Electronic Supplementary Material (ESI) for ChemComm.


Supporting Information for:

# Chalcogen-Atom Abstraction Reactions of Di-Iron Imidophosphorane Complexes

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## General Considerations

Unless otherwise stated, all reagents were obtained from commercial suppliers, and the syntheses and manipulations were conducted under argon with exclusion of dioxygen ($O_2$) and $H_2O$ using Schlenk techniques or in an inert atmosphere box (Vigor) under a dinitrogen (<0.1 ppm $O_2/H_2O$) atmosphere. All glassware was stored in an oven over-night (>8 h) at a temperature of ca. 160˚C prior to use. Celite and molecular sieves were dried under vacuum at a temperature >250 °C for a minimum of 24 h. $d_8$-THF was stored over 3 Å molecular sieves prior to use. Diethyl ether, *n*-pentane, *n*-hexane, and tetrahydrofuran (THF) were purged with UHP-grade argon (Airgas) and passed through columns containing Q-5 and molecular sieves in a solvent purification system (JC Meyer Solvent Systems). All solvents in the glovebox were stored in bottles over 3 Å molecular sieves. The anhydrous salts, $FeCl_2$ and $CoCl_2$, were purchased from Sigma Aldrich. The reagent K[NP(pip)$_3$] was prepared by published procedures.[1] NMR spectra were obtained on a Bruker Avance III 400 MHz spectrometer at 298 K, unless otherwise noted. $^1$H, $^{13}$C{$^1$H}, and $^{31}$P{$^1$H} NMR chemical shifts are reported in δ, parts per million. All NMR samples were prepared in $C_6D_6$ (unless otherwise noted) and $^1$H NMR are references to the residual $^1$H resonances of $C_6D_6$.[2] The peak position is listed, followed by the peak multiplicity, integration value, and proton assignment, where applicable. The multiplicity and shape are indicated by one or more of the following abbreviations: s (singlet); d (doublet); t (triplet); q (quartet); m (multiplet); br (broad). Evan's method magnetic susceptibility measurements were measured on the same instrument as all the other NMR spectra at the same temperature (298 K). To prepare an NMR sample for Evan's method measurements, first, a glass capillary with $C_6D_6$ was sealed under vacuum and inserted into a J. Young NMR tube. Then, a stock solution of a known concentration was made in a scintillation vial, and a known volume of this solution was transferred into a J. Young NMR tube with a $C_6D_6$ capillary in it. Evan's method experiments for each sample were done at least 3 times at the same temperature. To calculate a magnetic moment, diamagnetic corrections for the species and the solvent were accounted for using Pascal's constants.[3] Elemental analyses were determined at Robertson Microlit Laboratories (Ledgewood, NJ) and University of California, Berkeley, Microanalytical Facility (Berkeley, CA. Infrared (IR) samples were taken on a Bruker ALPHA FTIR spectrometer from 400 to 4000 cm$^{-1}$. IR samples were prepared as Nujol mulls sandwiched between two KBr plates. The peaks are listed in wavenumber [cm$^{-1}$] and intensity by using the following abbreviations: vw (very weak); w (weak); m (medium); s (strong); vs (very strong); br (broad). UV/visible/NIR spectroscopy was performed in Teflon-valve sealed quartz cuvettes with a 1 cm path length on a Hitachi UH4150 UV-vis-NIR scanning spectrophotometer between 2400-240 nm.

## Synthetic Procedures

### Synthesis of $[Fe_2(\mu_2\text{-}NP(pip)_3)_2(NP(pip)_3)_2]$ (1-Fe)

Inside a glovebox, 4 mL of THF was added to a 20-mL scintillation vial charged with $FeCl_2$ (0.099 g, 0.783 mmol, 2 equiv.) and a stir bar. A solution of $K[NP(pip)_3]$ (0.527 g, 1.567 mmol, 4 equiv.) in 12 mL of THF was then added to the vial and the reaction mixture was stirred for 24 hours. The mixture was reduced *in vacuo* to a residue and triturated three times with 4-6 mL of pentane. The mixture extracted into approximately 15 mL of *n*-pentane and the mixture was filtered through a pipet packed with glass filter paper and Celite. The filtrate was reduced *in vacuo* to a residue and triturated three times with 4-6 mL of pentane. The filtrate was then concentrated *in vacuo* until saturated and placed in the freezer at −35 °C for 24 hours, during which time, olive-green crystals formed. Decantation and removal of volatiles yielded the title compound in 79% yield (0.403 g). The product was recrystallized by placing a small 5-mL vial, containing the product as a concentrated pentane solution, inside a 20-mL scintillation vial with paratone oil covering the base at 25 °C to provide X-ray quality crystals. $^1$H NMR (400.13 MHz, $C_6D_6$, 295 K): δ 6.28 (br, m, 24H, terminal piperidinyl methylene C-*H*), 3.39 (br, m, 24H, bridging piperidinyl methylene C-*H*), 2.32 (br, m, 24H, bridging piperidinyl methylene C-*H*), 1.56 (br, m, 12H, bridging piperidinyl methylene C-*H*), 0.72 (br, m, 36H, terminal piperidinyl methylene C-*H*). All protons are accounted for. Evan's method magnetic moment, 2.28(9) B.M. $^{31}$P{$^1$H} NMR (161.98 MHz, $C_6D_6$, 295 K): No signals were observed. $^{13}$C{$^1$H} NMR (100.61 MHz, $C_6D_6$, 295 K): δ 67.78 (s, bridging piperidinyl methylene C-*H*), 55.89 (s, bridging piperidinyl methylene C-*H*), 34.13 (s, bridging piperidinyl methylene C-*H*), 31.41 (s, terminal piperidinyl methylene C-*H*), 28.31 (s, terminal piperidinyl methylene C-*H*), 26.61 (s, terminal piperidinyl methylene C-*H*). IR (cm$^{-1}$): ν 1557 (vw), 1540 (vw), 1461 (vs), 1377(s), 1331 (w), 1246 (m), 1215 (m), 1159 (s), 1124 (s), 1061 (w), 1028 (vs), 945 (w), 854 (w), 834 (vw), 809 (w), 719 (s). Elem. Anal. Found (calculated) for $C_{60}H_{120}Fe_2N_{16}P_4$: C 55.39 (55.38), H 9.49 (9.30), N 17.09 (17.22).

### Synthesis of $[Fe_2(\mu_2\text{-}O)(\mu_2\text{-}NP(pip)_3)_2(NP(pip)_3)_2]$ (2-Fe)

Inside a glovebox, 12 mL of $Et_2O$ was added to a 20-mL scintillation vial charged with $[Fe(NP(pip)_3)_2]_2$ (0.183 g, 0.141 mmol) and a stir bar. A balloon was connected to a lecture bottle containing $N_2O$ and was filled. Once the balloon was filled it was connected to the top of the vial containing the stirring solution of $[Fe(NP(pip)_3)_2]_2$ and the reaction mixture was stirred for 10 minutes. The mixture was passed through a pipette packed with glass filter paper. The filtrate was reduced *in vacuo* to a residue and triturated three times with 2-3 mL of $Et_2O$. Removal of volatiles yielded the title compound as a brown microcrystalline solid in 95% yield (0.176 g). To produce X-ray quality crystals, the product was recrystallized inside a 20-mL scintillation from a after allowing the solution to sit at -35 °C for 24 hours. $^1$H NMR (400.13 MHz, $C_6D_6$, 295 K): δ 2.03 (br, m, 72H, piperidinyl methylene C-*H*), 1.65 (br, m, 48H, piperidinyl methylene C-*H*). All protons are accounted for. Evan's method magnetic moment, 3.5(1) $\mu_B$. $^{31}$P{$^1$H} NMR (161.98 MHz, $C_6D_6$, 295 K): No signals were observed. $^{13}$C{$^1$H} NMR (100.61 MHz, $C_6D_6$, 295 K No signals were observed. IR (cm$^{-1}$): ν 1582 (vw), 1337 (s), 1298 (w), 1259 (m), 1157 (s), 1123 (s), 1062 (vs), 1027(s), 988 (vw), 944 (vs), 885 (vw), 854 (vw), 835 (vw), 800 (w), 660 (vw). Elem.

Anal. Found (calculated) for $C_{60}H_{120}Fe_2N_{16}P_4O$: C 54.52 (54.79), H 9.05 (9.18), N 16.99 (17.01).

**Synthesis of $[Fe_2(\mu\text{-}\kappa^1\text{:}\kappa^1\text{-}S_2)(\mu_2\text{-}NP(pip)_3)_2(NP(pip)_3)_2]$ (3-Fe)**
Inside a glovebox, 2 mL of THF was added to a 20-mL scintillation vial charged with $S_8$ (0.006 g, 0.021 mmol, 0.25 equiv.) and a stir bar. A solution of $[Fe(NP(pip)_3)_2]_2$ (0.111 g, 0.085 mmol, 1 equiv.) in 8 mL of THF was then added to the vial and the reaction mixture was stirred for 24 hours. The mixture was reduced *in vacuo* to a residue and triturated three times with 4-6 mL of pentane. The mixture was extracted into approximately 12 mL of *n*-pentane and the mixture was filtered through a pipet packed with glass filter paper and Celite. The filtrate was reduced *in vacuo* to a residue and triturated three times with 2-3 mL of pentane. The filtrate was then extracted in $Et_2O$ and concentrated *in vacuo* until saturated and placed in the freezer at −35 °C for 24 hours, during which time, dark brown crystals formed. Decantation and removal of volatiles yielded the title compound in 84% yield (0.101 g). The product was recrystallized by redissolving the crystallized product in $Et_2O$ and allowing a concentrated solution inside a 20-mL scintillation vial to sit at -35 °C for 24 hours to produce X-ray quality crystals. $^1$H NMR (400.13 MHz, $C_6D_6$, 295 K): δ 2.03 (br, m, 72H, piperidinyl methylene C-*H*), 1.65 (br, m, 48H, piperidinyl methylene C-*H*). Evan's method magnetic moment, 2.3(1) $\mu_B$. $^{31}P\{^1H\}$ NMR (161.98 MHz, $C_6D_6$, 295 K): No signals were observed. $^{13}C\{^1H\}$ NMR (100.61 MHz, $C_6D_6$, 295 K No signals were observed. IR ($cm^{-1}$): ν 1558 (vw), 1541 (vw), 1507 (vw), 1460 (s), 1377 (w), 1261 (w), 1212 (m), 1159 (m), 1104 (m), 1062 (w), 1026 (w), 950 (m), 802 (w), 721 (m). Elem. Anal. Found (calculated) for $C_{60}H_{120}Fe_2N_{16}P_4S_2$: C 52.45 (52.78), H 8.74 (8.86), N 16.02 (16.41).

**Synthesis of $[Fe_2(\mu\text{-}\kappa^1\text{:}\kappa^1\text{-}Se_2)(\mu_2\text{-}NP(pip)_3)_2(NP(pip)_3)_2]$ (4-Fe)**
Inside a glovebox, 2 mL of THF was added to a 20-mL scintillation vial charged with $Se^0$ (0.019 g, 0.237 mmol, 2 equiv.) and a stir bar. A solution of $[Fe(NP(pip)_3)_2]_2$ (0.154 g, 0.118 mmol, 1 equiv.) in 8 mL of THF was then added to the vial and the reaction mixture was stirred for 24 hours. The mixture was reduced *in vacuo* to a residue and triturated three times with 4-6 mL of pentane. The mixture was extracted into approximately 12 mL of *n*-pentane and the mixture was filtered through a pipet packed with glass filter paper and Celite. The filtrate was reduced *in vacuo* to a residue and triturated three times with 2-3 mL of pentane. The filtrate was then extracted in $Et_2O$ and concentrated *in vacuo* until saturated and placed in the freezer at −35 °C for 24 hours, during which time, dark brown crystals formed. Decantation and removal of volatiles yielded the title compound in 71% yield (0.112 g). The product was recrystallized by redissolving the crystallized product in hexanes and allowing a concentrated solution inside a 20-mL scintillation vial to sit at 25 °C for 24 hours to produce X-ray quality crystals. $^1$H NMR (400.13 MHz, $C_6D_6$, 295 K): No signals were observed. Evan's method magnetic moment, 2.8(1) $\mu_B$. $^{31}P\{^1H\}$ NMR (161.98 MHz, $C_6D_6$, 295 K): No signals were observed. $^{13}C\{^1H\}$ NMR (100.61 MHz, $C_6D_6$, 295 K No signals were observed. IR ($cm^{-1}$): ν 1540 (vw), 1460 (s), 1377 (s), 1261 (vw), 1212 (w), 1175 (m), 1062 (w), 948 (m), 854 (vw), 803 (w), 721 (m). Elem. Anal. Found (calculated) for $C_{60}H_{120}Fe_2N_{16}P_4Se_2$: C 47.85 (49.39), H 8.11 (8.29), N 13.37 (15.36). Elemental percentages consistently low on multiple burns. Powder XRD was used to confirm bulk purity (see Figure S38).

**Synthesis of $[Co_2(\mu_2\text{-}NP(pip)_3)_2(NP(pip)_3)_2]$ (1-Co)**

Inside a glovebox, 4 mL of THF was added to a 20-mL scintillation vial charged with $CoCl_2$ (0.072 g, 3.385 mmol, 2 equiv.) and a stir bar. A solution of $K[NP(pip)_3]$ (0.371 g, 1.1031 mmol, 4 equiv.) in 12 mL of THF was then added to the flask and the reaction mixture was stirred for 24 hours. The mixture was reduced *in vacuo* to a residue and triturated three times with 4-6 mL of pentane. The mixture extracted into approximately 15 mL of *n*-pentane and the mixture was filtered through a pipet packed with glass filter paper and Celite. The filtrate was reduced *in vacuo* to a residue and triturated three times with 4-6 mL of pentane. The filtrate was then concentrated *in vacuo* until saturated and placed in the freezer at −35 °C for 24 hours, during which time, dark purple crystals formed. Decantation and removal of volatiles yielded the title compound in 73% yield (0.263 g). The product was recrystallized by placing a small 5-mL vial, containing the product as a concentrated pentane solution, inside a 20-mL scintillation vial with paratone oil covering the base at 25 °C to provide X-ray quality crystals. $^1$H NMR (400.13 MHz, $C_6D_6$, 295 K): δ 6.43 (br, m, 24H, terminal piperidinyl methylene C-*H*), 5.89 (br, m, 24H, bridging piperidinyl methylene C-*H*), 1.23 (br, m, 24H, bridging piperidinyl methylene C-*H*), -0.14 (br, m, 12H, bridging piperidinyl methylene C-*H*), -0.47 (br, m, 36H, terminal piperidinyl methylene C-*H*). Evan's method magnetic moment, 2.8(1) $\mu_B$. $^{31}P\{^1H\}$ NMR (161.98 MHz, $C_6D_6$, 295 K): No signals were observed. $^{13}C\{^1H\}$ NMR (100.61 MHz, $C_6D_6$, 295 K): δ 82.04 (s, bridging piperidinyl methylene C-*H*), 58.05 (s, bridging piperidinyl methylene C-*H*), 36.34 (s, bridging piperidinyl methylene C-*H*), 31.20 (s, terminal piperidinyl methylene C-*H*), 28.47 (s, terminal piperidinyl methylene C-*H*), 26.85 (s, terminal piperidinyl methylene C-*H*). HSQC NMR allowed for correlation between the signals observed in the $^1$H and $^{13}C\{^1H\}$ spectra, however, it did not help to determine which signals corresponded to the terminal or piperidinyl atoms. IR ($cm^{-1}$): ν 1577 (vw), 1540 (vw), 1461 (s), 1376 (s), 1331 (w), 1259 (vw), 1214 (m),1162 (m), 1115 (m), 1059 (m), 1027 (m), 941 (s), 854 (w), 833 (w), 809 (w), 710 (m). Elem. Anal. Found (calculated) for $C_{60}H_{120}Co_2N_{16}P_4$: C 54.91 (55.12), H 9.31 (9.25), N 17.29 (17.14).

## NMR Spectra of Reported Compounds

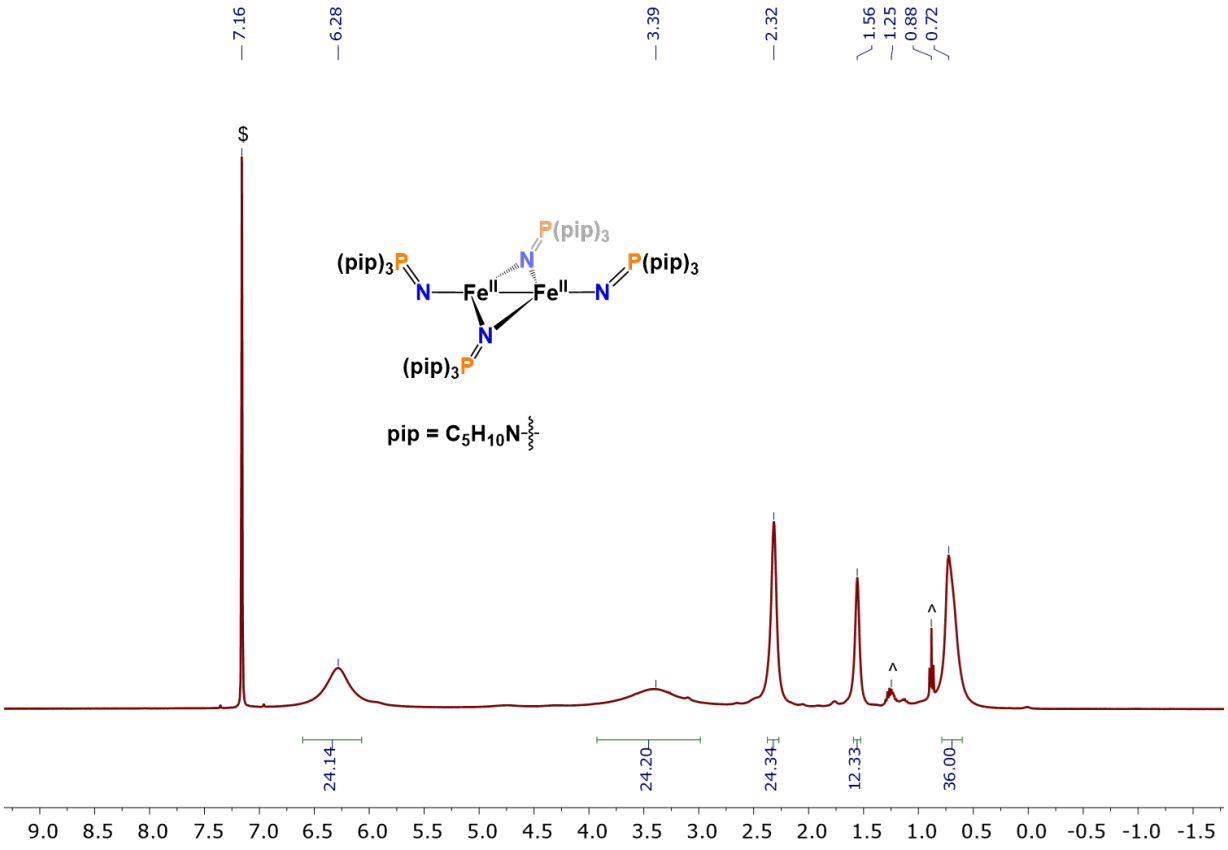
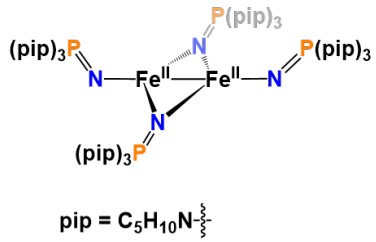



**Figure S1.** $^1$H NMR of **1-Fe** (400.13 MHz, $C_6D_6$, 295 K). Residual *n*-pentane noted as ^.



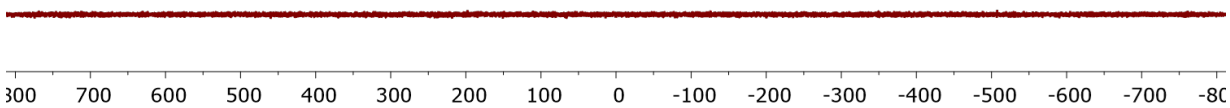




**Figure S2.** $^{31}P\{^{1}H\}$ NMR of **1-Fe** (161.98 MHz, $C_6D_6$, 295 K).

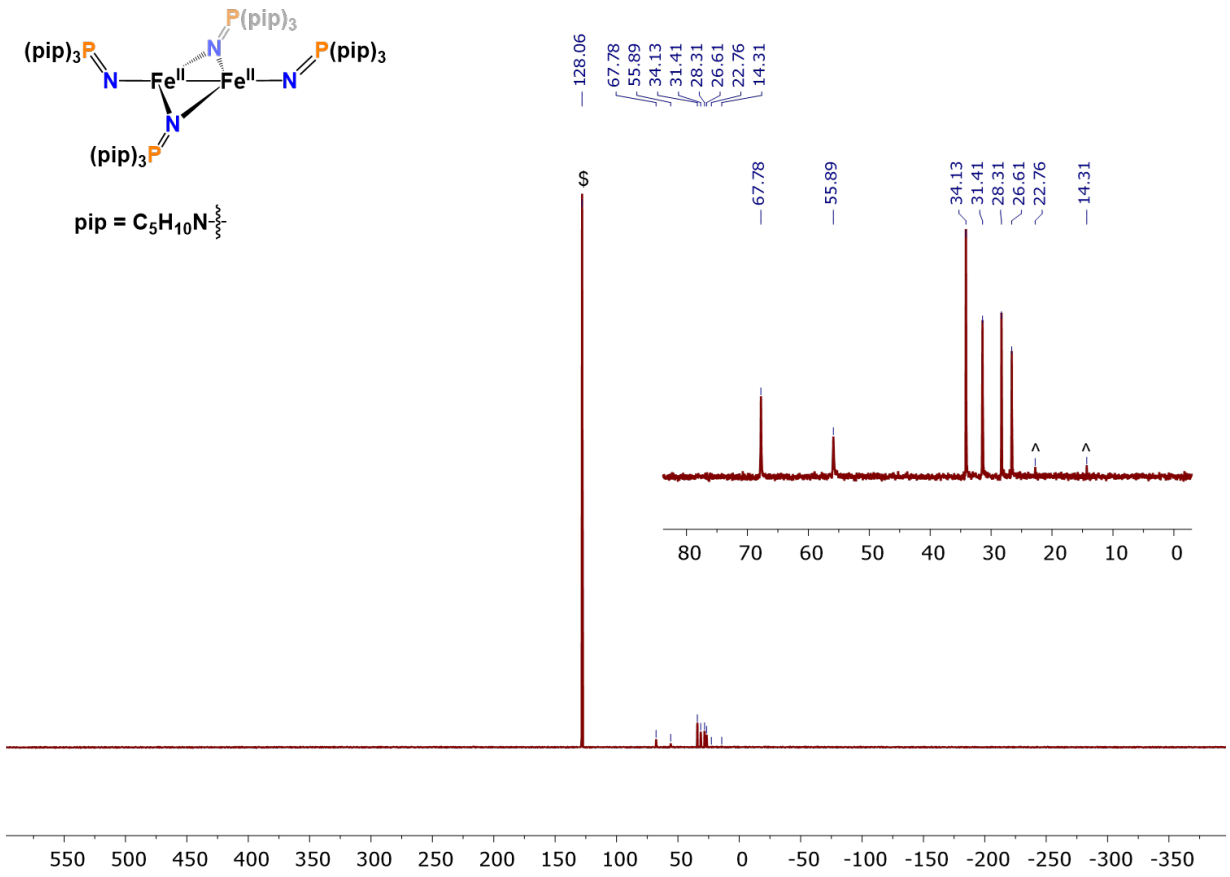



**Figure S3.** $^{13}C\{^{1}H\}$ NMR of **1-Fe** (100.61 MHz, $C_6D_6$, 295 K).

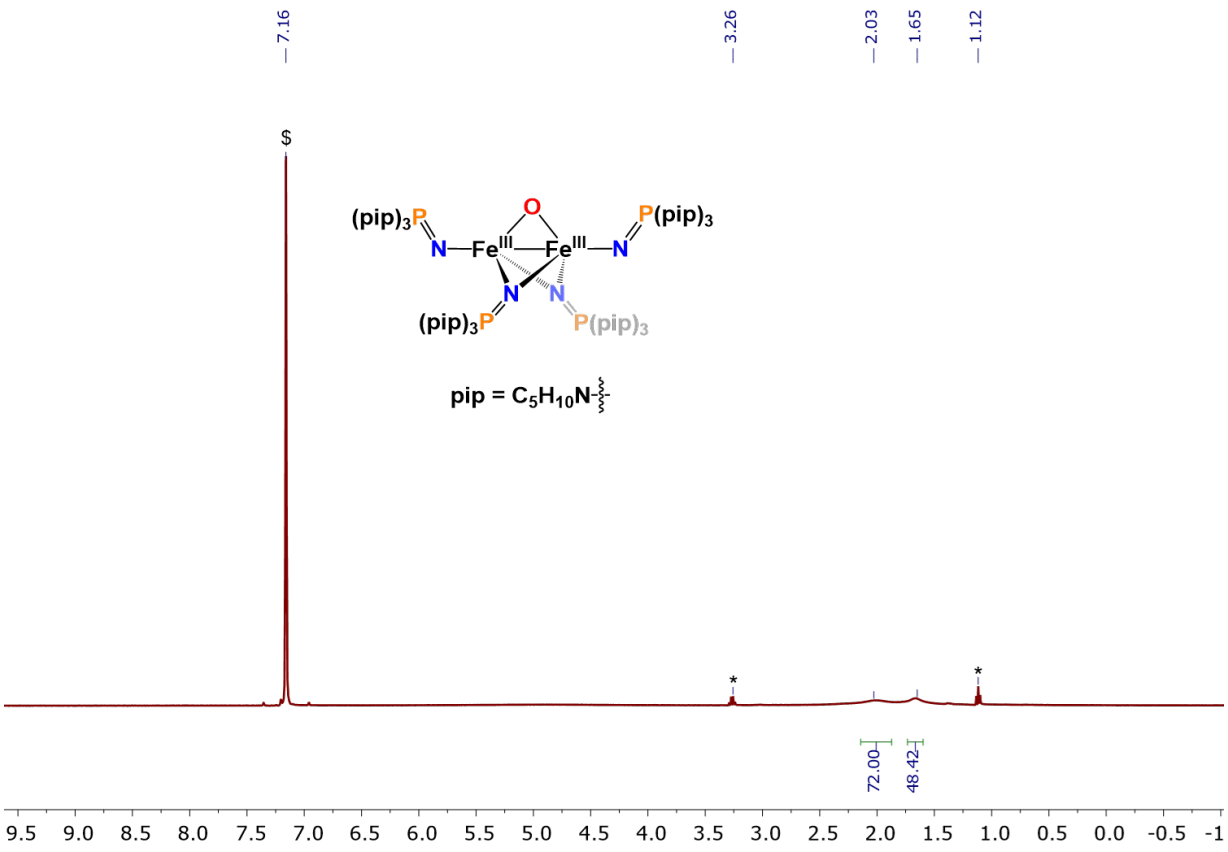
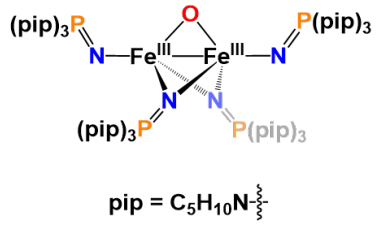



**Figure S4.** $^{1}$H NMR of **2-Fe** (400.13 MHz, $C_6D_6$, 295 K).



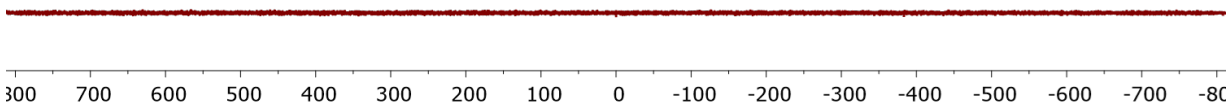




**Figure S5.** $^{31}P\{^{1}H\}$ NMR of **2-Fe** (161.98 MHz, $C_6D_6$, 295 K).

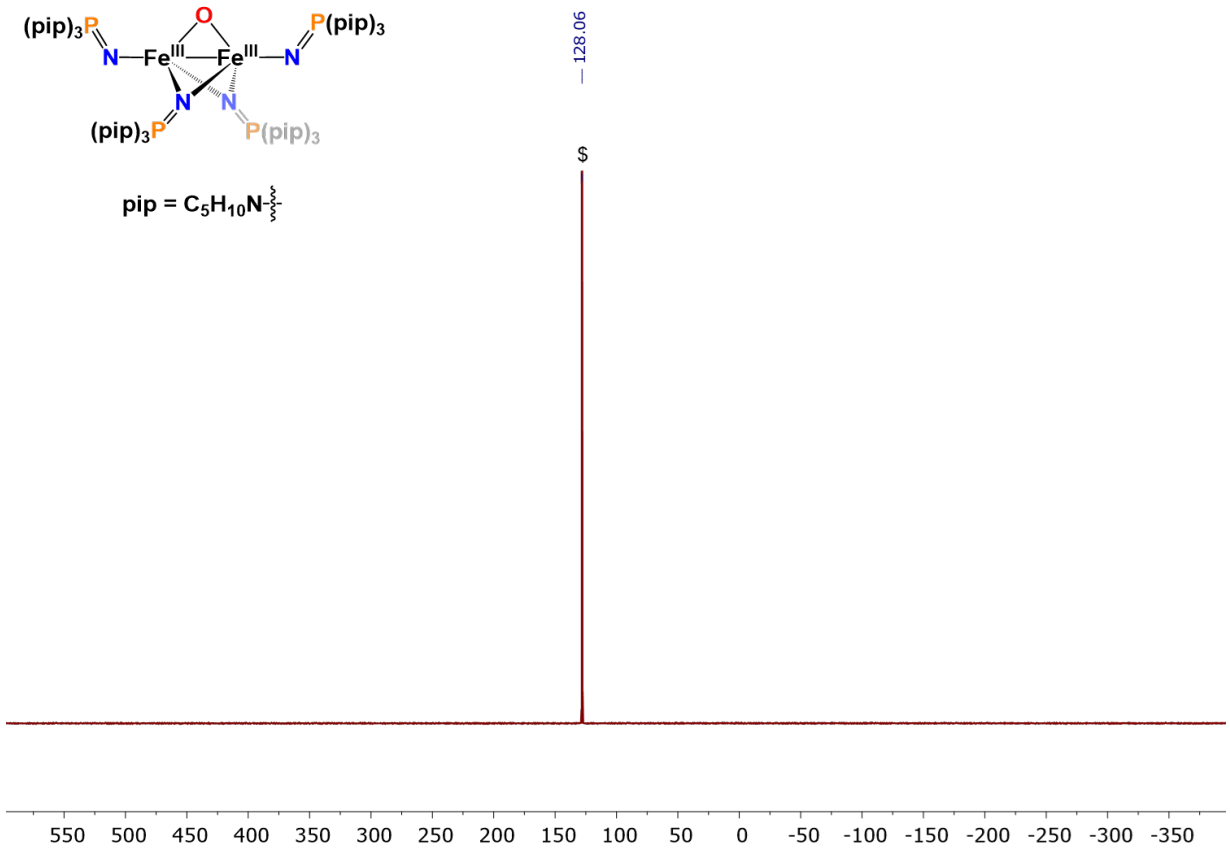



**Figure S6.** $^{13}C\{^{1}H\}$ NMR of **2-Fe** (100.61 MHz, $C_6D_6$, 295 K).

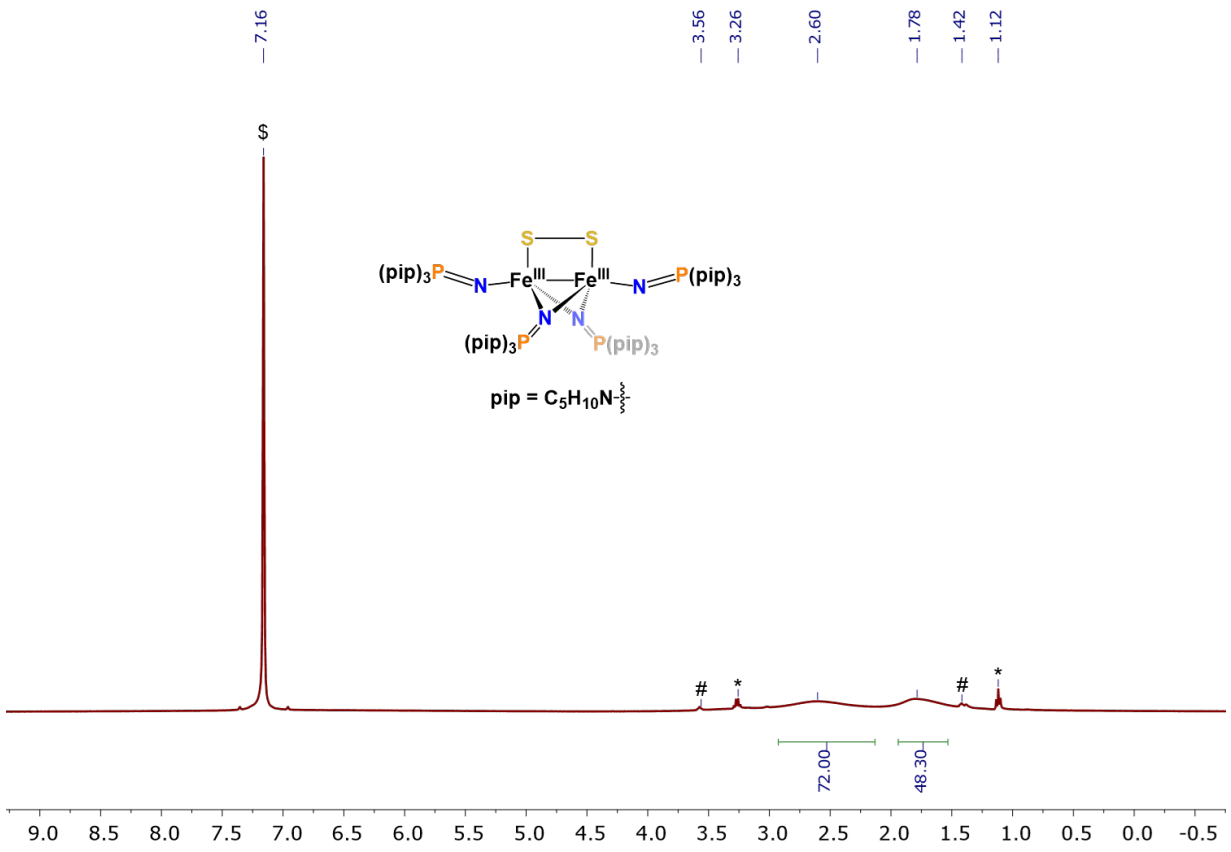



**Figure S7.** $^{1}$H NMR of **3-Fe** (400.13 MHz, $C_6D_6$, 295 K). Residual $Et_2O$ noted as ^. Residual THF noted as #.

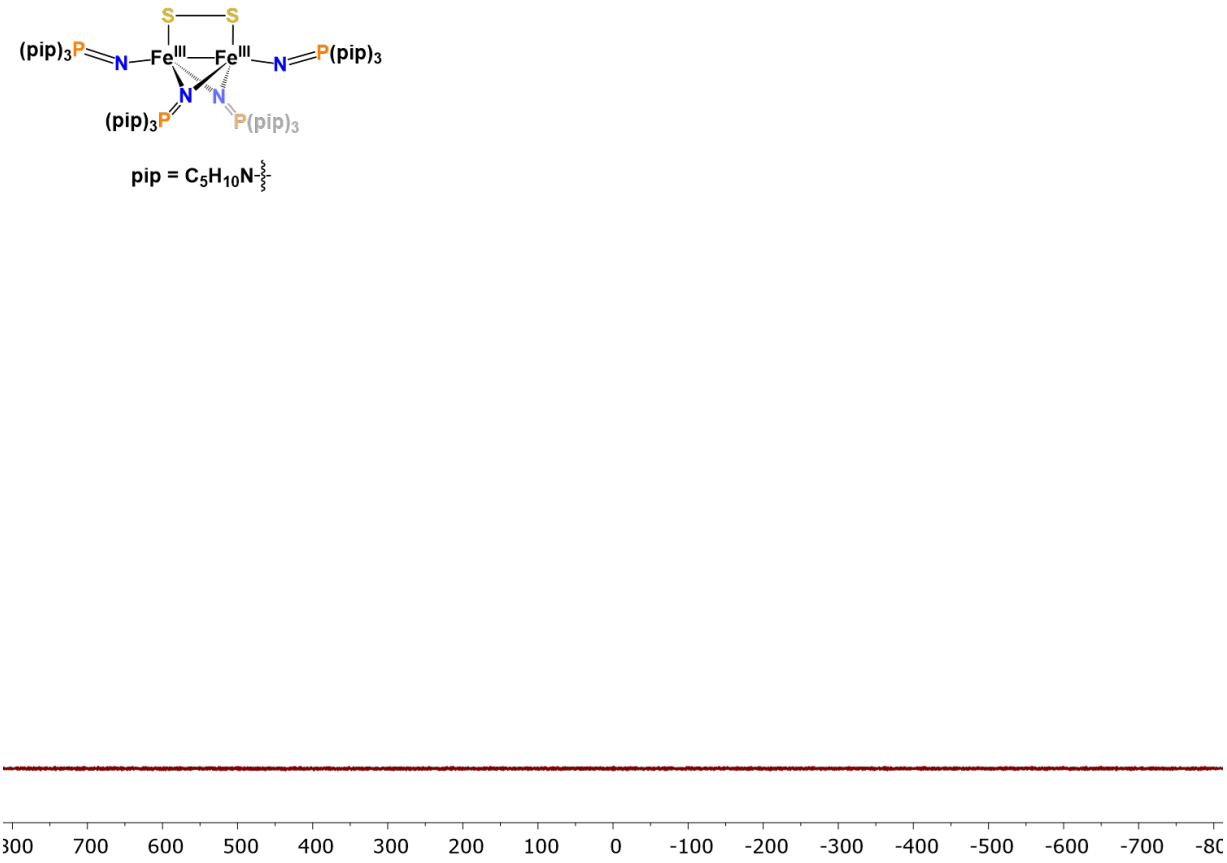



**Figure S8.** $^{31}P\{^{1}H\}$ NMR of **3-Fe** (161.98 MHz, $C_6D_6$, 295 K).

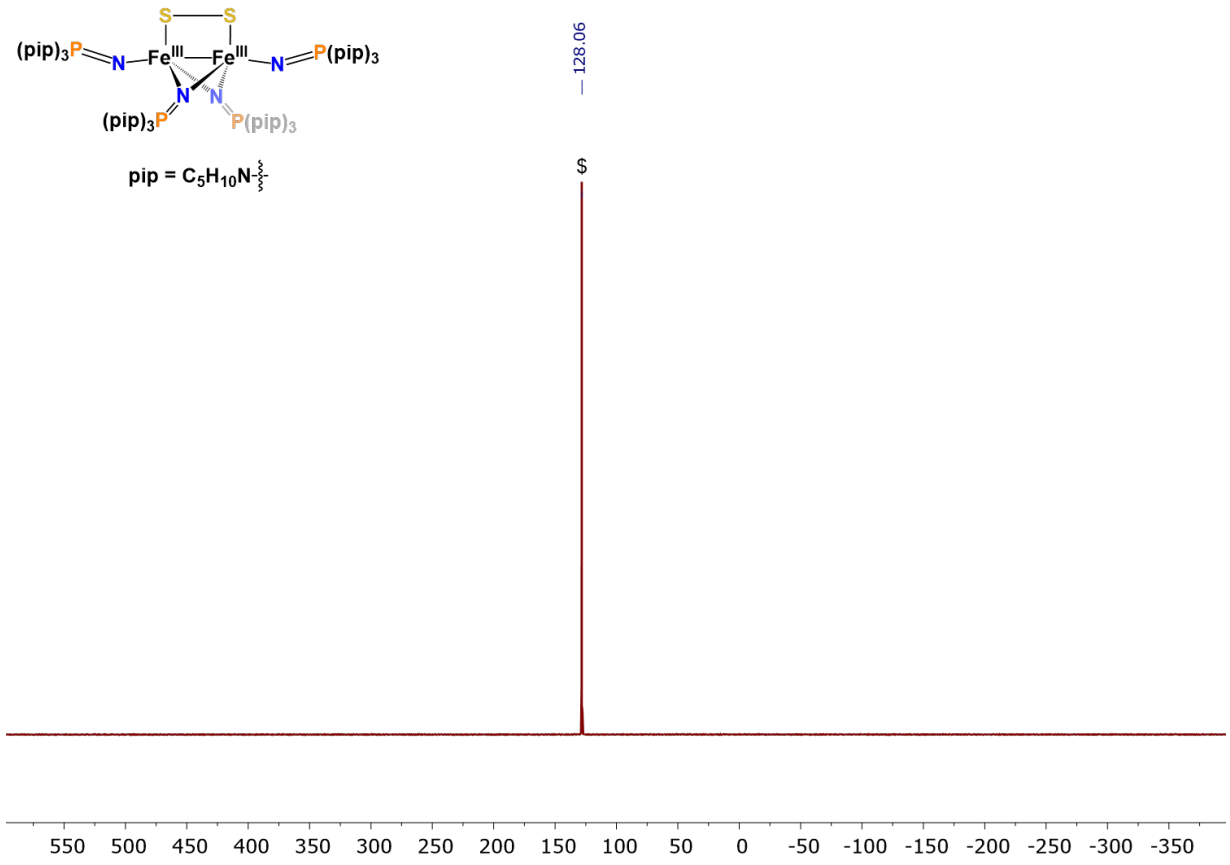



**Figure S9.** $^{13}C\{^{1}H\}$ NMR of **3-Fe** (400.13 MHz, $C_6D_6$, 295 K).

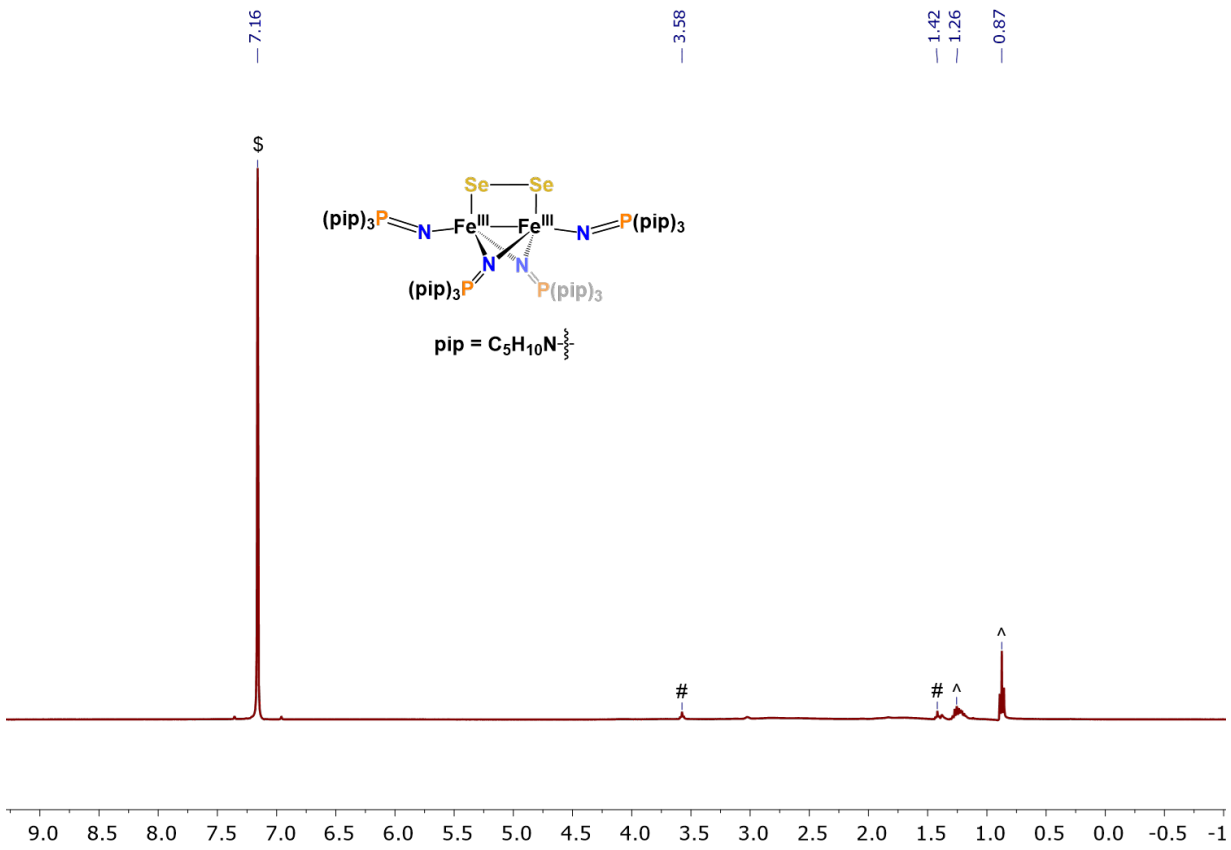
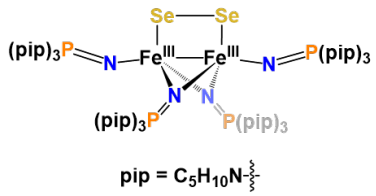



**Figure S10.** $^{1}$H NMR of **4-Fe** (400.13 MHz, $C_6D_6$, 295 K). Residual THF noted as *. Residual *n*-pentane noted as ^.



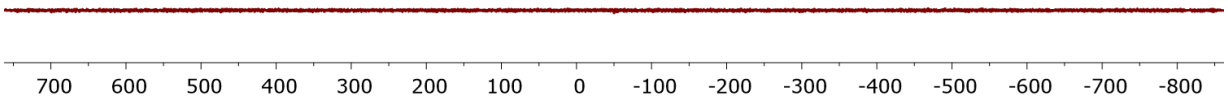




**Figure S11.** $^{31}P\{^{1}H\}$ NMR of **4-Fe** (100.61 MHz, $C_6D_6$, 295 K).

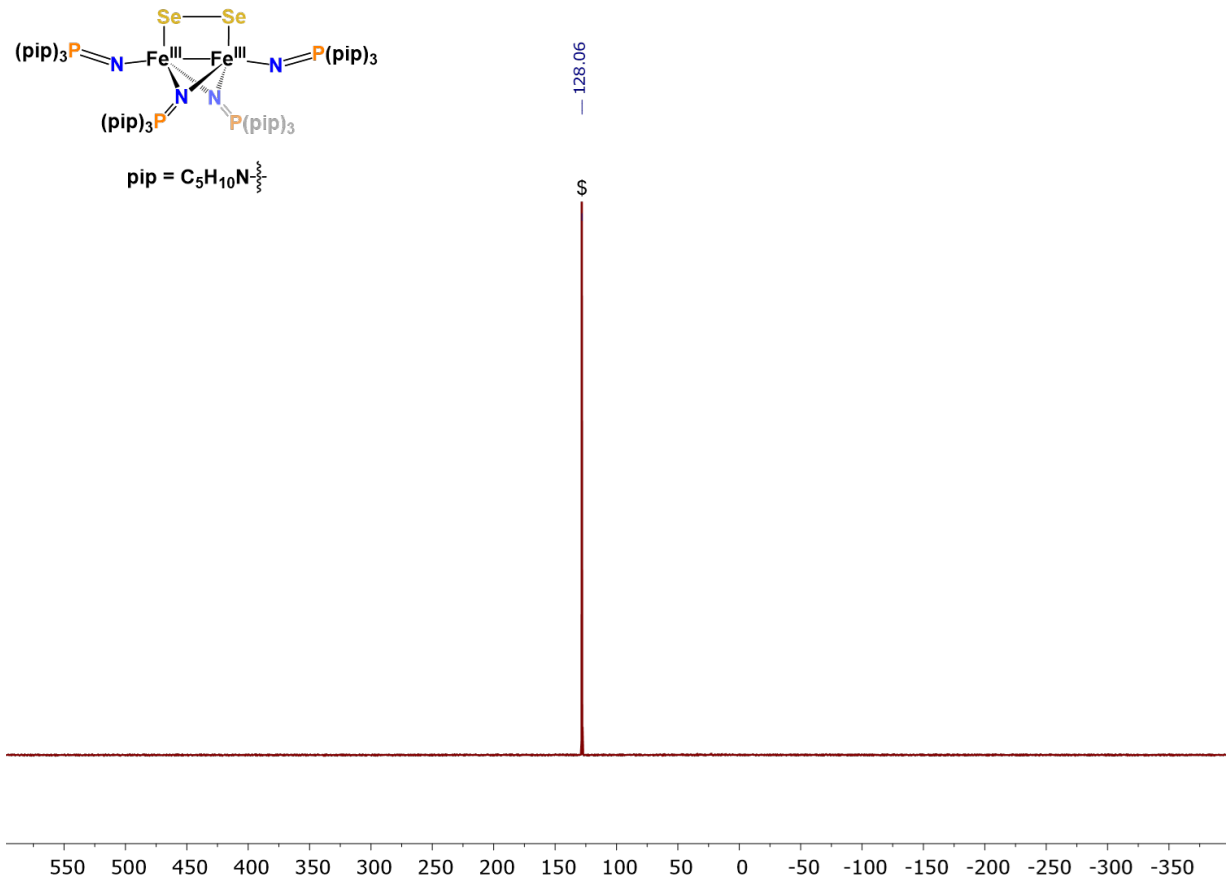



**Figure S12.** $^{13}C\{^{1}H\}$ NMR of **4-Fe** (161.98 MHz, $C_6D_6$, 295 K).

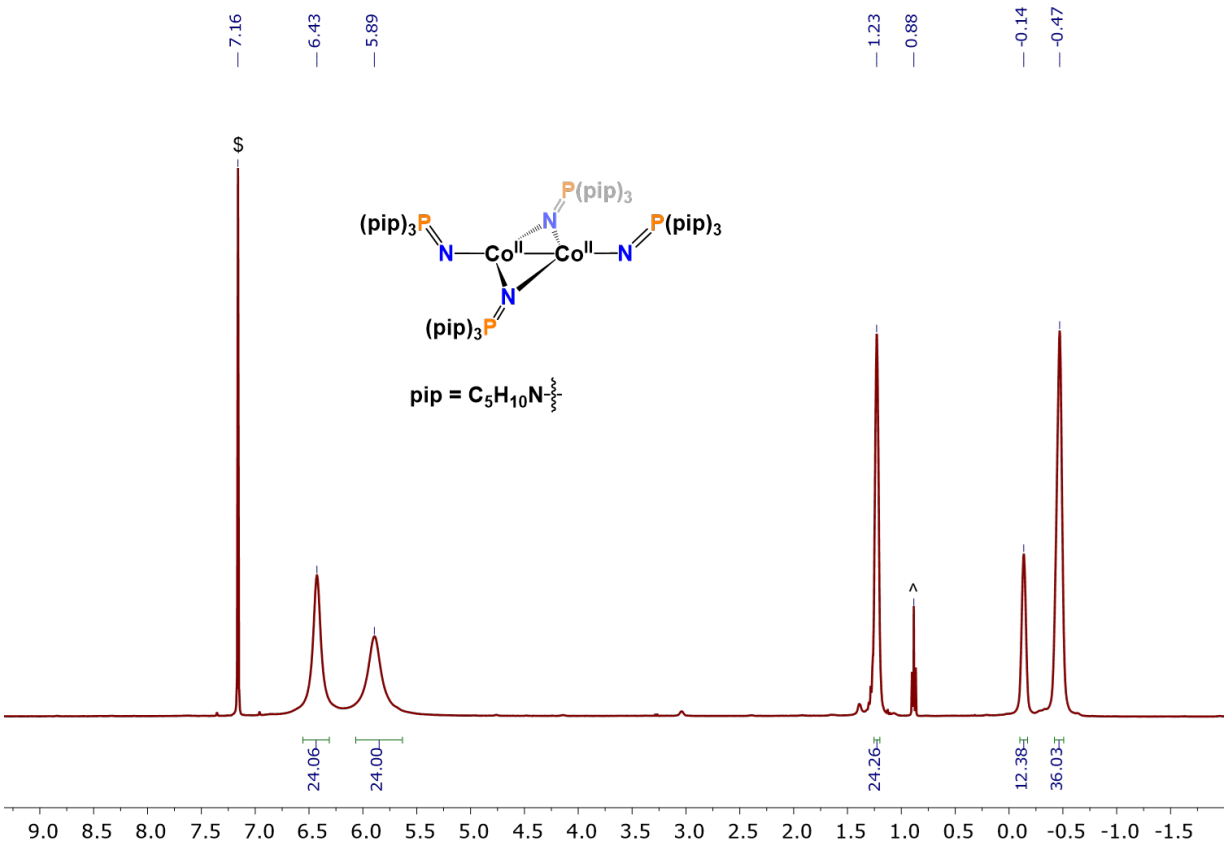
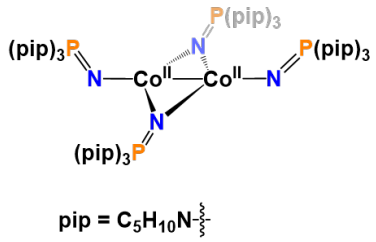



**Figure S13.** $^{1}$H NMR of **1-Co** (400.13 MHz, $C_6D_6$, 295 K). Residual *n*-pentane noted as ^.



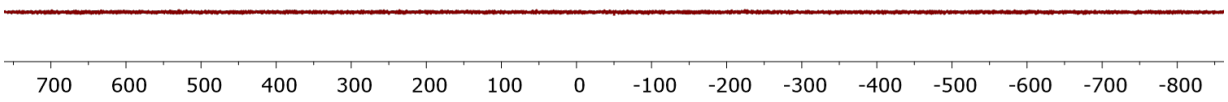




**Figure S14.** $^{31}P\{^{1}H\}$ NMR of **1-Co** (161.98 MHz, $C_6D_6$, 295 K).

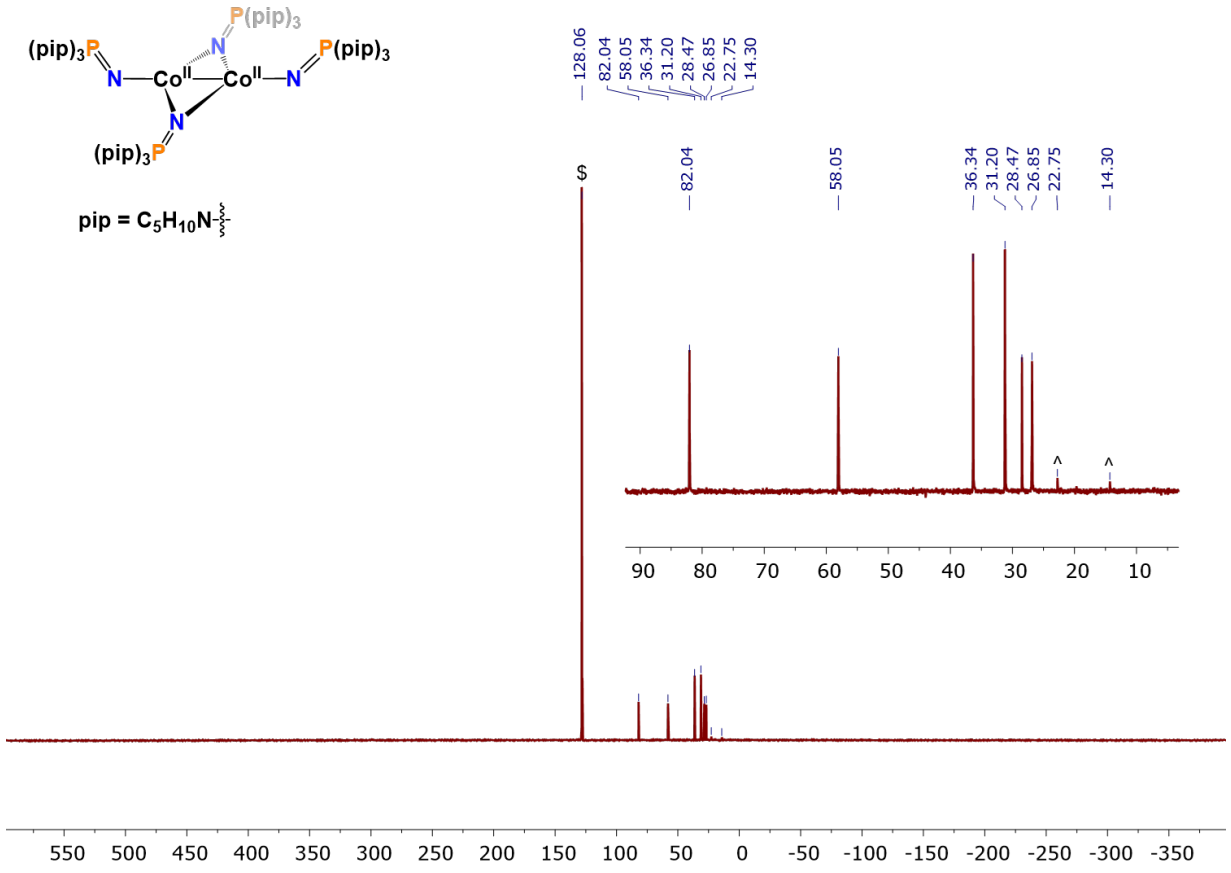



**Figure S15.** $^{13}C\{^{1}H\}$ NMR of **1-Co** (161.98 MHz, $C_6D_6$, 295 K).

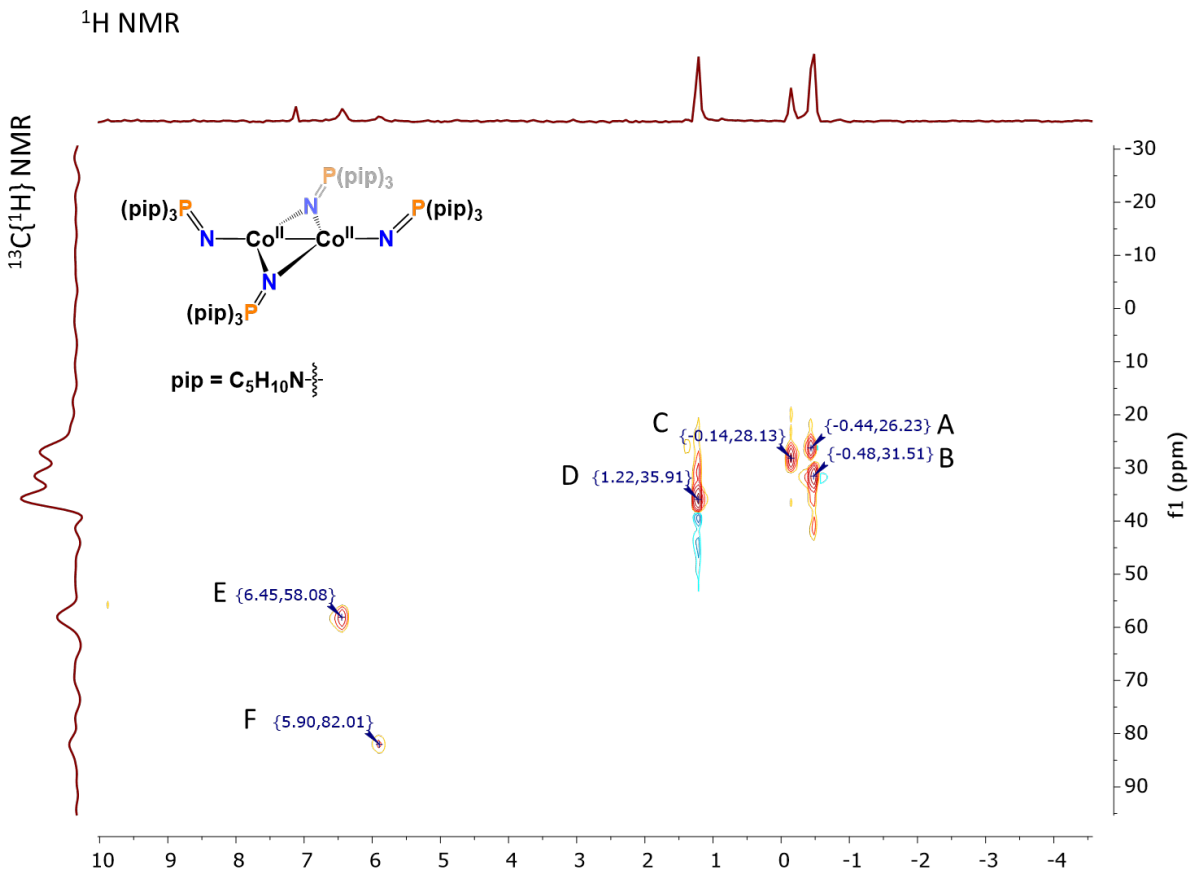



**Figure S16.** HSQC NMR of **1-Co** (161.98 MHz, $C_6D_6$, 295 K).

**UV-Vis-NIR Spectroscopy**

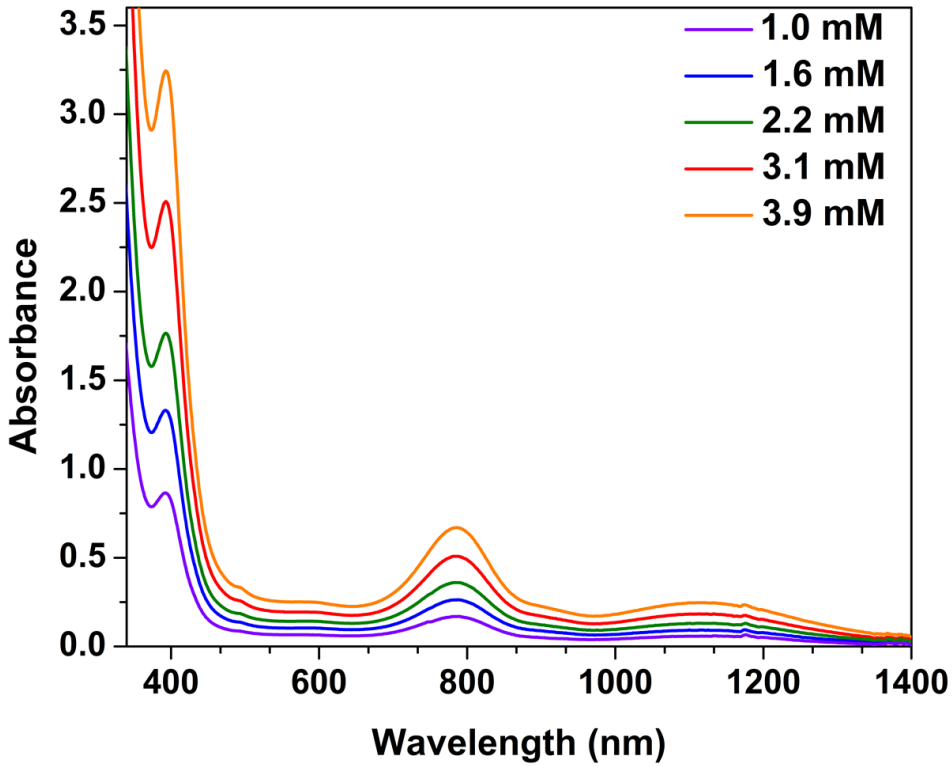



**Figure S17.** UV-Vis-NIR spectra of **1-Fe** in THF.

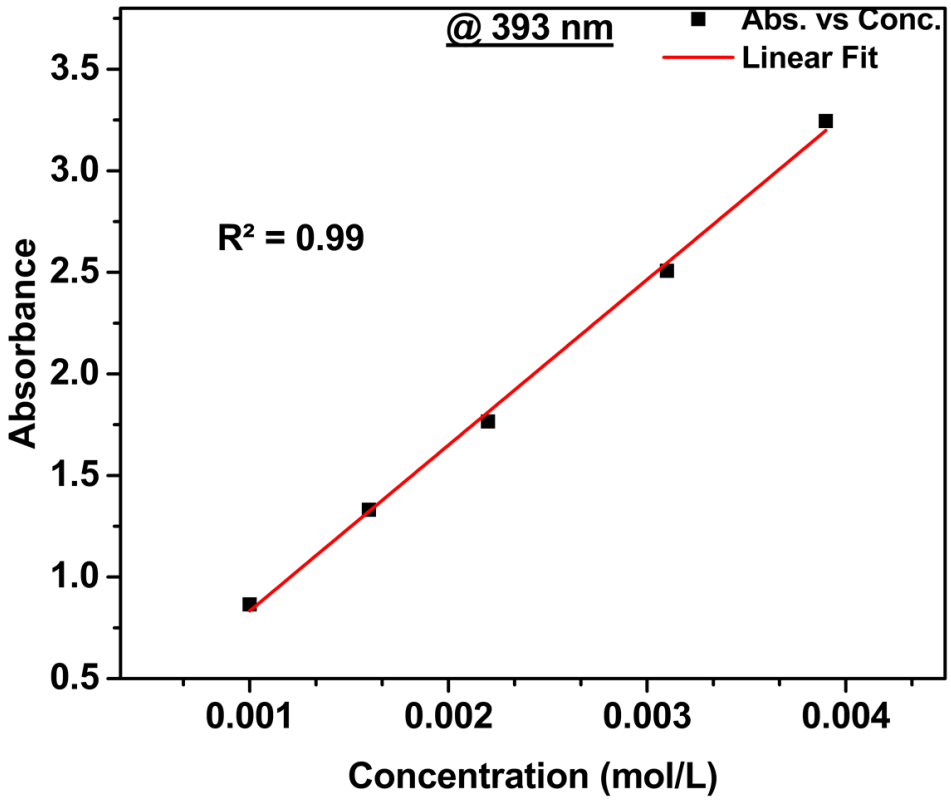



**Figure S18.** Linear regression of absorbance at 393 nm maximum where $\varepsilon$ = 816 $cm^{-1}M^{-1}$ for the UV-vis-NIR spectrum of **1-Fe**.

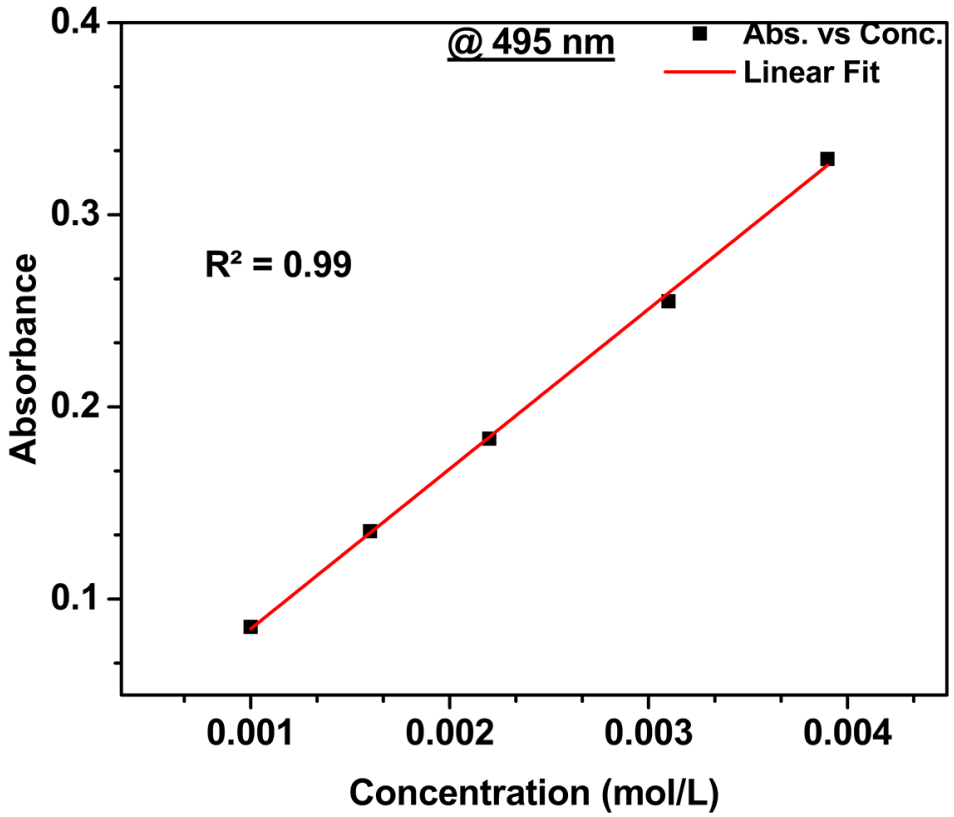



**Figure S19.** Linear regression of absorbance at 495 nm maximum where $\varepsilon$ = 83 $cm^{-1}M^{-1}$ for the UV-vis-NIR spectrum of **1-Fe**.

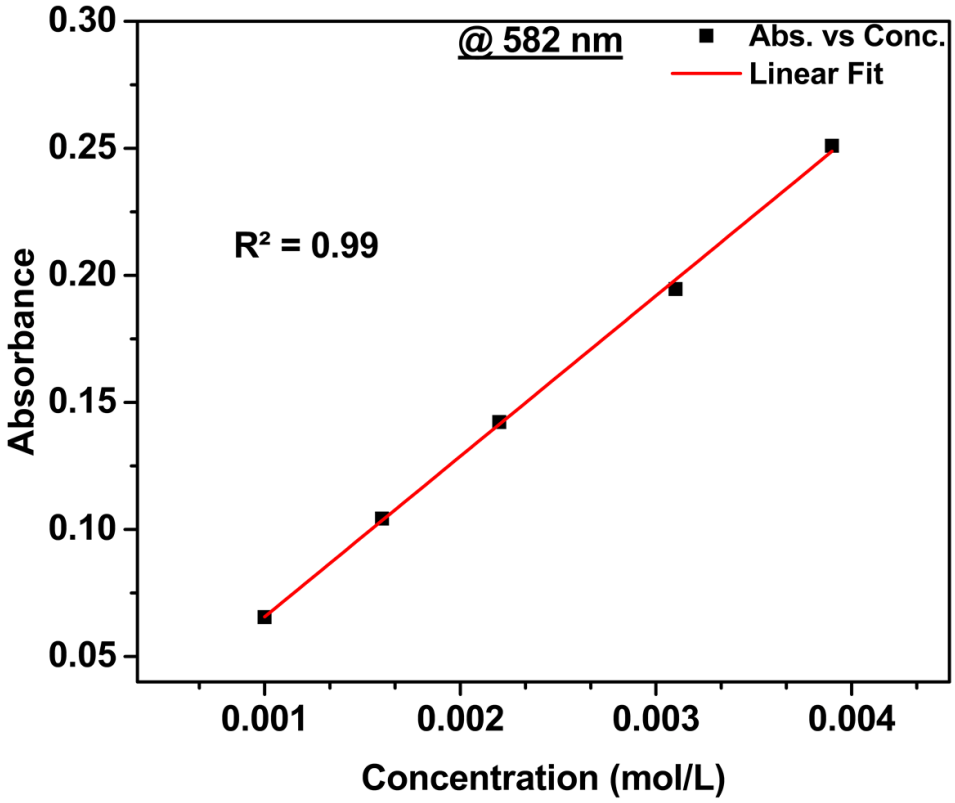



**Figure S20.** Linear regression of absorbance at 582 nm maximum where $\varepsilon$ = 63 $cm^{-1}M^{-1}$ for the UV-vis spectrum of **1-Fe**.

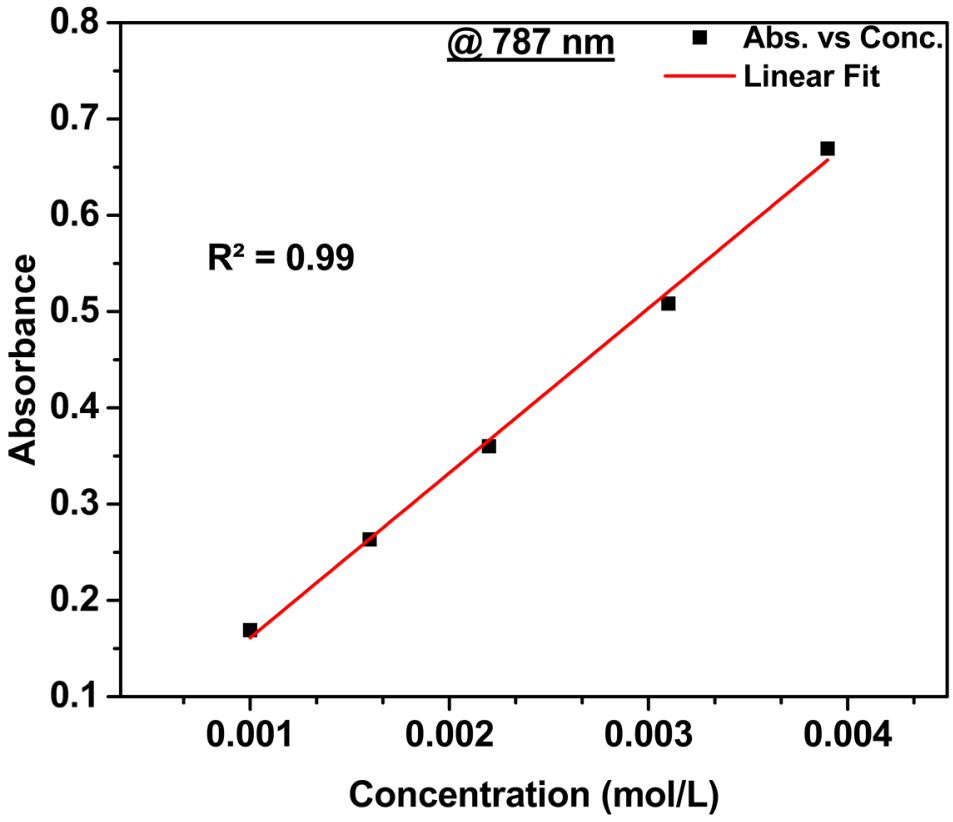



**Figure S21.** Linear regression of absorbance at 787 nm maximum where $\varepsilon$ = 171 $cm^{-1}M^{-1}$ for the UV-vis spectrum of **1-Fe**.

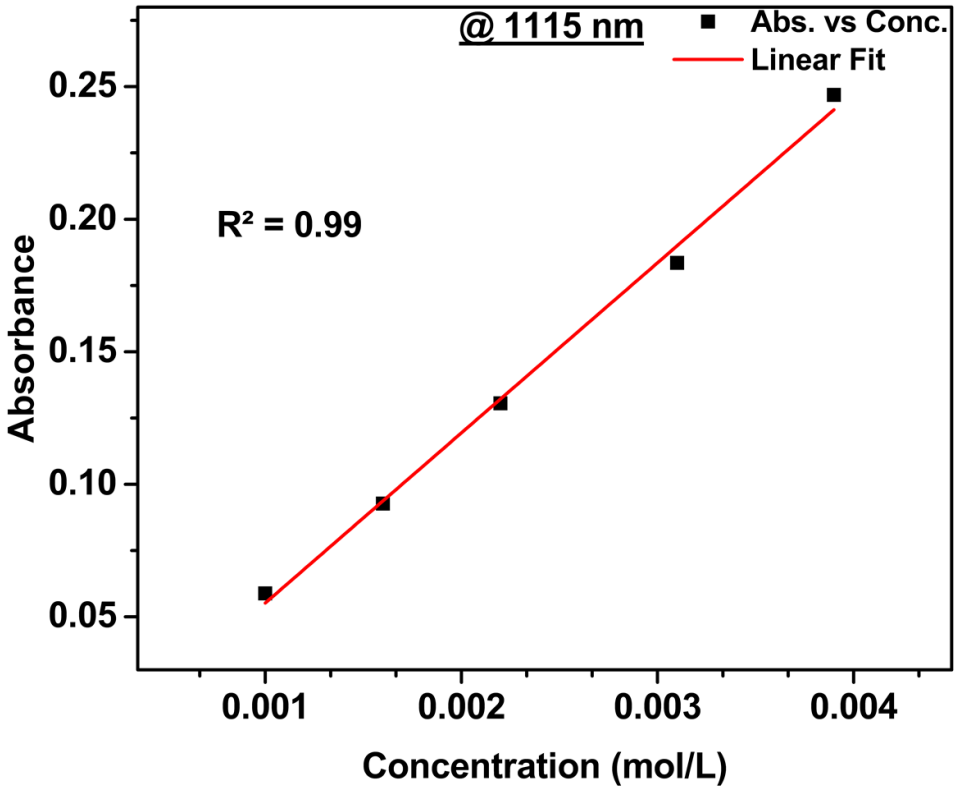



**Figure S22.** Linear regression of absorbance at 1115 nm maximum where $\varepsilon$ = 64 $cm^{-1}M^{-1}$ for the UV-vis spectrum of **1-Fe**.

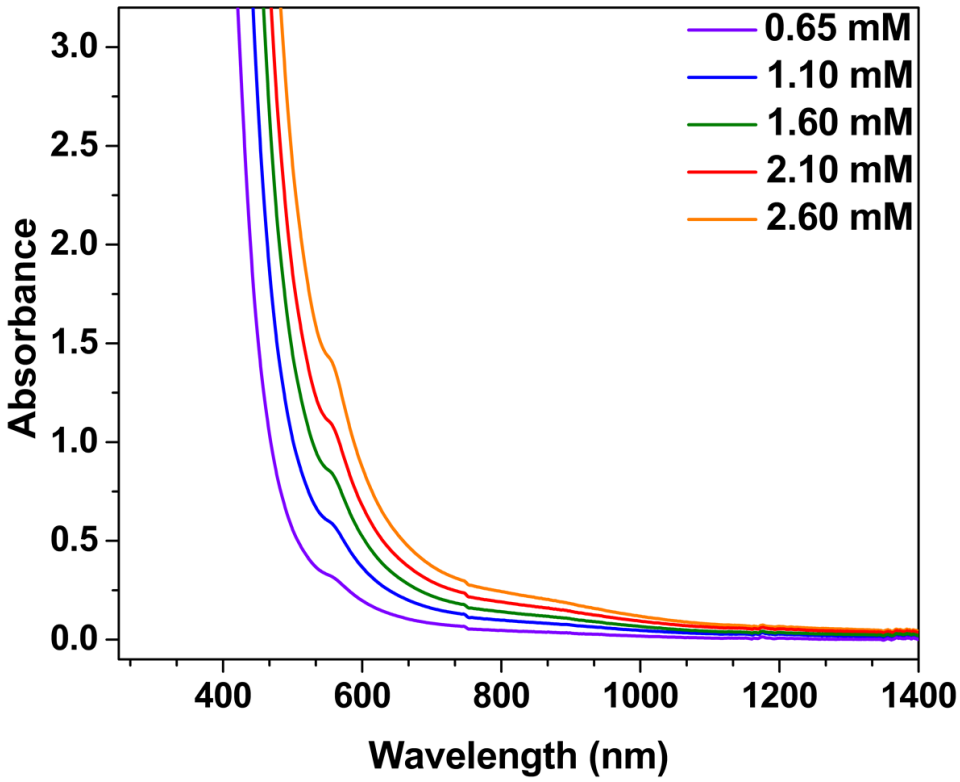



**Figure S23.** UV-Vis-NIR spectra of **2-Fe** in THF.

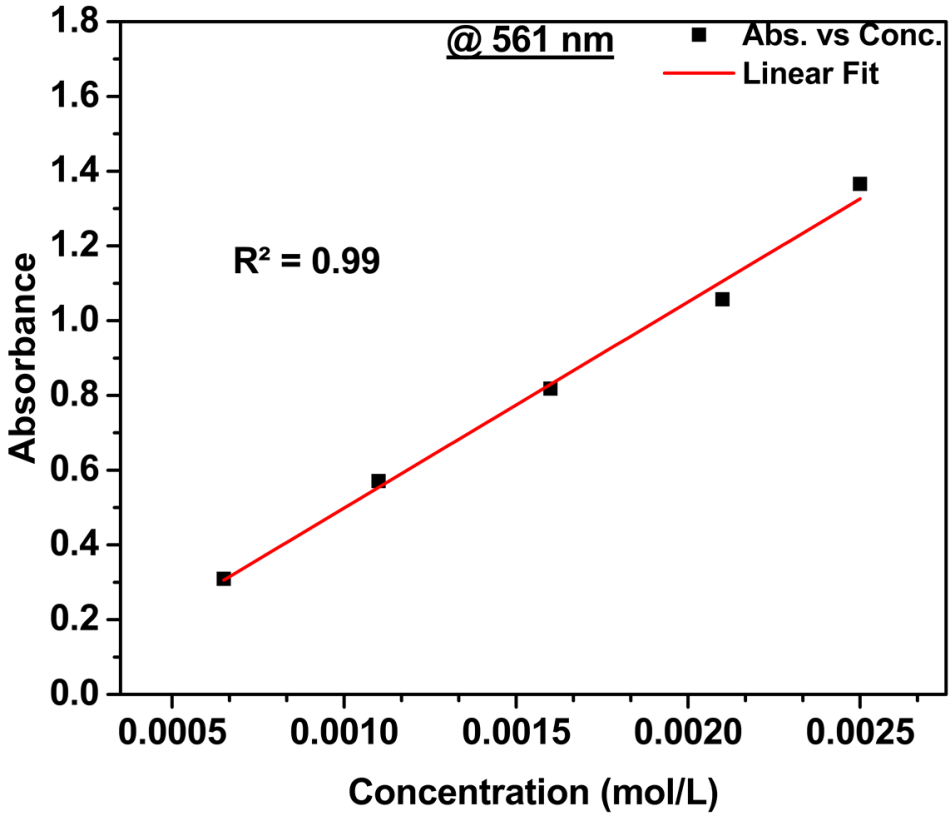



**Figure S24.** Linear regression of absorbance at 561 nm maximum where $\varepsilon$ = 552 $cm^{-1}M^{-1}$ for the UV-vis spectrum of **2-Fe**.

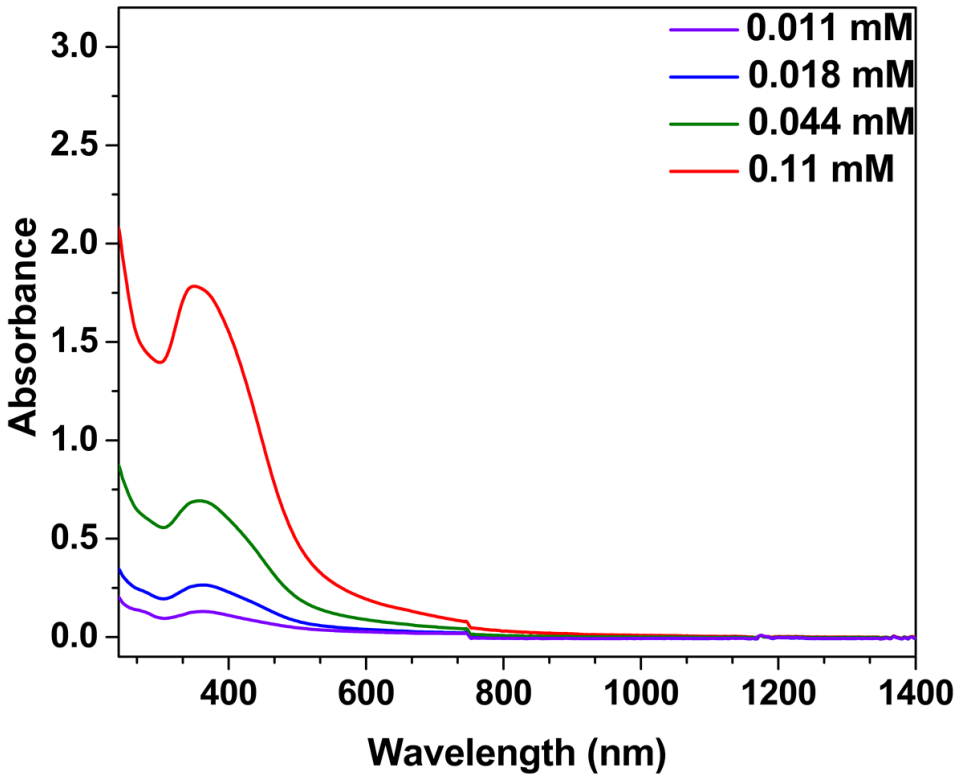



**Figure S25.** UV-Vis-NIR spectra of **3-Fe** in THF.

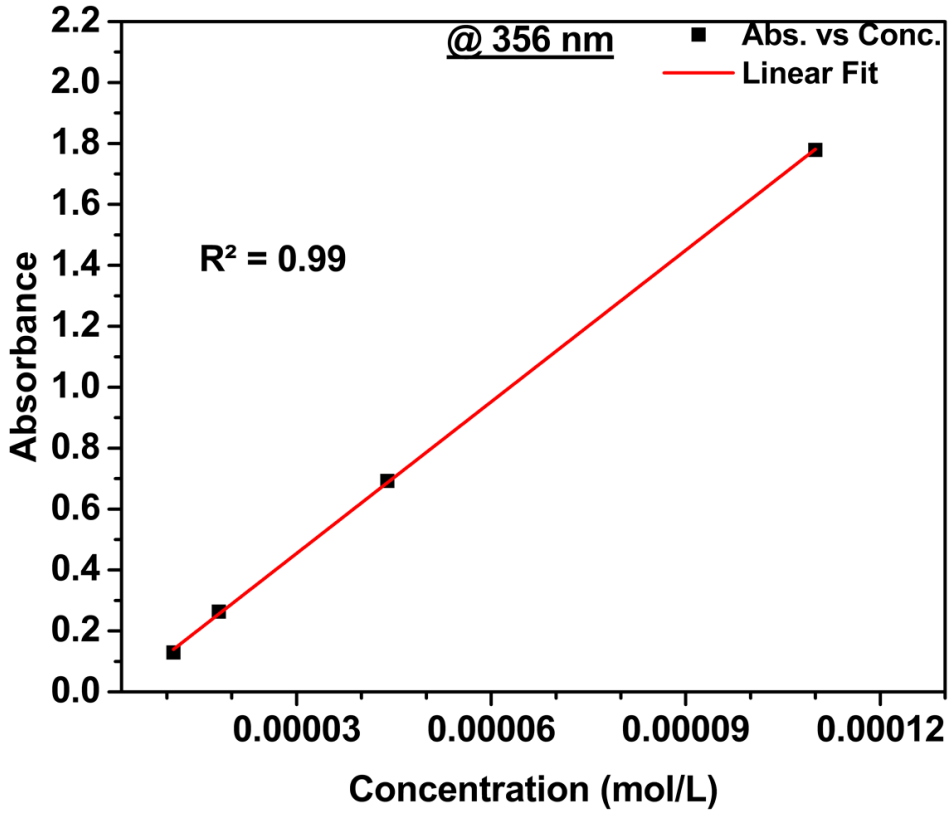



**Figure S26.** Linear regression of absorbance at 356 nm maximum where $\varepsilon$ = 16584 $cm^{-1}M^{-1}$ for the UV-vis spectrum of **3-Fe**.

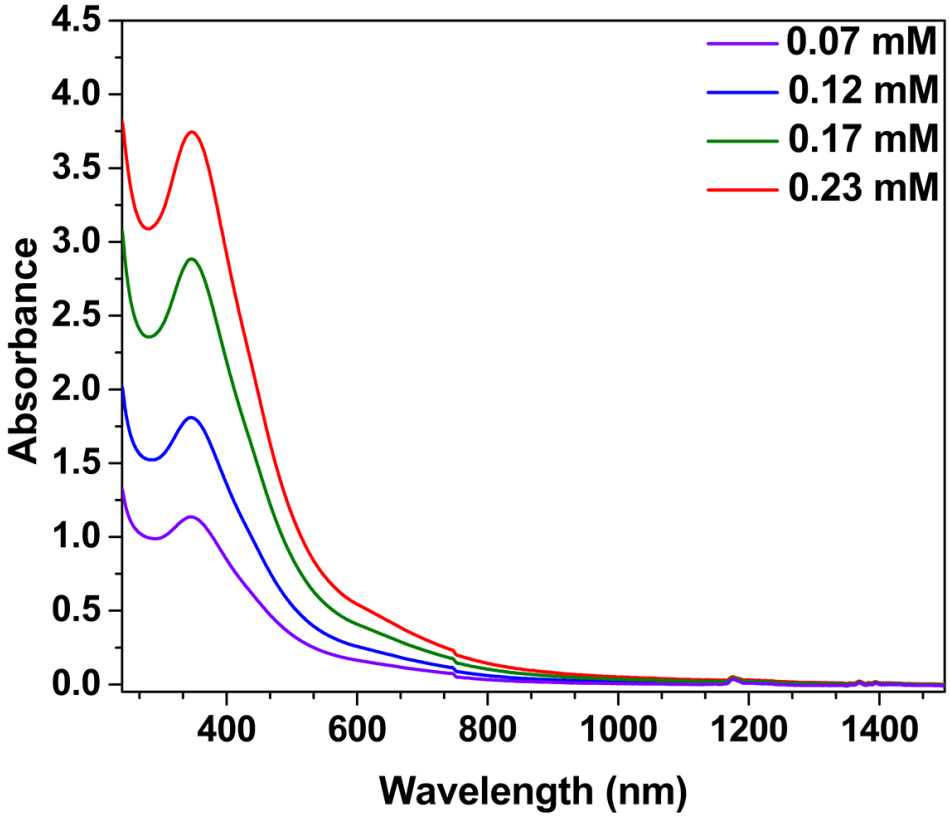



**Figure S27.** UV-Vis-NIR spectra of **4-Fe** in THF.

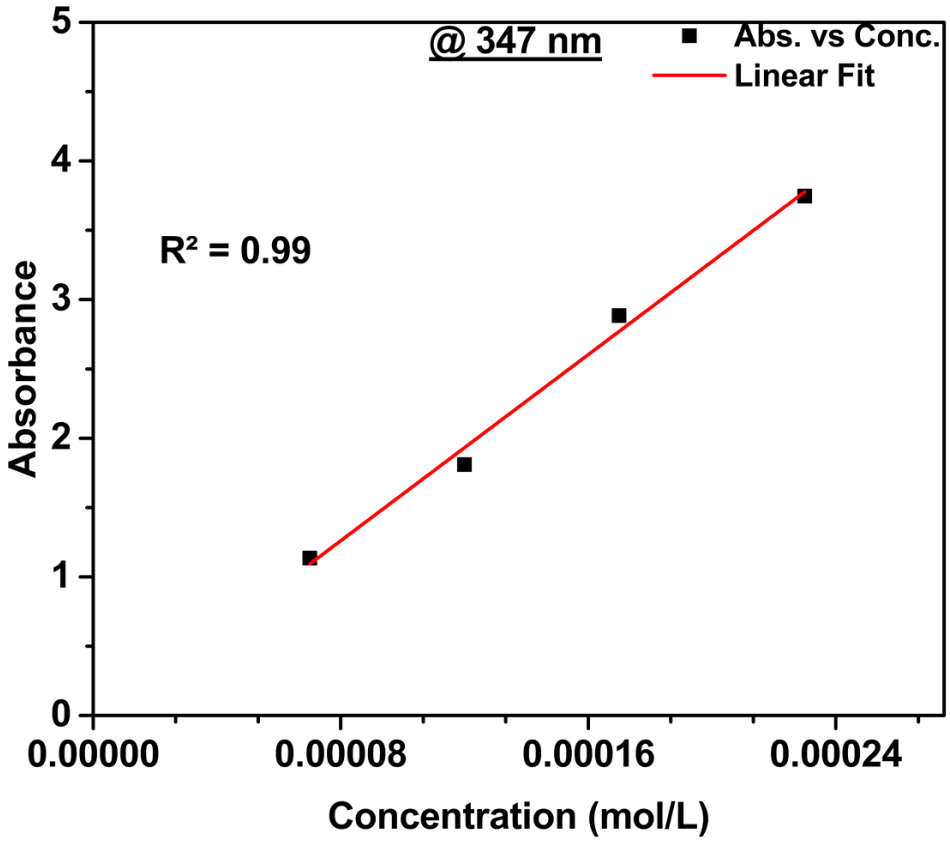



**Figure S28.** Linear regression of absorbance at 347 nm maximum where $\varepsilon$ = 16783 $cm^{-1}M^{-1}$ for the UV-vis spectrum of **4-Fe**.

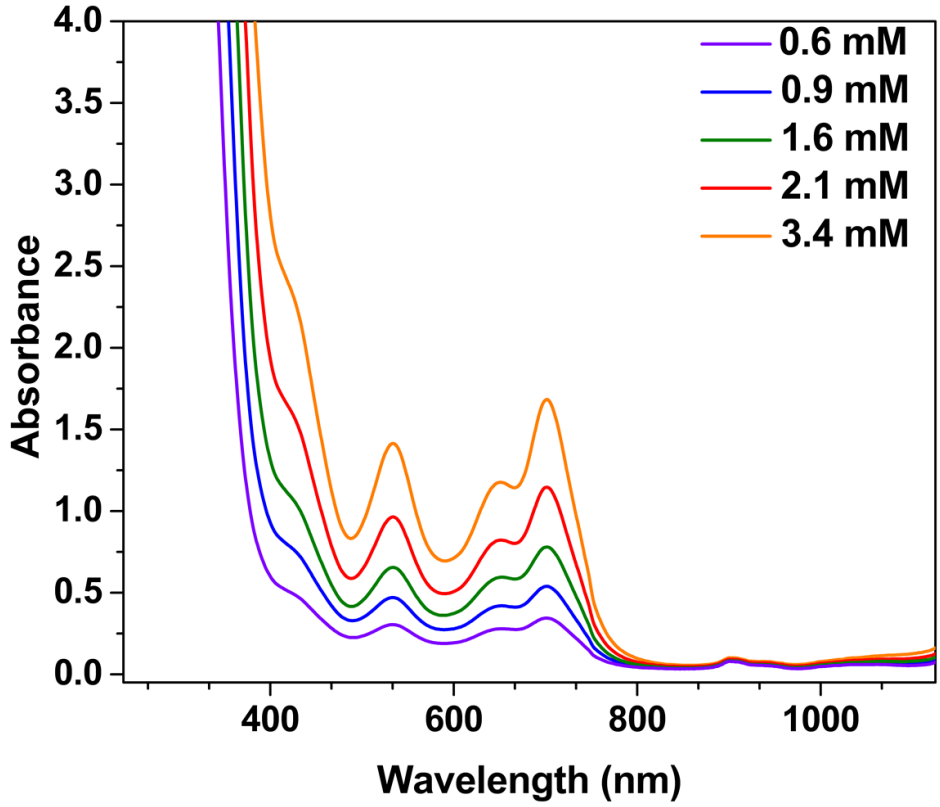



**Figure S29.** UV-Vis-NIR spectra of **1-Co** in THF.

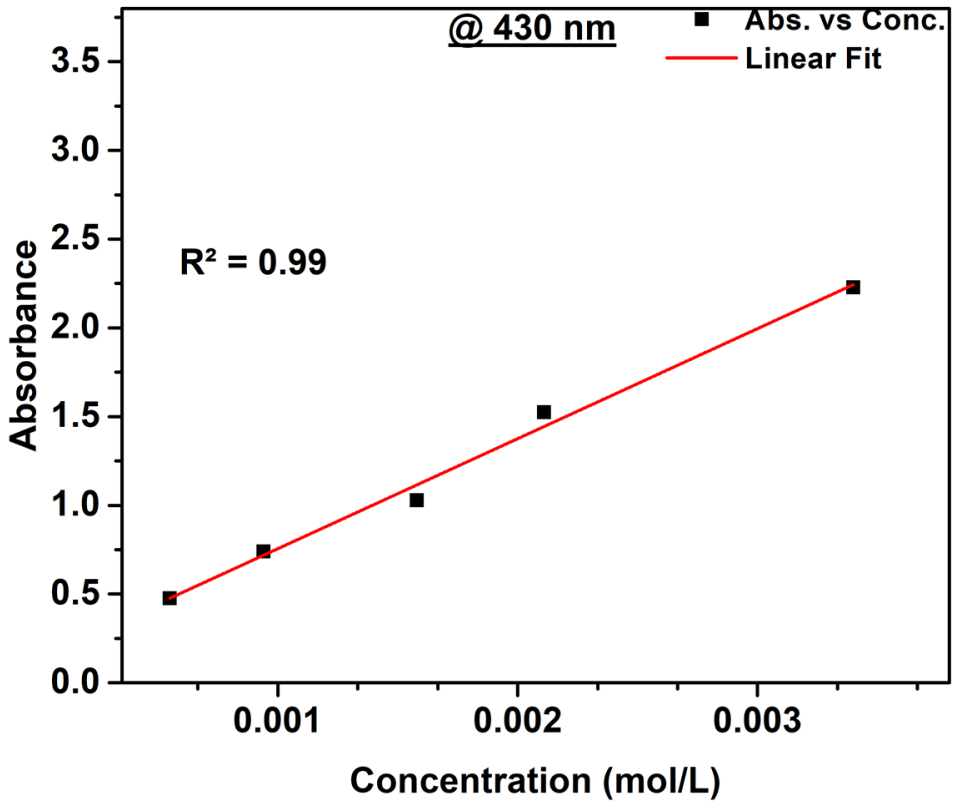



**Figure S30.** Linear regression of absorbance at 430 nm maximum where $\varepsilon$ = 620 $cm^{-1}M^{-1}$ for the UV-vis spectrum of **1-Co**.

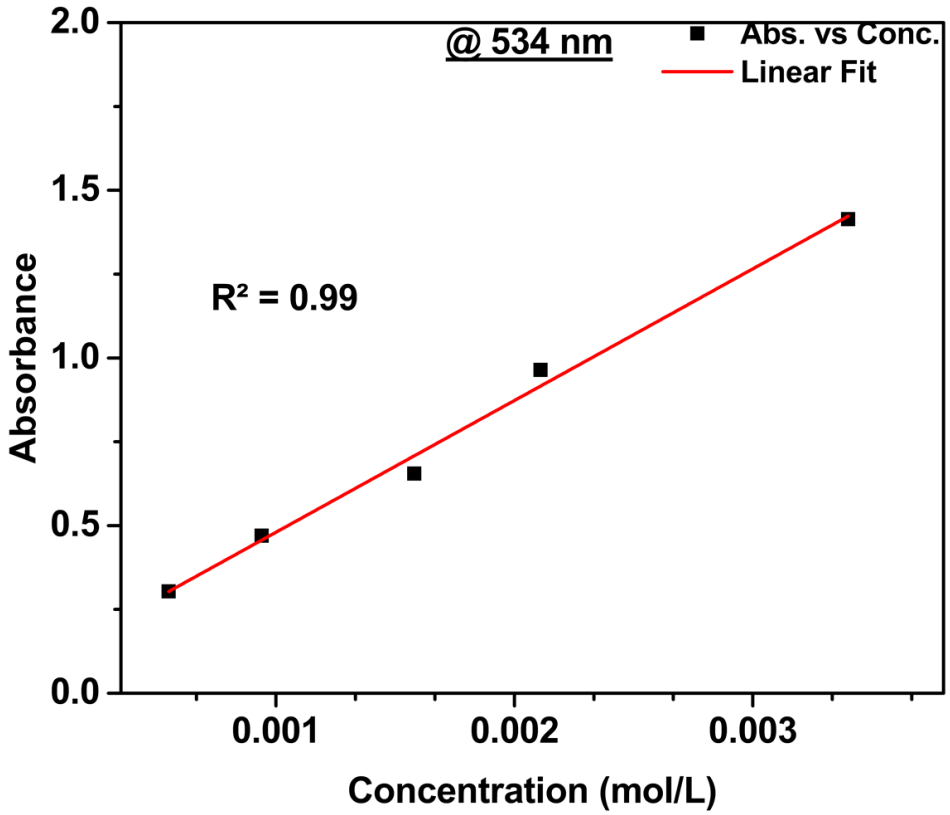



**Figure S31.** Linear regression of absorbance at 534 nm maximum where $\varepsilon$ = 393 $cm^{-1}M^{-1}$ for the UV-vis spectrum of **1-Co**.

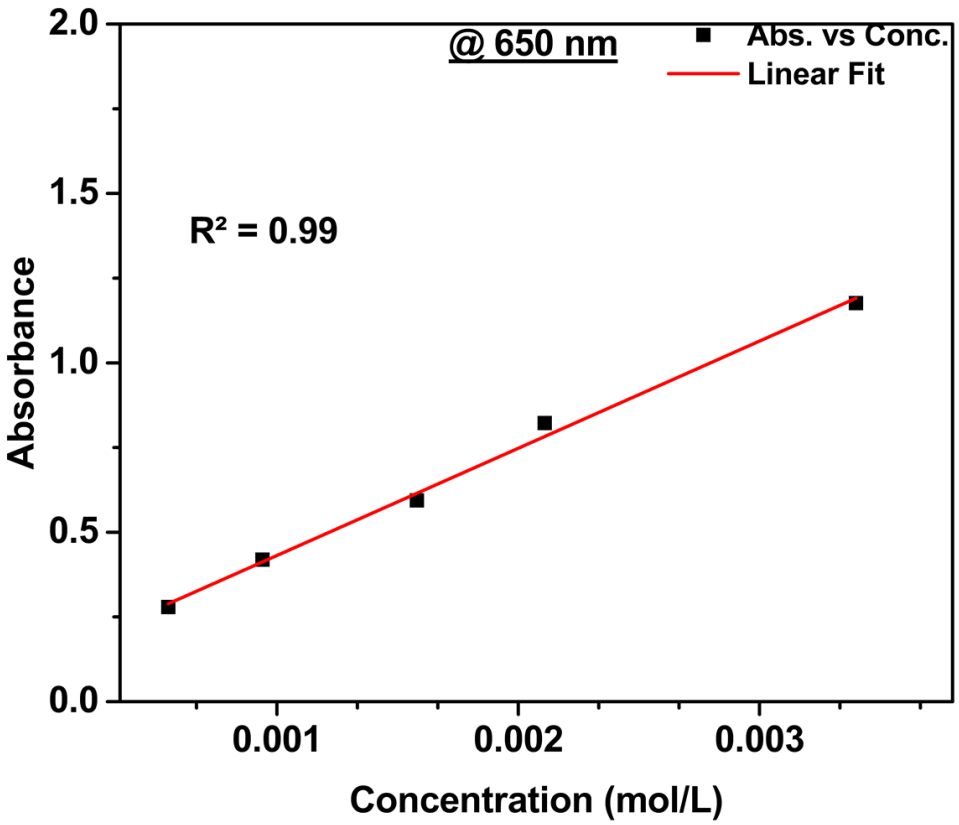



**Figure S32.** Linear regression of absorbance at 650 nm maximum where $\varepsilon$ = 316 $cm^{-1}M^{-1}$ for the UV-vis spectrum of **1-Co**.

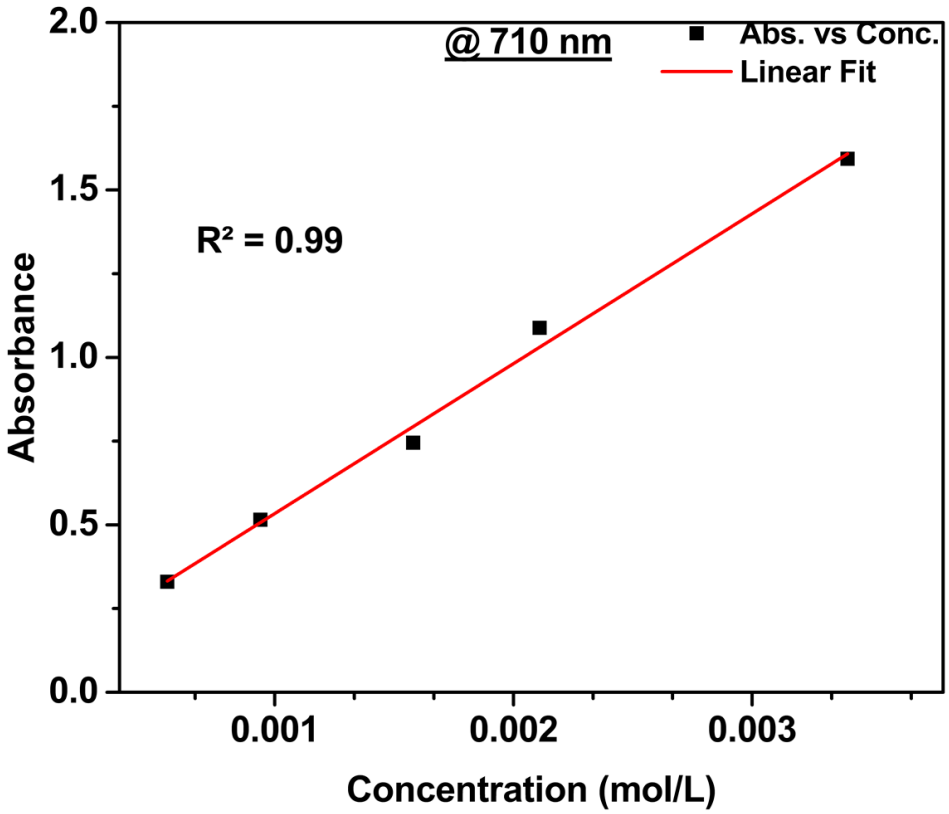



**Figure S33.** Linear regression of absorbance at 710 nm maximum where $\varepsilon$ = 448 $cm^{-1}M^{-1}$ for the UV-vis spectrum of **1-Co**.

## Calculated Energy Profile

All calculations were carried out with the Gaussian09 program[4] at the DFT level using the hybrid functional B3PW91.[5,6] For Fe, the relativistic energy-consistent pseudopotential of the Stuttgart-Köln ECP library was used in combination with its adapted segmented basis.[7] For all other atoms, a standard 6-31G** basis set was used.[8,9] Electronic energies and enthalpies were computed at T = 298 K in the gas phase. All stationary points have been identified as minima (number of imaginary frequencies Nimag = 0) or transition states (Nimag = 1) and IRC calculations were carried out from all transition states. All compounds were computed as singlet spin state, except the μ–$O^{2-}$ product that was computed as a triplet spin state.

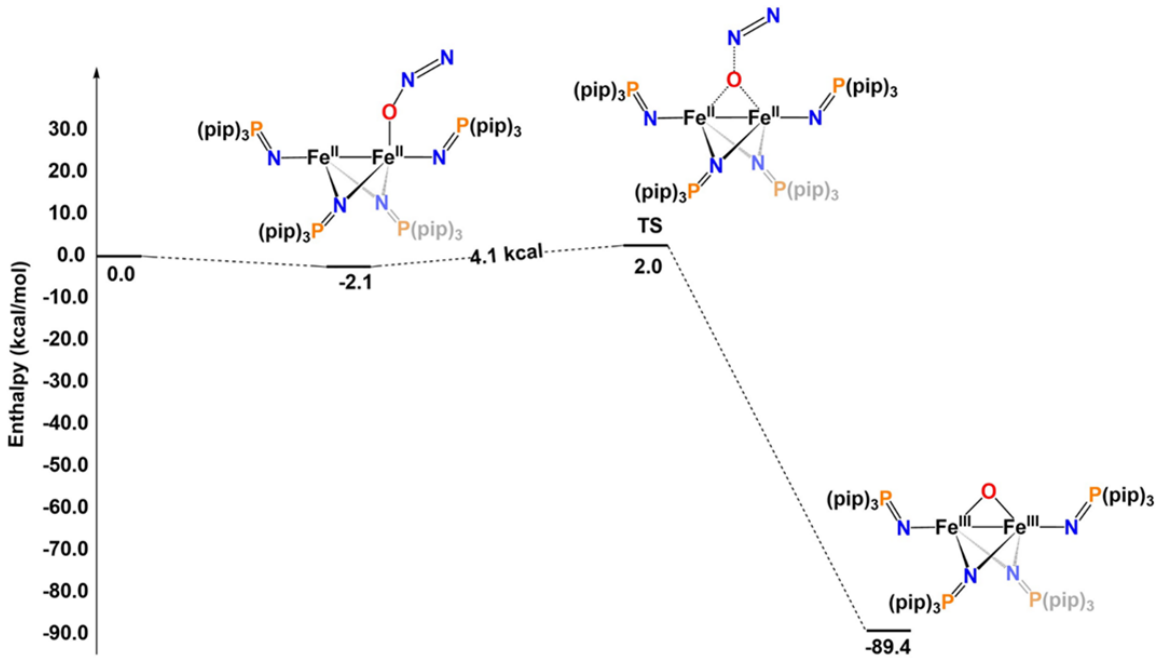
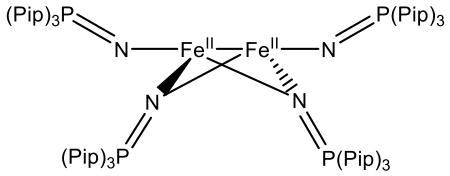



**Figure S34.** Calculated enthalpy profile for the reaction between **1-Fe** and $N_2O$ to produce **2-Fe**.

Cartesian coordinates of all optimized strcutures



| | | | |
|---|---|---|---|
| C | 14.27255900 | 7.34582700 | 18.32144200 |
| H | 13.91326900 | 8.31896700 | 17.93677100 |
| C | 14.38606400 | 7.43923500 | 19.84454300 |
| H | 14.83305400 | 6.51101500 | 20.22545000 |
| C | 13.00631100 | 7.64693400 | 20.47231700 |
| H | 12.62383000 | 8.63598000 | 20.17725200 |
| C | 12.03295300 | 6.56739700 | 19.99395600 |
| H | 12.34611200 | 5.59414500 | 20.39442000 |
| H | 11.02012700 | 6.76628400 | 20.36763500 |
| C | 12.00051000 | 6.48563400 | 18.46757300 |
| H | 11.34647400 | 5.68244600 | 18.11677100 |
| H | 11.58482200 | 7.43005500 | 18.06839000 |
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| H | 7.83550300 | 6.59816400 | 12.23564500 |
| C | 9.66132300 | 7.63163300 | 11.74892100 |
| H | 10.70253100 | 7.63708500 | 12.08828600 |
| H | 9.22235800 | 8.59916500 | 12.02475600 |
| C | 9.61811800 | 7.43053000 | 10.23303000 |
| H | 8.58340500 | 7.55154800 | 9.87812000 |
| H | 10.21704900 | 8.19516200 | 9.72234100 |
| C | 10.10999000 | 6.02817300 | 9.87090600 |
| H | 10.00536300 | 5.84328700 | 8.79374500 |
| H | 11.17587600 | 5.93121700 | 10.11734200 |
| C | 9.32207200 | 4.96951400 | 10.64282700 |
| H | 8.26642100 | 5.01492600 | 10.31840900 |
| H | 9.69511800 | 3.96502400 | 10.42131300 |
| C | 11.56667200 | 3.04437800 | 12.50216500 |
| H | 12.03169500 | 3.13616200 | 13.49881500 |
| H | 11.59959900 | 4.03086900 | 12.03433800 |
| C | 12.31855300 | 2.00996200 | 11.66670200 |
| H | 13.37110900 | 2.31003800 | 11.58469800 |
| H | 11.90150700 | 1.99818300 | 10.65011600 |
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| H | 8.30235000 | 1.83177000 | 11.27922600 |
| H | 7.27144400 | 3.09310900 | 10.59030100 |
| C | 6.16010800 | 1.48221400 | 11.47169300 |

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| H | 6.28648100 | 0.74195900 | 12.27311400 |
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| C | 3.97721900 | 7.65051800 | 12.59232500 |
| H | 3.34689700 | 6.84514700 | 12.99415500 |
| H | 4.22536100 | 7.38684200 | 11.55508700 |
| C | 3.21387900 | 8.97665700 | 12.63977500 |
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| H | 3.86435400 | 4.39871800 | 18.69488200 |
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| H | 11.46434400 | -0.94491000 | 18.53686200 |

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| H | 13.09064400 | 2.49014500 | 20.57665900 |
| H | 11.60028000 | 1.79250700 | 21.22382000 |
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| H | 11.92821500 | 3.12944500 | 18.47504300 |
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| H | 7.84345100 | 2.34780900 | 15.78591700 |
| C | 6.02965800 | 1.19173300 | 16.09700900 |
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| H | 5.42605000 | 2.10809500 | 16.11261000 |
| C | 5.44956700 | 0.18072900 | 17.08631000 |
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| H | 5.99142100 | -0.77325800 | 16.99277600 |
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| H | 4.97573900 | 1.59958800 | 18.64772200 |
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| C | 7.04989500 | 1.05995600 | 18.81298200 |
| H | 7.14213600 | 1.51996700 | 19.79905600 |
| H | 7.65005400 | 0.12976900 | 18.81242700 |
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| Fe | 8.29408800 | 5.40545300 | 16.00140600 |
| N | 12.24734200 | 4.43531900 | 16.07871500 |
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| N | 9.05534800 | 4.20314700 | 14.76975700 |
| N | 9.43901100 | 5.21065400 | 12.08232100 |
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| N | 6.71524100 | 6.18001900 | 15.54792900 |
| N | 4.95886600 | 8.14573100 | 14.78306100 |
| N | 4.45843800 | 6.58691900 | 17.17201800 |
| N | 9.24988000 | 4.34938900 | 17.29167600 |
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| N | 7.55172600 | 2.01093700 | 17.82575000 |
| P | 13.55363500 | 5.31718200 | 16.48021700 |
| P | 9.02765200 | 3.86284700 | 13.16691700 |
| P | 5.73037200 | 7.30538700 | 16.13595900 |
| P | 8.81116300 | 3.14599500 | 18.31026200 |
| C | 7.03608300 | 9.68980300 | 16.57425000 |
| H | 6.86513500 | 9.73746000 | 15.49473600 |
| C | 8.51947900 | 9.38794700 | 16.86795600 |

| | | | |
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| C | 7.55684000 | 9.03529400 | 19.16524400 |
| H | 7.70173600 | 8.58145600 | 20.15359000 |
| C | 6.19483700 | 8.59207800 | 18.60479900 |
| H | 5.39419600 | 9.18933500 | 19.07348300 |
| N | 6.11014300 | 8.71911300 | 17.14706500 |
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| H | 9.40370900 | 4.66302100 | 21.11489900 |
| H | 9.37333800 | 2.87981900 | 21.12734700 |
| C | 7.76245600 | 3.81498800 | 22.22573800 |
| H | 8.32447000 | 3.88348800 | 23.16666900 |
| H | 7.19990300 | 2.87166900 | 22.25019300 |
| C | 6.79351100 | 4.98779100 | 22.08357000 |
| H | 6.05262100 | 4.98040300 | 22.89330600 |
| H | 7.35195100 | 5.93196500 | 22.17529600 |
| C | 6.10814200 | 4.93660200 | 20.71872300 |
| H | 5.46734900 | 5.81420900 | 20.56798700 |
| H | 5.46285000 | 4.04930200 | 20.66564500 |
| C | 7.13609600 | 4.86318900 | 19.58937600 |
| H | 6.63261700 | 4.75751700 | 18.62395600 |
| H | 7.71190700 | 5.80539700 | 19.55086100 |
| N | 8.02275000 | 3.72073100 | 19.79313800 |
| H | 6.76628900 | 10.67835000 | 16.97629100 |
| H | 8.94620500 | 8.78077000 | 16.06172500 |
| H | 7.56824400 | 10.12352000 | 19.32017500 |
| H | 5.99991300 | 7.54880600 | 18.86804600 |
| H | 15.24772000 | 7.16977300 | 17.86659700 |
| H | 15.06165800 | 8.26343900 | 20.11016400 |
| H | 13.07581100 | 7.65165800 | 21.56763200 |
| C | 16.16535500 | 4.72856900 | 17.24135300 |
| H | 16.08096300 | 4.81251000 | 18.34125600 |
| H | 16.35284200 | 5.72938300 | 16.84150800 |
| C | 17.33726200 | 3.80737700 | 16.89230500 |
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| C | 17.05486500 | 2.36440200 | 17.31192800 |
| H | 17.87059400 | 1.70340200 | 16.99278900 |
| H | 17.01305600 | 2.30685100 | 18.41019000 |
| C | 15.71705800 | 1.90083800 | 16.73434700 |
| H | 15.78186200 | 1.84680300 | 15.63914500 |
| H | 15.46552800 | 0.89561700 | 17.09726400 |
| C | 14.59931900 | 2.86983900 | 17.11379100 |
| H | 13.65039800 | 2.58686700 | 16.65158200 |

| | | | |
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| H | 14.46088500 | 2.85244000 | 18.21113700 |
| N | 14.92950800 | 4.21723900 | 16.65753000 |
| C | 13.58341700 | 7.72440300 | 15.15384200 |
| H | 14.31546600 | 8.54664500 | 15.09132100 |
| H | 12.93607900 | 7.93461700 | 16.01051200 |
| C | 12.75621000 | 7.67355100 | 13.86977300 |
| H | 12.28186900 | 8.65052000 | 13.70665700 |
| H | 11.95549800 | 6.93343500 | 13.99874600 |
| C | 13.63302400 | 7.28590400 | 12.67841700 |
| H | 13.03407700 | 7.21185300 | 11.76217200 |
| H | 14.38138900 | 8.07436400 | 12.50142900 |
| C | 14.34430300 | 5.96354300 | 12.96443600 |
| H | 13.60349600 | 5.15825200 | 13.04313900 |
| H | 15.03085000 | 5.70264500 | 12.14748500 |
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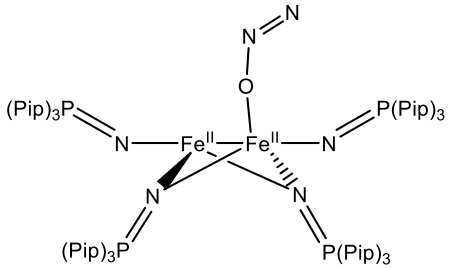


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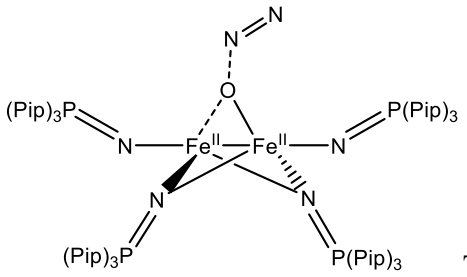


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| H | 1.89105300 | 4.59807200 | 8.49759400 |

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| H | 5.79779300 | 7.86129400 | 18.67153000 |
| H | 7.61671300 | 4.58510400 | 17.47792800 |

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| H | 9.40250500 | 5.53026200 | 12.62965000 |
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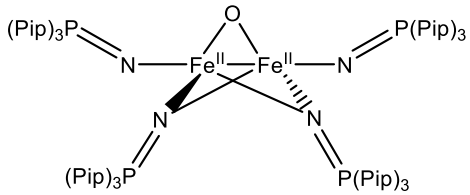


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| H | -1.17610200 | 3.01566400 | 19.05042600 |
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| C | -1.27865700 | 2.60615400 | 16.91621300 |
| H | -2.31608000 | 2.24750400 | 16.91176400 |
| H | -1.31637600 | 3.68062300 | 16.68577800 |
| C | -0.45494200 | 1.89506300 | 15.83979500 |

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| C | 1.01659900 | 2.30035300 | 15.91452000 |
| H | 1.13746500 | 3.37021400 | 15.67948500 |
| H | 1.61839500 | 1.74620000 | 15.19105900 |
| C | 4.31842700 | 1.72254900 | 20.01850000 |
| H | 4.96454600 | 2.46335600 | 19.54017100 |
| H | 3.71463000 | 2.25635400 | 20.77849900 |
| C | 5.11876200 | 0.61690500 | 20.70839400 |
| H | 5.73246100 | 1.04887400 | 21.51056400 |
| H | 5.80373900 | 0.16729700 | 19.97661600 |
| C | 4.18362800 | -0.45704400 | 21.27104700 |
| H | 4.75836000 | -1.28308700 | 21.70910600 |
| C | 3.23437300 | -0.97687200 | 20.18797000 |
| H | 2.50326300 | -1.67437200 | 20.61862000 |
| H | 3.80544000 | -1.52742700 | 19.42845200 |
| C | 2.49980400 | 0.18380200 | 19.51089200 |
| H | 1.83221100 | 0.65792800 | 20.25731000 |
| H | 1.86152100 | -0.16609900 | 18.69774600 |
| C | 5.08503800 | 0.87231400 | 15.73753600 |
| H | 5.42250000 | 1.91186200 | 15.71610100 |
| H | 5.71325800 | 0.32052000 | 16.46519000 |
| C | 5.23542100 | 0.23742000 | 14.35765800 |
| H | 4.70253800 | 0.86139600 | 13.62868300 |
| H | 6.29596400 | 0.23426000 | 14.07382200 |
| C | 4.66898900 | -1.18255200 | 14.34449000 |
| H | 5.28298500 | -1.82412800 | 14.99507400 |
| H | 4.71949400 | -1.61537200 | 13.33717600 |
| C | 3.22805700 | -1.17853900 | 14.85626400 |
| H | 2.83981300 | -2.20222100 | 14.94037500 |
| H | 2.58693800 | -0.64296500 | 14.14334400 |
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| H | 3.66061300 | -1.09468100 | 16.97645400 |
| H | 2.07976100 | -0.41602200 | 16.52391100 |
| C | 5.64548900 | 9.37952700 | 10.95552900 |
| H | 4.83982900 | 10.03554200 | 11.29886800 |
| H | 6.36716500 | 9.29244600 | 11.78769700 |
| C | 6.34121600 | 9.97034800 | 9.72929300 |
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| H | 6.77886300 | 10.94301000 | 9.98942100 |
| C | 7.41765600 | 9.01764900 | 9.20482000 |
| H | 8.23139600 | 8.95329200 | 9.94285800 |
| H | 7.86215600 | 9.40676100 | 8.28007200 |
| C | 6.83687300 | 7.61980400 | 8.98050900 |
| H | 7.62839500 | 6.91124300 | 8.70333200 |
| H | 6.11669800 | 7.64509700 | 8.15133300 |

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|---|---|---|---|
| C | 6.12466900 | 7.12108500 | 10.23785700 |
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| C | 2.43993600 | 5.17988000 | 11.74831500 |
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| H | 1.42602200 | 5.62498200 | 11.74795100 |
| C | 2.37612100 | 3.77353100 | 11.15748400 |
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| H | 1.99611400 | 2.80361100 | 9.24414400 |
| C | 2.85686300 | 4.77081900 | 8.90513400 |
| H | 3.87866500 | 4.37015600 | 8.85627200 |
| H | 2.50174500 | 4.88459900 | 7.87213400 |
| C | 2.89954300 | 6.14467100 | 9.57724300 |
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| Fe | 4.44588200 | 4.59188000 | 16.22254600 |
| Fe | 4.53494900 | 6.08285800 | 14.55906600 |
| N | 4.75920300 | 6.46068500 | 16.39910600 |
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| N | 4.16514900 | 3.34160900 | 17.49947700 |
| N | 1.52414200 | 2.00185800 | 17.26266000 |
| N | 3.45149600 | 1.15516300 | 18.99949100 |
| N | 3.68311900 | 0.85981800 | 16.14221800 |
| N | 4.29906700 | 7.40234800 | 13.34569500 |
| N | 5.07915800 | 8.07192700 | 10.61746000 |
| N | 3.35965600 | 6.00955800 | 10.96045000 |
| O | 3.22712500 | 4.92345600 | 14.96515300 |
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| P | 3.28418600 | 1.99306800 | 17.45446900 |
| P | 3.87312100 | 7.49957500 | 11.79397900 |
| C | 2.07941200 | 9.39508900 | 12.75092100 |
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| H | 2.54593900 | 10.39520300 | 12.84931300 |
| C | 0.56416700 | 9.55981100 | 12.62554500 |
| H | 0.09985200 | 8.56483000 | 12.64958200 |
| H | 0.17976800 | 10.12262500 | 13.48693000 |
| C | 0.20087100 | 10.27053900 | 11.31825800 |
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| C | 0.84458300 | 9.57108000 | 10.11745400 |
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| C | 5.61092100 | 10.73271800 | 15.93547500 |
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| C | 5.36503800 | 11.78776000 | 17.01480400 |
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| C | 5.20439300 | 11.12359700 | 18.38342700 |
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| C | 4.97832000 | 6.19847800 | 21.74900500 |
| H | 5.51386300 | 5.25517000 | 21.56580800 |
| H | 4.99586500 | 6.36602200 | 22.83349800 |
| C | 5.69797900 | 7.33248100 | 21.01655800 |

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| H | 6.05038200 | 7.99582900 | 18.97326300 |
| N | 4.17149200 | 7.08962800 | 19.12004300 |
| C | 7.58702700 | 3.83074400 | 17.54036100 |
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| C | 9.24718500 | 2.08239900 | 18.27085200 |
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| C | 9.52737600 | 8.90502300 | 15.35718100 |
| H | 8.76392200 | 9.51091900 | 15.86587100 |
| H | 10.38621400 | 9.56494800 | 15.17975600 |
| C | 9.92172200 | 7.73601300 | 16.25959600 |
| H | 10.77030400 | 7.19700300 | 15.81705400 |
| H | 10.24274600 | 8.09750900 | 17.24554400 |
| C | 8.76073400 | 6.75485100 | 16.43733900 |
| H | 7.94183700 | 7.23801200 | 16.99776600 |
| H | 9.10322500 | 5.88283900 | 16.99750200 |
| N | 8.30603800 | 6.30104400 | 15.12674800 |
| C | 7.08758100 | 3.79588000 | 12.39725400 |
| H | 6.13830200 | 3.53182200 | 12.86805200 |
| H | 6.88889800 | 4.64865500 | 11.72564100 |
| C | 7.66815300 | 2.64039100 | 11.58359500 |
| H | 7.75262800 | 1.75476600 | 12.22796100 |
| H | 6.97459900 | 2.38640700 | 10.77146100 |
| C | 9.04416600 | 3.00653300 | 11.02395500 |
| H | 8.93143600 | 3.82399300 | 10.29548300 |

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|---|---|---|---|
| H | 9.48391300 | 2.16050000 | 10.48067800 |
| C | 9.97427100 | 3.46197600 | 12.14939600 |
| H | 10.19402200 | 2.61189900 | 12.80981700 |
| H | 10.93363400 | 3.81031300 | 11.74445400 |
| C | 9.34186900 | 4.58756700 | 12.97317800 |
| H | 9.26990200 | 5.49483200 | 12.34544800 |
| H | 9.96652900 | 4.84378400 | 13.83184400 |
| N | 8.02147400 | 4.19078600 | 13.44780100 |
| H | 3.58919400 | -0.02059300 | 22.08843300 |

**Powder X-Ray Diffraction**

Laboratory PXRD was collected on a PANalytical X'Pert PRO Alpha-1 diffractometer with Cu Kα source in reflection geometry equipped with a fixed divergence slit of 1/8 “, a convergence slit of ¼ “and a working radius of 240 mm. The samples were homogenized by finely grinding them inside the glove box using an agate mortar for about ~15 min. To avoid the exposure of sample to atmospheric air, PANalytical domed sample holder equipped with stainless steel base and a polycarbonate dome with a 70% X-ray transmission. A 2θ range of 5–85° was used with a scan speed of 5 s and a step size of 0.1. Quantitative Rietveld refinements to the laboratory XRD data were carried out using Bruker TOPAS 5 suite.[10-12]

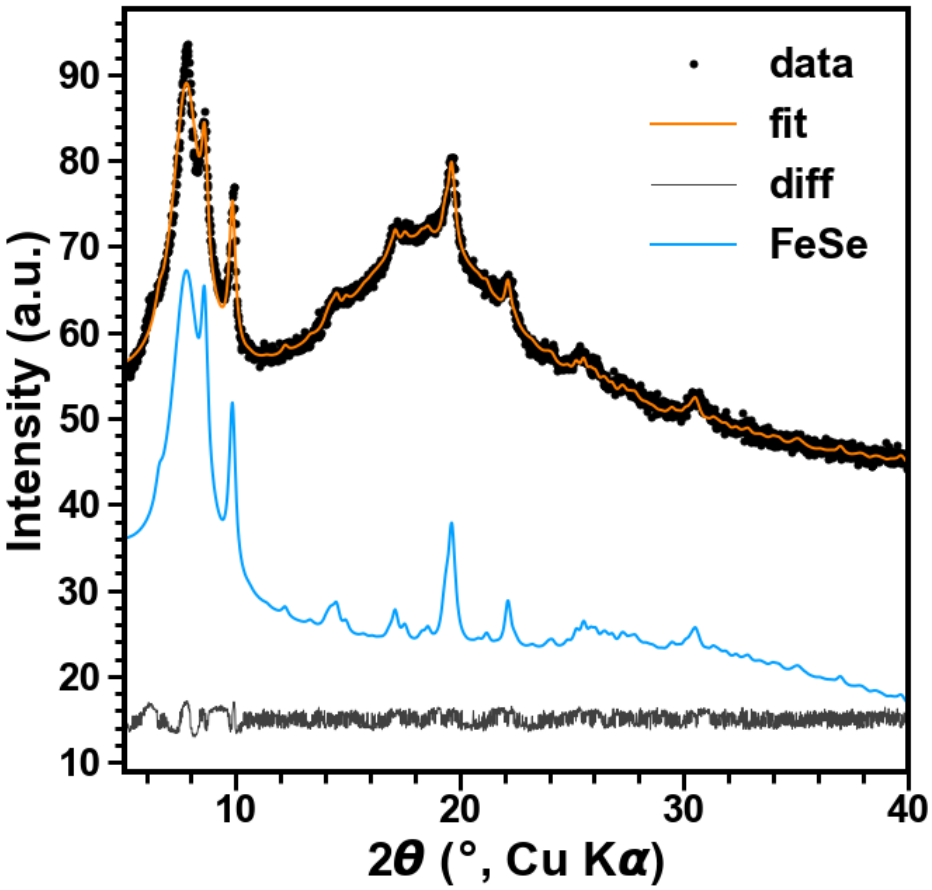


**Figure S35.** Laboratory powder X-ray diffraction patterns of **4-Fe** collected at 300 K. Phase purity was confirmed using Rietveld refinements. PXRD data is shown in black, Rietveld fits in orange and difference curves in light grey. No impurity phase was observed in the laboratory PXRD data. The broad hump around 2θ = 20° is due to the polycarbonate dome in the sample holder. The broad hump was modeled by introducing a peak in the background. Rietveld refinements were carried out using Topas v5.0.[10-12]

## Crystallographic Analyses

Crystals suitable for X-ray diffraction were covered in paratone oil in a glove box and transferred to the diffractometer in a 20-mL capped vial. Crystals were mounted on a loop with paratone oil on a Bruker D8 VENTURE diffractometer. The crystals were cooled and kept at T = 100(2) K during data collections. The structures were solved with the ShelXT structure solution program using the Intrinsic Phasing solution method and by using Olex2 as the graphical interface.[13,14] The model was refined with version 2014/7 of XL using Least Squares minimization.[15] Structures were visualized in Mercury and graphics were generated with POV-ray.[16,17]

**Table 1.** Relevant crystallographic metrics of **1-Fe**, **2-Fe**, **3-Fe**, **4-Fe**, and **1-Co**.

| **Compound/Metric** | **1-Fe** | **2-Fe** | **3-Fe** | **4-Fe** | **1-Co** |
|---|---|---|---|---|---|
| Avg. M–M dist. | 2.6114(5) Å | 2.3396(6) Å | 2.5964(4) Å | 2.6072(11) Å | 2.6264(17) |
| Avg. terminal Fe–$N_{imido}$ dist. | 1.8601(18) Å | 1.837(2) Å | 1.8281(9) Å | 1.822(3) Å | 1.799(7) |
| Avg. bridging Fe–$N_{imido}$ dist. | 1.9534(16) Å | 2.0265(2) Å | 1.9819(9) Å | 1.979(3) Å | 1.927(7) |
| Avg. terminal P–$N_{imido}$ dist. | 1.5340(14) Å | 1.5395(2) Å | 1.5429(10) Å | 1.541(3) Å | 1.584(8) |
| Avg. bridging P–$N_{imido}$ dist. | 1.5584(16) Å | 1.5475(2) Å | 1.5591(9) Å | 1.557(4) Å | 1.578(6) |
| Avg.terminal P–$N_{imido}$–M angle | 140.39(13)° | 138.35(15)° | 147.98(17)° | 147.7(2)° | 138.9(5) |
| Formal Shortness Ratio (FSR) | 1.05 | 0.94 | 1.05 | 1.05 | 1.07 |

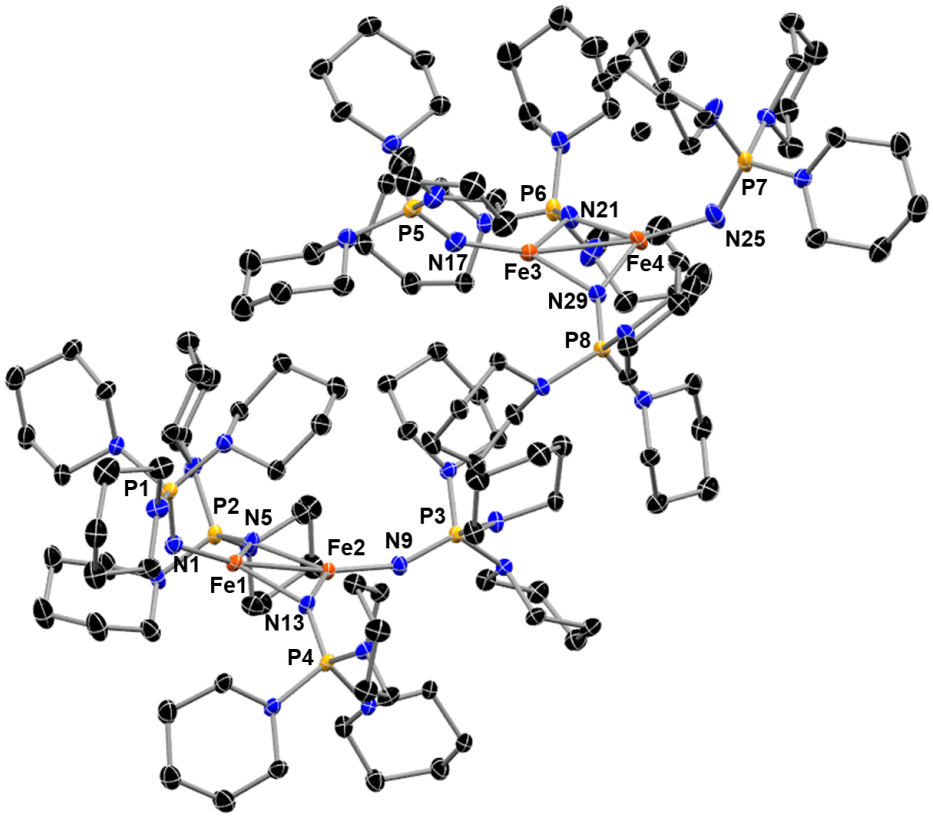


**Figure S36.** Molecular structure of **1-Fe** with thermal ellipsoids shown at 50% probability; H atoms are omitted for clarity.

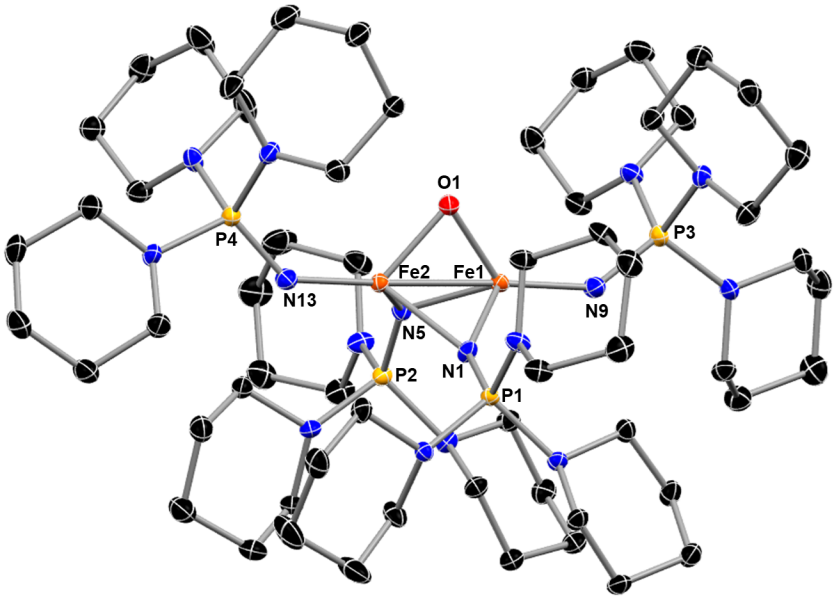


**Figure S37.** Molecular structure of **2-Fe** with thermal ellipsoids shown at 50% probability; H atoms are omitted for clarity.

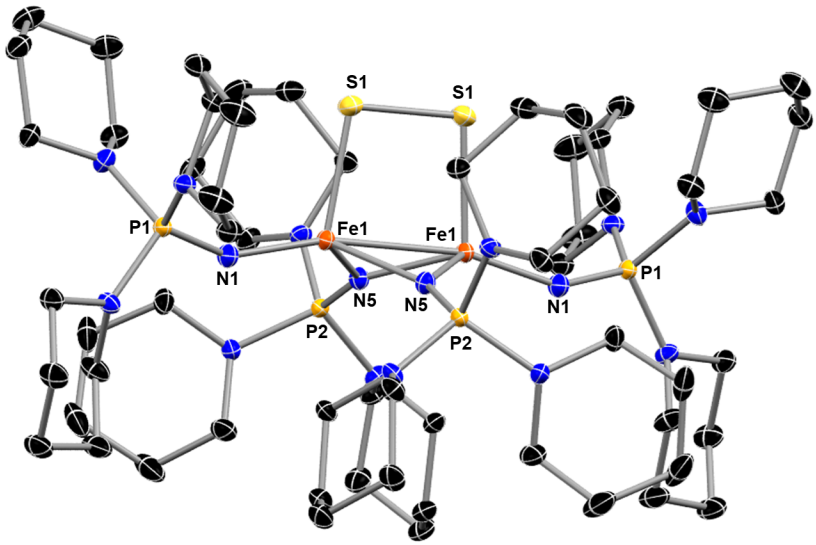


**Figure S38.** Molecular structure of **3-Fe** with thermal ellipsoids shown at 50% probability; H atoms are omitted for clarity.

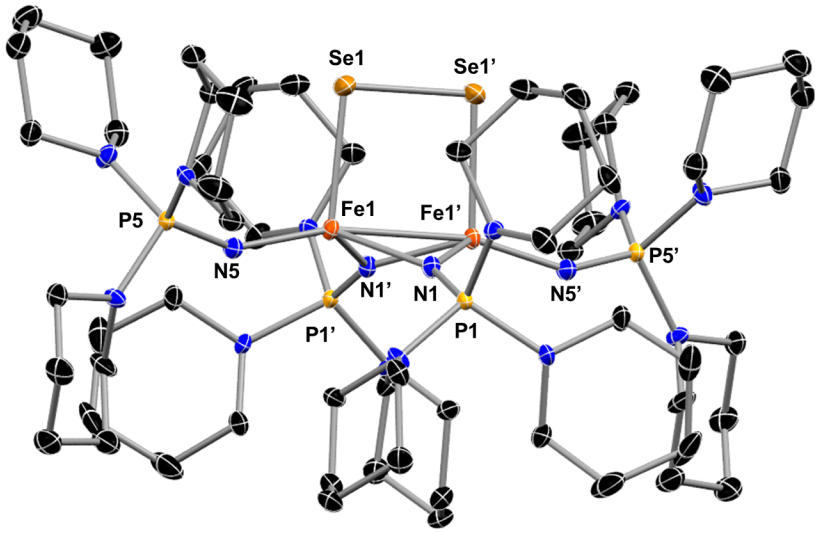


**Figure S39.** Molecular structure of **4-Fe** with thermal ellipsoids shown at 50% probability; H atoms are omitted for clarity.

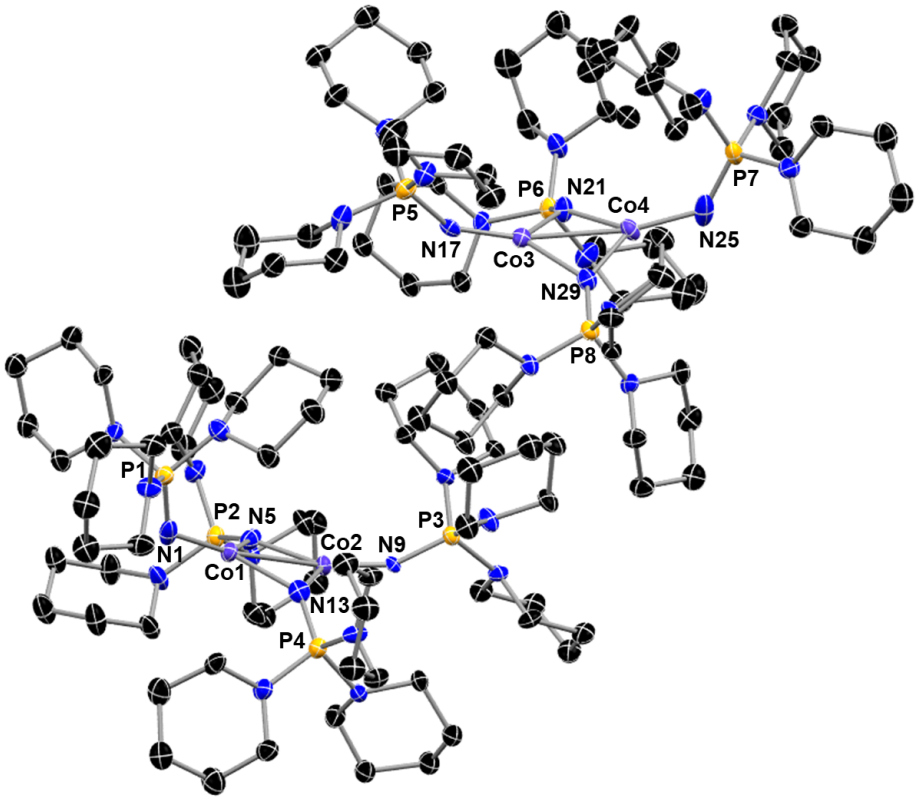


**Figure S40.** Molecular structure of **1-Co** with thermal ellipsoids shown at 50% probability; H atoms are omitted for clarity.

**Table S2.** Crystallographic Data and Structure Refinement for **1-Fe**, **2-Fe**, **3-Fe**, **4-Fe**, and **1-Co**.

| | **1-Fe** | **2-Fe** | **3-Fe** | **4-Fe** | **1-Co** |
|---|---|---|---|---|---|
| ***Empirical Formula*** | $C_{60}H_{120}Fe_2N_{16}P_4$ | $C_{60}H_{120}Fe_2N_{16}OP_4$ | $C_{120}H_{240}Fe_4N_{32}P_8S_4$ | $C_{120}H_{240}Fe_4N_{32}P_8Se_4$ | $C_{60}H_{120}Co_2N_{16}P_4$ |
| ***Formula Weight*** | 1301.29 | 1317.29 | 2730.83 | 1459.21 | 1307.45 |
| ***Temperature (K)*** | 100(2) | 100(2) | 99.99 | 100.0 | 100(2) |
| ***Crystal System*** | triclinic | triclinic | Monoclinic | Monoclinic | triclinic |
| ***Space Group*** | P-$\bar{1}$ | P-$\bar{1}$ | *C*2/*c* | *C*2/*c* | P-$\bar{1}$ |
| ***a/Å*** | 15.746(2) | 13.069(2) | 26.121(3) | 26.073(3) | 15.746(2) |
| ***b/Å*** | 20.493(3) | 13.560(2) | 9.9298(10) | 9.9415(9) | 20.493(3) |
| ***c/Å*** | 21.460(3) | 21.307(4) | 27.898(3) | 27.859(2) | 21.460(3) |
| ***α/°*** | 95.749(6) | 100.590(7) | 90 | 90 | 95.749(6) |
| ***β/°*** | 92.265(6) | 95.542(7) | 103.715(4) | 103.714(3) | 92.265(6) |
| ***γ/°*** | 90.151(6) | 109.567(6) | 90 | 90 | 90.151(6) |
| ***Volume/Å3*** | 6884.3(18) | 3445.9(10) | 7029.7(13) | 7015.3(11) | 6884.3(18) |
| ***Z*** | 4 | 2 | 2 | 4 | 4 |
| ***Z'*** | 2 | 1 | 0.25 | 0.5 | 2 |
| ***ρ(g/cm3)*** | 1.256 | 1.270 | 1.290 | 1.382 | 1.261 |
| ***μ(mm-1)*** | 0.564 | 0.565 | 0.612 | 15.592 | 0.624 |
| ***F(000)*** | 2816.0 | 1424.0 | 2944.0 | 3088.0 | 2824.0 |
| ***Crystal Size/mm3*** | 0.394 x 0.309 x 0.264 | 0.243 x 0.118 x 0.117 | 0.489 x 0.293 x 0.19 | 0.126 x 0.055 x 0.05 | 0.503 x 0.318 x 0.179 |
| ***Radiation*** | MoK$\alpha$ ($\lambda$=0.71073) | MoK$\alpha$ ($\lambda$=0.71073) | MoK$\alpha$ ($\lambda$=0.71073) | MoK$\alpha$ ($\lambda$=0.71073) | MoK$\alpha$ ($\lambda$=0.71073) |
| ***2θ range for data collection(°)*** | 3.818 to 61.016 | 4.512 to 58.26 | 4.404 to 71.258 | 3.848 to 55.01 | 4.484 to 51.364 |
| ***Index Ranges*** | -22 ≤ h ≤ 22, -29 ≤ k ≤25, -30 ≤ 1 ≤ 30 | -17 ≤ h ≤ 17, -18 ≤ k ≤18, -29 ≤ 1 ≤ 28 | -42 ≤ h ≤ 42, -16 ≤ k ≤16, -45 ≤ 1 ≤ 45 | -33 ≤ h ≤ 33, -12 ≤ k ≤12, -33 ≤ 1 ≤ 36 | -19 ≤ h ≤ 19, -24 ≤ k ≤24, -26 ≤ 1 ≤ 26 |
| ***Reflections Collected*** | 337894 | 43669 | 82455 | 47790 | 153159 |
| ***Independent Reflections*** | 42043 [Rint = 0.0892, Rsigma = 0.0474]] | 18470 [Rint = 0.0567, Rsigma = 0.0837]] | 16183 [Rint = 0.0692, Rsigma = 0.0528]] | 8028 [Rint = 0.1070, Rsigma = 0.0707]] | 25962 [Rint = 0.0949, Rsigma = 0.0592]] |
| ***Data/Restraints/ Parameters*** | 42043/20354/1651 | 18470/360/748 | 16183/0/380 | 8028/0/379 | 25962/20354/1653 |
| ***Goodness-of-Fit on F2*** | 1.054 | 1.030 | 1.039 | 1.062 | 1.593 |
| ***Final R Indexes [I>=2σ (I)]*** | R1=0.0491, wR2=0.1147 | R1=0.0587, wR2=0.1053 | R1=0.0377, wR2=0.0919 | R1=0.0633, wR2=0.1533 | R1=0.1141, wR2=0.3282 |
| ***Final R Indexes [all data]*** | R1=0.0641, wR2=0.1227 | R1=0.0952, wR2=0.1227 | R1=0.0537, wR2=0.1033 | R1=0.0925, wR2=0.1707 | R1=0.1445, wR2=0.3674 |
| ***Largest Diff. Peak/Hole/ (e Å3)*** | 1.13/-0.82 | 0.51/-0.57 | 0.55/-0.61 | 0.62/-1.02 | 2.55/-1.12 |
| ***Flack Parameter*** | - | - | - | - | - |
| ***Completeness to 2θ*** | 100 | 100 | 100 | 100 | 99 |

**Table S3.** Lengths for **1-Fe**

| Atom | Atom | Length/Å |
|---|---|---|
| Fe1 | Fe2 | 2.6164(5) |
| Fe1 | N1 | 1.8724(17) |
| Fe1 | N5 | 1.9370(15) |
| Fe1 | N13 | 1.9551(16) |
| Fe2 | N5 | 1.9233(15) |
| Fe2 | N9 | 1.8545(16) |
| Fe2 | N13 | 1.9710(15) |
| P1 | N1 | 1.5435(18) |
| P1 | N2_1 | 1.6678(13) |
| P1 | N2_4 | 1.6814(13) |
| P1 | N2_5 | 1.6955(14) |
| P3 | N9 | 1.5267(17) |
| P3 | N2_8 | 1.6861(12) |
| P3 | N2_9 | 1.6733(13) |
| P3 | N2_10 | 1.6981(13) |
| P4 | N13 | 1.5534(16) |
| P4 | N2_2 | 1.6720(13) |
| P4 | N2_3 | 1.6604(13) |
| P4 | N2_22 | 1.6738(13) |
| N5 | P2 | 1.5820(14) |
| Fe3 | Fe4 | 2.6064(5) |
| Fe3 | N17 | 1.8554(18) |
| Fe3 | N21 | 1.9570(17) |
| Fe3 | N29 | 1.9706(17) |
| Fe4 | N21 | 1.9533(17) |
| Fe4 | N25 | 1.8581(19) |
| Fe4 | N29 | 1.9596(16) |
| P5 | N17 | 1.5268(18) |
| P5 | N2_11 | 1.6858(14) |
| P5 | N2_12 | 1.6867(13) |
| P5 | N2_14 | 1.6957(13) |
| P7 | N25 | 1.539(2) |
| P7 | N2_16 | 1.647(2) |
| P7 | N2_17 | 1.716(2) |
| P7 | N2_18 | 1.6867(13) |
| P7 | N2_19 | 1.6634(13) |
| N21 | P6 | 1.5517(17) |
| N29 | P8 | 1.5465(16) |
| P2 | N2_6 | 1.6547(13) |

| Atom | Atom | Length/Å |
|---|---|---|
| C3_9 | C4_9 | 1.5240(14) |
| C4_9 | C5_9 | 1.5214(14) |
| N2_10 | C1_10 | 1.4694(13) |
| N2_10 | C5_10 | 1.4712(13) |
| C1_10 | C2_10 | 1.5180(14) |
| C2_10 | C3_10 | 1.5269(14) |
| C3_10 | C4_10 | 1.5248(14) |
| C4_10 | C5_10 | 1.5216(14) |
| N2_11 | C1_11 | 1.4700(13) |
| N2_11 | C5_11 | 1.4716(13) |
| C1_11 | C2_11 | 1.5195(14) |
| C2_11 | C3_11 | 1.5253(14) |
| C3_11 | C4_11 | 1.5239(15) |
| C4_11 | C5_11 | 1.5231(14) |
| N2_12 | C1_12 | 1.4676(13) |
| N2_12 | C5_12 | 1.4664(14) |
| C1_12 | C2_12 | 1.5172(14) |
| C2_12 | C3_12 | 1.5284(15) |
| C3_12 | C4_12 | 1.5212(15) |
| C4_12 | C5_12 | 1.5166(14) |
| N2_13 | C1_13 | 1.4729(13) |
| N2_13 | C5_13 | 1.4724(13) |
| C1_13 | C2_13 | 1.5210(13) |
| C2_13 | C3_13 | 1.5265(14) |
| C3_13 | C4_13 | 1.5239(14) |
| C4_13 | C5_13 | 1.5230(14) |
| N2_14 | C1_14 | 1.4697(13) |
| N2_14 | C5_14 | 1.4692(13) |
| C1_14 | C2_14 | 1.5211(14) |
| C2_14 | C3_14 | 1.5287(14) |
| C3_14 | C4_14 | 1.5234(14) |
| C4_14 | C5_14 | 1.5189(14) |
| N2_15 | C1_15 | 1.4701(13) |
| N2_15 | C5_15 | 1.4715(13) |
| C1_15 | C2_15 | 1.5204(14) |
| C2_15 | C3_15 | 1.5252(14) |
| C3_15 | C4_15 | 1.5241(14) |
| C4_15 | C5_15 | 1.5224(14) |
| N2_16 | C1_16 | 1.4744(15) |

| | | | | | |
|---|---|---|---|---|---|
| P2 | N2_7 | 1.6665(13) | N2_16 | C5_16 | 1.4759(15) |
| P2 | N2_24 | 1.6571(13) | C1_16 | C2_16 | 1.5232(15) |
| P6 | N2_15 | 1.6641(13) | C2_16 | C3_16 | 1.5271(15) |
| P6 | N2_20 | 1.6617(13) | C3_16 | C4_16 | 1.5231(16) |
| P6 | N2_25 | 1.6527(15) | C4_16 | C5_16 | 1.5239(15) |
| P8 | N2_13 | 1.6703(12) | N2_17 | C1_17 | 1.4762(15) |
| P8 | N2_21 | 1.6789(13) | N2_17 | C5_17 | 1.4764(15) |
| P8 | N2_23 | 1.6827(13) | C1_17 | C2_17 | 1.5203(15) |
| N2_1 | C1_1 | 1.4643(13) | C2_17 | C3_17 | 1.5280(15) |
| N2_1 | C5_1 | 1.4655(13) | C3_17 | C4_17 | 1.5242(15) |
| C1_1 | C2_1 | 1.5196(14) | C4_17 | C5_17 | 1.5218(15) |
| C2_1 | C3_1 | 1.5260(14) | N2_18 | C1_18 | 1.4693(13) |
| C3_1 | C4_1 | 1.5232(14) | N2_18 | C5_18 | 1.4702(13) |
| C4_1 | C5_1 | 1.5205(14) | C1_18 | C2_18 | 1.5212(14) |
| N2_2 | C1_2 | 1.4681(13) | C2_18 | C3_18 | 1.5273(14) |
| N2_2 | C5_2 | 1.4689(13) | C3_18 | C4_18 | 1.5233(14) |
| C1_2 | C2_2 | 1.5206(14) | C4_18 | C5_18 | 1.5203(14) |
| C2_2 | C3_2 | 1.5262(14) | N2_19 | C1_19 | 1.4628(13) |
| C3_2 | C4_2 | 1.5230(14) | N2_19 | C5_19 | 1.4651(13) |
| C4_2 | C5_2 | 1.5196(14) | C1_19 | C2_19 | 1.5183(14) |
| N2_3 | C1_3 | 1.4627(13) | C2_19 | C3_19 | 1.5270(14) |
| N2_3 | C5_3 | 1.4665(13) | C3_19 | C4_19 | 1.5244(15) |
| C1_3 | C2_3 | 1.5198(14) | C4_19 | C5_19 | 1.5209(14) |
| C2_3 | C3_3 | 1.5262(14) | N2_20 | C1_20 | 1.4667(13) |
| C3_3 | C4_3 | 1.5229(14) | N2_20 | C5_20 | 1.4656(13) |
| C4_3 | C5_3 | 1.5231(14) | C1_20 | C2_20 | 1.5200(14) |
| N2_4 | C1_4 | 1.4677(13) | C2_20 | C3_20 | 1.5255(14) |
| N2_4 | C5_4 | 1.4701(13) | C3_20 | C4_20 | 1.5238(15) |
| C1_4 | C2_4 | 1.5192(14) | C4_20 | C5_20 | 1.5220(15) |
| C2_4 | C3_4 | 1.5262(14) | N2_21 | C1_21 | 1.4689(13) |
| C3_4 | C4_4 | 1.5238(14) | N2_21 | C5_21 | 1.4694(13) |
| C4_4 | C5_4 | 1.5219(14) | C1_21 | C2_21 | 1.5199(14) |
| N2_5 | C1_5 | 1.4705(13) | C2_21 | C3_21 | 1.5269(14) |
| N2_5 | C5_5 | 1.4716(13) | C3_21 | C4_21 | 1.5241(14) |
| C1_5 | C2_5 | 1.5204(14) | C4_21 | C5_21 | 1.5231(14) |
| C2_5 | C3_5 | 1.5272(15) | N2_22 | C1_22 | 1.4717(13) |
| C3_5 | C4_5 | 1.5237(14) | N2_22 | C5_22 | 1.4725(13) |
| C4_5 | C5_5 | 1.5217(14) | C1_22 | C2_22 | 1.5206(14) |
| N2_6 | C1_6 | 1.4650(13) | C2_22 | C3_22 | 1.5272(14) |
| N2_6 | C5_6 | 1.4640(13) | C3_22 | C4_22 | 1.5231(14) |
| C1_6 | C2_6 | 1.5208(14) | C4_22 | C5_22 | 1.5226(13) |

| | | | | | |
|---|---|---|---|---|---|
| C2_6 | C3_6 | 1.5266(14) | N2_23 | C1_23 | 1.4701(13) |
| C3_6 | C4_6 | 1.5224(14) | N2_23 | C5_23 | 1.4715(13) |
| C4_6 | C5_6 | 1.5208(14) | C1_23 | C2_23 | 1.5223(13) |
| N2_7 | C1_7 | 1.4711(13) | C2_23 | C3_23 | 1.5282(14) |
| N2_7 | C5_7 | 1.4697(13) | C3_23 | C4_23 | 1.5238(14) |
| C1_7 | C2_7 | 1.5220(14) | C4_23 | C5_23 | 1.5217(14) |
| C2_7 | C3_7 | 1.5271(14) | N2_24 | C1_24 | 1.4643(13) |
| C3_7 | C4_7 | 1.5220(14) | N2_24 | C5_24 | 1.4666(13) |
| C4_7 | C5_7 | 1.5222(14) | C1_24 | C2_24 | 1.5220(14) |
| N2_8 | C1_8 | 1.4707(13) | C2_24 | C3_24 | 1.5273(14) |
| N2_8 | C5_8 | 1.4719(13) | C3_24 | C4_24 | 1.5223(14) |
| C1_8 | C2_8 | 1.5225(14) | C4_24 | C5_24 | 1.5220(14) |
| C2_8 | C3_8 | 1.5271(14) | N2_25 | C1_25 | 1.4617(13) |
| C3_8 | C4_8 | 1.5222(14) | N2_25 | C5_25 | 1.4669(13) |
| C4_8 | C5_8 | 1.5210(14) | C1_25 | C2_25 | 1.5179(14) |
| N2_9 | C1_9 | 1.4642(13) | C2_25 | C3_25 | 1.5262(15) |
| N2_9 | C5_9 | 1.4652(13) | C3_25 | C4_25 | 1.5216(15) |
| C1_9 | C2_9 | 1.5210(14) | C4_25 | C5_25 | 1.5210(15) |
| C2_9 | C3_9 | 1.5269(14) | | | |

**Table S4.** Angles for **1-Fe**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| N1 | Fe1 | Fe2 | 169.60(6) | N2_7 | C5_7 | C4_7 | 109.69(12) |
| N1 | Fe1 | N5 | 133.57(7) | C1_8 | N2_8 | P3 | 116.72(9) |
| N1 | Fe1 | N13 | 131.47(7) | C1_8 | N2_8 | C5_8 | 110.19(12) |
| N5 | Fe1 | Fe2 | 47.11(5) | C5_8 | N2_8 | P3 | 117.40(10) |
| N5 | Fe1 | N13 | 94.78(6) | N2_8 | C1_8 | C2_8 | 109.64(11) |
| N13 | Fe1 | Fe2 | 48.47(4) | C1_8 | C2_8 | C3_8 | 110.27(12) |
| N5 | Fe2 | Fe1 | 47.55(4) | C4_8 | C3_8 | C2_8 | 110.17(12) |
| N5 | Fe2 | N13 | 94.71(7) | C5_8 | C4_8 | C3_8 | 111.86(12) |
| N9 | Fe2 | Fe1 | 169.10(6) | N2_8 | C5_8 | C4_8 | 110.78(12) |
| N9 | Fe2 | N5 | 135.02(7) | C1_9 | N2_9 | P3 | 122.53(11) |
| N9 | Fe2 | N13 | 130.07(7) | C1_9 | N2_9 | C5_9 | 112.35(12) |
| N13 | Fe2 | Fe1 | 47.95(5) | C5_9 | N2_9 | P3 | 125.10(10) |
| N1 | P1 | N2_1 | 112.15(8) | N2_9 | C1_9 | C2_9 | 110.84(12) |
| N1 | P1 | N2_4 | 112.03(8) | C1_9 | C2_9 | C3_9 | 111.16(13) |
| N1 | P1 | N2_5 | 121.98(9) | C4_9 | C3_9 | C2_9 | 110.35(13) |
| N2_1 | P1 | N2_4 | 108.22(9) | C5_9 | C4_9 | C3_9 | 111.08(13) |
| N2_1 | P1 | N2_5 | 101.05(8) | N2_9 | C5_9 | C4_9 | 111.48(12) |
| N2_4 | P1 | N2_5 | 99.95(7) | C1_10 | N2_10 | P3 | 113.55(9) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N9 | P3 | N2_8 | 117.83(9) | C1_10 | N2_10 | C5_10 | 111.03(12) |
| N9 | P3 | N2_9 | 114.09(8) | C5_10 | N2_10 | P3 | 121.76(10) |
| N9 | P3 | N2_10 | 113.99(8) | N2_10 | C1_10 | C2_10 | 111.81(12) |
| N2_8 | P3 | N2_10 | 99.90(7) | C1_10 | C2_10 | C3_10 | 111.54(12) |
| N2_9 | P3 | N2_8 | 101.71(7) | C4_10 | C3_10 | C2_10 | 109.20(12) |
| N2_9 | P3 | N2_10 | 107.65(8) | C5_10 | C4_10 | C3_10 | 110.20(12) |
| N13 | P4 | N2_2 | 113.28(8) | N2_10 | C5_10 | C4_10 | 110.46(12) |
| N13 | P4 | N2_3 | 110.03(8) | C1_11 | N2_11 | P5 | 116.15(11) |
| N13 | P4 | N2_22 | 117.83(8) | C1_11 | N2_11 | C5_11 | 110.25(13) |
| N2_2 | P4 | N2_22 | 100.63(7) | C5_11 | N2_11 | P5 | 117.52(11) |
| N2_3 | P4 | N2_2 | 109.78(8) | N2_11 | C1_11 | C2_11 | 110.53(13) |
| N2_3 | P4 | N2_22 | 104.57(7) | C1_11 | C2_11 | C3_11 | 112.11(14) |
| P1 | N1 | Fe1 | 126.45(11) | C4_11 | C3_11 | C2_11 | 110.10(14) |
| Fe2 | N5 | Fe1 | 85.34(6) | C5_11 | C4_11 | C3_11 | 109.97(14) |
| P2 | N5 | Fe1 | 135.33(10) | N2_11 | C5_11 | C4_11 | 109.69(12) |
| P2 | N5 | Fe2 | 133.92(10) | C1_12 | N2_12 | P5 | 120.24(11) |
| P3 | N9 | Fe2 | 151.87(12) | C5_12 | N2_12 | P5 | 122.73(11) |
| Fe1 | N13 | Fe2 | 83.58(6) | C5_12 | N2_12 | C1_12 | 112.07(13) |
| P4 | N13 | Fe1 | 137.95(10) | N2_12 | C1_12 | C2_12 | 111.03(14) |
| P4 | N13 | Fe2 | 128.44(10) | C1_12 | C2_12 | C3_12 | 110.49(14) |
| N17 | Fe3 | Fe4 | 161.95(6) | C4_12 | C3_12 | C2_12 | 109.68(14) |
| N17 | Fe3 | N21 | 132.99(7) | C5_12 | C4_12 | C3_12 | 111.62(15) |
| N17 | Fe3 | N29 | 132.08(7) | N2_12 | C5_12 | C4_12 | 111.86(14) |
| N21 | Fe3 | Fe4 | 48.14(5) | C1_13 | N2_13 | P8 | 118.68(10) |
| N21 | Fe3 | N29 | 94.26(7) | C5_13 | N2_13 | P8 | 116.69(9) |
| N29 | Fe3 | Fe4 | 48.28(5) | C5_13 | N2_13 | C1_13 | 110.66(12) |
| N21 | Fe4 | Fe3 | 48.26(5) | N2_13 | C1_13 | C2_13 | 109.75(11) |
| N21 | Fe4 | N29 | 94.73(7) | C1_13 | C2_13 | C3_13 | 111.41(12) |
| N25 | Fe4 | Fe3 | 166.27(8) | C4_13 | C3_13 | C2_13 | 110.85(12) |
| N25 | Fe4 | N21 | 132.22(8) | C5_13 | C4_13 | C3_13 | 110.69(12) |
| N25 | Fe4 | N29 | 132.99(8) | N2_13 | C5_13 | C4_13 | 110.02(11) |
| N29 | Fe4 | Fe3 | 48.64(5) | C1_14 | N2_14 | P5 | 122.48(10) |
| N17 | P5 | N2_11 | 117.76(10) | C5_14 | N2_14 | P5 | 114.24(10) |
| N17 | P5 | N2_12 | 113.98(9) | C5_14 | N2_14 | C1_14 | 111.37(13) |
| N17 | P5 | N2_14 | 113.96(9) | N2_14 | C1_14 | C2_14 | 110.28(12) |
| N2_11 | P5 | N2_12 | 101.10(8) | C1_14 | C2_14 | C3_14 | 110.20(13) |
| N2_11 | P5 | N2_14 | 99.94(7) | C4_14 | C3_14 | C2_14 | 109.33(13) |
| N2_12 | P5 | N2_14 | 108.46(9) | C5_14 | C4_14 | C3_14 | 111.47(13) |
| N25 | P7 | N2_16 | 120.92(17) | N2_14 | C5_14 | C4_14 | 112.02(13) |
| N25 | P7 | N2_17 | 123.74(17) | C1_15 | N2_15 | P6 | 120.08(10) |
| N25 | P7 | N2_18 | 111.79(10) | C1_15 | N2_15 | C5_15 | 111.04(12) |

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|---|---|---|---|---|---|---|---|
| N25 | P7 | N2_19 | 111.04(9) | C5_15 | N2_15 | P6 | 116.28(10) |
| N2_16 | P7 | N2_18 | 101.18(12) | N2_15 | C1_15 | C2_15 | 109.75(12) |
| N2_16 | P7 | N2_19 | 102.33(13) | C1_15 | C2_15 | C3_15 | 111.25(13) |
| N2_18 | P7 | N2_17 | 99.57(12) | C4_15 | C3_15 | C2_15 | 111.31(13) |
| N2_19 | P7 | N2_17 | 100.77(13) | C5_15 | C4_15 | C3_15 | 110.42(12) |
| N2_19 | P7 | N2_18 | 108.49(9) | N2_15 | C5_15 | C4_15 | 109.27(12) |
| P5 | N17 | Fe3 | 151.84(13) | C1_16 | N2_16 | P7 | 113.0(2) |
| Fe4 | N21 | Fe3 | 83.60(6) | C1_16 | N2_16 | C5_16 | 109.48(19) |
| P6 | N21 | Fe3 | 131.66(10) | C5_16 | N2_16 | P7 | 109.3(2) |
| P6 | N21 | Fe4 | 136.11(11) | N2_16 | C1_16 | C2_16 | 108.17(17) |
| P7 | N25 | Fe4 | 131.41(15) | C1_16 | C2_16 | C3_16 | 110.81(17) |
| Fe4 | N29 | Fe3 | 83.09(6) | C4_16 | C3_16 | C2_16 | 110.64(17) |
| P8 | N29 | Fe3 | 130.37(10) | C3_16 | C4_16 | C5_16 | 110.76(17) |
| P8 | N29 | Fe4 | 145.73(11) | N2_16 | C5_16 | C4_16 | 108.54(17) |
| N5 | P2 | N2_6 | 111.65(8) | C1_17 | N2_17 | P7 | 123.6(2) |
| N5 | P2 | N2_7 | 117.23(8) | C1_17 | N2_17 | C5_17 | 109.54(17) |
| N5 | P2 | N2_24 | 112.46(9) | C5_17 | N2_17 | P7 | 125.6(2) |
| N2_6 | P2 | N2_7 | 105.60(8) | N2_17 | C1_17 | C2_17 | 110.60(19) |
| N2_6 | P2 | N2_24 | 108.42(8) | C1_17 | C2_17 | C3_17 | 110.70(17) |
| N2_24 | P2 | N2_7 | 100.60(7) | C4_17 | C3_17 | C2_17 | 109.33(17) |
| N21 | P6 | N2_15 | 117.01(9) | C5_17 | C4_17 | C3_17 | 110.85(18) |
| N21 | P6 | N2_20 | 112.53(9) | N2_17 | C5_17 | C4_17 | 110.50(19) |
| N21 | P6 | N2_25 | 112.38(9) | C1_18 | N2_18 | P7 | 122.04(10) |
| N2_20 | P6 | N2_15 | 100.73(8) | C1_18 | N2_18 | C5_18 | 111.15(13) |
| N2_25 | P6 | N2_15 | 104.72(9) | C5_18 | N2_18 | P7 | 114.87(10) |
| N2_25 | P6 | N2_20 | 108.49(9) | N2_18 | C1_18 | C2_18 | 110.51(12) |
| N29 | P8 | N2_13 | 118.34(8) | C1_18 | C2_18 | C3_18 | 110.66(13) |
| N29 | P8 | N2_21 | 112.19(8) | C4_18 | C3_18 | C2_18 | 109.85(13) |
| N29 | P8 | N2_23 | 110.69(8) | C5_18 | C4_18 | C3_18 | 110.99(14) |
| N2_13 | P8 | N2_21 | 100.87(7) | N2_18 | C5_18 | C4_18 | 110.96(13) |
| N2_13 | P8 | N2_23 | 102.62(7) | C1_19 | N2_19 | P7 | 125.13(11) |
| N2_21 | P8 | N2_23 | 111.45(8) | C1_19 | N2_19 | C5_19 | 112.94(12) |
| C1_1 | N2_1 | P1 | 121.60(11) | C5_19 | N2_19 | P7 | 120.79(11) |
| C1_1 | N2_1 | C5_1 | 112.84(12) | N2_19 | C1_19 | C2_19 | 110.90(13) |
| C5_1 | N2_1 | P1 | 125.15(11) | C1_19 | C2_19 | C3_19 | 110.58(13) |
| N2_1 | C1_1 | C2_1 | 110.68(13) | C4_19 | C3_19 | C2_19 | 110.47(14) |
| C1_1 | C2_1 | C3_1 | 111.03(13) | C5_19 | C4_19 | C3_19 | 110.72(14) |
| C4_1 | C3_1 | C2_1 | 110.57(13) | N2_19 | C5_19 | C4_19 | 110.09(13) |
| C5_1 | C4_1 | C3_1 | 110.91(13) | C1_20 | N2_20 | P6 | 119.90(10) |
| N2_1 | C5_1 | C4_1 | 110.78(13) | C5_20 | N2_20 | P6 | 125.97(11) |
| C1_2 | N2_2 | P4 | 124.97(10) | C5_20 | N2_20 | C1_20 | 111.90(12) |

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|---|---|---|---|---|---|---|---|
| C1_2 | N2_2 | C5_2 | 111.28(12) | N2_20 | C1_20 | C2_20 | 110.81(13) |
| C5_2 | N2_2 | P4 | 117.40(10) | C1_20 | C2_20 | C3_20 | 111.02(13) |
| N2_2 | C1_2 | C2_2 | 110.26(13) | C4_20 | C3_20 | C2_20 | 110.15(13) |
| C1_2 | C2_2 | C3_2 | 110.81(13) | C5_20 | C4_20 | C3_20 | 110.54(14) |
| C4_2 | C3_2 | C2_2 | 110.37(13) | N2_20 | C5_20 | C4_20 | 109.96(13) |
| C5_2 | C4_2 | C3_2 | 111.50(13) | C1_21 | N2_21 | P8 | 121.13(10) |
| N2_2 | C5_2 | C4_2 | 110.35(13) | C1_21 | N2_21 | C5_21 | 111.78(12) |
| C1_3 | N2_3 | P4 | 123.13(11) | C5_21 | N2_21 | P8 | 121.22(10) |
| C1_3 | N2_3 | C5_3 | 112.77(12) | N2_21 | C1_21 | C2_21 | 110.53(12) |
| C5_3 | N2_3 | P4 | 124.08(10) | C1_21 | C2_21 | C3_21 | 111.17(13) |
| N2_3 | C1_3 | C2_3 | 111.10(12) | C4_21 | C3_21 | C2_21 | 110.18(13) |
| C1_3 | C2_3 | C3_3 | 111.42(13) | C5_21 | C4_21 | C3_21 | 110.59(13) |
| C4_3 | C3_3 | C2_3 | 110.60(12) | N2_21 | C5_21 | C4_21 | 110.56(12) |
| C3_3 | C4_3 | C5_3 | 110.23(12) | C1_22 | N2_22 | P4 | 116.90(10) |
| N2_3 | C5_3 | C4_3 | 110.21(12) | C1_22 | N2_22 | C5_22 | 110.76(11) |
| C1_4 | N2_4 | P1 | 114.22(10) | C5_22 | N2_22 | P4 | 117.84(10) |
| C1_4 | N2_4 | C5_4 | 111.80(12) | N2_22 | C1_22 | C2_22 | 110.41(12) |
| C5_4 | N2_4 | P1 | 121.57(10) | C1_22 | C2_22 | C3_22 | 110.67(12) |
| N2_4 | C1_4 | C2_4 | 110.62(12) | C4_22 | C3_22 | C2_22 | 110.60(12) |
| C1_4 | C2_4 | C3_4 | 110.96(13) | C5_22 | C4_22 | C3_22 | 111.28(12) |
| C4_4 | C3_4 | C2_4 | 110.25(13) | N2_22 | C5_22 | C4_22 | 109.46(12) |
| C5_4 | C4_4 | C3_4 | 110.13(13) | C1_23 | N2_23 | P8 | 121.84(10) |
| N2_4 | C5_4 | C4_4 | 110.11(12) | C1_23 | N2_23 | C5_23 | 111.32(11) |
| C1_5 | N2_5 | P1 | 112.35(10) | C5_23 | N2_23 | P8 | 115.27(9) |
| C1_5 | N2_5 | C5_5 | 110.24(12) | N2_23 | C1_23 | C2_23 | 109.73(11) |
| C5_5 | N2_5 | P1 | 115.35(10) | C1_23 | C2_23 | C3_23 | 110.78(12) |
| N2_5 | C1_5 | C2_5 | 110.83(12) | C4_23 | C3_23 | C2_23 | 110.36(12) |
| C1_5 | C2_5 | C3_5 | 111.00(13) | C5_23 | C4_23 | C3_23 | 111.01(12) |
| C4_5 | C3_5 | C2_5 | 109.54(13) | N2_23 | C5_23 | C4_23 | 110.96(12) |
| C5_5 | C4_5 | C3_5 | 110.76(13) | C1_24 | N2_24 | P2 | 126.50(11) |
| N2_5 | C5_5 | C4_5 | 110.69(12) | C1_24 | N2_24 | C5_24 | 112.33(12) |
| C1_6 | N2_6 | P2 | 122.15(11) | C5_24 | N2_24 | P2 | 119.73(10) |
| C5_6 | N2_6 | P2 | 125.82(11) | N2_24 | C1_24 | C2_24 | 110.24(13) |
| C5_6 | N2_6 | C1_6 | 111.98(12) | C1_24 | C2_24 | C3_24 | 110.42(14) |
| N2_6 | C1_6 | C2_6 | 109.84(13) | C4_24 | C3_24 | C2_24 | 110.47(13) |
| C1_6 | C2_6 | C3_6 | 110.25(14) | C5_24 | C4_24 | C3_24 | 111.11(13) |
| C4_6 | C3_6 | C2_6 | 110.55(14) | N2_24 | C5_24 | C4_24 | 110.38(13) |
| C5_6 | C4_6 | C3_6 | 110.78(14) | C1_25 | N2_25 | P6 | 125.45(12) |
| N2_6 | C5_6 | C4_6 | 110.47(13) | C1_25 | N2_25 | C5_25 | 111.89(14) |
| C1_7 | N2_7 | P2 | 117.15(10) | C5_25 | N2_25 | P6 | 122.62(13) |
| C5_7 | N2_7 | P2 | 120.73(10) | N2_25 | C1_25 | C2_25 | 110.19(14) |

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|---|---|---|---|---|---|---|---|
| C5_7 | N2_7 | C1_7 | 111.43(12) | C1_25 | C2_25 | C3_25 | 110.95(15) |
| N2_7 | C1_7 | C2_7 | 109.86(12) | C4_25 | C3_25 | C2_25 | 110.65(15) |
| C1_7 | C2_7 | C3_7 | 110.57(13) | C5_25 | C4_25 | C3_25 | 110.46(15) |
| C4_7 | C3_7 | C2_7 | 111.12(13) | N2_25 | C5_25 | C4_25 | 110.15(14) |
| C3_7 | C4_7 | C5_7 | 111.32(13) | | | | |

**Table S5.** Lengths for **2-Fe**.

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| C1 | C2 | 1.518(4) | C41 | N12 | 1.472(4) |
| C1 | N2 | 1.476(3) | C42 | C43 | 1.528(4) |
| C2 | C3 | 1.524(5) | C43 | C44 | 1.526(4) |
| C3 | C4 | 1.521(5) | C44 | C45 | 1.523(4) |
| C4 | C5 | 1.522(4) | C45 | N12 | 1.473(3) |
| C5 | N2 | 1.480(3) | C46 | C47 | 1.521(4) |
| C6 | C7 | 1.520(4) | C46 | N14 | 1.462(3) |
| C6 | N3 | 1.462(3) | C47 | C48 | 1.527(4) |
| C7 | C8 | 1.524(4) | C48 | C49 | 1.517(5) |
| C8 | C9 | 1.520(4) | C49 | C50 | 1.530(4) |
| C9 | C10 | 1.530(4) | C50 | N14 | 1.468(3) |
| C10 | N3 | 1.462(3) | C51 | C52 | 1.519(4) |
| C11 | C12 | 1.517(4) | C51 | N15 | 1.479(4) |
| C11 | N4 | 1.479(3) | C52 | C53 | 1.528(4) |
| C12 | C13 | 1.518(4) | C53 | C54 | 1.522(4) |
| C13 | C14 | 1.525(4) | C54 | C55 | 1.517(4) |
| C14 | C15 | 1.523(4) | C55 | N15 | 1.477(3) |
| C15 | N4 | 1.473(3) | C56 | C57 | 1.518(4) |
| C16 | C17 | 1.515(4) | C56 | N16 | 1.464(3) |
| C16 | N6 | 1.470(3) | C57 | C58 | 1.521(4) |
| C17 | C18 | 1.531(4) | C58 | C59 | 1.519(5) |
| C18 | C19 | 1.522(4) | C59 | C60 | 1.528(5) |
| C19 | C20 | 1.529(4) | C60 | N16 | 1.458(4) |
| C20 | N6 | 1.469(3) | Fe1 | Fe2 | 2.3396(6) |
| C21 | C22 | 1.522(4) | Fe1 | N1 | 2.015(2) |
| C21 | N7 | 1.479(3) | Fe1 | N5 | 2.030(2) |
| C22 | C23 | 1.530(4) | Fe1 | N9 | 1.833(2) |
| C23 | C24 | 1.525(4) | Fe1 | O1 | 1.8485(18) |
| C24 | C25 | 1.522(4) | Fe2 | N1 | 2.046(2) |
| C25 | N7 | 1.482(3) | Fe2 | N5 | 2.015(2) |
| C26 | C27 | 1.516(4) | Fe2 | N13 | 1.841(2) |
| C26 | N8 | 1.452(4) | Fe2 | O1 | 1.8538(18) |
| C27 | C28 | 1.539(5) | N1 | P1 | 1.539(2) |

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| C28 | C29 | 1.524(5) | N2 | P1 | 1.679(2) |
| C29 | C30 | 1.510(4) | N3 | P1 | 1.664(2) |
| C30 | N8 | 1.464(4) | N4 | P1 | 1.682(2) |
| C31 | C32 | 1.530(4) | N5 | P2 | 1.556(2) |
| C31 | N10 | 1.473(3) | N6 | P2 | 1.674(2) |
| C32 | C33 | 1.520(4) | N7 | P2 | 1.671(2) |
| C33 | C34 | 1.524(4) | N8 | P2 | 1.658(2) |
| C34 | C35 | 1.530(4) | N9 | P3 | 1.540(2) |
| C35 | N10 | 1.482(3) | N10 | P3 | 1.688(2) |
| C36 | C37 | 1.529(4) | N11 | P3 | 1.663(2) |
| C36 | N11 | 1.449(3) | N12 | P3 | 1.681(2) |
| C37 | C38 | 1.527(4) | N13 | P4 | 1.539(2) |
| C38 | C39 | 1.527(4) | N14 | P4 | 1.684(2) |
| C39 | C40 | 1.520(4) | N15 | P4 | 1.674(2) |
| C40 | N11 | 1.458(3) | N16 | P4 | 1.676(2) |
| C41 | C42 | 1.514(4) | | | |

**Table S6.** Angles for **2-Fe**.

| Atom | Atom | Atom | Angle/˚ | Atom | Atom | Atom | Angle/˚ |
|---|---|---|---|---|---|---|---|
| N2 | C1 | C2 | 110.1(2) | N13 | Fe2 | N5 | 126.88(10) |
| C1 | C2 | C3 | 111.6(2) | N13 | Fe2 | O1 | 127.01(9) |
| C4 | C3 | C2 | 109.9(3) | O1 | Fe2 | Fe1 | 50.71(6) |
| C3 | C4 | C5 | 110.6(3) | O1 | Fe2 | N1 | 87.73(9) |
| N2 | C5 | C4 | 108.7(2) | O1 | Fe2 | N5 | 88.60(8) |
| N3 | C6 | C7 | 110.5(2) | Fe1 | N1 | Fe2 | 70.35(7) |
| C6 | C7 | C8 | 111.1(2) | P1 | N1 | Fe1 | 147.79(14) |
| C9 | C8 | C7 | 111.1(2) | P1 | N1 | Fe2 | 135.94(13) |
| C8 | C9 | C10 | 110.3(2) | C1 | N2 | C5 | 110.8(2) |
| N3 | C10 | C9 | 110.5(2) | C1 | N2 | P1 | 115.05(17) |
| N4 | C11 | C12 | 111.0(2) | C5 | N2 | P1 | 116.12(17) |
| C11 | C12 | C13 | 111.6(2) | C6 | N3 | P1 | 123.83(18) |
| C12 | C13 | C14 | 109.6(2) | C10 | N3 | C6 | 112.4(2) |
| C15 | C14 | C13 | 109.7(2) | C10 | N3 | P1 | 123.72(18) |
| N4 | C15 | C14 | 110.6(2) | C11 | N4 | P1 | 114.60(17) |
| N6 | C16 | C17 | 110.7(2) | C15 | N4 | C11 | 111.3(2) |
| C16 | C17 | C18 | 111.2(2) | C15 | N4 | P1 | 121.20(17) |
| C19 | C18 | C17 | 110.5(2) | Fe2 | N5 | Fe1 | 70.69(7) |
| C18 | C19 | C20 | 111.0(2) | P2 | N5 | Fe1 | 130.97(13) |
| N6 | C20 | C19 | 109.7(2) | P2 | N5 | Fe2 | 136.39(13) |
| N7 | C21 | C22 | 110.0(2) | C16 | N6 | P2 | 116.00(17) |
| C21 | C22 | C23 | 111.3(2) | C20 | N6 | C16 | 111.4(2) |

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|---|---|---|---|---|---|---|---|
| C24 | C23 | C22 | 109.9(2) | C20 | N6 | P2 | 124.11(18) |
| C25 | C24 | C23 | 110.6(2) | C21 | N7 | C25 | 110.4(2) |
| N7 | C25 | C24 | 109.9(2) | C21 | N7 | P2 | 117.66(17) |
| N8 | C26 | C27 | 110.2(2) | C25 | N7 | P2 | 117.67(18) |
| C26 | C27 | C28 | 111.0(3) | C26 | N8 | C30 | 113.3(2) |
| C29 | C28 | C27 | 110.1(3) | C26 | N8 | P2 | 123.97(19) |
| C30 | C29 | C28 | 110.2(3) | C30 | N8 | P2 | 122.7(2) |
| N8 | C30 | C29 | 111.6(2) | P3 | N9 | Fe1 | 141.17(15) |
| N10 | C31 | C32 | 110.5(2) | C31 | N10 | C35 | 110.8(2) |
| C33 | C32 | C31 | 110.8(2) | C31 | N10 | P3 | 115.74(18) |
| C32 | C33 | C34 | 109.6(2) | C35 | N10 | P3 | 114.54(18) |
| C33 | C34 | C35 | 110.8(2) | C36 | N11 | C40 | 112.7(2) |
| N10 | C35 | C34 | 110.3(2) | C36 | N11 | P3 | 122.70(18) |
| N11 | C36 | C37 | 111.2(2) | C40 | N11 | P3 | 124.55(19) |
| C38 | C37 | C36 | 110.3(2) | C41 | N12 | C45 | 112.3(2) |
| C37 | C38 | C39 | 110.4(2) | C41 | N12 | P3 | 115.29(18) |
| C40 | C39 | C38 | 110.9(2) | C45 | N12 | P3 | 122.29(19) |
| N11 | C40 | C39 | 110.9(2) | P4 | N13 | Fe2 | 135.53(14) |
| N12 | C41 | C42 | 110.8(2) | C46 | N14 | C50 | 112.6(2) |
| C41 | C42 | C43 | 111.4(2) | C46 | N14 | P4 | 118.26(18) |
| C44 | C43 | C42 | 109.5(2) | C50 | N14 | P4 | 120.89(18) |
| C45 | C44 | C43 | 111.0(3) | C51 | N15 | P4 | 119.17(18) |
| N12 | C45 | C44 | 110.5(2) | C55 | N15 | C51 | 110.3(2) |
| N14 | C46 | C47 | 110.9(2) | C55 | N15 | P4 | 116.89(18) |
| C46 | C47 | C48 | 110.7(2) | C56 | N16 | P4 | 120.96(18) |
| C49 | C48 | C47 | 110.3(3) | C60 | N16 | C56 | 112.7(2) |
| C48 | C49 | C50 | 111.1(3) | C60 | N16 | P4 | 124.9(2) |
| N14 | C50 | C49 | 109.7(2) | Fe1 | O1 | Fe2 | 78.39(7) |
| N15 | C51 | C52 | 109.8(2) | N1 | P1 | N2 | 117.46(12) |
| C51 | C52 | C53 | 111.2(2) | N1 | P1 | N3 | 112.82(12) |
| C54 | C53 | C52 | 109.9(2) | N1 | P1 | N4 | 112.56(11) |
| C55 | C54 | C53 | 110.4(3) | N2 | P1 | N4 | 100.68(11) |
| N15 | C55 | C54 | 109.9(2) | N3 | P1 | N2 | 102.97(11) |
| N16 | C56 | C57 | 110.9(2) | N3 | P1 | N4 | 109.27(12) |
| C56 | C57 | C58 | 110.1(3) | N5 | P2 | N6 | 112.29(12) |
| C59 | C58 | C57 | 110.6(3) | N5 | P2 | N7 | 119.91(12) |
| C58 | C59 | C60 | 111.4(3) | N5 | P2 | N8 | 110.06(12) |
| N16 | C60 | C59 | 111.2(3) | N7 | P2 | N6 | 101.81(11) |
| N1 | Fe1 | Fe2 | 55.43(6) | N8 | P2 | N6 | 109.47(12) |
| N1 | Fe1 | N5 | 87.78(9) | N8 | P2 | N7 | 102.46(12) |
| N5 | Fe1 | Fe2 | 54.35(6) | N9 | P3 | N10 | 120.45(12) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N9 | Fe1 | Fe2 | 177.24(7) | N9 | P3 | N11 | 108.82(12) |
| N9 | Fe1 | N1 | 121.86(9) | N9 | P3 | N12 | 113.07(12) |
| N9 | Fe1 | N5 | 126.24(10) | N11 | P3 | N10 | 103.22(12) |
| N9 | Fe1 | O1 | 130.99(9) | N11 | P3 | N12 | 110.64(12) |
| O1 | Fe1 | Fe2 | 50.91(6) | N12 | P3 | N10 | 99.95(12) |
| O1 | Fe1 | N1 | 88.78(8) | N13 | P4 | N14 | 109.57(12) |
| O1 | Fe1 | N5 | 88.29(9) | N13 | P4 | N15 | 120.40(12) |
| N1 | Fe2 | Fe1 | 54.22(6) | N13 | P4 | N16 | 112.91(12) |
| N5 | Fe2 | Fe1 | 54.95(6) | N15 | P4 | N14 | 100.14(12) |
| N5 | Fe2 | N1 | 87.36(9) | N15 | P4 | N16 | 101.06(12) |
| N13 | Fe2 | Fe1 | 177.60(7) | N16 | P4 | N14 | 111.97(12) |
| N13 | Fe2 | N1 | 126.31(9) | | | | |

**Table S7.** Lengths for **3-Fe**.

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| C1 | C2 | 1.5257(17) | C21 | N7 | 1.4677(13) |
| C1 | N2 | 1.4730(13) | C22 | C23 | 1.5301(19) |
| C2 | C3 | 1.5242(19) | C23 | C24 | 1.5245(18) |
| C3 | C4 | 1.5280(18) | C24 | C25 | 1.5262(15) |
| C4 | C5 | 1.5239(18) | C25 | N7 | 1.4666(14) |
| C5 | N2 | 1.4686(14) | C26 | C27 | 1.5266(16) |
| C6 | C7 | 1.5259(16) | C26 | N8 | 1.4785(14) |
| C6 | N3 | 1.4669(14) | C27 | C28 | 1.524(2) |
| C7 | C8 | 1.5257(17) | C28 | C29 | 1.528(2) |
| C8 | C9 | 1.5295(18) | C29 | C30 | 1.5314(18) |
| C9 | C10 | 1.5208(18) | C30 | N8 | 1.4623(14) |
| C10 | N3 | 1.4628(14) | Fe1 | Fe11 | 2.5964(4) |
| C11 | C12 | 1.5249(16) | Fe1 | N1 | 1.8281(9) |
| C11 | N4 | 1.4664(14) | Fe1 | N5 | 1.9911(9) |
| C12 | C13 | 1.5270(19) | Fe1 | N51 | 1.9727(9) |
| C13 | C14 | 1.5296(19) | Fe1 | S1 | 2.3258(4) |
| C14 | C15 | 1.5249(16) | N1 | P1 | 1.5429(10) |
| C15 | N4 | 1.4610(15) | N2 | P1 | 1.6784(9) |
| C16 | C17 | 1.5319(15) | N3 | P1 | 1.6782(9) |
| C16 | N6 | 1.4718(13) | N4 | P1 | 1.6691(9) |
| C17 | C18 | 1.5286(19) | N5 | P2 | 1.5591(9) |
| C18 | C19 | 1.5291(17) | N6 | P2 | 1.6594(9) |
| C19 | C20 | 1.5268(16) | N7 | P2 | 1.6617(9) |
| C20 | N6 | 1.4630(14) | N8 | P2 | 1.6734(9) |
| C21 | C22 | 1.5266(16) | S1 | S11 | 2.0847(6) |

[1] 1-X,+Y,3/2-Z

**Table S8.** Angles for **3-Fe**.

| Atom | Atom | Atom | Angle/˚ |
|---|---|---|---|
| N2 | C1 | C2 | 109.13(9) |
| C3 | C2 | C1 | 110.80(10) |
| C2 | C3 | C4 | 111.06(10) |
| C5 | C4 | C3 | 110.89(11) |
| N2 | C5 | C4 | 109.91(10) |
| N3 | C6 | C7 | 110.23(9) |
| C8 | C7 | C6 | 110.76(10) |
| C7 | C8 | C9 | 109.63(9) |
| C10 | C9 | C8 | 111.30(10) |
| N3 | C10 | C9 | 110.75(10) |
| N4 | C11 | C12 | 111.16(9) |
| C11 | C12 | C13 | 111.26(10) |
| C12 | C13 | C14 | 110.58(10) |
| C15 | C14 | C13 | 110.76(11) |
| N4 | C15 | C14 | 110.66(10) |
| N6 | C16 | C17 | 112.29(9) |
| C18 | C17 | C16 | 111.47(10) |
| C17 | C18 | C19 | 110.14(10) |
| C20 | C19 | C18 | 110.02(10) |
| N6 | C20 | C19 | 111.61(9) |
| N7 | C21 | C22 | 110.19(9) |
| C21 | C22 | C23 | 110.58(10) |
| C24 | C23 | C22 | 110.21(10) |
| C23 | C24 | C25 | 111.56(10) |
| N7 | C25 | C24 | 111.90(9) |
| N8 | C26 | C27 | 109.84(9) |
| C28 | C27 | C26 | 110.64(11) |
| C27 | C28 | C29 | 110.49(11) |
| C28 | C29 | C30 | 110.55(11) |
| N8 | C30 | C29 | 109.60(11) |
| N1 | Fe1 | Fe11 | 166.79(3) |
| N1 | Fe1 | N5 | 125.49(4) |
| N1 | Fe1 | N51 | 123.97(4) |
| N1 | Fe1 | S1 | 109.51(3) |
| N5 | Fe1 | Fe11 | 48.77(3) |
| N51 | Fe1 | Fe11 | 49.39(3) |
| N51 | Fe1 | N5 | 87.97(4) |
| N51 | Fe1 | S1 | 102.48(3) |
| N5 | Fe1 | S1 | 103.37(3) |
| S1 | Fe1 | Fe11 | 83.672(8) |
| P1 | N1 | Fe1 | 147.98(6) |
| C1 | N2 | P1 | 119.09(7) |
| C5 | N2 | C1 | 110.52(8) |
| C5 | N2 | P1 | 116.84(7) |
| C6 | N3 | P1 | 125.36(7) |
| C10 | N3 | C6 | 112.84(8) |
| C10 | N3 | P1 | 117.97(8) |
| C11 | N4 | P1 | 122.24(8) |
| C15 | N4 | C11 | 114.02(9) |
| C15 | N4 | P1 | 122.21(8) |
| Fe11 | N5 | Fe1 | 81.84(3) |
| P2 | N5 | Fe11 | 137.85(5) |
| P2 | N5 | Fe1 | 140.17(6) |
| C16 | N6 | P2 | 123.62(8) |
| C20 | N6 | C16 | 113.47(8) |
| C20 | N6 | P2 | 122.89(7) |
| C21 | N7 | P2 | 120.38(7) |
| C25 | N7 | C21 | 113.34(8) |
| C25 | N7 | P2 | 125.76(7) |
| C26 | N8 | P2 | 119.16(7) |
| C30 | N8 | C26 | 110.40(9) |
| C30 | N8 | P2 | 119.69(7) |
| N1 | P1 | N2 | 120.75(5) |
| N1 | P1 | N3 | 110.82(5) |
| N1 | P1 | N4 | 111.95(5) |
| N3 | P1 | N2 | 99.49(5) |
| N4 | P1 | N2 | 102.27(5) |
| N4 | P1 | N3 | 110.62(5) |
| N5 | P2 | N6 | 110.15(5) |
| N5 | P2 | N7 | 112.28(5) |
| N5 | P2 | N8 | 117.76(5) |
| N6 | P2 | N7 | 110.75(5) |
| N6 | P2 | N8 | 104.74(5) |
| N7 | P2 | N8 | 100.60(5) |
| S11 | S1 | Fe1 | 96.302(8) |

[1] 1-X,+Y,3/2-Z

**Table S9.** Lengths for **4-Fe**.

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| Se1 | Se11 | 2.3532(8) | N8 | C26 | 1.463(5) |
| Se1 | Fe1 | 2.4582(8) | C1 | C2 | 1.520(6) |
| Fe1 | Fe11 | 2.6072(11) | C15 | C14 | 1.524(6) |
| Fe1 | N1 | 1.969(3) | C10 | C9 | 1.536(6) |
| Fe1 | N11 | 1.989(3) | C5 | C4 | 1.522(6) |
| Fe1 | N5 | 1.822(3) | C11 | C12 | 1.536(7) |
| P2 | N5 | 1.541(3) | C20 | C19 | 1.504(6) |
| P2 | N6 | 1.675(4) | C16 | C17 | 1.529(7) |
| P2 | N7 | 1.665(4) | C2 | C3 | 1.527(7) |
| P2 | N8 | 1.677(3) | C25 | C24 | 1.517(6) |
| P1 | N1 | 1.557(4) | C9 | C8 | 1.526(7) |
| P1 | N2 | 1.660(3) | C7 | C6 | 1.523(6) |
| P1 | N4 | 1.673(3) | C7 | C8 | 1.527(7) |
| P1 | N3 | 1.658(3) | C17 | C18 | 1.525(7) |
| N2 | C1 | 1.472(5) | C19 | C18 | 1.523(7) |
| N2 | C5 | 1.459(5) | C4 | C3 | 1.528(6) |
| N4 | C15 | 1.481(5) | C30 | C29 | 1.524(6) |
| N4 | C11 | 1.459(6) | C29 | C28 | 1.504(7) |
| N3 | C10 | 1.474(5) | C14 | C13 | 1.512(8) |
| N3 | C6 | 1.463(5) | C12 | C13 | 1.530(7) |
| N6 | C20 | 1.470(5) | C26 | C27 | 1.513(7) |
| N6 | C16 | 1.469(5) | C28 | C27 | 1.519(6) |
| N7 | C25 | 1.465(6) | C24 | C23 | 1.515(7) |
| N7 | C21 | 1.466(5) | C21 | C22 | 1.511(6) |
| N8 | C30 | 1.460(5) | C23 | C22 | 1.519(7) |

[1] 1-X,+Y,3/2-Z

**Table S10.** Angles for **4-Fe**.

| Atom | Atom | Atom | Angle/˚ | Atom | Atom | Atom | Angle/˚ |
|---|---|---|---|---|---|---|---|
| Se11 | Se1 | Fe1 | 92.929(16) | C16 | N6 | C20 | 110.3(3) |
| Se1 | Fe1 | Fe11 | 87.008(16) | C25 | N7 | P2 | 122.2(3) |
| N1 | Fe1 | Se1 | 103.53(10) | C25 | N7 | C21 | 113.8(3) |
| N11 | Fe1 | Se1 | 105.18(10) | C21 | N7 | P2 | 122.6(3) |
| N11 | Fe1 | Fe11 | 48.46(10) | C30 | N8 | P2 | 125.3(3) |
| N1 | Fe1 | Fe11 | 49.12(10) | C30 | N8 | C26 | 112.6(3) |
| N1 | Fe1 | N11 | 88.39(15) | C26 | N8 | P2 | 117.9(3) |
| N5 | Fe1 | Se1 | 106.51(11) | N2 | C1 | C2 | 112.0(3) |
| N5 | Fe1 | Fe11 | 166.47(11) | N4 | C15 | C14 | 109.1(4) |
| N5 | Fe1 | N1 | 124.48(15) | N3 | C10 | C9 | 109.3(4) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N5 | Fe1 | N11 | 125.63(15) | N2 | C5 | C4 | 111.6(4) |
| N5 | P2 | N6 | 120.46(18) | N4 | C11 | C12 | 109.7(4) |
| N5 | P2 | N7 | 112.21(19) | N6 | C20 | C19 | 110.0(4) |
| N5 | P2 | N8 | 110.64(18) | N6 | C16 | C17 | 109.5(4) |
| N6 | P2 | N8 | 99.70(17) | C1 | C2 | C3 | 111.9(4) |
| N7 | P2 | N6 | 102.10(18) | N7 | C25 | C24 | 110.3(4) |
| N7 | P2 | N8 | 110.80(18) | C8 | C9 | C10 | 110.4(4) |
| N1 | P1 | N2 | 110.35(18) | C6 | C7 | C8 | 110.9(4) |
| N1 | P1 | N4 | 117.89(18) | N3 | C6 | C7 | 112.1(4) |
| N1 | P1 | N3 | 112.07(18) | C18 | C17 | C16 | 110.9(4) |
| N2 | P1 | N4 | 104.90(18) | C20 | C19 | C18 | 111.0(4) |
| N3 | P1 | N2 | 110.59(18) | C19 | C18 | C17 | 110.6(4) |
| N3 | P1 | N4 | 100.44(17) | C5 | C4 | C3 | 109.8(4) |
| Fe1 | N1 | Fe11 | 82.41(13) | N8 | C30 | C29 | 110.4(3) |
| P1 | N1 | Fe1 | 137.3(2) | C28 | C29 | C30 | 110.9(4) |
| P1 | N1 | Fe11 | 140.3(2) | C9 | C8 | C7 | 110.2(4) |
| C1 | N2 | P1 | 123.5(3) | C13 | C14 | C15 | 111.0(4) |
| C5 | N2 | P1 | 122.9(3) | C2 | C3 | C4 | 109.8(4) |
| C5 | N2 | C1 | 113.6(3) | C13 | C12 | C11 | 110.1(4) |
| C15 | N4 | P1 | 119.4(3) | N8 | C26 | C27 | 110.9(4) |
| C11 | N4 | P1 | 119.3(3) | C29 | C28 | C27 | 110.6(4) |
| C11 | N4 | C15 | 110.3(3) | C23 | C24 | C25 | 111.5(4) |
| P2 | N5 | Fe1 | 147.7(2) | C14 | C13 | C12 | 110.7(4) |
| C10 | N3 | P1 | 120.2(3) | N7 | C21 | C22 | 110.9(4) |
| C6 | N3 | P1 | 126.0(3) | C24 | C23 | C22 | 109.9(4) |
| C6 | N3 | C10 | 113.0(3) | C21 | C22 | C23 | 111.8(4) |
| C20 | N6 | P2 | 120.0(3) | C26 | C27 | C28 | 111.3(4) |
| C16 | N6 | P2 | 116.9(3) | | | | |

[1] 1-X,+Y,3/2-Z

**Table S11.** Lengths for **1-Co**.

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| Co1 | N1 | 1.823(8) | C4_9 | C5_9 | 1.525(3) |
| Co1 | N5 | 1.866(7) | N2_10 | C1_10 | 1.470(3) |
| Co1 | N13 | 1.929(8) | N2_10 | C5_10 | 1.472(3) |
| Co2 | N5 | 1.874(6) | C1_10 | C2_10 | 1.520(3) |
| Co2 | N9 | 1.776(6) | C2_10 | C3_10 | 1.527(3) |
| Co2 | N13 | 1.963(7) | C3_10 | C4_10 | 1.527(3) |
| P1 | N1 | 1.579(9) | C4_10 | C5_10 | 1.525(3) |
| P1 | N2_1 | 1.669(3) | N2_11 | C1_11 | 1.471(3) |
| P1 | N2_4 | 1.675(3) | N2_11 | C5_11 | 1.473(3) |
| P1 | N2_5 | 1.673(3) | C1_11 | C2_11 | 1.521(3) |

| | | | | | |
|---|---|---|---|---|---|
| P3 | N9 | 1.573(6) | C2_11 | C3_11 | 1.526(3) |
| P3 | N2_8 | 1.677(3) | C3_11 | C4_11 | 1.526(3) |
| P3 | N2_9 | 1.667(3) | C4_11 | C5_11 | 1.526(3) |
| P3 | N2_10 | 1.683(3) | N2_12 | C1_12 | 1.471(3) |
| P4 | N13 | 1.566(8) | N2_12 | C5_12 | 1.472(3) |
| P4 | N2_2 | 1.666(3) | C1_12 | C2_12 | 1.521(3) |
| P4 | N2_3 | 1.662(3) | C2_12 | C3_12 | 1.527(3) |
| P4 | N2_22 | 1.667(3) | C3_12 | C4_12 | 1.526(3) |
| N5 | P2 | 1.654(3) | C4_12 | C5_12 | 1.525(3) |
| Co3 | N17 | 1.797(7) | N2_13 | C1_13 | 1.471(3) |
| Co3 | N21 | 1.944(8) | N2_13 | C5_13 | 1.472(3) |
| Co3 | N29 | 1.954(7) | C1_13 | C2_13 | 1.521(3) |
| Co4 | N21 | 1.950(7) | C2_13 | C3_13 | 1.526(3) |
| Co4 | N25 | 1.801(8) | C3_13 | C4_13 | 1.526(3) |
| Co4 | N29 | 1.939(7) | C4_13 | C5_13 | 1.525(3) |
| P5 | N17 | 1.586(7) | N2_14 | C1_14 | 1.471(3) |
| P5 | N2_11 | 1.670(3) | N2_14 | C5_14 | 1.471(3) |
| P5 | N2_12 | 1.675(3) | C1_14 | C2_14 | 1.522(3) |
| P5 | N2_14 | 1.682(3) | C2_14 | C3_14 | 1.528(3) |
| P7 | N25 | 1.597(10) | C3_14 | C4_14 | 1.527(3) |
| P7 | N2_16 | 1.666(3) | C4_14 | C5_14 | 1.524(3) |
| P7 | N2_17 | 1.675(3) | N2_15 | C1_15 | 1.471(3) |
| P7 | N2_18 | 1.676(3) | N2_15 | C5_15 | 1.472(3) |
| P7 | N2_19 | 1.667(3) | C1_15 | C2_15 | 1.522(3) |
| N21 | P6 | 1.535(7) | C2_15 | C3_15 | 1.526(3) |
| N29 | P8 | 1.557(7) | C3_15 | C4_15 | 1.526(3) |
| P2 | N2_6 | 1.658(3) | C4_15 | C5_15 | 1.526(3) |
| P2 | N2_7 | 1.663(3) | N2_16 | C1_16 | 1.472(3) |
| P2 | N2_24 | 1.664(3) | N2_16 | C5_16 | 1.472(3) |
| P6 | N2_15 | 1.662(3) | C1_16 | C2_16 | 1.522(3) |
| P6 | N2_20 | 1.663(3) | C2_16 | C3_16 | 1.527(3) |
| P6 | N2_25 | 1.662(3) | C3_16 | C4_16 | 1.526(3) |
| P8 | N2_13 | 1.665(3) | C4_16 | C5_16 | 1.525(3) |
| P8 | N2_21 | 1.673(3) | N2_17 | C1_17 | 1.472(3) |
| P8 | N2_23 | 1.674(3) | N2_17 | C5_17 | 1.473(3) |
| N2_1 | C1_1 | 1.471(3) | C1_17 | C2_17 | 1.522(3) |
| N2_1 | C5_1 | 1.472(3) | C2_17 | C3_17 | 1.527(3) |
| C1_1 | C2_1 | 1.522(3) | C3_17 | C4_17 | 1.526(3) |
| C2_1 | C3_1 | 1.527(3) | C4_17 | C5_17 | 1.525(3) |
| C3_1 | C4_1 | 1.526(3) | N2_18 | C1_18 | 1.471(3) |
| C4_1 | C5_1 | 1.525(3) | N2_18 | C5_18 | 1.472(3) |

| | | | | | |
|---|---|---|---|---|---|
| N2_2 | C1_2 | 1.471(3) | C1_18 | C2_18 | 1.521(3) |
| N2_2 | C5_2 | 1.472(3) | C2_18 | C3_18 | 1.527(3) |
| C1_2 | C2_2 | 1.522(3) | C3_18 | C4_18 | 1.527(3) |
| C2_2 | C3_2 | 1.527(3) | C4_18 | C5_18 | 1.525(3) |
| C3_2 | C4_2 | 1.526(3) | N2_19 | C1_19 | 1.470(3) |
| C4_2 | C5_2 | 1.525(3) | N2_19 | C5_19 | 1.472(3) |
| N2_3 | C1_3 | 1.470(3) | C1_19 | C2_19 | 1.521(3) |
| N2_3 | C5_3 | 1.471(3) | C2_19 | C3_19 | 1.527(3) |
| C1_3 | C2_3 | 1.521(3) | C3_19 | C4_19 | 1.527(3) |
| C2_3 | C3_3 | 1.527(3) | C4_19 | C5_19 | 1.526(3) |
| C3_3 | C4_3 | 1.526(3) | N2_20 | C1_20 | 1.470(3) |
| C4_3 | C5_3 | 1.525(3) | N2_20 | C5_20 | 1.471(3) |
| N2_4 | C1_4 | 1.471(3) | C1_20 | C2_20 | 1.521(3) |
| N2_4 | C5_4 | 1.472(3) | C2_20 | C3_20 | 1.526(3) |
| C1_4 | C2_4 | 1.521(3) | C3_20 | C4_20 | 1.527(3) |
| C2_4 | C3_4 | 1.527(3) | C4_20 | C5_20 | 1.526(3) |
| C3_4 | C4_4 | 1.527(3) | N2_21 | C1_21 | 1.471(3) |
| C4_4 | C5_4 | 1.525(3) | N2_21 | C5_21 | 1.472(3) |
| N2_5 | C1_5 | 1.471(3) | C1_21 | C2_21 | 1.521(3) |
| N2_5 | C5_5 | 1.472(3) | C2_21 | C3_21 | 1.527(3) |
| C1_5 | C2_5 | 1.521(3) | C3_21 | C4_21 | 1.527(3) |
| C2_5 | C3_5 | 1.527(3) | C4_21 | C5_21 | 1.525(3) |
| C3_5 | C4_5 | 1.526(3) | N2_22 | C1_22 | 1.471(3) |
| C4_5 | C5_5 | 1.524(3) | N2_22 | C5_22 | 1.473(3) |
| N2_6 | C1_6 | 1.469(3) | C1_22 | C2_22 | 1.522(3) |
| N2_6 | C5_6 | 1.470(3) | C2_22 | C3_22 | 1.527(3) |
| C1_6 | C2_6 | 1.521(3) | C3_22 | C4_22 | 1.526(3) |
| C2_6 | C3_6 | 1.527(3) | C4_22 | C5_22 | 1.525(3) |
| C3_6 | C4_6 | 1.526(3) | N2_23 | C1_23 | 1.471(3) |
| C4_6 | C5_6 | 1.525(3) | N2_23 | C5_23 | 1.472(3) |
| N2_7 | C1_7 | 1.472(3) | C1_23 | C2_23 | 1.522(3) |
| N2_7 | C5_7 | 1.472(3) | C2_23 | C3_23 | 1.527(3) |
| C1_7 | C2_7 | 1.522(3) | C3_23 | C4_23 | 1.527(3) |
| C2_7 | C3_7 | 1.526(3) | C4_23 | C5_23 | 1.524(3) |
| C3_7 | C4_7 | 1.526(3) | N2_24 | C1_24 | 1.470(3) |
| C4_7 | C5_7 | 1.525(3) | N2_24 | C5_24 | 1.471(3) |
| N2_8 | C1_8 | 1.472(3) | C1_24 | C2_24 | 1.522(3) |
| N2_8 | C5_8 | 1.473(3) | C2_24 | C3_24 | 1.527(3) |
| C1_8 | C2_8 | 1.522(3) | C3_24 | C4_24 | 1.527(3) |
| C2_8 | C3_8 | 1.527(3) | C4_24 | C5_24 | 1.526(3) |
| C3_8 | C4_8 | 1.526(3) | N2_25 | C1_25 | 1.470(3) |

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|---|---|---|---|---|---|
| C4_8 | C5_8 | 1.524(3) | N2_25 | C5_25 | 1.471(3) |
| N2_9 | C1_9 | 1.470(3) | C1_25 | C2_25 | 1.521(3) |
| N2_9 | C5_9 | 1.471(3) | C2_25 | C3_25 | 1.526(3) |
| C1_9 | C2_9 | 1.521(3) | C3_25 | C4_25 | 1.526(3) |
| C2_9 | C3_9 | 1.527(3) | C4_25 | C5_25 | 1.525(3) |
| C3_9 | C4_9 | 1.526(3) | | | |

**Table S12.** Angles for **1-Co**.

| Atom | Atom | Atom | Angle/˚ | Atom | Atom | Atom | Angle/˚ |
|---|---|---|---|---|---|---|---|
| N1 | Co1 | N5 | 134.6(3) | C4_8 | C3_8 | C2_8 | 109.9(3) |
| N1 | Co1 | N13 | 132.8(3) | C5_8 | C4_8 | C3_8 | 111.3(3) |
| N5 | Co1 | N13 | 92.6(3) | N2_8 | C5_8 | C4_8 | 110.8(3) |
| N5 | Co2 | N13 | 91.2(3) | C1_9 | N2_9 | P3 | 123.6(4) |
| N9 | Co2 | N5 | 138.8(3) | C1_9 | N2_9 | C5_9 | 111.4(2) |
| N9 | Co2 | N13 | 129.8(3) | C5_9 | N2_9 | P3 | 124.9(4) |
| N1 | P1 | N2_1 | 112.2(3) | N2_9 | C1_9 | C2_9 | 110.6(3) |
| N1 | P1 | N2_4 | 111.7(3) | C1_9 | C2_9 | C3_9 | 110.9(3) |
| N1 | P1 | N2_5 | 122.1(4) | C4_9 | C3_9 | C2_9 | 110.0(3) |
| N2_1 | P1 | N2_4 | 107.8(3) | C5_9 | C4_9 | C3_9 | 111.0(3) |
| N2_1 | P1 | N2_5 | 101.4(3) | N2_9 | C5_9 | C4_9 | 110.5(3) |
| N2_5 | P1 | N2_4 | 100.2(3) | C1_10 | N2_10 | P3 | 114.0(3) |
| N9 | P3 | N2_8 | 118.3(3) | C1_10 | N2_10 | C5_10 | 111.2(2) |
| N9 | P3 | N2_9 | 111.3(3) | C5_10 | N2_10 | P3 | 120.9(3) |
| N9 | P3 | N2_10 | 114.3(3) | N2_10 | C1_10 | C2_10 | 111.4(3) |
| N2_8 | P3 | N2_10 | 100.9(3) | C1_10 | C2_10 | C3_10 | 111.4(3) |
| N2_9 | P3 | N2_8 | 102.1(3) | C2_10 | C3_10 | C4_10 | 109.4(3) |
| N2_9 | P3 | N2_10 | 108.7(3) | C5_10 | C4_10 | C3_10 | 110.5(3) |
| N13 | P4 | N2_2 | 113.1(4) | N2_10 | C5_10 | C4_10 | 110.6(3) |
| N13 | P4 | N2_3 | 110.7(3) | C1_11 | N2_11 | P5 | 117.1(4) |
| N13 | P4 | N2_22 | 117.9(4) | C1_11 | N2_11 | C5_11 | 110.8(3) |
| N2_2 | P4 | N2_22 | 101.6(3) | C5_11 | N2_11 | P5 | 118.2(4) |
| N2_3 | P4 | N2_2 | 108.5(3) | N2_11 | C1_11 | C2_11 | 110.6(3) |
| N2_3 | P4 | N2_22 | 104.2(3) | C1_11 | C2_11 | C3_11 | 111.3(3) |
| P1 | N1 | Co1 | 124.0(5) | C2_11 | C3_11 | C4_11 | 110.1(3) |
| Co1 | N5 | Co2 | 89.59(18) | C5_11 | C4_11 | C3_11 | 110.6(3) |
| P2 | N5 | Co1 | 134.2(5) | N2_11 | C5_11 | C4_11 | 109.9(3) |
| P2 | N5 | Co2 | 130.7(4) | C1_12 | N2_12 | P5 | 120.3(4) |
| P3 | N9 | Co2 | 153.8(4) | C1_12 | N2_12 | C5_12 | 111.2(3) |
| Co1 | N13 | Co2 | 85.2(3) | C5_12 | N2_12 | P5 | 122.7(4) |
| P4 | N13 | Co1 | 137.4(5) | N2_12 | C1_12 | C2_12 | 110.8(3) |
| P4 | N13 | Co2 | 126.1(4) | C1_12 | C2_12 | C3_12 | 111.1(3) |

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|---|---|---|---|---|---|---|---|
| N17 | Co3 | N21 | 134.5(3) | C4_12 | C3_12 | C2_12 | 109.8(3) |
| N17 | Co3 | N29 | 132.9(3) | C5_12 | C4_12 | C3_12 | 111.0(3) |
| N21 | Co3 | N29 | 92.5(3) | N2_12 | C5_12 | C4_12 | 110.7(3) |
| N25 | Co4 | N21 | 132.7(3) | C1_13 | N2_13 | P8 | 119.6(3) |
| N25 | Co4 | N29 | 134.6(3) | C1_13 | N2_13 | C5_13 | 110.9(2) |
| N29 | Co4 | N21 | 92.7(3) | C5_13 | N2_13 | P8 | 116.9(3) |
| N17 | P5 | N2_11 | 115.9(3) | N2_13 | C1_13 | C2_13 | 110.4(3) |
| N17 | P5 | N2_12 | 113.3(3) | C1_13 | C2_13 | C3_13 | 111.3(3) |
| N17 | P5 | N2_14 | 115.0(3) | C4_13 | C3_13 | C2_13 | 110.3(3) |
| N2_11 | P5 | N2_12 | 100.7(3) | C5_13 | C4_13 | C3_13 | 111.1(3) |
| N2_11 | P5 | N2_14 | 100.1(3) | N2_13 | C5_13 | C4_13 | 110.1(3) |
| N2_12 | P5 | N2_14 | 110.3(3) | C1_14 | N2_14 | P5 | 122.3(4) |
| N25 | P7 | N2_16 | 122.3(7) | C1_14 | N2_14 | C5_14 | 111.2(2) |
| N25 | P7 | N2_17 | 122.8(5) | C5_14 | N2_14 | P5 | 113.9(4) |
| N25 | P7 | N2_18 | 110.9(4) | N2_14 | C1_14 | C2_14 | 110.9(3) |
| N25 | P7 | N2_19 | 109.7(4) | C1_14 | C2_14 | C3_14 | 110.9(3) |
| N2_16 | P7 | N2_18 | 101.2(6) | C4_14 | C3_14 | C2_14 | 109.5(3) |
| N2_16 | P7 | N2_19 | 102.9(6) | C5_14 | C4_14 | C3_14 | 110.9(3) |
| N2_17 | P7 | N2_18 | 100.8(4) | N2_14 | C5_14 | C4_14 | 111.1(3) |
| N2_19 | P7 | N2_17 | 102.7(4) | C1_15 | N2_15 | P6 | 120.9(3) |
| N2_19 | P7 | N2_18 | 109.1(3) | C1_15 | N2_15 | C5_15 | 110.9(3) |
| P5 | N17 | Co3 | 149.1(4) | C5_15 | N2_15 | P6 | 117.1(3) |
| Co3 | N21 | Co4 | 84.5(3) | N2_15 | C1_15 | C2_15 | 110.2(3) |
| P6 | N21 | Co3 | 131.2(5) | C1_15 | C2_15 | C3_15 | 111.3(3) |
| P6 | N21 | Co4 | 134.6(5) | C4_15 | C3_15 | C2_15 | 110.3(3) |
| P7 | N25 | Co4 | 128.7(6) | C5_15 | C4_15 | C3_15 | 110.8(3) |
| Co4 | N29 | Co3 | 84.5(3) | N2_15 | C5_15 | C4_15 | 110.0(3) |
| P8 | N29 | Co3 | 130.0(4) | C1_16 | N2_16 | P7 | 113.1(9) |
| P8 | N29 | Co4 | 145.5(5) | C1_16 | N2_16 | C5_16 | 110.8(3) |
| N5 | P2 | N2_6 | 111.6(4) | C5_16 | N2_16 | P7 | 108.2(9) |
| N5 | P2 | N2_7 | 118.1(4) | N2_16 | C1_16 | C2_16 | 110.4(3) |
| N5 | P2 | N2_24 | 112.2(3) | C1_16 | C2_16 | C3_16 | 111.2(3) |
| N2_6 | P2 | N2_7 | 105.8(3) | C4_16 | C3_16 | C2_16 | 110.2(3) |
| N2_6 | P2 | N2_24 | 107.5(3) | C5_16 | C4_16 | C3_16 | 110.9(3) |
| N2_7 | P2 | N2_24 | 100.6(3) | N2_16 | C5_16 | C4_16 | 110.2(3) |
| N21 | P6 | N2_15 | 117.0(4) | C1_17 | N2_17 | P7 | 121.9(6) |
| N21 | P6 | N2_20 | 113.4(4) | C1_17 | N2_17 | C5_17 | 110.7(3) |
| N21 | P6 | N2_25 | 112.9(4) | C5_17 | N2_17 | P7 | 126.4(6) |
| N2_15 | P6 | N2_20 | 99.9(3) | N2_17 | C1_17 | C2_17 | 110.7(3) |
| N2_25 | P6 | N2_15 | 104.7(3) | C1_17 | C2_17 | C3_17 | 111.2(3) |
| N2_25 | P6 | N2_20 | 107.8(3) | C4_17 | C3_17 | C2_17 | 109.9(3) |

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|---|---|---|---|---|---|---|---|
| N29 | P8 | N2_13 | 117.5(4) | C5_17 | C4_17 | C3_17 | 110.9(3) |
| N29 | P8 | N2_21 | 112.2(3) | N2_17 | C5_17 | C4_17 | 110.4(3) |
| N29 | P8 | N2_23 | 112.4(3) | C1_18 | N2_18 | P7 | 121.7(4) |
| N2_13 | P8 | N2_21 | 100.5(3) | C1_18 | N2_18 | C5_18 | 111.0(3) |
| N2_13 | P8 | N2_23 | 102.2(3) | C5_18 | N2_18 | P7 | 115.4(4) |
| N2_21 | P8 | N2_23 | 111.1(3) | N2_18 | C1_18 | C2_18 | 110.8(3) |
| C1_1 | N2_1 | P1 | 122.2(4) | C1_18 | C2_18 | C3_18 | 111.1(3) |
| C1_1 | N2_1 | C5_1 | 111.2(2) | C4_18 | C3_18 | C2_18 | 109.7(3) |
| C5_1 | N2_1 | P1 | 125.7(4) | C5_18 | C4_18 | C3_18 | 110.9(3) |
| N2_1 | C1_1 | C2_1 | 110.5(3) | N2_18 | C5_18 | C4_18 | 110.6(3) |
| C1_1 | C2_1 | C3_1 | 111.0(3) | C1_19 | N2_19 | P7 | 125.2(4) |
| C4_1 | C3_1 | C2_1 | 109.9(3) | C1_19 | N2_19 | C5_19 | 111.2(2) |
| C5_1 | C4_1 | C3_1 | 110.9(3) | C5_19 | N2_19 | P7 | 122.1(4) |
| N2_1 | C5_1 | C4_1 | 110.5(3) | N2_19 | C1_19 | C2_19 | 110.7(3) |
| C1_2 | N2_2 | P4 | 124.4(3) | C1_19 | C2_19 | C3_19 | 111.1(3) |
| C1_2 | N2_2 | C5_2 | 111.0(2) | C4_19 | C3_19 | C2_19 | 110.0(3) |
| C5_2 | N2_2 | P4 | 118.2(3) | C5_19 | C4_19 | C3_19 | 110.8(3) |
| N2_2 | C1_2 | C2_2 | 110.3(3) | N2_19 | C5_19 | C4_19 | 110.1(3) |
| C1_2 | C2_2 | C3_2 | 111.1(3) | C1_20 | N2_20 | P6 | 119.5(4) |
| C4_2 | C3_2 | C2_2 | 110.1(3) | C1_20 | N2_20 | C5_20 | 111.3(2) |
| C5_2 | C4_2 | C3_2 | 110.8(3) | C5_20 | N2_20 | P6 | 127.2(4) |
| N2_2 | C5_2 | C4_2 | 110.3(3) | N2_20 | C1_20 | C2_20 | 110.8(3) |
| C1_3 | N2_3 | P4 | 124.8(3) | C1_20 | C2_20 | C3_20 | 111.4(3) |
| C1_3 | N2_3 | C5_3 | 111.5(2) | C2_20 | C3_20 | C4_20 | 109.9(3) |
| C5_3 | N2_3 | P4 | 123.8(3) | C5_20 | C4_20 | C3_20 | 110.6(3) |
| N2_3 | C1_3 | C2_3 | 110.8(3) | N2_20 | C5_20 | C4_20 | 110.3(3) |
| C1_3 | C2_3 | C3_3 | 111.3(3) | C1_21 | N2_21 | P8 | 120.8(3) |
| C4_3 | C3_3 | C2_3 | 110.1(3) | C1_21 | N2_21 | C5_21 | 111.0(2) |
| C5_3 | C4_3 | C3_3 | 110.7(3) | C5_21 | N2_21 | P8 | 122.0(3) |
| N2_3 | C5_3 | C4_3 | 110.3(3) | N2_21 | C1_21 | C2_21 | 110.7(3) |
| C1_4 | N2_4 | P1 | 113.9(3) | C1_21 | C2_21 | C3_21 | 111.2(3) |
| C1_4 | N2_4 | C5_4 | 110.9(2) | C4_21 | C3_21 | C2_21 | 109.9(3) |
| C5_4 | N2_4 | P1 | 122.3(3) | C5_21 | C4_21 | C3_21 | 110.7(3) |
| N2_4 | C1_4 | C2_4 | 110.6(3) | N2_21 | C5_21 | C4_21 | 110.4(3) |
| C1_4 | C2_4 | C3_4 | 111.1(3) | C1_22 | N2_22 | P4 | 117.3(3) |
| C4_4 | C3_4 | C2_4 | 109.9(3) | C1_22 | N2_22 | C5_22 | 110.7(2) |
| C5_4 | C4_4 | C3_4 | 110.9(3) | C5_22 | N2_22 | P4 | 119.1(3) |
| N2_4 | C5_4 | C4_4 | 110.5(3) | N2_22 | C1_22 | C2_22 | 110.5(3) |
| C1_5 | N2_5 | P1 | 112.3(3) | C1_22 | C2_22 | C3_22 | 111.2(3) |
| C1_5 | N2_5 | C5_5 | 110.9(3) | C4_22 | C3_22 | C2_22 | 110.2(3) |
| C5_5 | N2_5 | P1 | 115.4(4) | C5_22 | C4_22 | C3_22 | 111.1(3) |

| | | | |
|---|---|---|---|
| N2_5 | C1_5 | C2_5 | 110.7(3) |
| C1_5 | C2_5 | C3_5 | 111.2(3) |
| C4_5 | C3_5 | C2_5 | 109.9(3) |
| C5_5 | C4_5 | C3_5 | 111.0(3) |
| N2_5 | C5_5 | C4_5 | 110.6(3) |
| C1_6 | N2_6 | P2 | 122.5(4) |
| C1_6 | N2_6 | C5_6 | 111.7(2) |
| C5_6 | N2_6 | P2 | 125.8(4) |
| N2_6 | C1_6 | C2_6 | 110.6(3) |
| C1_6 | C2_6 | C3_6 | 111.0(3) |
| C4_6 | C3_6 | C2_6 | 110.1(3) |
| C5_6 | C4_6 | C3_6 | 111.0(3) |
| N2_6 | C5_6 | C4_6 | 110.4(3) |
| C1_7 | N2_7 | P2 | 118.0(3) |
| C1_7 | N2_7 | C5_7 | 110.8(3) |
| C5_7 | N2_7 | P2 | 121.2(3) |
| N2_7 | C1_7 | C2_7 | 110.3(3) |
| C1_7 | C2_7 | C3_7 | 111.2(3) |
| C4_7 | C3_7 | C2_7 | 110.2(3) |
| C5_7 | C4_7 | C3_7 | 111.0(3) |
| N2_7 | C5_7 | C4_7 | 110.1(3) |
| C1_8 | N2_8 | P3 | 118.0(3) |
| C1_8 | N2_8 | C5_8 | 110.7(2) |
| C5_8 | N2_8 | P3 | 117.7(3) |
| N2_8 | C1_8 | C2_8 | 110.4(3) |
| C1_8 | C2_8 | C3_8 | 110.8(3) |
| N2_22 | C5_22 | C4_22 | 110.2(2) |
| C1_23 | N2_23 | P8 | 122.4(3) |
| C1_23 | N2_23 | C5_23 | 111.1(2) |
| C5_23 | N2_23 | P8 | 115.0(3) |
| N2_23 | C1_23 | C2_23 | 110.7(3) |
| C1_23 | C2_23 | C3_23 | 111.0(3) |
| C4_23 | C3_23 | C2_23 | 109.8(3) |
| C5_23 | C4_23 | C3_23 | 111.0(3) |
| N2_23 | C5_23 | C4_23 | 110.7(3) |
| C1_24 | N2_24 | P2 | 126.8(4) |
| C1_24 | N2_24 | C5_24 | 111.3(2) |
| C5_24 | N2_24 | P2 | 120.5(4) |
| N2_24 | C1_24 | C2_24 | 110.5(3) |
| C1_24 | C2_24 | C3_24 | 111.1(3) |
| C4_24 | C3_24 | C2_24 | 110.0(3) |
| C5_24 | C4_24 | C3_24 | 110.8(3) |
| N2_24 | C5_24 | C4_24 | 110.3(3) |
| C1_25 | N2_25 | P6 | 125.2(4) |
| C1_25 | N2_25 | C5_25 | 111.4(3) |
| C5_25 | N2_25 | P6 | 123.4(4) |
| N2_25 | C1_25 | C2_25 | 110.7(3) |
| C1_25 | C2_25 | C3_25 | 111.4(3) |
| C4_25 | C3_25 | C2_25 | 110.2(3) |
| C5_25 | C4_25 | C3_25 | 110.8(3) |
| N2_25 | C5_25 | C4_25 | 110.3(3) |

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