2.20807500 | 0.09226000 | -2.92047600 | H | 0.37558300 | 3.99296500 | -2.25238500 |
| C | -0.38037800 | -0.67073300 | -2.33788300 | C | 2.64284100 | -0.15970800 | 0.06329100 |
| C | 1.35614800 | -0.27548900 | -3.97215700 | C | 4.01807500 | 0.14080700 | 0.06147800 |
| H | 3.23665800 | 0.39732200 | -3.13249300 | C | 2.27042900 | 1.46329700 | 1.74243100 |
| C | 0.04183900 | -0.66580300 | -3.67482400 | C | 4.51745500 | 1.12615800 | 0.92494600 |
| H | -1.39469400 | -0.97232800 | -2.07215700 | H | 4.69727300 | -0.39302900 | -0.60871900 |
| H | 1.71592100 | -0.25831400 | -5.00640300 | C | 3.62939900 | 1.79967700 | 1.77936400 |
| H | -0.65950000 | -0.96493100 | -4.46006100 | H | 1.53627700 | 1.96173300 | 2.38097100 |
| C | -2.76192700 | 0.18905200 | 0.15726200 | H | 5.58632700 | 1.36311600 | 0.92998400 |
| C | -4.13731700 | -0.05296300 | -0.01302800 | H | 3.97453200 | 2.57622500 | 2.46850900 |
| C | -2.34076400 | -2.13070800 | 0.30663700 | N | -0.61605900 | 1.34532600 | -0.38181400 |
| C | -4.61348600 | -1.37287900 | -0.02152300 | N | 1.78515400 | 0.50776600 | 0.90594000 |
| H | -4.83475300 | 0.78074900 | -0.13541000 | Co | -0.06603500 | -0.05581300 | 0.83773300 |
| C | -3.70055900 | -2.42811500 | 0.14105100 | H | -0.45630400 | 0.88956200 | 1.90584400 |
| H | -1.59756700 | -2.92049400 | 0.43115800 | H | -1.89846400 | -2.31446900 | 1.88732000 |
| H | -5.68260500 | -1.57269600 | -0.15104400 | H | -1.10922800 | -2.26180200 | -1.17368300 |
| H | -4.02708600 | -3.47291500 | 0.14269900 | N | 0.35695300 | -1.32400000 | 2.32275700 |
| N | 0.44276600 | -0.31039300 | -1.32482900 | H | 1.27108700 | -1.09571200 | 2.73948000 |
| N | -1.88044000 | -0.85368100 | 0.31124000 | H | -0.32455900 | -1.26180900 | 3.09245900 |
| Co | -0.01309700 | -0.28513900 | 0.58075100 | H | 0.41158000 | -2.30954100 | 2.02557900 |
| H | 1.92983500 | 0.57818800 | 2.86415700 | | | | |
| H | 0.99738800 | 2.59986500 | 0.56985200 | | | | |
| N | 0.68871700 | -2.08289000 | 0.77966600 | | | | |
| C | 1.19857900 | -3.13262300 | 0.88694500 | | | | |
| C | 1.81685900 | -4.44195300 | 1.02193900 | | | | |
| H | 2.90324000 | -4.33292100 | 1.19549800 | | | | |
| H | 1.37448500 | -4.98837300 | 1.87521300 | | | | |
| H | 1.66183100 | -5.03243000 | 0.10016200 | | | | |
| N | -0.42505400 | -0.23255300 | 2.55284100 | | | | |
| H | -1.38805800 | -0.55729700 | 2.73104800 | | | | |
| H | 0.18959200 | -0.85571600 | 3.09813400 | | | | |
| H | -0.35994300 | 0.71141900 | 2.96382300 | | | | |

[Co-H]²⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | 0.58253500 | -2.99618700 | -2.33631300 |
| C | -0.03267400 | -2.19700400 | -1.36190100 |
| C | 2.00164200 | -1.17207000 | -0.80413000 |
| C | 2.68306900 | -1.94246100 | -1.76437800 |
| C | 1.96527100 | -2.86650500 | -2.53808400 |
| H | -0.01564500 | -3.70131200 | -2.92114800 |
| H | 3.76003300 | -1.82724500 | -1.91476000 |

[Co-CO]³⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | 0.21590400 | 3.57758400 | 1.29131200 |
| C | -0.26791500 | 2.45917700 | 0.59751100 |
| C | 1.89325300 | 1.51072000 | 0.48498700 |
| C | 2.42915100 | 2.60931300 | 1.18038700 |
| C | 1.58563200 | 3.65378400 | 1.58881300 |
| H | -0.48082400 | 4.36832500 | 1.58744300 |
| H | 3.49901100 | 2.65302100 | 1.40407700 |
| H | 1.99454900 | 4.51357900 | 2.13053300 |
| C | -2.59227800 | 0.94916600 | -1.79547400 |
| C | -3.97257600 | 1.17933200 | -1.74286000 |
| C | -2.62894300 | -0.19218100 | 0.27457700 |
| C | -4.69816300 | 0.70124400 | -0.63877900 |
| H | -4.45896900 | 1.71862500 | -2.56217400 |
| C | -4.01743200 | 0.01290300 | 0.37613600 |
| H | -5.78042300 | 0.85683500 | -0.57082600 |
| H | -4.56859600 | -0.37060800 | 1.23951300 |
| N | -1.93144700 | 0.28858000 | -0.80919600 |
| N | 0.54897900 | 1.45195200 | 0.20090800 |
| C | -1.81137500 | -0.91417900 | 1.26002400 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -2.30240000 | -1.47983700 | 2.45034200 | C | 2.73155100 | 0.62666200 | -0.01516500 |
| C | 0.36644200 | -1.68786900 | 1.76276500 | C | 4.05803800 | 0.93935400 | 0.34481700 |
| C | -1.43002700 | -2.16389200 | 3.30985100 | C | 2.16299800 | 0.32538100 | 2.24436700 |
| H | -3.36234400 | -1.39156700 | 2.70536400 | C | 4.44123300 | 0.94434000 | 1.68737100 |
| C | -0.07512000 | -2.26877800 | 2.95972000 | H | 4.78970300 | 1.16335800 | -0.43840300 |
| H | 1.41109700 | -1.75933300 | 1.45654500 | C | 3.45962300 | 0.62203600 | 2.65313900 |
| H | -1.80610100 | -2.61200500 | 4.23592500 | H | 1.39023100 | 0.06249000 | 2.96923600 |
| H | 0.64344600 | -2.79739700 | 3.59424300 | H | 5.47047300 | 1.17746900 | 1.97836600 |
| C | 2.67169700 | 0.36010500 | 0.00130800 | H | 3.70257400 | 0.59109800 | 3.72070400 |
| C | 4.06302200 | 0.20729700 | 0.14739700 | N | -0.80334600 | 1.63302900 | 0.23906600 |
| C | 2.54432100 | -1.71422400 | -1.13520800 | N | 1.75833100 | 0.32991300 | 0.93472500 |
| C | 4.69829900 | -0.93525400 | -0.36294100 | Mn | 0.00562300 | -0.16296200 | 0.27108600 |
| H | 4.65099600 | 0.97834700 | 0.65376300 | H | -1.40790000 | -2.61775500 | -0.92655900 |
| C | 3.92593700 | -1.91155400 | -1.01399500 | H | -0.71689500 | -0.18857500 | -2.70236200 |
| H | 1.92163300 | -2.46093600 | -1.63463400 | N | -0.74107600 | -0.37976600 | 1.99194700 |
| H | 5.78151600 | -1.05884100 | -0.25532400 | C | -1.29197700 | -0.44809500 | 3.03506000 |
| H | 4.37560800 | -2.81906400 | -1.43028400 | C | -1.95462500 | -0.58553600 | 4.32810900 |
| N | -0.48000600 | -1.02460300 | 0.93767200 | H | -3.02395400 | -0.83529500 | 4.19703100 |
| N | 1.92804500 | -0.60663600 | -0.63719400 | H | -1.48535000 | -1.39456000 | 4.91844500 |
| Co | 0.00636200 | -0.17298700 | -0.77296800 | H | -1.88945500 | 0.35055200 | 4.91359400 |
| H | -2.01106600 | 1.30937300 | -2.64710800 | N | 0.52037400 | -2.11921600 | 0.21017200 |
| H | -1.32775300 | 2.36765100 | 0.35080000 | C | 1.19272200 | -2.76180400 | -0.81640500 |
| C | -0.48194200 | -1.71556100 | -1.64023900 | C | 0.12290900 | -3.10863000 | 1.09032100 |
| O | -0.84076600 | -2.67065200 | -2.16200400 | C | 1.21999100 | -4.14717500 | -0.59549600 |
| N | 0.45857100 | 0.77732400 | -2.50942400 | H | 1.62665100 | -2.20079700 | -1.64396700 |
| H | 0.28470800 | 1.79190000 | -2.43315700 | C | 0.53078000 | -4.37081500 | 0.63191100 |
| H | 1.46378000 | 0.67280400 | -2.72008500 | H | -0.44032100 | -2.86242900 | 1.99055800 |
| H | -0.03783800 | 0.44505500 | -3.35161200 | H | 1.69569400 | -4.89394300 | -1.23628700 |
| | | | | H | 0.36057500 | -5.32712300 | 1.13331600 |

L = Pyrrole

M = Mn

[Mn-S]⁰

| | x | y | z |
|---|-------------|-------------|-------------|
| C | 1.00432100 | 0.45064000 | -3.86435600 |
| C | 0.32645000 | 0.13570900 | -2.68636700 |
| C | 2.22726700 | 0.58148400 | -1.37779000 |
| C | 2.96479700 | 0.90886100 | -2.53601800 |
| C | 2.35831500 | 0.84297800 | -3.79211700 |
| H | 0.48037700 | 0.38040900 | -4.82300900 |
| H | 4.01162800 | 1.21522300 | -2.44417900 |
| H | 2.92247800 | 1.09253900 | -4.69708200 |
| C | -2.17795500 | -1.84160300 | -0.93867600 |
| C | -3.48448400 | -2.10012900 | -1.36306000 |
| C | -2.70428300 | 0.41162600 | -0.50211200 |
| C | -4.44071000 | -1.06476500 | -1.34391900 |
| H | -3.74516300 | -3.11029300 | -1.69521500 |
| C | -4.03730300 | 0.20273900 | -0.90994300 |
| H | -5.47343200 | -1.24212500 | -1.66307300 |
| H | -4.75124500 | 1.03256000 | -0.88846400 |
| N | -1.77419900 | -0.61210600 | -0.50079300 |
| N | 0.90351600 | 0.18907700 | -1.45331500 |
| C | -2.14524100 | 1.69962600 | -0.09232100 |
| C | -2.84938100 | 2.92058100 | -0.06944500 |
| C | -0.16811200 | 2.80013200 | 0.54741500 |
| C | -2.18819800 | 4.10533400 | 0.26924400 |
| H | -3.91302000 | 2.93838700 | -0.32834100 |
| C | -0.81132400 | 4.03753200 | 0.57377000 |
| H | 0.89283800 | 2.70390100 | 0.79506800 |
| H | -2.72574700 | 5.05912200 | 0.28990600 |
| H | -0.24094600 | 4.93453400 | 0.83693500 |

[Mn-H]⁻¹

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.54394900 | -0.09224100 | 3.76632800 |
| C | 0.02426500 | -0.21199900 | 2.49992900 |
| C | -1.99653300 | 0.39350700 | 1.44836900 |
| C | -2.62691800 | 0.51721500 | 2.70593900 |
| C | -1.90992100 | 0.27153400 | 3.88098800 |
| H | 0.06836300 | -0.29370500 | 4.65300100 |
| H | -3.68071100 | 0.81501600 | 2.75411200 |
| H | -2.39175300 | 0.36247800 | 4.86130900 |
| C | 2.24271200 | -2.06560600 | 0.03090000 |
| C | 3.56542600 | -2.46290900 | 0.19813200 |
| C | 2.88755800 | 0.19778600 | -0.13888000 |
| C | 4.60571500 | -1.49874500 | 0.18955500 |
| H | 3.78154600 | -3.52977700 | 0.32766900 |
| C | 4.24300600 | -0.16043800 | 0.01933300 |
| H | 5.65576000 | -1.78902900 | 0.31066600 |
| H | 5.00906400 | 0.62372100 | 0.00157300 |
| N | 1.86034600 | -0.75262000 | -0.14790200 |
| N | -0.66371100 | 0.00910000 | 1.33875300 |
| C | 2.39213200 | 1.54574600 | -0.31040800 |
| C | 3.17093200 | 2.72185700 | -0.30616700 |
| C | 0.43285800 | 2.82862200 | -0.58979800 |
| C | 2.56848900 | 3.97544400 | -0.44702600 |
| H | 4.25709500 | 2.64273200 | -0.18076100 |
| C | 1.15697000 | 4.01611200 | -0.58193900 |
| H | -0.65472600 | 2.82673900 | -0.70193600 |
| H | 3.16759000 | 4.89314000 | -0.44354600 |
| H | 0.62176200 | 4.96771400 | -0.68237600 |
| C | -2.59842100 | 0.68305300 | 0.16091800 |
| C | -3.94285700 | 1.05767900 | -0.04515800 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -2.17166500 | 0.87507300 | -2.15070600 | N | -0.85663500 | 1.62097600 | 0.51922700 |
| C | -4.40887300 | 1.35264800 | -1.32901700 | N | 1.85924500 | 0.39135500 | 0.79697800 |
| H | -4.62345600 | 1.10249600 | 0.81322400 | Mn | 0.02108400 | -0.17227100 | 0.54436000 |
| C | -3.48527200 | 1.25890600 | -2.40186600 | H | -1.55882800 | -2.75546100 | -0.02962100 |
| H | -1.43462500 | 0.76502500 | -2.95021100 | H | -1.27258400 | -0.23870400 | -2.30559700 |
| H | -5.45405500 | 1.63497800 | -1.49921700 | C | -0.31907600 | -0.31230300 | 2.27664500 |
| H | -3.79052000 | 1.46770900 | -3.43390700 | O | -0.58026500 | -0.32493200 | 3.43138800 |
| N | 1.00565400 | 1.58470600 | -0.47580400 | N | 0.57297800 | -2.09936500 | 0.37498300 |
| N | -1.68793700 | 0.58034600 | -0.89776600 | C | 0.85552500 | -2.78014700 | -0.80017600 |
| Mn | 0.07037200 | -0.09626300 | -0.48942800 | C | 0.51565800 | -3.05604700 | 1.37365500 |
| H | 0.30015800 | -0.16167400 | -2.06139300 | C | 0.96957400 | -4.15579500 | -0.55221700 |
| H | 1.42384300 | -2.78905300 | 0.02318800 | H | 0.96514000 | -2.25477300 | -1.74842200 |
| H | 1.06815200 | -0.51562200 | 2.36851000 | C | 0.75146800 | -4.33373600 | 0.84529900 |
| N | -0.58134300 | -2.00660900 | -0.73876600 | H | 0.31046800 | -2.77353000 | 2.40710100 |
| C | -1.08392100 | -2.84709100 | 0.23891100 | H | 1.20631300 | -4.92635500 | -1.29020100 |
| C | -0.46655600 | -2.76642300 | -1.88413000 | H | 0.78292100 | -5.26964300 | 1.40842600 |
| C | -1.28383800 | -4.13963000 | -0.27683200 | | | | |
| H | -1.27274600 | -2.47814400 | 1.24865800 | | | | |
| C | -0.88371800 | -4.08794000 | -1.64685600 | | | | |
| H | -0.07595300 | -2.31258000 | -2.79648300 | | | | |
| H | -1.68443700 | -5.00024600 | 0.26813700 | | | | |
| H | -0.90644800 | -4.90275600 | -2.37721800 | | | | |

[Mn-CO]⁰

| | x | y | z |
|---|-------------|-------------|-------------|
| C | 0.20648200 | 0.31270400 | -3.79978800 |
| C | -0.24034600 | 0.06667000 | -2.49919300 |
| C | 1.87492700 | 0.51764200 | -1.58694700 |
| C | 2.39179100 | 0.77306200 | -2.87835400 |
| C | 1.55801800 | 0.66826500 | -3.99273800 |
| H | -0.48627500 | 0.21376800 | -4.64128800 |
| H | 3.44281500 | 1.05065100 | -3.00220800 |
| H | 1.95023600 | 0.85894800 | -4.99761100 |
| C | -2.32023200 | -1.97461900 | -0.10363000 |
| C | -3.66219000 | -2.26881100 | -0.37356600 |
| C | -2.79172500 | 0.32485200 | 0.01888400 |
| C | -4.60015700 | -1.22433700 | -0.44749900 |
| H | -3.95825000 | -3.31254900 | -0.51868900 |
| C | -4.15391800 | 0.08775600 | -0.24809500 |
| H | -5.65679700 | -1.42676700 | -0.65291000 |
| H | -4.85872200 | 0.92360100 | -0.29430300 |
| N | -1.87707400 | -0.70114000 | 0.09313100 |
| N | 0.55973600 | 0.15650500 | -1.40790400 |
| C | -2.20530700 | 1.65231800 | 0.24441700 |
| C | -2.91891900 | 2.86584000 | 0.19656800 |
| C | -0.22068500 | 2.80434300 | 0.73297700 |
| C | -2.25389400 | 4.07554700 | 0.42363200 |
| H | -3.99125200 | 2.86005700 | -0.02113500 |
| C | -0.87315400 | 4.03869700 | 0.69563600 |
| H | 0.84859500 | 2.72868300 | 0.94822700 |
| H | -2.79791700 | 5.02521800 | 0.38997600 |
| H | -0.30302800 | 4.95482200 | 0.88050500 |
| C | 2.62470500 | 0.62448600 | -0.34414500 |
| C | 3.99461300 | 0.95448400 | -0.27322000 |
| C | 2.51715200 | 0.49056600 | 1.99910300 |
| C | 4.63611400 | 1.05214600 | 0.96111700 |
| H | 4.55520100 | 1.12267200 | -1.19829200 |
| C | 3.86478600 | 0.81195100 | 2.12128500 |
| H | 1.91284000 | 0.29250100 | 2.88649700 |
| H | 5.70048800 | 1.29922300 | 1.02565500 |
| H | 4.30864700 | 0.86234300 | 3.12099000 |

L = Pyrrole
M = Fe

[Fe-S]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -0.61067600 | -1.59279700 | -3.58515200 |
| C | -0.02011100 | -0.96763100 | -2.48135000 |
| C | -2.00430500 | -1.11523700 | -1.24049500 |
| C | -2.65682400 | -1.74429500 | -2.31740700 |
| C | -1.95828100 | -1.98198800 | -3.50613400 |
| H | -0.01994100 | -1.75804000 | -4.49112000 |
| H | -3.70409900 | -2.04471000 | -2.22422800 |
| H | -2.45460400 | -2.46470300 | -4.35401700 |
| C | 1.97824000 | 1.91349600 | -1.14528100 |
| C | 3.25311300 | 2.24735800 | -1.62500900 |
| C | 2.74634900 | -0.18433100 | -0.40369300 |
| C | 4.30252600 | 1.32520400 | -1.48960100 |
| H | 3.40821600 | 3.22302700 | -2.09548500 |
| C | 4.04505500 | 0.09592800 | -0.86636300 |
| H | 5.30784600 | 1.55916300 | -1.85497900 |
| H | 4.84905100 | -0.63393100 | -0.73467100 |
| N | 1.72132500 | 0.71572600 | -0.56005800 |
| N | -0.69285200 | -0.72100700 | -1.33046700 |
| C | 2.34966900 | -1.42484300 | 0.28705200 |
| C | 3.20125300 | -2.52170800 | 0.51853600 |
| C | 0.57808400 | -2.52985500 | 1.35600700 |
| C | 2.71207600 | -3.64798100 | 1.19176500 |
| H | 4.23817800 | -2.49730200 | 0.17114300 |
| C | 1.37383900 | -3.65084100 | 1.61935600 |
| H | -0.46934700 | -2.48768600 | 1.66742600 |
| H | 3.36298400 | -4.50845200 | 1.37709100 |
| H | 0.94501000 | -4.50745500 | 2.14821700 |
| C | -2.60627900 | -0.85993300 | 0.07300700 |
| C | -3.94288000 | -1.13735700 | 0.41310000 |
| C | -2.16898000 | -0.10306300 | 2.24745900 |
| C | -4.39262900 | -0.88409600 | 1.71370500 |
| H | -4.62924000 | -1.53697800 | -0.33876100 |
| C | -3.48291000 | -0.36437800 | 2.64954300 |
| H | -1.43652500 | 0.31721200 | 2.93943700 |
| H | -5.43208900 | -1.08565700 | 1.99100000 |
| H | -3.78479100 | -0.14765200 | 3.67870800 |
| N | 1.04308600 | -1.43551100 | 0.70623100 |
| N | -1.72257000 | -0.34054900 | 0.98839400 |
| Fe | -0.00107800 | 0.18586500 | 0.24608500 |

| | | | | | | | |
|---|-------------|-------------|-------------|----------------------|-------------|-------------|-------------|
| H | 1.12309500 | 2.59090800 | -1.22751500 | H | 1.10260000 | -0.50311000 | 2.39953100 |
| H | 1.01812900 | -0.62966900 | -2.51322900 | N | -0.60756500 | -1.95136900 | -0.69979900 |
| N | -0.87850100 | 1.85305600 | -0.34689100 | C | -1.11928000 | -2.77106400 | 0.29194300 |
| C | -1.24258300 | 2.18679200 | -1.64449300 | C | -0.48664800 | -2.72694800 | -1.83501300 |
| C | -1.16313500 | 2.95269700 | 0.43987300 | C | -1.31942600 | -4.06802400 | -0.20928700 |
| C | -1.74055200 | 3.49657500 | -1.68048700 | H | -1.31421800 | -2.39154700 | 1.29563500 |
| H | -1.12476400 | 1.48649400 | -2.47111900 | C | -0.91293500 | -4.03981500 | -1.57447900 |
| C | -1.69401300 | 3.98588700 | -0.34574200 | H | -0.08904800 | -2.29547500 | -2.75463400 |
| H | -0.98814500 | 2.93894100 | 1.51541300 | H | -1.72530800 | -4.91793200 | 0.34536100 |
| H | -2.10520200 | 4.02034500 | -2.56648000 | H | -0.93731300 | -4.86504200 | -2.29050100 |
| H | -2.01879300 | 4.96477600 | 0.01272200 | | | | |
| N | 0.62172700 | 1.01679900 | 1.83611300 | | | | |
| C | 1.10379800 | 1.53566700 | 2.77195300 | | | | |
| C | 1.67599800 | 2.22443200 | 3.92370500 | [Fe-CO] ⁺ | x | y | z |
| H | 1.24718000 | 3.23909200 | 4.00831100 | C | 0.09664200 | 0.44615200 | -3.78286500 |
| H | 1.46461500 | 1.67172500 | 4.85604200 | C | -0.32471900 | 0.13263600 | -2.48481900 |
| H | 2.77071500 | 2.31625200 | 3.81147500 | C | 1.76045700 | 0.70236700 | -1.58141800 |
| | | | C | 2.24938700 | 1.03344700 | -2.86032100 | |
| | | | C | 1.41089500 | 0.90260300 | -3.97327700 | |
| | | | H | -0.59377600 | 0.32206300 | -4.62232300 | |
| | | | H | 3.27580300 | 1.38844400 | -2.98515700 | |
| | | | H | 1.77859200 | 1.15144300 | -4.97399100 | |
| | | | C | -2.10433900 | -2.16973100 | -0.11296400 | |
| | | | C | -3.41838500 | -2.58643200 | -0.37637700 | |
| | | | C | -2.79189200 | 0.08061300 | 0.03038400 | |
| | | | C | -4.44322300 | -1.63121600 | -0.43665700 | |
| | | | H | -3.62043500 | -3.65150400 | -0.52324000 | |
| | | | C | -4.12572900 | -0.28084900 | -0.22890700 | |
| | | | H | -5.47782900 | -1.92950900 | -0.63494600 | |
| | | | H | -4.91025900 | 0.48025400 | -0.26004200 | |
| | | | N | -1.79669800 | -0.86195100 | 0.07576100 | |
| | | | N | 0.48036900 | 0.25522300 | -1.40526300 | |
| | | | C | -2.32892100 | 1.45916100 | 0.28303200 | |
| | | | C | -3.15738500 | 2.59681600 | 0.26637300 | |
| | | | C | -0.46539300 | 2.78220800 | 0.81921500 | |
| | | | C | -2.60773000 | 3.85642600 | 0.53574100 | |
| | | | H | -4.22411700 | 2.49933000 | 0.04640300 | |
| | | | C | -1.23575400 | 3.95135300 | 0.81834500 | |
| | | | H | 0.60533700 | 2.80286200 | 1.03999600 | |
| | | | H | -3.24188600 | 4.74871600 | 0.52861500 | |
| | | | H | -0.76248900 | 4.91260800 | 1.03956600 | |
| | | | C | 2.53548700 | 0.81164000 | -0.33628500 | |
| | | | C | 3.88967000 | 1.18902600 | -0.28017300 | |
| | | | C | 2.46610000 | 0.59331800 | 1.99618300 | |
| | | | C | 4.54042800 | 1.26428200 | 0.95633600 | |
| | | | H | 4.43633800 | 1.40792200 | -1.20146000 | |
| | | | C | 3.81004500 | 0.96306200 | 2.11606800 | |
| | | | H | 1.87936500 | 0.34145100 | 2.88199100 | |
| | | | H | 5.59631300 | 1.54700000 | 1.01211400 | |
| | | | H | 4.26897700 | 0.99933900 | 3.10848300 | |
| | | | N | -0.99009900 | 1.56294700 | 0.55658500 | |
| | | | N | 1.82296700 | 0.51847900 | 0.80176900 | |
| | | | Fe | 0.01235000 | -0.17070600 | 0.51205200 | |
| | | | H | -1.26923000 | -2.87220300 | -0.04726100 | |
| | | | H | -1.33046700 | -0.24979500 | -2.29496100 | |
| | | | C | -0.35218000 | -0.41808100 | 2.21024000 | |
| | | | O | -0.65780600 | -0.51008000 | 3.33403700 | |
| | | | N | 0.80480300 | -1.96252900 | 0.31295100 | |
| | | | C | 1.08278000 | -2.61211200 | -0.88220100 | |
| | | | C | 0.95963500 | -2.89851100 | 1.32267400 | |
| | | | C | 1.41470300 | -3.94988200 | -0.62856100 | |
| | | | H | 1.03783600 | -2.10114800 | -1.84203700 | |

| | | | | | | | |
|---|------------|-------------|-------------|---|------------|-------------|-------------|
| C | 1.33712900 | -4.13337200 | 0.77937000 | H | 1.21261800 | -1.02161100 | -2.69777800 |
| H | 0.80911700 | -2.63780400 | 2.37086200 | C | 2.39478100 | -3.48333500 | -0.78321700 |
| H | 1.70007000 | -4.69087200 | -1.37797400 | H | 1.23623200 | -3.01070500 | 1.07667300 |
| H | 1.54843000 | -5.04433900 | 1.34229600 | H | 2.92120300 | -3.11060100 | -2.95042100 |
| | | | | H | 2.93920000 | -4.39272000 | -0.52319100 |

L = Pyrrole

M = Co

[Co-S]²⁺

| | x | y | z |
|----|-------------|--------------|-------------|
| C | 0.41534900 | 2.14999200 | -3.28981000 |
| C | -0.11376100 | 1.28802200 | -2.32096700 |
| C | 1.85104300 | 1.41842800 | -1.03339800 |
| C | 2.43379600 | 2.28684300 | -1.97314100 |
| C | 1.71277400 | 2.65495500 | -3.11585400 |
| H | -0.18766700 | 2.40766800 | -4.16542600 |
| H | 3.44652800 | 2.66689700 | -1.81475700 |
| H | 2.15784600 | 3.32481700 | -3.85848300 |
| C | -1.92851100 | -1.78761400 | -1.49972600 |
| C | -3.18931100 | -2.06485300 | -2.04953900 |
| C | -2.76660300 | 0.12209200 | -0.38854400 |
| C | -4.26382300 | -1.21207600 | -1.75425500 |
| H | -3.31275300 | -2.93922400 | -2.69559200 |
| C | -4.05098200 | -0.10996200 | -0.91171300 |
| H | -5.25950300 | -1.40280100 | -2.16795600 |
| H | -4.88060600 | 0.55700900 | -0.66102300 |
| N | -1.72655600 | -0.71235100 | -0.70411200 |
| N | 0.58481500 | 0.92892900 | -1.21925600 |
| C | -2.41187300 | 1.22863300 | 0.52353500 |
| C | -3.30480200 | 2.22543000 | 0.95759800 |
| C | -0.67722800 | 2.17591100 | 1.79656200 |
| C | -2.85330300 | 3.21928100 | 1.83731300 |
| H | -4.34224600 | 2.22998300 | 0.61196500 |
| C | -1.51790200 | 3.19331300 | 2.26830100 |
| H | 0.37034900 | 2.11423100 | 2.10413700 |
| H | -3.53702700 | 4.00184900 | 2.18180600 |
| H | -1.12463700 | 3.94687800 | 2.95710500 |
| C | 2.49060600 | 0.97427000 | 0.21113600 |
| C | 3.79105500 | 1.31787600 | 0.61974900 |
| C | 2.16139900 | -0.277742200 | 2.17468500 |
| C | 4.27666000 | 0.84149400 | 1.84444000 |
| H | 4.42248600 | 1.94377500 | -0.01648400 |
| C | 3.44489100 | 0.03737900 | 2.63869600 |
| H | 1.48659100 | -0.91025100 | 2.75315400 |
| H | 5.29012300 | 1.09386700 | 2.17221400 |
| H | 3.78097800 | -0.35785000 | 3.60174200 |
| N | -1.11027700 | 1.22029200 | 0.94580900 |
| N | 1.69115800 | 0.18412200 | 0.99281600 |
| Co | -0.01338800 | -0.27776300 | 0.16962200 |
| H | -1.04800000 | -2.41178600 | -1.67909200 |
| H | -1.11061100 | 0.85931100 | -2.43447700 |
| N | -0.62416400 | -1.41065900 | 1.60743100 |
| C | -1.09998100 | -2.10922300 | 2.41547000 |
| C | -1.66757800 | -3.00045900 | 3.41753900 |
| H | -2.75042300 | -3.12772600 | 3.24183000 |
| H | -1.18042600 | -3.99028400 | 3.35844200 |
| H | -1.51829500 | -2.58621500 | 4.43020900 |
| N | 0.92016400 | -1.75770300 | -0.66844400 |
| C | 1.50709400 | -1.73919800 | -1.93365300 |
| C | 1.51360800 | -2.79311100 | 0.04730300 |
| C | 2.38652300 | -2.81555400 | -2.04586000 |

[Co-H]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -0.44504700 | 0.23005300 | 3.82340200 |
| C | 0.10995600 | -0.02963100 | 2.56262700 |
| C | -1.87883000 | 0.55958000 | 1.47521600 |
| C | -2.50077200 | 0.84153600 | 2.70655200 |
| C | -1.77517100 | 0.67389700 | 3.89374800 |
| H | 0.15524700 | 0.08037300 | 4.72578100 |
| H | -3.53805900 | 1.18598800 | 2.74187200 |
| H | -2.24398000 | 0.88528900 | 4.86028300 |
| C | 2.20182100 | -2.08595000 | 0.07127100 |
| C | 3.53823200 | -2.46163800 | 0.27491700 |
| C | 2.82372400 | 0.17503600 | -0.16586500 |
| C | 4.54187700 | -1.48263000 | 0.24895600 |
| H | 3.77334700 | -3.51685100 | 0.44230100 |
| C | 4.17821200 | -0.14701400 | 0.02687800 |
| H | 5.59294000 | -1.75112100 | 0.39663000 |
| H | 4.94132000 | 0.63574100 | -0.00005600 |
| N | 1.85130800 | -0.79202800 | -0.14080400 |
| N | -0.58355500 | 0.13045200 | 1.41628500 |
| C | 2.30773300 | 1.53167000 | -0.41124600 |
| C | 3.09909100 | 2.69233700 | -0.49127800 |
| C | 0.36337100 | 2.78581900 | -0.79990800 |
| C | 2.48853800 | 3.92882000 | -0.73369600 |
| H | 4.18394400 | 2.62916300 | -0.36920900 |
| C | 1.09374500 | 3.97678200 | -0.88803100 |
| H | -0.72282800 | 2.77484700 | -0.92130700 |
| H | 3.09223300 | 4.83939500 | -0.80267400 |
| H | 0.57171300 | 4.91921500 | -1.07832100 |
| C | -2.53280100 | 0.68814900 | 0.15619900 |
| C | -3.88488500 | 1.02829400 | -0.03353600 |
| C | -2.22177000 | 0.49530200 | -2.16939200 |
| C | -4.40479700 | 1.09939600 | -1.33233700 |
| H | -4.53087400 | 1.21931300 | 0.82773600 |
| C | -3.55891400 | 0.82869200 | -2.41874700 |
| H | -1.52472600 | 0.25783500 | -2.97583300 |
| H | -5.45754300 | 1.35388300 | -1.49176700 |
| H | -3.92281500 | 0.86087500 | -3.44982200 |
| N | 0.94786700 | 1.58731200 | -0.56987100 |
| N | -1.71468800 | 0.43612900 | -0.91469600 |
| Co | 0.06224300 | -0.16275000 | -0.49072600 |
| H | 0.41333200 | -0.29165100 | -1.91496600 |
| H | 1.38529800 | -2.81252900 | 0.07856500 |
| H | 1.13784600 | -0.39071600 | 2.45511600 |
| N | -0.60247700 | -1.95289500 | -0.62135000 |
| C | -1.06355800 | -2.73831600 | 0.42237400 |
| C | -0.46973800 | -2.76697300 | -1.73269300 |
| C | -1.23036000 | -4.05544700 | -0.02951500 |
| H | -1.25877400 | -2.32395700 | 1.41040200 |
| C | -0.85325500 | -4.07336300 | -1.40195900 |
| H | -0.10100800 | -2.37045800 | -2.67928300 |
| H | -1.60507600 | -4.89156200 | 0.56428800 |
| H | -0.86970700 | -4.92803000 | -2.08071900 |

[Co-CO]²⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 0.13995500 | 2.60711100 | -3.25994900 |
| C | -0.32345800 | 1.63625600 | -2.36045500 |
| C | 1.73052500 | 1.56861000 | -1.24344100 |
| C | 2.26503100 | 2.53925600 | -2.11223400 |
| C | 1.45998700 | 3.06462700 | -3.13284000 |
| H | -0.52479300 | 2.99057300 | -4.03980200 |
| H | 3.29531500 | 2.88759800 | -2.00087300 |
| H | 1.85981000 | 3.82068900 | -3.81619000 |
| C | -2.26197000 | -1.27425100 | -1.70492500 |
| C | -3.60287700 | -1.36847500 | -2.09661200 |
| C | -2.81965000 | 0.12988100 | 0.10625700 |
| C | -4.58056400 | -0.69681400 | -1.34409100 |
| H | -3.86651500 | -1.96265600 | -2.97672800 |
| C | -4.18190800 | 0.06454700 | -0.23741400 |
| H | -5.63852100 | -0.75916900 | -1.61842900 |
| H | -4.92598100 | 0.60625700 | 0.35285400 |
| N | -1.87785900 | -0.55150200 | -0.62168300 |
| N | 0.44577800 | 1.12436000 | -1.37575100 |
| C | -2.25896300 | 0.92166600 | 1.20994200 |
| C | -3.01802200 | 1.69359600 | 2.10573900 |
| C | -0.26921200 | 1.58036300 | 2.26843300 |
| C | -2.37059700 | 2.42656200 | 3.10891400 |
| H | -4.10797600 | 1.71978800 | 2.02335200 |
| C | -0.97151800 | 2.37125700 | 3.18697800 |
| H | 0.81866400 | 1.50931800 | 2.30853700 |
| H | -2.94980500 | 3.02827100 | 3.81636800 |
| H | -0.41870300 | 2.92637800 | 3.95053400 |
| C | 2.48098900 | 0.95204800 | -0.12864700 |
| C | 3.81656400 | 1.27145600 | 0.18446100 |
| C | 2.40874500 | -0.56230800 | 1.67473900 |
| C | 4.45298600 | 0.65153300 | 1.26701100 |
| H | 4.35848400 | 2.00723300 | -0.41538000 |
| C | 3.73314700 | -0.28111300 | 2.02911000 |
| H | 1.81536900 | -1.26816400 | 2.26044000 |
| H | 5.49114700 | 0.89741600 | 1.51272700 |
| H | 4.17892000 | -0.78857000 | 2.88980400 |
| N | -0.89005600 | 0.86720800 | 1.30015200 |
| N | 1.78839900 | 0.02971800 | 0.62004900 |
| Co | -0.05395800 | -0.34094300 | 0.02168900 |
| H | -1.46055500 | -1.77322000 | -2.25586800 |
| H | -1.34545000 | 1.25157200 | -2.42780100 |
| C | -0.28191700 | -1.87080200 | 1.14166200 |
| O | -0.60102700 | -2.09760300 | 2.27740400 |
| N | 0.59804000 | -1.95227300 | -0.98031400 |
| C | 1.77314100 | -2.40428000 | -1.38587700 |
| C | 0.08668600 | -2.91706600 | 0.00928700 |
| C | 2.10452500 | -3.68285700 | -0.78471900 |
| H | 2.39999100 | -1.82721100 | -2.07349300 |
| C | 1.11038500 | -3.98870600 | 0.11363200 |
| H | -0.90142200 | -3.32908400 | -0.28923600 |
| H | 2.98513300 | -4.28239400 | -1.02642600 |
| H | 1.01979300 | -4.88349600 | 0.73383700 |

L = Pyridine
M = Mn

[Mn-S]⁺

| | x | y | z |
|----|--------------|-------------|-------------|
| C | -0.222311400 | -1.36840000 | -3.75409400 |
| C | 0.20799400 | -0.71089600 | -2.59988700 |
| C | -1.62354100 | -1.50807100 | -1.36640300 |
| C | -2.11227500 | -2.18633100 | -2.50044700 |
| C | -1.41530900 | -2.11656800 | -3.71108000 |
| H | 0.36874500 | -1.29043400 | -4.67147500 |
| H | -3.03070300 | -2.77651700 | -2.42941800 |
| H | -1.78566300 | -2.63987800 | -4.59820300 |
| C | -1.60199800 | 2.05496900 | -1.36765000 |
| C | -2.55226400 | 3.04319400 | -1.64760600 |
| C | -1.91842300 | 2.29826900 | 0.91750500 |
| C | -3.21148600 | 3.68543400 | -0.58698200 |
| H | -2.76713100 | 3.29821900 | -2.69050800 |
| C | -2.87975100 | 3.29571700 | 0.72049600 |
| H | -1.64783900 | 1.97438700 | 1.92483900 |
| H | -3.96019100 | 4.46218200 | -0.77355100 |
| H | -3.36120100 | 3.75420800 | 1.59044200 |
| C | 1.68900400 | 2.37983300 | -0.91347700 |
| C | 2.86124400 | 3.00585500 | -1.34231400 |
| C | 2.83937400 | 0.39872800 | -0.41352500 |
| C | 4.07413100 | 2.29143500 | -1.31220700 |
| H | 2.81922400 | 4.04281100 | -1.69046100 |
| C | 4.05234000 | 0.97652000 | -0.83559500 |
| H | 5.01098700 | 2.75127900 | -1.64188200 |
| H | 4.97943700 | 0.39808900 | -0.78077200 |
| N | 1.64218300 | 1.09146500 | -0.46413800 |
| N | -0.47113300 | -0.74977300 | -1.41788000 |
| C | 2.70838000 | -0.95812700 | 0.12281300 |
| C | 3.75967500 | -1.89131200 | 0.22000400 |
| C | 1.20769800 | -2.50983900 | 1.04369500 |
| C | 3.51646400 | -3.16435400 | 0.74518300 |
| H | 4.76355200 | -1.62217700 | -0.12169600 |
| C | 2.20927400 | -3.47558600 | 1.16505500 |
| H | 0.18264300 | -2.71477900 | 1.36271100 |
| H | 4.32452600 | -3.89852300 | 0.82329600 |
| H | 1.96321300 | -4.45677900 | 1.58298600 |
| C | -2.22413000 | -1.56263100 | -0.03287300 |
| C | -3.41653600 | -2.23905600 | 0.28435700 |
| C | -1.93502400 | -0.95817100 | 2.21638900 |
| C | -3.87491000 | -2.27180900 | 1.60633600 |
| H | 3.98671200 | -2.73713400 | -0.50572000 |
| C | -3.10600400 | -1.62029000 | 2.59004200 |
| H | -1.31417800 | -0.44767400 | 2.95684500 |
| H | -4.80184100 | -2.79291200 | 1.86458600 |
| H | -3.40911500 | -1.62187800 | 3.64203100 |
| N | 1.42933000 | -1.26630100 | 0.53431000 |
| N | -1.26351100 | 1.66951700 | -0.10172600 |
| N | -1.47730500 | -0.90198700 | 0.92966200 |
| Mn | 0.05941700 | 0.13489200 | 0.27227300 |
| H | 0.73763400 | 2.91594300 | -0.91455800 |
| H | -1.07628600 | 1.54347900 | -2.17805100 |
| H | 1.12340500 | -0.11297400 | -2.60046300 |
| N | 0.50680800 | 0.85315600 | 1.97449700 |
| C | 0.90820700 | 1.28241900 | 2.99967300 |
| C | 1.41890700 | 1.80860000 | 4.26225100 |
| H | 2.22282700 | 2.54507800 | 4.08071300 |
| H | 0.61646300 | 2.30935100 | 4.83386600 |
| H | 1.83062300 | 0.99461800 | 4.88658400 |

[Mn-H]⁰

| | x | y | z | | x | y | z |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -0.19985900 | 0.62847800 | 3.81248600 | H | 0.71844600 | 1.57430700 | -3.97007800 |
| C | 0.21972100 | 0.17728300 | 2.56428000 | H | -1.04936700 | 0.43610700 | -4.57525000 |
| C | -1.66138000 | 1.12068200 | 1.50890500 | H | 2.38622300 | 2.57374400 | -3.02123200 |
| C | -2.13711900 | 1.59521300 | 2.74974500 | H | 0.91834900 | 1.99737100 | -4.95986200 |
| C | -1.41230200 | 1.35189600 | 3.91903800 | C | 1.55470200 | -2.22210700 | -1.00808400 |
| H | 0.41321600 | 0.41537500 | 4.69492300 | C | 2.50361600 | -3.22076700 | -1.25469900 |
| H | -3.06967200 | 2.16850200 | 2.78900400 | C | 2.11010800 | -2.15094100 | 1.24320700 |
| H | -1.76927900 | 1.71906500 | 4.88684100 | C | 3.28998800 | -3.70005300 | -0.19526100 |
| C | -1.96069900 | -2.12949100 | 0.29962400 | H | 2.61717200 | -3.61064400 | -2.27146800 |
| C | -2.71539200 | -3.30351300 | 0.20126900 | C | 3.07998700 | -3.14580300 | 1.07701800 |
| C | -0.61775400 | -2.76532500 | -1.49121400 | H | 1.92986100 | -1.71351400 | 2.22759800 |
| C | -2.39927600 | -4.25396200 | -0.78457600 | H | 4.04058600 | -4.48075900 | -0.35581800 |
| H | -3.54266200 | -3.46272500 | 0.90187200 | H | 3.65682400 | -3.47713100 | 1.94634000 |
| C | -1.31889800 | -3.96445200 | -1.63910300 | C | -1.64694500 | -2.64621300 | -0.05711600 |
| H | 0.21129600 | -2.49501800 | -2.14979200 | C | -2.81310600 | -3.37835600 | -0.29846900 |
| H | -2.97352100 | -5.18098200 | -0.88673100 | C | -2.84513800 | -0.63835000 | 0.09231100 |
| H | -1.01920200 | -4.65887600 | -2.43177700 | C | -4.04494300 | -2.70375000 | -0.35279900 |
| C | 1.89485200 | -2.29600400 | 0.49001400 | H | -2.74941300 | -4.46258600 | -0.43239200 |
| C | 3.12527400 | -2.89966300 | 0.72680800 | C | -4.05358100 | -1.31932400 | -0.14867600 |
| C | 2.93089800 | -0.28592200 | -0.15936200 | H | -4.97827400 | -3.24520900 | -0.53631500 |
| C | 4.32023800 | -2.17846800 | 0.49299600 | H | -4.99880500 | -0.76928000 | -0.16305300 |
| H | 3.14735200 | -3.93023200 | 1.09811600 | N | -1.63577900 | -1.29784800 | 0.12470700 |
| C | 4.20025100 | -0.85589300 | 0.05818700 | N | 0.21696200 | 0.48423500 | -1.41918200 |
| H | 5.30243800 | -2.63108100 | 0.66210700 | C | -2.74571600 | 0.80173600 | 0.37051600 |
| H | 5.09605100 | -0.24948200 | -0.11382700 | C | -3.83521100 | 1.69388600 | 0.37380000 |
| N | 1.74829000 | -1.01071300 | 0.01435000 | C | -1.28484700 | 2.53065800 | 0.98030500 |
| N | -0.48054700 | 0.39199100 | 1.40617900 | C | -3.62904900 | 3.04062700 | 0.69270200 |
| C | 2.68673100 | 1.08593000 | -0.55927200 | H | -4.83949800 | 1.33607400 | 0.12951400 |
| C | 3.67693200 | 2.06120400 | -0.80276800 | C | -2.32614100 | 3.46337800 | 1.00697700 |
| C | 0.99738300 | 2.65791700 | -1.01552700 | H | -0.25861800 | 2.81812500 | 1.22215300 |
| C | 3.31062400 | 3.35985800 | -1.16133300 | H | -4.46751200 | 3.74416300 | 0.70138300 |
| H | 4.73399500 | 1.79283700 | -0.70599500 | H | -2.11163400 | 4.50302700 | 1.27263800 |
| C | 1.93346000 | 3.66000000 | -1.26103200 | C | 2.03394300 | 1.63514500 | -0.39790200 |
| H | -0.07459400 | 2.85524500 | -1.09057400 | C | 3.18975900 | 2.43878700 | -0.36982900 |
| H | 4.07170600 | 4.12361200 | -1.35306800 | C | 2.14860700 | 1.34575000 | 1.92665500 |
| H | 1.58681000 | 4.66414000 | -1.52718700 | C | 3.83913500 | 2.69667300 | 0.84133500 |
| C | -2.29463700 | 1.34872800 | 0.21822800 | H | 3.58384600 | 2.85771000 | -1.30044100 |
| C | -3.53478100 | 1.99443600 | 0.02231900 | C | 3.29370400 | 2.13866200 | 2.01277000 |
| C | -2.04742900 | 1.07157100 | -2.10816100 | H | 1.70572400 | 0.91195700 | 2.82607900 |
| C | -4.03255100 | 2.18322000 | -1.26848500 | H | 4.74031400 | 3.31645200 | 0.87353800 |
| H | -4.10505100 | 2.34149700 | 0.89055200 | H | 3.74892100 | 2.31179200 | 2.99299900 |
| C | -3.26134600 | 1.70927700 | -2.35527700 | N | -1.47182000 | 1.22293400 | 0.66575300 |
| H | -1.42026100 | 0.68114500 | -2.91369900 | N | 1.33539300 | -1.67437900 | 0.22384700 |
| H | -4.99462600 | 2.68065000 | -1.43070500 | N | 1.50383300 | 1.06845500 | 0.75065800 |
| H | -3.60250400 | 1.82852600 | -3.38910000 | Mn | -0.02685700 | -0.15415300 | 0.53162200 |
| N | 1.33632800 | 1.37667100 | -0.68025500 | H | -0.67613000 | -3.14211300 | 0.00776100 |
| N | -0.91114000 | -1.83183500 | -0.52846300 | H | 0.93223100 | -1.83871000 | -1.81978500 |
| N | -1.53979700 | 0.87301000 | -0.85010700 | H | -1.41357900 | -0.48723500 | -2.27676100 |
| Mn | 0.10053500 | -0.11051000 | -0.41671200 | C | -0.19799000 | -0.50244000 | 2.25819000 |
| H | 0.27824100 | -0.31858500 | -1.98544900 | O | -0.36024700 | -0.69552700 | 3.41307200 |
| H | 0.96339800 | -2.83549600 | 0.67542200 | | | | |
| H | -2.18405900 | -1.38677200 | 1.06975200 | | | | |
| H | 1.14795300 | -0.39045800 | 2.44844800 | | | | |

L = Pyridine

M = Fe

[Fe-S]²⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.15984400 | -1.26803800 | -3.77387500 |
| C | 0.25087500 | -0.62205800 | -2.60181100 |
| C | -1.56863100 | -1.48226800 | -1.39796500 |
| C | -2.03743800 | -2.14994600 | -2.54447100 |
| C | -1.33087500 | -2.04215800 | -3.74868400 |

[Mn-CO]⁺

| | x | y | z |
|---|-------------|------------|-------------|
| C | -0.37156500 | 0.70998100 | -3.76099400 |
| C | -0.58178200 | 0.19474800 | -2.47810200 |
| C | 1.27150400 | 1.34068300 | -1.61543500 |
| C | 1.54185800 | 1.89223800 | -2.88554800 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | 0.43365500 | -1.15883100 | -4.68658600 | H | -0.52678500 | -0.59001300 | 4.70125400 |
| H | -2.94478700 | -2.75822100 | -2.49528900 | H | 2.80627100 | -2.51856700 | 2.70919800 |
| H | -1.68433500 | -2.55750400 | -4.64731500 | H | 1.51421900 | -2.09479700 | 4.81173800 |
| C | -1.53844400 | 2.09739600 | -1.36324400 | C | 1.93973700 | 2.10763100 | 0.50881800 |
| C | -2.46989300 | 3.10377600 | -1.64453400 | C | 2.74999400 | 3.24927500 | 0.48011700 |
| C | -1.94992500 | 2.25684500 | 0.91714700 | C | 0.86864500 | 2.73261000 | -1.45927400 |
| C | -3.16865900 | 3.70648400 | -0.58698200 | C | 2.60370600 | 4.16909000 | -0.56940600 |
| H | -2.63893500 | 3.40273500 | -2.68377600 | H | 3.48258100 | 3.40595000 | 1.27841200 |
| C | -2.89685200 | 3.26854500 | 0.71815100 | C | 1.63837100 | 3.89774000 | -1.55245600 |
| H | -1.72196700 | 1.89830400 | 1.92274900 | H | 0.11244500 | 2.48140500 | -2.20674900 |
| H | -3.90411100 | 4.49540100 | -0.77505400 | H | 3.22366600 | 5.07019600 | -0.62081300 |
| H | -3.41056800 | 3.70052100 | 1.58263700 | H | 1.47761000 | 4.57660600 | -2.39605300 |
| C | 1.70993400 | 2.39374500 | -0.81685200 | C | -1.84210300 | 2.37640000 | 0.45735200 |
| C | 2.89885500 | 3.00036700 | -1.24114300 | C | -3.07306900 | 2.99813000 | 0.68322200 |
| C | 2.80506800 | 0.36243900 | -0.39925300 | C | -2.88857800 | 0.38675600 | -0.20814800 |
| C | 4.08115500 | 2.24378200 | -1.25299900 | C | -4.25998400 | 2.28601700 | 0.43468700 |
| H | 2.88839000 | 4.04920200 | -1.55267300 | H | -3.09274000 | 4.03002100 | 1.04751200 |
| C | 4.03025600 | 0.91256300 | -0.81974500 | C | -4.15621800 | 0.96251300 | -0.00752500 |
| H | 5.02788700 | 2.68371900 | -1.58224700 | H | -5.24005700 | 2.74727900 | 0.59080200 |
| H | 4.94204500 | 0.30939000 | -0.79923500 | H | -5.05869600 | 0.37349200 | -0.19545100 |
| N | 1.64386300 | 1.09726900 | -0.42156800 | N | -1.72361900 | 1.09765800 | -0.00191400 |
| N | -0.43484300 | -0.70821400 | -1.43315300 | N | 0.40339900 | -0.45045500 | 1.43396800 |
| C | 2.64246900 | -1.00642100 | 0.12008300 | C | -2.65225700 | -0.99700800 | -0.62161600 |
| C | 3.67790100 | -1.95584300 | 0.20377300 | C | -3.65906400 | -1.94161400 | -0.89431700 |
| C | 1.12721300 | -2.52340900 | 1.07012900 | C | -0.99019700 | -2.59147300 | -1.05697600 |
| C | 3.41509800 | -3.22292200 | 0.73965100 | C | -3.30914200 | -3.24597200 | -1.25857000 |
| H | 4.68327000 | -1.70994200 | -0.14893200 | H | -4.71202900 | -1.65450800 | -0.82171300 |
| C | 2.11549900 | -3.50896200 | 1.18553700 | C | -1.94448300 | -3.57442300 | -1.33348800 |
| H | 0.10466100 | -2.71005100 | 1.40554100 | H | 0.07711700 | -2.81300200 | -1.11855400 |
| H | 4.21109600 | -3.97108200 | 0.80876700 | H | -4.08178000 | -3.98994600 | -1.47639800 |
| H | 1.86036200 | -4.48183500 | 1.61625100 | H | -1.61439400 | -4.58131700 | -1.60700100 |
| C | -2.19537500 | -1.56443900 | -0.06945200 | C | 2.17605500 | -1.43955400 | 0.18833800 |
| C | -3.37315500 | -2.27778100 | 0.21817900 | C | 3.37853800 | -2.14522100 | -0.00940700 |
| C | -1.96978700 | -0.95692800 | 2.18430400 | C | 2.05375300 | -0.94228200 | -2.10727000 |
| C | -3.85324500 | -2.32251600 | 1.53356100 | C | 3.92222700 | -2.24647500 | -1.29509000 |
| H | -3.91428000 | -2.79447500 | -0.57928800 | H | 3.88890700 | -2.60682900 | 0.84110200 |
| C | -3.13122700 | -1.65542000 | 2.53618600 | C | 3.24332400 | -1.63137700 | -2.36245000 |
| H | -1.37688700 | -0.43044900 | 2.93597600 | H | 1.48621100 | -0.44968000 | -2.90039700 |
| H | -4.76925500 | -2.87252500 | 1.77111200 | H | 4.85703500 | -2.79128100 | -1.46111200 |
| H | -3.45750000 | -1.67076300 | 3.58050600 | H | 3.62738000 | -1.68068100 | -3.38597000 |
| N | 1.37183900 | -1.29753000 | 0.54692500 | N | -1.31627300 | -1.31646700 | -0.71462700 |
| N | -1.26341800 | 1.66633000 | -0.09983900 | N | 1.00213700 | 1.83102700 | -0.44132200 |
| N | -1.50220800 | -0.89733300 | 0.91128200 | N | 1.51307200 | -0.83923200 | -0.86143100 |
| Fe | 0.04494900 | 0.14241600 | 0.27355000 | Fe | -0.08995900 | 0.15593300 | -0.42269600 |
| H | 0.77411100 | 2.95509300 | -0.78450900 | H | -0.33006100 | 0.43634100 | -1.90504400 |
| H | -0.98248000 | 1.61620100 | -2.17127500 | H | -0.90455700 | 2.90502300 | 0.64121400 |
| H | 1.15098700 | -0.00293000 | -2.58865000 | H | 2.02798500 | 1.38148000 | 1.32004900 |
| N | 0.50540700 | 0.85771600 | 1.98646000 | H | -1.16206800 | 0.41868000 | 2.49374900 |
| C | 0.91409100 | 1.28748100 | 3.00013600 | | | | |
| C | 1.41810500 | 1.82290900 | 4.25992700 | | | | |
| H | 2.25058400 | 2.52369200 | 4.07072700 | | | | |
| H | 0.62009100 | 2.36503800 | 4.79764100 | | | | |
| H | 1.78579400 | 1.00550100 | 4.90537800 | | | | |

[Fe-H]⁺

| | x | y | z |
|---|-------------|-------------|------------|
| C | 0.07173800 | -0.80095900 | 3.80951900 |
| C | -0.28972900 | -0.23623600 | 2.58183000 |
| C | 1.50909300 | -1.26737900 | 1.48877300 |
| C | 1.92742700 | -1.86697400 | 2.69264900 |
| C | 1.20382700 | -1.63385500 | 3.86862500 |

[Fe-CO]²⁺

| | x | y | z |
|---|-------------|-------------|------------|
| C | -0.32365500 | -0.54715800 | 3.78424800 |
| C | -0.56507200 | -0.08390600 | 2.48467500 |
| C | 1.27783900 | -1.25804600 | 1.63479600 |
| C | 1.57941800 | -1.75399600 | 2.91742400 |
| C | 0.77333000 | -1.39472800 | 4.00534200 |
| H | -0.98605500 | -0.24371600 | 4.60050600 |
| H | 2.43144300 | -2.42239100 | 3.06730600 |
| H | 0.99595900 | -1.77502000 | 5.00746300 |
| C | 1.50886300 | 2.27612300 | 0.93877000 |
| C | 2.45943100 | 3.28321300 | 1.14341800 |

| | | | | | | | |
|--------------------------------------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | 2.13953000 | 2.04103400 | -1.28733400 | C | 4.26221700 | -0.79047900 | -0.05668500 |
| C | 3.28139400 | 3.67888800 | 0.07691100 | H | 3.91927000 | -1.03332400 | -2.18773900 |
| H | 2.54515800 | 3.74508700 | 2.13199300 | C | 3.68302100 | -0.54871400 | 1.19140800 |
| C | 3.11109000 | 3.04021000 | -1.16074400 | H | 1.80189400 | -0.17037500 | 2.19359600 |
| H | 1.99424800 | 1.53662200 | -2.24528600 | H | 4.29694300 | -0.50597800 | 2.09538800 |
| H | 4.03205900 | 4.46532900 | 0.20611600 | C | -0.29515000 | -2.89666200 | -0.59511400 |
| H | 3.71740600 | 3.30908600 | -2.03120600 | C | -0.80262900 | -4.14077400 | -0.99005700 |
| C | -1.66121400 | 2.63132500 | 0.00535100 | C | -2.44789200 | -1.98177900 | -0.43129900 |
| C | -2.84373500 | 3.35094900 | 0.21755600 | C | -2.19152000 | -4.29678500 | -1.12009600 |
| C | -2.82862700 | 0.59490100 | -0.09334600 | H | -0.11323500 | -4.96723700 | -1.18730900 |
| C | -4.05970200 | 2.65362500 | 0.28464000 | C | -3.01948700 | -3.20472200 | -0.82917600 |
| H | -2.80187000 | 4.43970200 | 0.31643800 | H | -2.62406100 | -5.25319000 | -1.43064500 |
| C | -4.04852300 | 1.26190900 | 0.12179400 | H | -4.10558000 | -3.30843400 | -0.90156100 |
| H | -5.00371900 | 3.18391700 | 0.44558300 | N | -1.08572100 | -1.82403600 | -0.33882000 |
| H | -4.98697100 | 0.70164800 | 0.14615400 | N | -0.50230500 | 0.81676800 | -1.47237200 |
| N | -1.63946600 | 1.28165100 | -0.12806300 | C | -3.22123300 | -0.78587000 | -0.05500000 |
| N | 0.21586300 | -0.41807400 | 1.42900200 | C | -4.62491400 | -0.69749600 | -0.10189400 |
| C | -2.70371300 | -0.85315400 | -0.33816300 | C | -3.07642700 | 1.40256600 | 0.77619500 |
| C | -3.78067000 | -1.75849900 | -0.33147700 | H | -5.22045200 | -1.54296500 | -0.45706200 |
| C | -1.21352000 | -2.57791300 | -0.90404700 | C | -4.46909800 | 1.55002600 | 0.75955400 |
| C | -3.55218200 | -3.10939200 | -0.62403400 | H | -2.42884400 | 2.21278800 | 1.11778200 |
| H | -4.79255900 | -1.41235200 | -0.10423500 | H | -4.91655400 | 2.49061400 | 1.09446100 |
| C | -2.24535300 | -3.52474700 | -0.92126100 | C | 0.20547000 | 2.67798500 | -0.15658100 |
| H | -0.18392500 | -2.86046700 | -1.13382500 | C | 0.64780900 | 3.99086200 | 0.08799900 |
| H | -4.38254800 | -3.82259500 | -0.62678200 | C | 0.19262300 | 2.21557200 | 2.14344000 |
| H | -2.01789300 | -4.56612100 | -1.16762600 | C | 0.86618600 | 4.41485100 | 1.40559300 |
| C | 2.02737500 | -1.60068900 | 0.41266500 | H | 0.82213400 | 4.67912500 | -0.74368000 |
| C | 3.17273800 | -2.41742500 | 0.39107300 | C | 0.62451800 | 3.51125300 | 2.45277300 |
| C | 2.10670800 | -1.37968000 | -1.92295500 | H | -0.01394700 | 1.48497900 | 2.92935300 |
| C | 3.79498300 | -2.71433200 | -0.82855600 | H | 1.21230700 | 5.43293000 | 1.61003400 |
| H | 3.58048600 | -2.81909500 | 1.32264000 | H | 0.76747900 | 3.79850100 | 3.49889300 |
| C | 3.24465100 | -2.19082000 | -2.00835500 | N | -2.45507000 | 0.26629000 | 0.37780300 |
| H | 1.65180000 | -0.96736500 | -2.82712900 | N | 1.49353500 | -0.40802300 | 0.14061800 |
| H | 4.68805600 | -3.34664200 | -0.85609800 | N | -0.00961800 | 1.79104900 | 0.87003300 |
| H | 3.68284100 | -2.40117400 | -2.98864100 | Fe | -0.50008600 | -0.03287100 | 0.30067800 |
| N | -1.42806900 | -1.27286200 | -0.61366500 | H | 0.77911400 | -2.74513200 | -0.47331400 |
| N | 1.33377500 | 1.64947500 | -0.25931900 | H | 1.44024800 | -0.67908700 | -1.93401000 |
| N | 1.50219700 | -1.07564800 | -0.74389000 | H | -1.19317200 | -0.80273200 | -2.58899100 |
| Fe | -0.03578200 | 0.14632800 | -0.50264100 | N | -0.57119300 | -0.76838000 | 2.06774000 |
| H | -0.69870400 | 3.14090800 | -0.07076300 | C | -0.71498000 | -1.29560100 | 3.10730500 |
| H | 0.85745500 | 1.95748000 | 1.75527500 | C | -0.89172700 | -1.94933000 | 4.39917400 |
| H | -1.40420200 | 0.58505300 | 2.27512300 | H | -1.08370800 | -3.02781200 | 4.25758400 |
| C | -0.28059800 | 0.50111100 | -2.21195900 | H | 0.01482500 | -1.83398400 | 5.01950400 |
| O | -0.51287000 | 0.71537000 | -3.33267400 | H | -1.74751800 | -1.50698600 | 4.93947500 |
| L = p-NO₂-Pyridine | | | | | | | |
| M = Fe | | | | | | | |
| [Fe-S]²⁺ | | | | | | | |
| | x | y | z | | | | |
| C | -0.85239500 | 0.92331500 | -3.86666600 | | | | |
| C | -0.87621900 | 0.24158500 | -2.64410200 | | | | |
| C | -0.10611200 | 2.13162900 | -1.48724500 | | | | |
| C | -0.05217800 | 2.86792400 | -2.68524100 | | | | |
| C | -0.42492800 | 2.26053900 | -3.89102100 | | | | |
| H | -1.16355700 | 0.40613800 | -4.77932500 | | | | |
| H | 0.27152700 | 3.91231800 | -2.67599400 | | | | |
| H | -0.38842300 | 2.82254900 | -4.82958900 | | | | |
| C | 2.09497300 | -0.64483500 | -1.06070700 | | | | |
| C | 3.47200900 | -0.84379400 | -1.20791700 | | | | |
| C | 2.29733100 | -0.36242700 | 1.24051400 | | | | |
| [Fe-H]⁺ | | | | | | | |
| | x | y | z | | | | |
| C | 1.38842800 | 0.73677600 | 3.77745100 | | | | |
| C | 1.08435400 | 0.06509400 | 2.58826500 | | | | |
| C | 0.72082400 | 2.08114400 | 1.45036800 | | | | |
| C | 1.01905200 | 2.81887600 | 2.61250200 | | | | |
| C | 1.35691500 | 2.14259700 | 3.79131400 | | | | |
| H | 1.64630100 | 0.16441600 | 4.67390100 | | | | |
| H | 0.99533500 | 3.91247800 | 2.59496000 | | | | |
| H | 1.59285800 | 2.70116900 | 4.70265800 | | | | |
| C | -2.25289500 | 0.36060300 | 0.61031300 | | | | |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -3.64605700 | 0.27302800 | 0.66191200 | C | -2.35004100 | -0.17024000 | -1.39405800 |
| C | -2.14081800 | -1.16023500 | -1.15567200 | C | -4.26945300 | -0.75817800 | -0.09207900 |
| H | -4.22404300 | 0.84806200 | 1.38983900 | H | -3.84800900 | -1.32379000 | 1.96209300 |
| C | -3.52806200 | -1.31417100 | -1.17053900 | H | -1.89816500 | 0.14863400 | -2.33552100 |
| H | -1.50295700 | -1.69295200 | -1.86416000 | C | 0.24858400 | -3.01199800 | -0.08945800 |
| H | -4.01429000 | -1.98117100 | -1.88700600 | C | 0.73511200 | -4.31031300 | 0.10745200 |
| C | -0.03827600 | -2.85054400 | 0.64426400 | C | 2.42126700 | -2.11795200 | -0.10619600 |
| C | 0.29370800 | -4.18318100 | 0.90501800 | C | 2.12085900 | -4.50702800 | 0.20925200 |
| C | 2.10118900 | -2.40732800 | -0.20590800 | H | 0.03201300 | -5.14632300 | 0.16836200 |
| C | 1.57927000 | -4.64705800 | 0.57709100 | C | 2.96941400 | -3.39783100 | 0.09557300 |
| H | -0.45271000 | -4.84242000 | 1.35885800 | H | 2.53671400 | -5.50837700 | 0.35982200 |
| C | 2.48997400 | -3.73913900 | 0.02523100 | H | 4.05314200 | -3.53216400 | 0.14841200 |
| H | 1.86851200 | -5.68687900 | 0.75806300 | N | 1.06200000 | -1.92975900 | -0.17538400 |
| H | 3.50490000 | -4.06287100 | -0.22287500 | N | 0.59505100 | 0.51092600 | 1.43325300 |
| N | 0.82660000 | -1.96211100 | 0.07711100 | C | 3.21712800 | -0.89221000 | -0.29619900 |
| N | 0.75321800 | 0.70667300 | 1.43934500 | C | 4.62226800 | -0.83866300 | -0.25099500 |
| C | 2.97896800 | -1.35765100 | -0.72771600 | C | 3.11320300 | 1.40053300 | -0.79851900 |
| C | 4.32301600 | -1.54338000 | -1.10047000 | C | 5.27785400 | 0.37609900 | -0.49026500 |
| C | 3.11150800 | 0.92130400 | -1.25350300 | H | 5.20284400 | -1.73971400 | -0.03592100 |
| C | 5.07269900 | -0.45675800 | -1.56324300 | C | 4.50877800 | 1.51476600 | -0.77412600 |
| H | 4.77854900 | -2.53519300 | -1.03029800 | H | 2.48010900 | 2.26226300 | -1.02034500 |
| C | 4.45171800 | 0.80151200 | -1.63323600 | H | 6.37084700 | 0.42913100 | -0.46272900 |
| H | 2.59895100 | 1.88345500 | -1.30747100 | H | 4.97441600 | 2.48329300 | -0.97918900 |
| H | 6.11789800 | -0.58785900 | -1.86036300 | C | -0.08543600 | 2.58257200 | 0.45302600 |
| H | 4.99283700 | 1.68672000 | -1.98107800 | C | -0.48864100 | 3.93053400 | 0.45683700 |
| C | 0.35067700 | 2.67171300 | 0.15304800 | C | -0.19851300 | 2.52620000 | -1.89135300 |
| C | 0.15182600 | 4.04743000 | -0.07471400 | C | -0.75259500 | 4.58323900 | -0.75464100 |
| C | -0.15081700 | 2.19521400 | -2.09626500 | H | -0.59710000 | 4.47037300 | 1.40137000 |
| C | -0.20808100 | 4.49520600 | -1.35106900 | C | -0.59525100 | 3.86766600 | -1.95152200 |
| H | 0.27032100 | 4.76226200 | 0.74492800 | H | -0.05948500 | 1.94920300 | -2.80924700 |
| C | -0.36302800 | 3.54820200 | -2.37912500 | H | -1.06894400 | 5.63113000 | -0.76261800 |
| H | -0.25133100 | 1.41933800 | -2.85907200 | H | -0.77521600 | 4.33217900 | -2.92575600 |
| H | -0.36865200 | 5.56145300 | -1.53970000 | N | 2.47507600 | 0.23031000 | -0.55885400 |
| H | -0.64636300 | 3.84830000 | -3.39254800 | N | -1.50517400 | -0.38540900 | -0.34459200 |
| N | 2.36860200 | -0.12813900 | -0.81439400 | N | 0.04837600 | 1.88002300 | -0.72076300 |
| N | -1.48349300 | -0.33786000 | -0.27782500 | Fe | 0.50532600 | -0.03745500 | -0.51685900 |
| N | 0.20216100 | 1.74861100 | -0.85957600 | H | -0.82211600 | -2.82395300 | -0.19067100 |
| Fe | 0.46433700 | -0.11624200 | -0.38560900 | H | -1.37620200 | -0.96825900 | 1.66246600 |
| H | 0.31251300 | -0.53136000 | -1.84594300 | H | 1.24792100 | -1.29468300 | 2.24549500 |
| H | -1.02864500 | -2.46295400 | 0.89161000 | C | 0.54074800 | -0.41784700 | -2.23936700 |
| H | -1.71548400 | 1.00662100 | 1.30715900 | O | 0.63332500 | -0.69448900 | -3.36610200 |
| H | 1.10024700 | -1.02806900 | 2.53469900 | C | -3.73613300 | -0.34373200 | -1.31449100 |
| C | -4.28367400 | -0.58030200 | -0.24617400 | H | -4.38160200 | -0.16507900 | -2.17929000 |
| N | -5.75928500 | -0.70755100 | -0.22831000 | N | -5.75114800 | -0.95532200 | 0.04571200 |
| O | -6.37629200 | -0.02980900 | 0.61334700 | O | -6.43439600 | -0.71046700 | -0.95634800 |
| O | -6.27078600 | -1.48410700 | -1.05455500 | O | -6.15316200 | -1.34320100 | 1.15069800 |

L = m-NO₂-Pyridine

M = Fe

[Fe-CO]²⁺

| | x | y | z |
|---|-------------|-------------|------------|
| C | 1.02349900 | 0.21433800 | 3.79611500 |
| C | 0.97849900 | -0.26095800 | 2.47923800 |
| C | 0.25588100 | 1.81746700 | 1.66595700 |
| C | 0.27374200 | 2.35513400 | 2.96696400 |
| C | 0.65778400 | 1.54670700 | 4.04483100 |
| H | 1.33815100 | -0.45308000 | 4.60401400 |
| H | -0.00192100 | 3.39881000 | 3.14018700 |
| H | 0.67621800 | 1.95329400 | 5.06112400 |
| C | -2.06205100 | -0.79384000 | 0.83157800 |
| C | -3.43608500 | -0.99432900 | 1.00389500 |

[Fe-S]²⁺

| | x | y | z |
|---|-------------|-------------|------------|
| C | 1.97721200 | 1.88208400 | 3.29362300 |
| C | 1.64882700 | 0.91480900 | 2.33653100 |
| C | 0.38301200 | 2.45688700 | 1.10072700 |
| C | 0.67244800 | 3.47102400 | 2.03248800 |
| C | 1.47506600 | 3.18472400 | 3.14380600 |
| H | 2.61645800 | 1.60988900 | 4.13892100 |
| H | 0.28088600 | 4.48152100 | 1.88674600 |
| H | 1.70936500 | 3.96529500 | 3.87451900 |
| C | -1.62149600 | -0.35591600 | 2.11270300 |

| | | | | | | | |
|----|--------------|--------------|-------------|----|-------------|-------------|-------------|
| C | -2.86614300 | -0.52972000 | 2.73192800 | H | -3.36986200 | -2.31480300 | 4.17741900 |
| C | -2.53544300 | -0.67770000 | 0.00373800 | C | 1.84416400 | -1.47354400 | 1.12358800 |
| C | -4.00144200 | -0.79042100 | 1.94888200 | C | 3.13473600 | -1.94168100 | 1.40205700 |
| H | -2.93968100 | -0.45954000 | 3.82150100 | C | 2.65158900 | 0.10214500 | -0.38792800 |
| C | -3.80029700 | -0.86092000 | 0.56736400 | H | 3.26777100 | -2.75571300 | 2.12127000 |
| H | -2.41384500 | -0.73473300 | -1.07733500 | C | 3.95875200 | -0.32377300 | -0.13924500 |
| C | 0.73024900 | -2.63189100 | 1.39629700 | H | 2.44355300 | 0.90206300 | -1.10025000 |
| C | 1.45215600 | -3.73972600 | 1.85722600 | C | 0.98532700 | 2.36163800 | 1.21261600 |
| C | 2.60197500 | -1.78245800 | 0.26798300 | C | 1.12855200 | 3.70515800 | 1.57017100 |
| C | 2.80745800 | -3.85850200 | 1.51147200 | C | -0.91534400 | 2.83103200 | -0.07618400 |
| H | 0.95097700 | -4.49323600 | 2.47224200 | C | 0.21916300 | 4.65077000 | 1.06527200 |
| C | 3.38256100 | -2.87003100 | 0.70233400 | H | 1.94729700 | 3.99889800 | 2.23431800 |
| H | 3.40365100 | -4.70962500 | 1.85551100 | C | -0.81811500 | 4.19756200 | 0.24256900 |
| H | 4.43112500 | -2.951113800 | 0.40313000 | H | 0.31012500 | 5.71222700 | 1.31540900 |
| N | 1.28329700 | -1.65520800 | 0.63353700 | H | -1.55479900 | 4.90368700 | -0.15126300 |
| N | 0.86035400 | 1.17868800 | 1.26259800 | N | 0.00223000 | 1.90883800 | 0.38301700 |
| C | 3.08835700 | -0.71036700 | -0.61713700 | N | -1.19824900 | -0.64081900 | 1.38027300 |
| C | 4.40738200 | -0.60885400 | -1.09682100 | C | -1.98225100 | 2.23314600 | -0.88061600 |
| C | 2.47220500 | 1.21861800 | -1.80073300 | C | -3.04326300 | 2.94611800 | -1.46854100 |
| H | 5.16049000 | -1.34513100 | -0.80316600 | C | -2.83270200 | 0.21425000 | -1.71092300 |
| C | 3.76589800 | 1.37168100 | -2.31468400 | C | -4.02175500 | 2.26206100 | -2.19743500 |
| H | 1.67768600 | 1.92129500 | -2.06075900 | H | -3.10001000 | 4.03262700 | -1.35706300 |
| H | 3.98505700 | 2.20869400 | -2.98435600 | C | -3.91297700 | 0.86592300 | -2.31298000 |
| C | -0.40405400 | 2.65141100 | -0.12766400 | H | -2.71543600 | -0.86781000 | -1.79455700 |
| C | -1.01646200 | 3.86040800 | -0.50427300 | H | -4.85032300 | 2.80462000 | -2.66321100 |
| C | -1.13756800 | 1.62253100 | -2.10425500 | H | -4.65270600 | 0.27966700 | -2.86666000 |
| C | -1.70926800 | 3.93794200 | -1.72002500 | C | -1.29806600 | -2.53955100 | -0.05408900 |
| H | -0.95591900 | 4.73663100 | 0.14714800 | C | -1.59041000 | -3.86746700 | -0.42177300 |
| C | -1.76421100 | 2.79784900 | -2.53727500 | C | -0.19622900 | -2.18182700 | -2.10294500 |
| H | -1.15289500 | 0.71723500 | -2.71553800 | C | -1.17014900 | -4.35260000 | -1.66553800 |
| H | -2.19277400 | 4.871170600 | -2.02393500 | H | -2.13903000 | -4.51852700 | 0.26527200 |
| H | -2.28645500 | 2.80842000 | -3.49872800 | C | -0.45745000 | -3.49089700 | -2.51904400 |
| N | 2.12962500 | 0.20561800 | -0.96846500 | H | 0.34559400 | -1.46974200 | -2.73025600 |
| N | -1.43732600 | -0.42970100 | 0.76150600 | H | -1.39073000 | -5.38282200 | -1.96259700 |
| N | -0.47253700 | 1.53396900 | -0.92395200 | H | -0.10526000 | -3.82381100 | -3.50015600 |
| Fe | 0.35446400 | -0.08454400 | -0.15408600 | N | -1.86917200 | 0.86784100 | -1.00952100 |
| H | -0.32874700 | -2.51670700 | 1.63610700 | N | 1.58199200 | -0.46570400 | 0.23922300 |
| H | -0.73009600 | -0.15214300 | 2.71075400 | N | -0.60510600 | -1.69639000 | -0.89755200 |
| H | 2.01619900 | -0.11049600 | 2.42484000 | Fe | -0.25682300 | 0.09544000 | -0.24397400 |
| N | -0.10588300 | -1.23248100 | -1.61796600 | H | 0.35358700 | 0.48317800 | -1.58802900 |
| C | -0.30250200 | -1.99238100 | -2.49138400 | H | 1.67507900 | 1.60533500 | 1.59376300 |
| C | -0.56382700 | -2.93139500 | -3.57588500 | H | 0.97356500 | -1.90740700 | 1.62053300 |
| H | -0.176662200 | -3.93250400 | -3.31568000 | H | -1.09330300 | 1.03400700 | 2.61096200 |
| H | -1.65030200 | -3.01133300 | -3.75942900 | C | 4.23730300 | -1.36237700 | 0.75887500 |
| H | -0.07147000 | -2.59326800 | -4.50493200 | H | 5.26647800 | -1.68747900 | 0.93231900 |
| C | 4.75437300 | 0.44334200 | -1.95395000 | N | 5.07256100 | 0.34969500 | -0.86197000 |
| H | 5.77699000 | 0.53419200 | -2.33361300 | O | 4.77309400 | 1.27329300 | -1.63719200 |
| H | -4.99786200 | -0.93375900 | 2.37766500 | O | 6.22049900 | -0.06125900 | -0.63120600 |
| N | -4.94397800 | -1.13578200 | -0.35245400 | | | | |
| O | -6.05834900 | -1.26348700 | 0.16496000 | | | | |
| O | -4.67939200 | -1.21238900 | -1.56584800 | | | | |

[Fe-H]⁺

| | x | y | z |
|---|-------------|-------------|------------|
| C | -2.26404500 | -0.54063100 | 3.55475300 |
| C | -1.49513500 | 0.01919500 | 2.52889700 |
| C | -1.68117700 | -1.91930900 | 1.22500400 |
| C | -2.46300900 | -2.54093100 | 2.21814700 |
| C | -2.76079000 | -1.84704900 | 3.39740100 |
| H | -2.46997500 | 0.04154500 | 4.45834400 |
| H | -2.84306700 | -3.55584100 | 2.06800400 |

[Fe-CO]²⁺

| | x | y | z |
|---|-------------|-------------|------------|
| C | 1.83432300 | 0.82666800 | 3.61131100 |
| C | 1.55872400 | 0.16744600 | 2.40650100 |
| C | 0.26611700 | 1.96204200 | 1.62376200 |
| C | 0.50018600 | 2.67548000 | 2.81456500 |
| C | 1.28984700 | 2.10357000 | 3.82060800 |
| H | 2.46331300 | 0.34213800 | 4.36413500 |
| H | 0.07858100 | 3.67440100 | 2.95504400 |
| H | 1.48103600 | 2.64966800 | 4.74998500 |
| C | -1.61122800 | -1.15376700 | 1.68981200 |
| C | -2.83953900 | -1.54961000 | 2.23407900 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -2.57062800 | -0.75038600 | -0.38839900 | C | -1.61573900 | 2.13110100 | -1.43505600 |
| C | -3.98894200 | -1.54466600 | 1.42854200 | C | -2.52554600 | 3.14967100 | -1.74054700 |
| H | -2.88922200 | -1.85715900 | 3.28312800 | C | -1.98044600 | 2.39681900 | 0.84869300 |
| H | -2.48097800 | -0.43826800 | -1.42997000 | C | -3.18656000 | 3.81467000 | -0.69558800 |
| C | 0.80075200 | -3.00267100 | 0.36937100 | H | -2.70888900 | 3.40934400 | -2.78787300 |
| C | 1.57137000 | -4.16028900 | 0.53222300 | C | -2.90352800 | 3.42436200 | 0.62256300 |
| C | 2.67312700 | -1.75835600 | -0.31166400 | H | -1.73863100 | 2.07062500 | 1.86280000 |
| C | 2.94888800 | -4.10000800 | 0.27054800 | H | -3.90360500 | 4.61541300 | -0.90345700 |
| H | 1.08875000 | -5.08993300 | 0.84812400 | H | -3.39041600 | 3.90633600 | 1.47604100 |
| C | 3.50040300 | -2.88665100 | -0.16139700 | C | 1.83337300 | 2.32517800 | -1.03224200 |
| H | 3.58169200 | -4.98599700 | 0.38403400 | C | 3.02194900 | 2.88295400 | -1.51678700 |
| H | 4.56637200 | -2.82470800 | -0.39606400 | C | 2.91117500 | 0.30772100 | -0.47982400 |
| N | 1.33156300 | -1.81678400 | -0.02144900 | C | 4.19521600 | 2.11213500 | -1.48378800 |
| N | 0.78762700 | 0.70951800 | 1.43284000 | H | 3.02007100 | 3.90511600 | -1.90715500 |
| C | 3.13042500 | -0.45308500 | -0.81957400 | C | 4.13477800 | 0.81610600 | -0.95620300 |
| C | 4.46095500 | -0.15516600 | -1.16624400 | H | 5.14304400 | 2.51439500 | -1.85514800 |
| C | 2.44343100 | 1.69528200 | -1.47563900 | H | 5.04078700 | 0.20595500 | -0.90969000 |
| C | 4.77647300 | 1.10782100 | -1.68384400 | N | 1.76143900 | 1.06335200 | -0.53511600 |
| H | 5.24640000 | -0.90484700 | -1.03881700 | N | -0.54743400 | -0.82817100 | -1.46363900 |
| C | 3.74751800 | 2.04778900 | -1.84532000 | C | 2.75147700 | -1.03209700 | 0.11917400 |
| H | 1.61558700 | 2.39805100 | -1.59034000 | C | 3.79487800 | -1.96868600 | 0.24667300 |
| H | 5.80708900 | 1.34951400 | -1.96242600 | C | 1.25538100 | -2.52786500 | 1.15016500 |
| H | 3.94112400 | 3.04351100 | -2.25513600 | C | 3.54890800 | -3.21229900 | 0.84195300 |
| C | -0.50771500 | 2.48005000 | 0.48082800 | H | 4.79740500 | -1.73023400 | -0.11830800 |
| C | -1.15595500 | 3.72861100 | 0.46514200 | C | 2.25401200 | -3.49585800 | 1.30438800 |
| C | -1.18218200 | 2.07166900 | -1.73159000 | H | 0.23358300 | -2.70302500 | 1.49640800 |
| C | -1.83584700 | 4.14752700 | -0.68647100 | H | 4.35501700 | -3.94583400 | 0.94260100 |
| H | -1.13319300 | 4.37235800 | 1.34865300 | H | 2.01245700 | -4.45183100 | 1.77854000 |
| C | -1.84147200 | 3.30470300 | -1.80814700 | C | -2.29020500 | -1.63117000 | -0.01309300 |
| H | -1.16529300 | 1.40014900 | -2.59389100 | C | -3.46050400 | -2.34234800 | 0.31195000 |
| H | -2.34670900 | 5.11541900 | -0.70731900 | C | -2.06581300 | -0.93412900 | 2.22333900 |
| H | -2.34889100 | 3.58585500 | -2.73587400 | C | -3.93550600 | -2.34141200 | 1.62976500 |
| N | 2.13484200 | 0.47794600 | -0.96832700 | H | -4.00220300 | -2.89512600 | -0.46032400 |
| N | -1.45837200 | -0.76091700 | 0.39129700 | C | -3.21916600 | -1.62838500 | 2.60488700 |
| N | -0.53079600 | 1.64987400 | -0.61474000 | H | -1.47379600 | -0.36766500 | 2.94715800 |
| Fe | 0.33604400 | -0.11398400 | -0.36240700 | H | -4.84557300 | -2.89078000 | 1.89022200 |
| H | -0.27683300 | -3.01816200 | 0.54499500 | H | -3.54467200 | -1.60460600 | 3.64928800 |
| H | -0.70920700 | -1.14826600 | 2.30566900 | N | 1.48523800 | -1.32340400 | 0.56944200 |
| H | 1.95836800 | -0.83077300 | 2.20763500 | N | -1.32979400 | 1.74935900 | -0.15795000 |
| C | -0.00017300 | -0.73134800 | -1.98279300 | N | -1.60217400 | -0.92176400 | 0.94616100 |
| O | -0.15570100 | -1.15652900 | -3.05432300 | Ru | 0.04568600 | 0.15204300 | 0.26041400 |
| C | -3.82154800 | -1.12890900 | 0.10500700 | H | 0.89947800 | 2.89293100 | -1.02869600 |
| H | -4.97434200 | -1.84492700 | 1.79822000 | H | -1.09005300 | 1.59332600 | -2.22851800 |
| N | -4.99209600 | -1.07243400 | -0.82525100 | H | 1.00668000 | -0.17042400 | -2.68553600 |
| O | -6.07288900 | -1.46977900 | -0.37862700 | N | 0.56637900 | 0.99988500 | 2.03932500 |
| O | -4.77566100 | -0.62335800 | -1.96268400 | C | 0.96342400 | 1.47143700 | 3.04037300 |
| | | | | C | 1.45763800 | 2.05472000 | 4.28293800 |
| | | | | H | 2.28781800 | 2.75254500 | 4.07362900 |
| | | | | H | 0.65387700 | 2.61160900 | 4.79648100 |
| | | | | H | 1.82507500 | 1.26294800 | 4.95983000 |

L = pyridine

M = Ru

[Ru-S]²⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.34542800 | -1.47195400 | -3.78979300 |
| C | 0.10263900 | -0.78482200 | -2.65703100 |
| C | -1.68580900 | -1.59661000 | -1.35771700 |
| C | -2.18557500 | -2.30300300 | -2.46806500 |
| C | -1.51662600 | -2.24140900 | -3.69672100 |
| H | 0.21858900 | -1.39923500 | -4.72454300 |
| H | -3.09226400 | -2.90628100 | -2.37266900 |
| H | -1.89995700 | -2.78913500 | -4.56330200 |

[Ru-H]⁺

| | x | y | z |
|---|-------------|-------------|------------|
| C | 0.31802700 | -0.94485900 | 3.88412400 |
| C | -0.10196600 | -0.35633600 | 2.68653900 |
| C | 1.65216600 | -1.34570700 | 1.48085300 |
| C | 2.13025400 | -1.96485100 | 2.65472400 |
| C | 1.46021200 | -1.76530100 | 3.86767700 |
| H | -0.24009200 | -0.76186700 | 4.80768600 |
| H | 3.01381900 | -2.60871800 | 2.62237600 |
| H | 1.82088500 | -2.24439100 | 4.78358300 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | 2.00787000 | 2.18296200 | 0.56260100 | C | 3.11579500 | 3.23247900 | -1.07822800 |
| C | 2.81885500 | 3.32357400 | 0.58728000 | H | 2.01305300 | 1.75190400 | -2.21568800 |
| C | 0.99372900 | 2.86388300 | -1.42075600 | H | 4.02297100 | 4.61432900 | 0.34070500 |
| C | 2.70174800 | 4.27320200 | -0.43963700 | H | 3.69555000 | 3.56363100 | -1.94529700 |
| H | 3.52948900 | 3.45665300 | 1.40936800 | C | -1.80431300 | 2.63134200 | 0.18858700 |
| C | 1.76601700 | 4.03024300 | -1.45781400 | C | -2.99032900 | 3.32042900 | 0.46797600 |
| H | 0.26256400 | 2.63208800 | -2.19870100 | C | -2.94623800 | 0.57907200 | -0.00192300 |
| H | 3.32239700 | 5.17520800 | -0.44721600 | C | -4.19380900 | 2.60020500 | 0.51844900 |
| H | 1.63117600 | 4.73188100 | -2.28719200 | H | -2.96223000 | 4.40176600 | 0.63160700 |
| C | -1.98097000 | 2.42131400 | 0.46341300 | C | -4.16780600 | 1.21996100 | 0.27823800 |
| C | -3.20880400 | 3.02019000 | 0.75229300 | H | -5.14175900 | 3.10507100 | 0.73000600 |
| C | -3.01925900 | 0.38827200 | -0.10259500 | H | -5.09951400 | 0.64878400 | 0.29601400 |
| C | -4.39025200 | 2.27276900 | 0.59601600 | N | -1.77103600 | 1.29289800 | -0.02814900 |
| H | -3.23198600 | 4.06042500 | 1.09175600 | N | 0.31653800 | -0.53938100 | 1.51795500 |
| C | -4.28342200 | 0.94451800 | 0.17044600 | C | -2.82246800 | -0.86076600 | -0.31351700 |
| H | -5.36975500 | 2.71310200 | 0.80643000 | C | -3.90618100 | -1.75902900 | -0.32744600 |
| H | -5.18403800 | 0.33551900 | 0.05097400 | C | -1.35667900 | -2.58772000 | -0.95880600 |
| N | -1.86299000 | 1.13417700 | 0.02886200 | C | -3.69557100 | -3.10119500 | -0.66993000 |
| N | 0.53949900 | -0.54049200 | 1.50551800 | H | -4.91305900 | -1.41471800 | -0.07746500 |
| C | -2.79746500 | -1.00092400 | -0.52202000 | C | -2.39751900 | -3.52303600 | -0.99557900 |
| C | -3.82293200 | -1.94160800 | -0.73775400 | H | -0.32962900 | -2.86669400 | -1.20730300 |
| C | -1.17540000 | -2.61824900 | -1.05802400 | H | -4.53471500 | -3.80385900 | -0.68704300 |
| C | -3.50653200 | -3.24857500 | -1.12218200 | H | -2.18546300 | -4.55828400 | -1.27863400 |
| H | -4.86844100 | -1.64844700 | -0.60776500 | C | 2.11866800 | -1.68201200 | 0.39474300 |
| C | -2.15190600 | -3.59158700 | -1.27943300 | C | 3.26207100 | -2.50159600 | 0.34116600 |
| H | -0.11226300 | -2.83902200 | -1.18095500 | C | 2.21438400 | -1.37444900 | -1.93728100 |
| H | -4.29838300 | -3.98394000 | -1.29551800 | C | 3.88970700 | -2.75542700 | -0.88509000 |
| H | -1.84897500 | -4.60048400 | -1.57601800 | H | 3.66748300 | -2.94065500 | 1.25638500 |
| C | 2.27328000 | -1.50872600 | 0.15020000 | C | 3.34976300 | -2.18470100 | -2.04740400 |
| C | 3.46542700 | -2.22734300 | -0.07072600 | H | 1.76515000 | -0.91913400 | -2.82332200 |
| C | 2.11231200 | -1.04248600 | -2.15461600 | H | 4.78058000 | -3.38969400 | -0.93020500 |
| C | 3.98378600 | -2.35105400 | -1.36409900 | H | 3.79418200 | -2.35721300 | -3.03225800 |
| H | 3.99128800 | -2.68498100 | 0.77188700 | N | -1.55523300 | -1.29094600 | -0.62141400 |
| C | 3.28785000 | -1.74673000 | -2.42619300 | N | 1.40083400 | 1.74891800 | -0.21218500 |
| H | 1.53352200 | -0.55420800 | -2.94205400 | N | 1.60338300 | -1.11387800 | -0.74984400 |
| H | 4.91060000 | -2.90626600 | -1.53972400 | Ru | -0.04207700 | 0.16760600 | -0.49702700 |
| H | 3.64837000 | -1.81412000 | -3.45724900 | H | -0.84551200 | 3.15158500 | 0.12306200 |
| N | -1.47137500 | -1.34121600 | -0.69222600 | H | 0.96228900 | 1.92650100 | 1.82523500 |
| N | 1.09550300 | 1.93563700 | -0.42169200 | H | -1.27761700 | 0.42782500 | 2.44513200 |
| N | 1.59830300 | -0.91122300 | -0.89723700 | C | -0.28151700 | 0.59956300 | -2.30845600 |
| Ru | -0.10561500 | 0.18099600 | -0.45961600 | O | -0.44441400 | 0.83167200 | -3.44144900 |
| H | -0.39849900 | 0.54537400 | -2.02145100 | | | | |
| H | -1.04163200 | 2.96963800 | 0.56710900 | | | | |
| H | 2.07199900 | 1.43195200 | 1.35385500 | | | | |
| H | -0.98329600 | 0.29304700 | 2.64746400 | | | | |

**L = pyridine
M = Co**

[Ru-CO]²⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.15452400 | -0.76735000 | 3.87886500 |
| C | -0.43268600 | -0.24809300 | 2.60928000 |
| C | 1.38556300 | -1.38819300 | 1.64537600 |
| C | 1.71828500 | -1.94014600 | 2.89830400 |
| C | 0.94612900 | -1.62694500 | 4.02456800 |
| H | -0.78948000 | -0.50048500 | 4.72894200 |
| H | 2.57079800 | -2.61654300 | 2.99857800 |
| H | 1.19894300 | -2.05295100 | 5.00083300 |
| C | 1.58399400 | 2.31494300 | 1.01474900 |
| C | 2.50905100 | 3.33820400 | 1.25041000 |
| C | 2.17061000 | 2.21302200 | -1.23794400 |
| C | 3.29354200 | 3.81249700 | 0.18716000 |
| H | 2.60575000 | 3.75117700 | 2.25934800 |

[Co-S]³⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.15522900 | -1.20172400 | -3.78218300 |
| C | 0.26239900 | -0.57300200 | -2.60186800 |
| C | -1.57127200 | -1.45006300 | -1.40537700 |
| C | -2.03957900 | -2.09600600 | -2.56385900 |
| C | -1.33001200 | -1.97044000 | -3.76619400 |
| H | 0.43877200 | -1.08084400 | -4.69351300 |
| H | -2.94981600 | -2.70122200 | -2.52564100 |
| H | -1.68551500 | -2.47051700 | -4.67331800 |
| C | -1.54721800 | 2.09097000 | -1.34207300 |
| C | -2.46748100 | 3.11556100 | -1.59266900 |
| C | -1.91101300 | 2.24340800 | 0.96059000 |
| C | -3.13345700 | 3.72132200 | -0.51499500 |
| H | -2.65239900 | 3.42543200 | -2.62624800 |
| C | -2.84342200 | 3.27235400 | 0.78305100 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | -1.67124600 | 1.87752600 | 1.95981700 | C | -1.82633600 | -3.82312800 | -1.51894500 |
| H | -3.85988300 | 4.52359300 | -0.68300800 | H | -0.31567400 | -2.44186700 | -2.25897100 |
| H | -3.33096400 | 3.70866200 | 1.66068000 | H | -3.35425300 | -4.98372000 | -0.48772300 |
| C | 1.68492900 | 2.39783500 | -0.79946600 | H | -1.75423300 | -4.48155300 | -2.39019500 |
| C | 2.87861200 | 2.99990700 | -1.22104200 | C | 1.80049600 | -2.43776300 | 0.42012400 |
| C | 2.77754600 | 0.34422100 | -0.40849700 | C | 3.03006400 | -3.06744400 | 0.65013100 |
| C | 4.05486000 | 2.23413700 | -1.24502100 | C | 2.86285900 | -0.44388300 | -0.22821400 |
| H | 2.87349500 | 4.05266600 | -1.52031400 | C | 4.21525200 | -2.35376300 | 0.41369300 |
| C | 4.00186800 | 0.89610900 | -0.82767400 | H | 3.04605700 | -4.10274600 | 1.00343600 |
| H | 5.00323800 | 2.67318600 | -1.57260700 | C | 4.12641500 | -1.02593700 | -0.02369100 |
| H | 4.91226600 | 0.29022900 | -0.81950300 | H | 5.19292200 | -2.81994300 | 0.57189400 |
| N | 1.62808100 | 1.09626300 | -0.42486900 | H | 5.03571100 | -0.44621100 | -0.20407500 |
| N | -0.43262200 | -0.68392600 | -1.44238300 | N | 1.70939200 | -1.15769900 | -0.01888400 |
| C | 2.660616100 | -1.02792700 | 0.09621600 | N | -0.34562100 | 0.48875500 | 1.46709700 |
| C | 3.63380200 | -1.98482200 | 0.18239300 | C | 2.63663800 | 0.94479600 | -0.65233900 |
| C | 1.06797900 | -2.55226000 | 1.02790300 | C | 3.65389800 | 1.87432400 | -0.93168700 |
| C | 3.35776500 | -3.25534400 | 0.70766800 | C | 0.98959700 | 2.55102900 | -1.12417900 |
| H | 4.64441800 | -1.74274400 | -0.15829000 | C | 3.31458800 | 3.17714100 | -1.31805200 |
| C | 2.05477800 | -3.54123800 | 1.14297100 | H | 4.70438100 | 1.58201400 | -0.85202700 |
| H | 0.04386900 | -2.73934100 | 1.35596000 | C | 1.95774800 | 3.52141900 | -1.41090800 |
| H | 4.15022500 | -4.00791300 | 0.77786900 | H | -0.07449000 | 2.78147700 | -1.19865600 |
| H | 1.79247700 | -4.51597500 | 1.56588600 | H | 4.09664200 | 3.90904100 | -1.54346400 |
| C | -2.19546800 | -1.54593100 | -0.07873400 | H | 1.64134400 | 4.52580500 | -1.70739300 |
| C | -3.36989300 | -2.26184600 | 0.21435100 | C | -2.11301700 | 1.47696700 | 0.19098300 |
| C | -1.95229500 | -0.94872700 | 2.18808300 | C | -3.29759100 | 2.21058700 | -0.00641300 |
| C | -3.83850500 | -2.31222100 | 1.53543900 | C | -2.06836500 | 0.88861600 | -2.09414000 |
| H | -3.91689200 | -2.77681500 | -0.58050100 | C | -3.87013000 | 2.27715500 | -1.28416900 |
| C | -3.11221700 | -1.65251700 | 2.54013800 | H | -3.77520900 | 2.72154600 | 0.83407800 |
| H | -1.35494600 | -0.42876000 | 2.93991200 | C | -3.24497200 | 1.60515500 | -2.34641500 |
| H | -4.75300800 | -2.86450600 | 1.77632500 | H | -1.54146300 | 0.35160300 | -2.88650300 |
| H | -3.43109400 | -1.67706500 | 3.58688300 | H | -4.79242700 | 2.84445200 | -1.44568500 |
| N | 1.33552000 | -1.32848200 | 0.51500200 | H | -3.65540800 | 1.62905600 | -3.36024900 |
| N | -1.26144400 | 1.65544500 | -0.08202800 | N | 1.31305400 | 1.28954400 | -0.75353400 |
| N | -1.50673100 | -0.89042100 | 0.90957700 | N | -1.05322500 | -1.81545100 | -0.40354600 |
| Co | 0.03754900 | 0.13733100 | 0.25805600 | N | -1.51136800 | 0.82641500 | -0.85875100 |
| H | 0.75325800 | 2.96438200 | -0.75635900 | Co | 0.07854000 | -0.18420400 | -0.42448000 |
| H | -1.01611800 | 1.61096900 | -2.16620900 | H | 0.34244300 | -0.48622200 | -1.83976500 |
| H | 1.16428900 | 0.04165800 | -2.58207000 | H | 0.85816000 | -2.96183800 | 0.58893600 |
| N | 0.54592300 | 0.83270800 | 1.99222000 | H | -1.91665500 | -1.38028500 | 1.44905000 |
| C | 0.99351000 | 1.24455500 | 2.99325200 | H | 1.20401900 | -0.40146300 | 2.53248600 |
| C | 1.53346700 | 1.75913700 | 4.24221700 | | | | |
| H | 2.33456300 | 2.49187000 | 4.03460600 | | | | |
| H | 0.73992500 | 2.26037700 | 4.82602600 | | | | |
| H | 1.95245400 | 0.93340800 | 4.84574000 | | | | |

[Co-H]²⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | 0.01999600 | 0.90064500 | 3.81958700 |
| C | 0.35413500 | 0.28436500 | 2.60510900 |
| C | -1.42299500 | 1.33365500 | 1.49162600 |
| C | -1.81250400 | 1.98798200 | 2.67510900 |
| C | -1.08186700 | 1.76957100 | 3.85240100 |
| H | 0.61568800 | 0.70066900 | 4.71528600 |
| H | -2.67063800 | 2.66587800 | 2.68376700 |
| H | -1.37069100 | 2.27216000 | 4.78113600 |
| C | -1.91313800 | -2.08641600 | 0.61648600 |
| C | -2.74885600 | -3.20989700 | 0.62193100 |
| C | -1.01889700 | -2.68178000 | -1.45807900 |
| C | -2.71067600 | -4.09820200 | -0.46395500 |
| H | -3.41648200 | -3.37644000 | 1.47295300 |

[Co-CO]³⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.28151400 | -0.49431900 | 3.78799300 |
| C | -0.55105600 | -0.05757100 | 2.48376600 |
| C | 1.31582200 | -1.22311000 | 1.63346700 |
| C | 1.63752900 | -1.68374200 | 2.92318400 |
| C | 0.83486000 | -1.31594400 | 4.01286700 |
| H | -0.94172100 | -0.18734400 | 4.60536900 |
| H | 2.50445100 | -2.33259100 | 3.07722700 |
| H | 1.07523100 | -1.67123500 | 5.02064700 |
| C | 1.51650900 | 2.26745400 | 0.92522500 |
| C | 2.45177800 | 3.29822800 | 1.07853000 |
| C | 2.08313600 | 2.01474800 | -1.33179700 |
| C | 3.22648600 | 3.69774200 | -0.02257900 |
| H | 2.56207500 | 3.77400500 | 2.05850200 |
| C | 3.03172500 | 3.03994700 | -1.24771700 |
| H | 1.93131100 | 1.49027200 | -2.27799300 |
| H | 3.96321700 | 4.50293200 | 0.07127300 |
| H | 3.60211800 | 3.31138000 | -2.14203900 |
| C | -1.64576400 | 2.61830200 | 0.02506100 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -2.83539800 | 3.33169800 | 0.22219700 | C | -0.94477400 | 4.68507500 | -0.00585500 |
| C | -2.81578600 | 0.56502000 | -0.08181500 | H | -2.90237800 | 3.95118200 | -0.59253500 |
| C | -4.04976600 | 2.62870200 | 0.27580400 | C | 0.34802800 | 4.30577700 | 0.38701300 |
| H | -2.79757800 | 4.42136900 | 0.31890300 | H | 1.64988100 | 2.60536700 | 0.79416900 |
| C | -4.03655700 | 1.23459200 | 0.11796300 | H | -1.21649700 | 5.74160900 | -0.09557000 |
| H | -4.99742300 | 3.15794900 | 0.42291500 | H | 1.11630300 | 5.05100400 | 0.61401900 |
| H | -4.97573400 | 0.67445800 | 0.13451800 | C | 2.82261700 | 0.00262900 | -0.22249700 |
| N | -1.63216900 | 1.26626600 | -0.09908700 | C | 4.21457900 | 0.00412900 | -0.01518600 |
| N | 0.23306300 | -0.40395000 | 1.43340000 | C | 2.44250900 | 0.00607400 | 2.09239700 |
| C | -2.68101600 | -0.88124600 | -0.31772000 | C | 4.72189000 | 0.00665900 | 1.29030800 |
| C | -3.74944300 | -1.79616400 | -0.32812600 | H | 4.89926300 | 0.00338600 | -0.86783700 |
| C | -1.16012000 | -2.61205100 | -0.84447000 | C | 3.81543200 | 0.00771700 | 2.36350600 |
| C | -3.50506800 | -3.14873100 | -0.60799600 | H | 1.70712400 | 0.00682000 | 2.89931800 |
| H | -4.76882800 | -1.45603800 | -0.12462500 | H | 5.80230400 | 0.00783900 | 1.46566000 |
| C | -2.19035700 | -3.56189600 | -0.87433500 | H | 4.16068500 | 0.00977300 | 3.40180200 |
| H | -0.12610800 | -2.89445000 | -1.05047600 | N | -0.24638200 | 1.96835100 | 0.22323100 |
| H | -4.33199000 | -3.86673700 | -0.62413200 | N | 1.93700700 | 0.00347000 | 0.83031400 |
| H | -1.95202200 | -4.60432000 | -1.10808100 | Fe | 0.02605600 | 0.00060300 | 0.31842600 |
| C | 2.04722300 | -1.57531900 | 0.40758300 | H | -0.97904600 | -0.00176000 | -2.57614300 |
| C | 3.19378700 | -2.38909200 | 0.35868900 | C | -1.51105200 | -2.33854800 | -0.15889400 |
| C | 2.06543100 | -1.36874200 | -1.94538400 | C | -1.87720600 | -3.68936100 | -0.27802900 |
| C | 3.78358500 | -2.68991600 | -0.87781800 | C | 0.66329200 | -2.93839800 | 0.49342000 |
| H | 3.62635900 | -2.78655700 | 1.28134400 | C | -0.93188200 | -4.68711000 | 0.00082600 |
| C | 3.20366800 | -2.17826800 | -2.05006100 | H | -2.89131000 | -3.95935600 | -0.58743200 |
| H | 1.58880800 | -0.96853300 | -2.84419200 | C | 0.35974500 | -4.30371800 | 0.39361700 |
| H | 4.67830600 | -3.31999600 | -0.92474100 | H | 1.65673700 | -2.59915700 | 0.79893900 |
| H | 3.61707700 | -2.39720500 | -3.03990100 | H | -1.20067200 | -5.74450800 | -0.08752300 |
| N | -1.40051600 | -1.30791500 | -0.56812100 | H | 1.12997500 | -5.04652400 | 0.62192800 |
| N | 1.32452800 | 1.62893400 | -0.26461900 | N | -0.24097000 | -1.96814900 | 0.22630300 |
| N | 1.50146800 | -1.06754400 | -0.74614800 | N | -0.59032900 | 0.00114400 | 2.13337400 |
| Co | -0.03074000 | 0.12825600 | -0.44594100 | C | -1.05222800 | 0.00142900 | 3.21160700 |
| H | -0.68499800 | 3.13200400 | -0.03994800 | C | -1.61298000 | 0.00176100 | 4.55787100 |
| H | 0.90253200 | 1.94711200 | 1.76877700 | H | -2.24212500 | -0.89289800 | 4.71066000 |
| H | -1.40473400 | 0.59121600 | 2.27461900 | H | -0.80633300 | -0.00339500 | 5.31226100 |
| C | -0.37593700 | 0.50804300 | -2.19919200 | H | -2.23366400 | 0.90177700 | 4.71375100 |
| O | -0.68843800 | 0.72983600 | -3.28068100 | | | | |

[Fe(tpy)(bpy)(H)]⁺

[Fe(tpy)(bpy)(S)]²⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | 0.73488200 | -0.00248900 | -3.90971900 |
| C | 0.11010200 | -0.00146600 | -2.65719600 |
| C | 2.17360400 | 0.00047600 | -1.54200400 |
| C | 2.85975400 | -0.00063500 | -2.77033500 |
| C | 2.13709200 | -0.00216700 | -3.96959300 |
| H | 0.12389700 | -0.00352800 | -4.81728500 |
| H | 3.95296100 | -0.00028100 | -2.79037800 |
| H | 2.65931400 | -0.00305100 | -4.93152200 |
| C | -2.40458800 | -1.19522900 | -0.41989700 |
| C | -3.75850100 | -1.22391400 | -0.79996600 |
| C | -2.40798500 | 1.18856300 | -0.42150600 |
| C | -4.43380400 | -0.00660400 | -0.99321000 |
| H | -4.28197300 | -2.17391100 | -0.94023100 |
| C | -3.76194200 | 1.21289500 | -0.80162700 |
| H | -5.48748100 | -0.00827800 | -1.28938800 |
| H | -4.28807600 | 2.16121600 | -0.94327300 |
| N | -1.76741800 | -0.00232600 | -0.25203000 |
| N | 0.80127500 | -0.00009700 | -1.49018700 |
| C | -1.51758700 | 2.33471700 | -0.16217500 |
| C | -1.88745000 | 3.68435700 | -0.28308100 |
| C | 0.65534800 | 2.94142300 | 0.48862100 |

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.58386400 | -0.00069100 | 3.77262700 |
| C | 0.01559200 | -0.00041100 | 2.50819000 |
| C | -2.06758600 | -0.00096200 | 1.43266300 |
| C | -2.73459900 | -0.00126000 | 2.67307900 |
| C | -1.98734100 | -0.00111600 | 3.85720000 |
| H | 0.04107200 | -0.00057900 | 4.67096500 |
| H | -3.82780900 | -0.00164100 | 2.71398500 |
| H | -2.49081800 | -0.00135800 | 4.82925400 |
| C | 2.55265800 | -1.19066600 | -0.15468300 |
| C | 3.94651800 | -1.21287400 | 0.01668600 |
| C | 2.55128000 | 1.19335400 | -0.15466300 |
| C | 4.64553100 | 0.00255700 | 0.10988100 |
| H | 4.48353000 | -2.16487700 | 0.06541100 |
| C | 3.94510500 | 1.21719100 | 0.01671900 |
| H | 5.73192000 | 0.00319000 | 0.24047600 |
| H | 4.48101600 | 2.16980800 | 0.06549500 |
| N | 1.87490800 | 0.00096500 | -0.21911600 |
| N | -0.69820800 | -0.00051500 | 1.35632100 |
| C | 1.63887400 | 2.32515700 | -0.32019700 |
| C | 2.00820200 | 3.68177000 | -0.29527500 |
| C | -0.60336200 | 2.90146700 | -0.71040400 |
| C | 1.03435600 | 4.66818900 | -0.48613100 |
| H | 3.05386000 | 3.95759200 | -0.12758400 |
| C | -0.29667400 | 4.26559800 | -0.69679500 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | -1.62583000 | 2.55369100 | -0.87774400 | C | -4.06194200 | 0.00132500 | -2.03852400 |
| H | 1.30597700 | 5.72839800 | -0.47214900 | H | -2.05585400 | 0.00109400 | -2.85812100 |
| H | -1.09486900 | 4.99792900 | -0.85213600 | H | -5.91190300 | 0.00130000 | -0.88622700 |
| C | -2.72670000 | -0.00118800 | 0.11699200 | H | -4.53827300 | 0.00158400 | -3.02356700 |
| C | -4.12015000 | -0.00147100 | -0.08298300 | N | 0.26271900 | 1.97835900 | -0.43236700 |
| C | -2.36045500 | -0.00141900 | -2.20639100 | N | -1.99572600 | 0.00082900 | -0.76506900 |
| C | -4.63643500 | -0.00172700 | -1.38437100 | Fe | -0.02169900 | 0.00005900 | -0.52206100 |
| H | -4.79697200 | -0.00147000 | 0.77663300 | H | 1.31942600 | -0.00023100 | 2.29030700 |
| C | -3.73469900 | -0.00172500 | -2.46408800 | C | 0.32860800 | -0.00007800 | -2.25598600 |
| H | -1.62040800 | -0.00140800 | -3.01022700 | O | 0.58428200 | -0.00007300 | -3.38985200 |
| H | -5.71796600 | -0.00192600 | -1.55308500 | C | 1.56636900 | -2.34008100 | -0.17892400 |
| H | -4.08617600 | -0.00194500 | -3.50045300 | C | 1.94850000 | -3.68889800 | -0.10097000 |
| N | 0.33062000 | 1.93144600 | -0.53185000 | C | -0.66169200 | -2.95024300 | -0.61233600 |
| N | -1.84341100 | -0.00111200 | -0.94410700 | C | 0.98417400 | -4.69078000 | -0.28651400 |
| Fe | 0.05239900 | -0.00010300 | -0.50619300 | H | 2.99046800 | -3.95510000 | 0.09933200 |
| H | 1.10414100 | -0.00008500 | 2.39283000 | C | -0.34195700 | -4.31421700 | -0.54614900 |
| C | 1.64154100 | -2.32348800 | -0.32025700 | H | -1.68079000 | -2.61596100 | -0.82301900 |
| C | 2.01234000 | -3.67969700 | -0.29532300 | H | 1.26697500 | -5.74687100 | -0.23336500 |
| C | -0.60007700 | -2.90228200 | -0.71061500 | H | -1.12676900 | -5.06031900 | -0.70233200 |
| C | 1.03960500 | -4.66718000 | -0.48624800 | N | 0.26120600 | -1.97853900 | -0.43249500 |
| H | 3.05829900 | -3.95435300 | -0.12757600 | | | | |
| C | -0.29185900 | -4.26605400 | -0.69700100 | | | | |
| H | -1.62290400 | -2.55561800 | -0.87809200 | | | | |
| H | 1.31239500 | -5.72708900 | -0.47228800 | | | | |
| H | -1.08922800 | -4.99927900 | -0.85239400 | | | | |
| N | 0.33283100 | -1.93119700 | -0.53198600 | | | | |
| H | 0.33440400 | 0.00017000 | -2.00683400 | | | | |

[Fe(tpy)(bpy)(CO)]²⁺

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.22578900 | 0.00059700 | 3.81658900 |
| C | 0.24665600 | 0.00019200 | 2.49841100 |
| C | -1.93068400 | 0.00067800 | 1.63045600 |
| C | -2.47052200 | 0.00108400 | 2.93057100 |
| C | -1.61167900 | 0.00104500 | 4.03707200 |
| H | 0.48595400 | 0.00054500 | 4.64746800 |
| H | -3.55334600 | 0.00149200 | 3.08083800 |
| H | -2.01884100 | 0.00137600 | 5.05320600 |
| C | 2.48044900 | -1.19402900 | -0.01307700 |
| C | 3.86493200 | -1.22066200 | 0.23488500 |
| C | 2.48134900 | 1.19207900 | -0.01308500 |
| C | 4.55385500 | -0.00175800 | 0.35477600 |
| H | 4.40124000 | -2.16920500 | 0.32686700 |
| C | 3.86585000 | 1.21764400 | 0.23495300 |
| H | 5.63255000 | -0.00219000 | 0.54065000 |
| H | 4.40280600 | 2.16580600 | 0.32713500 |
| N | 1.83672700 | -0.00075100 | -0.12928400 |
| N | -0.57638200 | 0.00023100 | 1.42330400 |
| C | 1.56825300 | 2.33884800 | -0.17910700 |
| C | 1.95145700 | 3.68739700 | -0.10134600 |
| C | -0.65941500 | 2.95078300 | -0.61230000 |
| C | 0.98794600 | 4.68999500 | -0.28696500 |
| H | 2.99364300 | 3.95279200 | 0.09892700 |
| C | -0.33851100 | 4.31450100 | -0.54638600 |
| H | -1.67883200 | 2.61730800 | -0.82270400 |
| H | 1.27161200 | 5.74587000 | -0.23402700 |
| H | -1.12270400 | 5.06127000 | -0.70254900 |
| C | -2.73450900 | 0.00081500 | 0.39634900 |
| C | -4.14177900 | 0.00093400 | 0.37111300 |
| C | -2.66524700 | 0.00110000 | -1.95136900 |
| C | -4.81771300 | 0.00119400 | -0.85560500 |
| H | -4.70901400 | 0.00080100 | 1.30577600 |

[Ru(tpy)(bpy)(S)]²⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| Ru | -0.04617700 | 0.00000400 | 0.32922300 |
| N | 1.84435600 | -0.00002100 | -0.30835900 |
| C | -0.52983800 | 3.08503800 | 0.46598100 |
| H | -1.53109700 | 2.79231900 | 0.79407100 |
| C | -0.16583300 | 4.43238000 | 0.34070600 |
| C | 1.13485700 | 4.74669300 | -0.08155000 |
| H | 1.45366700 | 5.78815800 | -0.18987800 |
| C | 2.02549400 | 3.70129700 | -0.36474100 |
| H | 3.04385700 | 3.92452600 | -0.69571800 |
| C | 1.60701700 | 2.36699400 | -0.22310400 |
| C | 2.47327800 | 1.19910600 | -0.49880100 |
| C | 3.81549800 | 1.21873400 | -0.91946000 |
| H | 4.34003900 | 2.16486000 | -1.07875600 |
| C | 4.48198800 | -0.00005400 | -1.13011400 |
| H | 5.52643200 | -0.00006700 | -1.45705000 |
| C | 3.81546700 | -1.21882500 | -0.91946100 |
| H | 4.33998400 | -2.16496400 | -1.07875700 |
| C | 2.47324700 | -1.19916400 | -0.49880300 |
| N | -2.08422800 | 0.00002400 | 0.84702500 |
| C | -0.29013100 | 0.00001300 | -2.72206400 |
| H | 0.80096200 | 0.00000700 | -2.66262300 |
| C | -0.94764100 | 0.00002000 | -3.95587600 |
| H | -0.36236500 | 0.00001900 | -4.88019400 |
| C | -2.35156600 | 0.00002600 | -3.97537500 |
| H | -2.90086800 | 0.00003000 | -4.92202700 |
| C | -3.04133300 | 0.00002800 | -2.75735400 |
| H | -4.13443000 | 0.00003400 | -2.75202800 |
| C | -2.32911700 | 0.00002200 | -1.54292000 |
| C | -2.96463300 | 0.00002700 | -0.21306000 |
| C | -4.35701200 | 0.00003400 | -0.00162400 |
| H | -5.04394900 | 0.00003600 | -0.85215500 |
| C | -4.86568900 | 0.00003900 | 1.30283500 |
| H | -5.94640600 | 0.00004400 | 1.47563400 |
| C | -3.96204100 | 0.00003700 | 2.37886300 |
| H | -4.30956800 | 0.00004000 | 3.41640100 |
| C | -2.58977100 | 0.00002900 | 2.10982700 |
| H | -1.85029900 | 0.00002700 | 2.91429200 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| N | -0.95118800 | 0.00001300 | -1.53507900 | C | -0.17581400 | -2.19003200 | -3.69766100 |
| C | 1.60695700 | -2.36702900 | -0.22310500 | C | -0.69048100 | 0.44021700 | -3.05923600 |
| C | 2.02539900 | -3.70134300 | -0.36474500 | C | -0.38114900 | -1.27350200 | -4.73488800 |
| C | -0.52991100 | -3.08501900 | 0.46599500 | H | 0.02964200 | -3.24058900 | -3.92360600 |
| C | 1.13473900 | -4.74671700 | -0.08154700 | C | -0.64321700 | 0.06829900 | -4.40555900 |
| H | 3.04375500 | -3.92459700 | -0.69572800 | H | -0.89747100 | 1.47082200 | -2.75800700 |
| C | -0.16594000 | -4.43236900 | 0.34071900 | H | -0.33961600 | -1.59883300 | -5.77910800 |
| H | -1.53115800 | -2.79227300 | 0.79409500 | H | -0.81352500 | 0.82269900 | -5.17980200 |
| H | 1.45352200 | -5.78818900 | -0.18987600 | N | -0.49348000 | -0.43827500 | -2.04053200 |
| H | -0.89565300 | -5.21386600 | 0.57289800 | H | -0.81352500 | 0.82269900 | 5.17980200 |
| N | 0.32251500 | -2.06759700 | 0.19501500 | N | -0.49348000 | -0.43827500 | 2.04053200 |
| H | -0.89552800 | 5.21389400 | 0.57287600 | | | | |
| N | 0.32256500 | 2.06759400 | 0.19501100 | | | | |
| N | 0.64830800 | 0.00000800 | 2.25125800 | | | | |
| C | 1.63399400 | -0.00001900 | 4.69237900 | | | | |
| H | 1.29818100 | 0.89776100 | 5.24108900 | | | | |
| H | 1.29805800 | -0.89771900 | 5.24114700 | | | | |
| H | 2.73804700 | -0.00009600 | 4.66119900 | | | | |
| C | 1.09257000 | -0.00002800 | 3.33826400 | | | | |

[Ru(tpy)(bpy)(H)]⁺

| | x | y | z | | x | y | z |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| Ru | -0.52048500 | -0.04798900 | 0.00000000 | Ru | -0.03407400 | 0.00001100 | -0.53205500 |
| H | -2.10752300 | -0.41759700 | 0.00000000 | N | 1.92331700 | -0.00004000 | -0.05999300 |
| N | -0.14460000 | -1.97969400 | 0.00000000 | C | -0.51748000 | -3.10069100 | -0.60668800 |
| C | -0.69048100 | 0.44021700 | 3.05923600 | H | -1.54489000 | -2.81285100 | -0.84610600 |
| H | -0.89747100 | 1.47082200 | 2.75800700 | C | -0.13383000 | -4.44686000 | -0.52433600 |
| C | -0.64321700 | 0.06829900 | 4.40555900 | C | 1.20099600 | -4.75288800 | -0.22291200 |
| C | -0.38114900 | -1.27350200 | 4.73488800 | H | 1.53658700 | -5.79256700 | -0.15522700 |
| H | -0.33961600 | -1.59883300 | 5.77910800 | C | 2.10755300 | -3.70286900 | -0.01307300 |
| C | -0.17581400 | -2.19003200 | 3.69766100 | H | 3.15358900 | -3.92196500 | 0.21896000 |
| H | 0.02964200 | -3.24058900 | 3.92360600 | C | 1.66922000 | -2.37150200 | -0.10890800 |
| C | -0.23454600 | -1.76330800 | 2.35800200 | C | 2.55577900 | -1.19968400 | 0.08624400 |
| C | -0.04898200 | -2.64808000 | 1.19938500 | C | 3.92902900 | -1.21988700 | 0.39273700 |
| C | 0.17799900 | -4.03446800 | 1.21539900 | H | 4.46585700 | -2.16497900 | 0.51036600 |
| H | 0.25180000 | -4.57284300 | 2.16472300 | C | 4.61023500 | -0.00011200 | 0.54015600 |
| C | 0.29742500 | -4.72851100 | 0.00000000 | H | 5.68000400 | -0.00014100 | 0.77183300 |
| H | 0.47136500 | -5.80873300 | 0.00000000 | C | 3.92908900 | 1.21969800 | 0.39276400 |
| C | 0.17799900 | -4.03446800 | -1.21539900 | H | 4.46596200 | 2.16476200 | 0.51041500 |
| H | 0.25180000 | -4.57284300 | -2.16472300 | C | 2.55583800 | 1.19956900 | 0.08627200 |
| C | -0.04898200 | -2.64808000 | -1.19938500 | N | -2.14104000 | 0.00005700 | -0.76105000 |
| N | -0.97794800 | 1.99133000 | 0.00000000 | C | 0.05285800 | -0.00006000 | 2.61410100 |
| C | 2.64006100 | 0.29912500 | 0.00000000 | H | 1.13235400 | -0.00008500 | 2.43791400 |
| H | 2.59998600 | -0.79527500 | 0.00000000 | C | -0.46562900 | -0.00006600 | 3.91357000 |
| C | 3.86033300 | 0.98282800 | 0.00000000 | H | 0.21351900 | -0.00009700 | 4.77125100 |
| H | 4.80036900 | 0.42250000 | 0.00000000 | C | -1.85959800 | -0.00003400 | 4.07908800 |
| C | 3.84361700 | 2.38879200 | 0.00000000 | H | -2.30561300 | -0.00004000 | 5.07879400 |
| H | 4.77686400 | 2.96114700 | 0.00000000 | C | -2.67778000 | 0.00000600 | 2.94245200 |
| C | 2.61032100 | 3.04993600 | 0.00000000 | H | -3.76433200 | 0.00003100 | 3.05958000 |
| H | 2.57994400 | 4.14306300 | 0.00000000 | C | -2.09716700 | 0.00001200 | 1.65854900 |
| C | 1.41473800 | 2.30108900 | 0.00000000 | C | -2.87825500 | 0.00005000 | 0.40402200 |
| C | 0.06487000 | 2.89816100 | 0.00000000 | C | -4.28645900 | 0.00007600 | 0.36961400 |
| C | -0.17650200 | 4.28705700 | 0.00000000 | H | -4.85944800 | 0.00006900 | 1.30034000 |
| H | 0.66317000 | 4.98775400 | 0.00000000 | C | -4.96037800 | 0.00010900 | -0.85766900 |
| C | -1.48790600 | 4.77322100 | 0.00000000 | H | -6.05445700 | 0.00012800 | -0.88881500 |
| H | -1.68121200 | 5.85054100 | 0.00000000 | C | -4.20339100 | 0.00011500 | -2.03970500 |
| C | -2.54592100 | 3.84589200 | 0.00000000 | H | -4.67804800 | 0.00014000 | -3.02555300 |
| H | -3.59080300 | 4.17128100 | 0.00000000 | C | -2.80779000 | 0.00008800 | -1.94933700 |
| C | -2.25379000 | 2.48042100 | 0.00000000 | H | -2.19120800 | 0.00009100 | -2.85164300 |
| H | -3.03950100 | 1.72113500 | 0.00000000 | N | -0.73300900 | -0.00002000 | 1.51015000 |
| N | 1.44062000 | 0.93000000 | 0.00000000 | C | 1.66933400 | 2.37143500 | -0.10885200 |
| C | -0.23454600 | -1.76330800 | -2.35800200 | C | 2.10773200 | 3.70277800 | -0.01299100 |
| | | | | C | -0.51733300 | 3.10074100 | -0.60660600 |
| | | | | C | 1.20122600 | 4.75284500 | -0.22280300 |
| | | | | H | 3.15378000 | 3.92181800 | 0.21904300 |
| | | | | C | -0.13361700 | 4.44688900 | -0.52422700 |
| | | | | H | -1.54475800 | 2.81295600 | -0.84602700 |
| | | | | H | 1.53686700 | 5.79250700 | -0.15509800 |
| | | | | H | -0.87471600 | 5.23220800 | -0.70035000 |
| | | | | N | 0.35052600 | 2.08289900 | -0.40483800 |

| | | | |
|---|-------------|-------------|-------------|
| H | -0.87496600 | -5.23214000 | -0.70047800 |
| N | 0.35042700 | -2.08289600 | -0.40489200 |
| C | 0.33823900 | -0.00000600 | -2.38215800 |
| O | 0.53389000 | 0.00014300 | -3.53127800 |

4. Other Intermediates

Ferrocene (Cp_2Fe)

| | x | y | z |
|----|-------------|-------------|-------------|
| C | 0.00000000 | 1.64888800 | -1.22637400 |
| C | -1.16597000 | 1.64997300 | -0.37879000 |
| C | -0.72037400 | 1.64876700 | 0.99226000 |
| C | 0.72130300 | 1.64850500 | 0.99200900 |
| C | 1.16649400 | 1.64864900 | -0.37922000 |
| H | -0.00041300 | 1.62024200 | -2.31773500 |
| H | -2.20414100 | 1.62271900 | -0.71571500 |
| H | -1.36174700 | 1.61929400 | 1.87524700 |
| H | 1.36293300 | 1.61931100 | 1.87473000 |
| H | 2.20441600 | 1.62004600 | -0.71654600 |
| Fe | 0.00000000 | 0.00000000 | 0.00005500 |
| C | 0.72037400 | -1.64876700 | 0.99226000 |
| C | -0.72130300 | -1.64850500 | 0.99200900 |
| C | 1.16597000 | -1.64997300 | -0.37879000 |
| H | 1.36174700 | -1.61929400 | 1.87524700 |
| C | -1.16649400 | -1.64864900 | -0.37922000 |
| H | -1.36293300 | -1.61931100 | 1.87473000 |
| C | 0.00000000 | -1.64888800 | -1.22637400 |
| H | 2.20414100 | -1.62271900 | -0.71571500 |
| H | -2.20441600 | -1.62004600 | -0.71654600 |
| H | 0.00041300 | -1.62024200 | -2.31773500 |

Ferrocenium (Cp_2Fe^+)

| | x | y | z |
|----|--------------|-------------|-------------|
| C | 1.74968900 | -1.16349600 | -0.37505200 |
| C | 1.79843700 | -0.00754200 | -1.22003100 |
| C | 1.75101700 | 1.15878000 | -0.38952100 |
| C | 1.67844000 | 0.72901500 | 0.98359400 |
| C | 1.677766700 | -0.71647700 | 0.99273300 |
| H | 1.73788200 | -2.20164300 | -0.71294000 |
| H | 1.80969400 | -0.01426800 | -2.31209700 |
| H | 1.73936300 | 2.19267700 | -0.74022700 |
| H | 1.64251300 | 1.37967700 | 1.85926400 |
| H | 1.64165800 | -1.35600900 | 1.87656800 |
| Fe | 0.00000000 | -0.00016200 | 0.00608400 |
| C | -1.67844100 | 0.72901100 | 0.98359600 |
| C | -1.75101800 | 1.15878100 | -0.38951700 |
| C | -1.677766700 | -0.71648200 | 0.99273000 |
| H | -1.64251300 | 1.37967000 | 1.85926900 |
| C | -1.79843700 | -0.00753800 | -1.22003100 |
| H | -1.73936500 | 2.19267900 | -0.74021900 |
| C | -1.74968800 | -1.16349500 | -0.37505600 |
| H | -1.64165700 | -1.35601700 | 1.87656300 |
| H | -1.80969400 | -0.01426000 | -2.31209700 |
| H | -1.73787900 | -2.20164100 | -0.71294800 |

Phenol

| | x | y | z |
|---|-------------|-------------|-------------|
| C | 1.14079400 | -1.22718500 | -0.00006900 |
| C | -0.26450300 | -1.20893800 | 0.00014900 |
| C | -0.94593500 | 0.02337000 | 0.00046400 |
| C | -0.22405300 | 1.23206200 | 0.00001700 |
| C | 1.17811200 | 1.19936200 | -0.00001800 |
| C | 1.87010800 | -0.02635100 | -0.00003800 |
| H | 1.66405900 | -2.19042600 | -0.00019500 |

| | | | |
|---|-------------|-------------|-------------|
| H | -0.82954000 | -2.15088200 | 0.00012300 |
| H | -0.77337000 | 2.17932100 | -0.00028400 |
| H | 1.73530300 | 2.14341100 | -0.00018100 |
| H | 2.96523100 | -0.04434800 | -0.00037800 |
| O | -2.32341400 | 0.11259400 | -0.00004500 |
| H | -2.70151300 | -0.79174900 | -0.00174700 |

Phenoxyde Anion

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -1.11067700 | -1.21050300 | -0.00000800 |
| C | 0.28969600 | -1.22057900 | -0.00006800 |
| C | 1.08584100 | -0.00001500 | 0.00008500 |
| C | 0.28968500 | 1.22057900 | -0.00006100 |
| C | -1.11067400 | 1.21051300 | -0.00000600 |
| C | -1.84356600 | -0.00000400 | 0.00005100 |
| H | -1.65425400 | -2.16986200 | -0.00002100 |
| H | 0.84030100 | -2.17273800 | -0.00006100 |
| H | 0.84033800 | 2.17270900 | -0.00008600 |
| H | -1.65427200 | 2.16986000 | -0.00002400 |
| H | -2.94178000 | 0.00000600 | 0.00006500 |
| O | 2.37098000 | 0.00001000 | 0.00002100 |

Formate

| | x | y | z |
|---|-------------|-------------|------------|
| C | 0.00000000 | 0.31989600 | 0.00000000 |
| H | 0.00086900 | 1.47020200 | 0.00000000 |
| O | 1.15288400 | -0.21227100 | 0.00000000 |
| O | -1.15299300 | -0.21142700 | 0.00000000 |

CO₂

| | x | y | z |
|---|------------|------------|-------------|
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| O | 0.00000000 | 0.00000000 | 1.18139400 |
| O | 0.00000000 | 0.00000000 | -1.18139400 |

CO

| | x | y | z |
|---|------------|------------|-------------|
| C | 0.00000000 | 0.00000000 | -0.65663200 |
| O | 0.00000000 | 0.00000000 | 0.49247400 |

Bicarbonate

| | x | y | z |
|---|-------------|-------------|-------------|
| C | -0.16308000 | 0.06914700 | 0.00010300 |
| O | 0.09264800 | 1.31202000 | -0.00003000 |
| O | 1.04383800 | -0.77308300 | -0.00002300 |
| O | -1.23326000 | -0.57916500 | -0.00002800 |
| H | 1.75266500 | -0.09305900 | 0.00002500 |

Acetonitrile

| | x | y | z |
|---|-------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | 0.27757800 |
| N | 0.00000000 | 0.00000000 | 1.45163700 |
| C | 0.00000000 | 0.00000000 | -1.18619500 |
| H | 0.00000000 | 1.03488800 | -1.56992100 |
| H | 0.89624000 | -0.51744400 | -1.56992100 |
| H | -0.89624000 | -0.51744400 | -1.56992100 |

[Fe(bpy2PYMe)S]²⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -2.36442900 | -1.30338200 | -2.66749100 |
| C | -1.83319300 | -0.65637500 | -1.53892600 |
| C | 0.10960600 | -2.01672200 | -1.64974000 |
| C | -0.37494600 | -2.68927200 | -2.78309900 |
| C | -1.60262800 | -2.28576100 | -3.32574900 |
| H | -3.36768900 | -1.06591100 | -3.02762100 |
| H | 0.17503600 | -3.52965400 | -3.21566100 |
| H | -1.99852000 | -2.77786900 | -4.21967000 |
| C | -2.64543000 | 0.27551700 | -0.59077700 |
| C | -2.57130600 | -0.38622200 | 0.81051600 |
| C | -3.71509600 | -0.76034700 | 1.53689600 |
| C | -1.19643700 | -1.23260000 | 2.51739100 |
| C | -3.58150500 | -1.38505000 | 2.78577700 |
| H | -4.71214500 | -0.57248400 | 1.13532200 |
| C | -2.29437100 | -1.63275100 | 3.28271400 |
| H | -0.17346600 | -1.40774700 | 2.85826200 |
| H | -4.47052100 | -1.67899400 | 3.35306200 |
| H | -2.13486800 | -2.13219000 | 4.24296300 |
| C | -1.94491800 | 1.64675300 | -0.53730600 |
| C | -2.55674000 | 2.87700300 | -0.83126500 |
| C | 0.18553100 | 2.66503900 | -0.53916300 |
| C | -1.76548000 | 4.03595700 | -0.91090800 |
| H | -3.63163100 | 2.93868200 | -1.01374000 |
| C | -0.37209600 | 3.92393000 | -0.81606100 |
| H | -2.23000200 | 5.00636600 | -1.11235900 |
| H | 0.26733000 | 4.79280900 | -0.99514600 |
| N | -0.61769700 | 1.58817600 | -0.27580100 |
| N | -0.56526500 | -0.94080400 | -1.14051400 |
| C | 1.60075600 | 2.29190800 | -0.68083100 |
| C | 2.63429000 | 3.18879900 | -1.00228500 |
| C | 3.05783500 | 0.46951500 | -0.87824700 |
| C | 3.91548700 | 2.69364300 | -1.27899700 |
| H | 2.43607400 | 4.26362600 | -1.04841000 |
| C | 4.12419300 | 1.30668500 | -1.23353500 |
| H | 3.19882100 | -0.61163800 | -0.81746100 |
| H | 4.73076800 | 3.37693800 | -1.53716600 |
| H | 5.09994700 | 0.86870400 | -1.46397500 |
| C | 1.22606900 | -2.43120600 | -0.78474300 |
| C | 2.07255600 | -3.52668700 | -1.03000200 |
| C | 2.23861700 | -2.06404000 | 1.30387800 |
| C | 3.01724400 | -3.89938400 | -0.06337300 |
| H | 1.98778700 | -4.08879200 | -1.96475600 |
| C | 3.09162300 | -3.16165700 | 1.13025200 |
| H | 2.28929000 | -1.44240400 | 2.20242200 |
| H | 3.67912300 | -4.75376000 | -0.23686600 |
| H | 3.80521900 | -3.42292700 | 1.91750100 |
| N | 1.81848300 | 0.93519700 | -0.59548800 |
| N | -1.32300900 | -0.61321300 | 1.31523600 |
| N | 1.32307500 | -1.69006000 | 0.37562300 |
| Fe | 0.26490500 | -0.02169200 | 0.29540400 |
| C | -4.09839900 | 0.41903600 | -1.07842500 |
| H | -4.59756800 | -0.56129800 | -1.14278900 |
| H | -4.68804700 | 1.05127900 | -0.39487000 |
| H | -4.13337900 | 0.88468500 | -2.07721500 |
| N | 0.96140600 | 0.78758400 | 1.90353400 |
| C | 1.32568100 | 1.33913500 | 2.87308900 |
| C | 1.77307400 | 2.02312900 | 4.08108200 |
| H | 1.20782000 | 2.96195400 | 4.21909900 |

| | | | |
|---|------------|------------|------------|
| H | 1.61228300 | 1.38446300 | 4.96763600 |
| H | 2.84833800 | 2.26444700 | 4.01058100 |

[Fe(bpy2PYMe)S]⁺

| | x | y | z |
|----|-------------|-------------|-------------|
| C | -2.28496900 | -1.25131900 | -2.74195600 |
| C | -1.79403300 | -0.65085600 | -1.57618700 |
| C | 0.19872500 | -1.95660800 | -1.69168300 |
| C | -0.23542000 | -2.55703200 | -2.89696000 |
| C | -1.45769100 | -2.16769500 | -3.44252100 |
| H | -3.29430600 | -1.04320500 | -3.10188900 |
| H | 0.36412700 | -3.33787600 | -3.37488300 |
| H | -1.81093100 | -2.61501000 | -4.37718100 |
| C | -2.64356800 | 0.21707800 | -0.60429600 |
| C | -2.55886600 | -0.47939500 | 0.77817800 |
| C | -3.69696000 | -0.91125700 | 1.48296800 |
| C | -1.17903400 | -1.32851900 | 2.48197300 |
| C | -3.56022100 | -1.56538800 | 2.71578200 |
| H | -4.69385200 | -0.74451700 | 1.06992000 |
| C | -2.27150800 | -1.78460900 | 3.22261400 |
| H | -0.15308900 | -1.48135600 | 2.82531700 |
| H | -4.44658100 | -1.90363300 | 3.26250100 |
| H | -2.10614000 | -2.30570900 | 4.17050900 |
| C | -1.98797200 | 1.60845800 | -0.50278900 |
| C | -2.63221000 | 2.82213200 | -0.77160700 |
| C | 0.12321900 | 2.68799100 | -0.43835400 |
| C | -1.87070300 | 4.01820400 | -0.77274300 |
| H | -3.70094500 | 2.85483700 | -0.99203100 |
| C | -0.48307500 | 3.94569500 | -0.65315400 |
| H | -2.36344100 | 4.98174300 | -0.93698000 |
| H | 0.13236500 | 4.84315100 | -0.76998200 |
| N | -0.66631500 | 1.57481300 | -0.20530000 |
| N | -0.52623200 | -0.90444100 | -1.16220300 |
| C | 1.52204500 | 2.35192600 | -0.62939800 |
| C | 2.53783500 | 3.26850000 | -0.98654200 |
| C | 3.01891900 | 0.55430600 | -0.89057200 |
| C | 3.81306100 | 2.80037800 | -1.30633500 |
| H | 2.31342300 | 4.33880900 | -1.03001500 |
| C | 4.05697100 | 1.41108100 | -1.27567200 |
| H | 3.17797300 | -0.52539800 | -0.83658000 |
| H | 4.60465200 | 3.50166400 | -1.59040900 |
| H | 5.03492300 | 0.99479400 | -1.53408300 |
| C | 1.26638700 | -2.38972300 | -0.81612100 |
| C | 2.13071300 | -3.48641900 | -1.05365200 |
| C | 2.27858200 | -2.03729200 | 1.29155000 |
| C | 3.06835100 | -3.85880200 | -0.09270900 |
| H | 2.04810900 | -4.04438400 | -1.99185500 |
| C | 3.14018300 | -3.12130400 | 1.11624200 |
| H | 2.32322000 | -1.42165400 | 2.19597200 |
| H | 3.73352200 | -4.71034400 | -0.26830100 |
| H | 3.85797600 | -3.37836900 | 1.90065700 |
| N | 1.78458800 | 0.99245600 | -0.55613300 |
| N | -1.30919100 | -0.67968600 | 1.29559300 |
| N | 1.35738800 | -1.65637500 | 0.36953800 |
| Fe | 0.26428500 | -0.01400100 | 0.33243000 |
| C | -4.09870300 | 0.32594200 | -1.09236300 |
| H | -4.56430500 | -0.66878400 | -1.18471500 |
| H | -4.70829400 | 0.92648000 | -0.39683400 |
| H | -4.14004200 | 0.81459600 | -2.07943900 |
| N | 0.93483300 | 0.76163100 | 1.93030300 |
| C | 1.30631100 | 1.28832700 | 2.91293700 |
| C | 1.76580600 | 1.95683700 | 4.12606800 |

| | | | | | | | | |
|-----------------------------------|-------------|-------------|-------------|--|----|-------------|-------------|-------------|
| H | 1.19464300 | 2.88801100 | 4.29024800 | | C | x | y | z |
| H | 1.63030400 | 1.30457700 | 5.00701800 | | C | -2.31440300 | -2.20407500 | -2.00474500 |
| H | 2.83673100 | 2.21299300 | 4.04109100 | | C | -1.74132600 | -1.26262300 | -1.14424400 |
| [Fe(bpy2PYMe)]⁺ | | | | | | | | |
| | x | y | z | | C | 0.38935400 | -2.28799200 | -1.38651000 |
| C | -2.42221400 | -1.87050600 | -2.15289800 | | C | -0.14649600 | -3.25999900 | -2.25079800 |
| C | -1.81298500 | -1.04246800 | -1.19996000 | | C | -1.49409900 | -3.18356000 | -2.61678100 |
| C | 0.24682400 | -2.18809400 | -1.48958500 | | H | -3.39161700 | -2.20895000 | -2.19025400 |
| C | -0.31466100 | -3.03016900 | -2.46238900 | | H | 0.48290600 | -4.08202900 | -2.60813600 |
| C | -1.65193600 | -2.83691000 | -2.83242300 | | H | -1.92808700 | -3.91493500 | -3.30642300 |
| H | -3.49054700 | -1.78607800 | -2.36539700 | | C | -2.53241200 | -0.29676300 | -0.23576900 |
| H | 0.27438400 | -3.83974600 | -2.90388300 | | C | -2.05185900 | -0.55108400 | 1.22778700 |
| H | -2.11255700 | -3.46841700 | -3.59821800 | | C | -2.91962200 | -0.99587900 | 2.24129800 |
| C | -2.55409500 | -0.04533700 | -0.28051700 | | C | -0.26493800 | -0.54920800 | 2.76869600 |
| C | -2.20426800 | -0.41326400 | 1.19617900 | | C | -2.44373800 | -1.22450300 | 3.54110000 |
| C | -3.18220100 | -0.79312600 | 2.13434800 | | H | -3.97535300 | -1.17155700 | 2.02098000 |
| C | -0.53454100 | -0.63598400 | 2.83545000 | | C | -1.08167600 | -0.99787800 | 3.80595300 |
| C | -2.81167300 | -1.09776900 | 3.45231800 | | H | 0.79809200 | -0.34157600 | 2.92287700 |
| H | -4.23392200 | -0.85445900 | 1.84666700 | | H | -3.12355100 | -1.56947700 | 4.32758700 |
| C | -1.45732900 | -1.01542200 | 3.81211600 | | H | -0.65481800 | -1.15492100 | 4.80200800 |
| H | 0.53327800 | -0.55172700 | 3.06284800 | | C | -2.17109400 | 1.16181700 | -0.55127300 |
| H | -3.57107400 | -1.39177400 | 4.18430600 | | C | -3.10954500 | 2.15513800 | -0.84625600 |
| H | -1.11750300 | -1.23605500 | 4.82862400 | | C | -0.41656000 | 2.76701400 | -0.50209800 |
| C | -2.01378200 | 1.37412400 | -0.52267000 | | C | -2.68123200 | 3.49869100 | -0.97721600 |
| C | -2.82319100 | 2.46721300 | -0.85721300 | | H | -4.16751800 | 1.90784500 | -0.95938900 |
| C | -0.10326000 | 2.77772000 | -0.48110500 | | C | -1.33655100 | 3.80256400 | -0.77512800 |
| C | -2.25408800 | 3.74592000 | -1.00933500 | | H | -3.40413200 | 4.28923100 | -1.20549700 |
| H | -3.89797000 | 2.33647200 | -0.99839000 | | H | -0.98871900 | 4.83941700 | -0.82298300 |
| C | -0.88131000 | 3.90109600 | -0.80799800 | | N | -0.83915600 | 1.44278500 | -0.43833300 |
| H | -2.88131100 | 4.60361200 | -1.27096500 | | N | -0.38298200 | -1.20647400 | -0.97484400 |
| H | -0.41442400 | 4.88569100 | -0.90158200 | | C | 0.99457400 | 2.90318000 | -0.28573600 |
| N | -0.66323700 | 1.52149500 | -0.35576600 | | C | 1.71460800 | 4.11648900 | -0.40225600 |
| N | -0.47208900 | -1.12941400 | -0.97339200 | | C | 3.00266300 | 1.72918400 | 0.05690400 |
| C | 1.33148500 | 2.77839600 | -0.25205900 | | C | 3.09821900 | 4.13517000 | -0.27838600 |
| C | 2.16660100 | 3.90595200 | -0.38419000 | | H | 1.16533700 | 5.04191600 | -0.60790100 |
| C | 3.18100500 | 1.43154500 | 0.25944000 | | C | 3.75151300 | 2.88734100 | -0.07042000 |
| C | 3.54169200 | 3.78131600 | -0.17991400 | | H | 3.50939500 | 0.77265100 | 0.19415600 |
| H | 1.73518100 | 4.87389800 | -0.65540800 | | H | 3.66440900 | 5.06825000 | -0.36351900 |
| C | 4.05699000 | 2.50877900 | 0.14102600 | | H | 4.84357100 | 2.82084000 | -0.01412600 |
| H | 3.56504200 | 0.43485800 | 0.48436900 | | C | 1.68221800 | -2.28971600 | -0.74130500 |
| H | 4.20200200 | 4.64841000 | -0.28024000 | | C | 2.67163400 | -3.28279000 | -0.88410000 |
| H | 5.12918400 | 2.34927700 | 0.29089100 | | C | 2.92102000 | -1.27647800 | 0.98681600 |
| C | 1.51861200 | -2.36306200 | -0.79397300 | | C | 3.81253800 | -3.26483800 | -0.07880600 |
| C | 2.42515100 | -3.42062900 | -0.99910900 | | H | 2.52504400 | -4.08099700 | -1.62012000 |
| C | 2.71416900 | -1.66780600 | 1.10913800 | | C | 3.91319900 | -2.24869100 | 0.90452800 |
| C | 3.49205200 | -3.60245300 | -0.11330400 | | H | 2.96467000 | -0.49698000 | 1.75442900 |
| H | 2.27435700 | -4.11023300 | -1.83526500 | | H | 4.58607300 | -4.03268400 | -0.18095400 |
| C | 3.61420900 | -2.72811700 | 0.98524300 | | H | 4.75136200 | -2.22003900 | 1.60913800 |
| H | 2.78932600 | -0.96114000 | 1.94255600 | | N | 1.62394200 | 1.67701000 | 0.00845800 |
| H | 4.20078100 | -4.42384400 | -0.25797100 | | N | -0.72095900 | -0.32653600 | 1.50334600 |
| H | 4.40241100 | -2.85883100 | 1.73300200 | | N | 1.83424800 | -1.21596700 | 0.14854200 |
| N | 1.82987200 | 1.53275400 | 0.09025900 | | Fe | 0.45515200 | 0.12031400 | 0.03903100 |
| N | -0.88818100 | -0.34301100 | 1.55737900 | | C | -4.04560800 | -0.54298600 | -0.37561300 |
| N | 1.70414100 | -1.43814800 | 0.22262600 | | H | -4.30043000 | -1.59117600 | -0.14737200 |
| Fe | 0.47156000 | 0.07385300 | 0.12306700 | | H | -4.62166100 | 0.10790900 | 0.30275100 |
| C | -4.07270200 | -0.11591800 | -0.52602600 | | H | -4.37685500 | -0.33178700 | -1.40610600 |
| H | -4.45135500 | -1.13840400 | -0.36371300 | | | | | |
| H | -4.62194900 | 0.56037400 | 0.14907600 | | | | | |
| H | -4.31475000 | 0.17204800 | -1.56232400 | | | | | |

Fe(bpy2PYMe)]⁰